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GESELLSCHAFT für
ANGEWANDTE MATHEMATIK und MECHANIK e.V.
INTERNATIONAL ASSOCIATION of APPLIED MATHEMATICS and MECHANICS

89th Annual Meeting

of the International Association of
Applied Mathematics and Mechanics

March 19-23, 2018
Munich, Germany

Foto: Albert Scharger (TUM)

Book of Abstracts

Technische Universität München

Contents

Plenary Lectures

Ludwig Prandtl Memorial Lecture 2018

Date 19.03.2018 14:00–15:00
Room Audimax
Chair Heike Faßbender (Institut Computational Mathematics, Technische Universität Braunschweig)

Global Linear Stability Theory in Aerospace Applications

Vassilios Theofilis (*Mechanical, Materials & Aerospace Eng, University of Liverpool*)

Laminar-turbulent flow transition prediction remains one of the main scientific and technological frontiers in fluid mechanics research, recent advances holding promise of major improvements in performance of components of current and future aerospace systems. Linear (and nonlinear) stability theory forms the cornerstone of flow transition prediction and is rooted in the work on boundary layer stability and transition performed in the first half of last century by Tollmien, Schlichting, Görtler and others, under the auspices of Ludwig Prandtl. Today, achieving natural laminar flow on commercial aircraft is synonymous with controlling Tollmien-Schlichting instability waves, as well as crossflow and Görtler vortices, all of which develop in boundary layers on aircraft wings, engine nacelles and fins. In supersonic and hypersonic flow, choice of materials and design of optimal thermal protection systems relies on knowledge of the state, laminar or turbulent, of the flow in the different phases of the vehicle mission. In the latter part of last century, the classic linear stability theory founded in Göttingen has been substantially expanded in scope by developments in two key areas: global linear stability theory, which extends the classic analysis to flows with multiple inhomogeneous spatial directions (as opposed to the single such direction in the boundary layer), and non-modal / transient growth theory, which has unravelled the potential of fluid flows to sustain strong non-modal growth of small-amplitude perturbations that can lead flow to transition while by-passing eigenmode growth. The presentation will highlight results of global modal and non-modal instability analysis in flows of aerospace interest. Numerical solution of two-dimensional global eigenvalue problems will be introduced in the context of instability in the boundary layer at the leading edge of swept wings, where eigenmodes additional to those postulated by Görtler over half a century ago have been discovered and modeled. Instability and transition in separated flows will be discussed in some detail, following the discovery, also by global modal analysis, of a previously unknown class of self-excited stationary three-dimensional flow instability mechanism that can lead separated flow to transition through a scenario different to the well-known Kelvin-Helmholtz instability. Separation bubbles in the adverse pressure gradient flat plate boundary layer, in flow over stalled airfoils and wings, as well as in a cascade of low-pressure turbine blades will be monitored in this context, and the connection of global transient growth to laminar-turbulent transition on airfoils, wings, and turbine blades will be highlighted. Flow instability in a lateral-wall bounded three-dimensional cavity (modeling three-dimensional imperfections of a flat surface or flow in an aircraft bay) will be presented and results of numerical solution of the three-dimensional eigenvalue problem will be contrasted with those obtained in over-simplified analyses. The presentation will close with a brief discussion of instability of shock-induced laminar separation bubbles in hypersonic flows, where it will be shown that oscillations of the entire shock system that develops on a vehicle are intimately connected with linear amplification of flow instabilities, especially those developing in the separation region. Throughout the talk it will be argued that, seemingly unrelated technological issues, such as increased authority over aerodynamic control surfaces or adequate heat-shield protection, can be resolved through better understanding of the physical mechanisms of instability of the underlying spatially inhomogeneous flows. Continuous progress in algorithms

for the solution of multi-dimensional eigenvalue and singular value problems, alongside ever increasing computing hardware capabilities, permit unraveling such physical mechanisms in the framework of the global linear theory that extends and completes the classic stability analysis proposed by Prandtl's disciples.

Richard von Mises Lecture

Date 21.03.2018 10:30–11:30
Room Audimax
Chair Heike Faßbender (Institut Computational Mathematics, Technische Universität Braunschweig)

To be announced

Plenary Lecture 1

Date 19.03.2018 15:00–16:00
Room Audimax
Chair Kai-Uwe Bletzinger (Lehrstuhl für Statik, Technical University of Munich)

Phase-field modeling and computation of fracture and fatigue

Laura De Lorenzis (*Institute of Applied Mechanics, TU Braunschweig*)

The talk discusses recent research results obtained in the group of the speaker in the framework of the phase-field approach to fracture, and the recent extensions to fracture in partially saturated porous media and to fatigue. Applications include the study of desiccation phenomena in soils and shrinkage in cementitious materials, as well as the investigation of fatigue phenomena in brittle materials. The first steps towards mesoscale modeling of fracture in concrete are also discussed.

Plenary Lecture 2

Date 20.03.2018 11:00–12:00
Room Audimax
Chair Michael Ulbrich (Fakultät für Mathematik, Technische Universität München)

Selection and adaptation of computational models in the presence of uncertainty: Predictive models of tumor growth and random heterogeneous materials

Tinsley Oden (*ICES, University of Texas at Austin*)

In this presentation, we describe a general Bayesian framework for selecting, calibrating, validating, and optimizing computational models of the behavior of complex, physical systems in the presence of uncertainties. The selection and adaptive control of models is based on the calculation of model plausibilities as weighted values of model evidences, on estimates of sensitivity of outputs to the choice of model parameters, and on a posteriori estimates of modeling and

discretization error in quantities of interest. As an added benefit, the estimation of moments in modeling error between high-fidelity models and sequences of surrogate models can be used to significantly improve the efficiency of solvers, such as Multi Level Monte Carlo methods.
To demonstrate the theory and predictive paradigm, the problems of designing and selecting predictive models of the growth or decline of ava scular heterogeneous tumors in living tissue are explored and example applications using in vitro laboratory data are discussed . In addition, the estimation and control of modeling error and adaptive multiscale modeling of random heterogeneous media are also discussed.

Plenary Lecture 3

Date 20.03.2018 12:00–13:00
Room Audimax
Chair Wolfgang A. Wall (Institute for Computational Mechanics, Technical University of Munich)

On the continuum mechanical modelling of polymerphysical phenomena

Alexander Lion (*Universität der Bundeswehr München*)

Amorphous and semicrystalline polymers are applied in nearly all disciplines of engineering and daily life. For short-term applications under usual temperature conditions they exhibit a certain number of advantages but during larger times their mechanical material properties undergo significant changes. Caused by their chemical structure polymeric materials behave completely different in comparison with metals. They exhibit moderate characteristic temperatures which characterise glass transitions, melting and crystallisation regions or the onset of chemical ageing and diffusion processes. If, during the production of a polymer part or in a certain application, such a temperature is exceeded their mechanical material properties can change enormously. In consequence, detailed experimental investigations, the physical understanding, the constitutive representation in continuum mechanics or thermodynamics and the numerical simulation of polymers and parts which are made of them are essential and define big challenges in scientific research. In this presentation, three important polymerphysical phenomena, namely the glass transition, crystallisation and melting as well as the diffusion of fluids in polymers are highlighted in detail. The formulation of the constitutive models is done in accordance with the basic laws of thermodynamics. To this end, the physical motivation and all fundamental ideas as well as the related assumptions and constitutive theories are presented and discussed. The main properties of the different approaches are visualised using simulations and are discussed in the context of experimental data.

Plenary Lecture 4

Date 22.03.2018 11:00–12:00
Room Audimax
Chair Barbara Wohlmuth (Technische Universität München)

Hierarchical energy based modeling and numerical simulation for coupled multi-physics and multi-scale systems

Volker Mehrmann (*TU Berlin*)

We discuss an energy based modeling approach to deal with coupled systems from different physical domains that act on widely different scales. Each physical system is modeled via a model hierarchy (ranging from detailed models for simulation to reduced models for control and optimization) of port-Hamiltonian systems. The systems are coupled via a network of uni-physics nodes coupled via power conserving interconnections so that the full system stays port-Hamiltonian. Using this very flexible approach, it is possible to control the accuracy of each component seperately and to the need of the application. Error controlled model reduction and Galerkin projection as in Finite Element Modeling work in an analogous way. We will demonstrate the approach with real world examples from gas transport optimization, power grid modeling, and the analysis of disk brake squeal.

Plenary Lecture 5

Date 22.03.2018 12:00–13:00
Room Audimax
Chair Oliver Junge (TUM Technische Universität München)

Image compression with partial differential equations

Joachim Weickert (*Univ. d. Saarlandes*)

Partial differential equations (PDEs) are widely used to model processes in engineering. In this talk we will see that they also have a high potential for lossy compression of digital images. The idea sounds temptingly simple: We keep only a few pixels and reconstruct the remaining data with PDE-based interpolation. However, this gives rise to several difficult and interrelated problems, e.g.: - Which data should be kept? - What are the most useful PDEs? - How can the selected data be encoded efficiently? - What are efficient numerical algorithms? Solving these problems requires to combine ideas from different mathematical disciplines such as mathematical modelling, optimisation, interpolation and approximation, and numerical methods for PDEs. After careful engineering we will end up with compression methods that can beat current standards such as JPEG. Since the talk is intended for a broad audience, we focus on the main ideas, and no specific knowledge in image processing is required.

Plenary Lecture 6

Date 22.03.2018 16:30–17:30
Room Audimax
Chair Fabian Duddeck (Computational Mechanics, Technical University of Munich)

Particles - an option for unusual computations

Peter Eberhard (*Institute of Engineering and Computational Mechanics, University of Stuttgart*)

Simulation became an indispensible tool in the modern design process and there are several well established methods available like the finite element method or grid-based computational fluid dynamics. However, there are situations where these well investigated methods have weaknesses or can even not be applied at all.
For these challenging problems meshless methods can be an interesting alternative enriching and completing the toolbox of the engineer. In this talk two methods, the Discrete Element Method (DEM) and Smoothed Particle Hydrodynamics (SPH), are introduced.
The methods are illustrated by a number of applications from different fields of engineering. Examples from fluid dynamics, from fluid-structure interaction, from material processing and others are presented and challenges and limitations are shown. Although the presented methods are quite young compared to some of the well established computation methods they clearly already show their high potential. However, also some numerical problems and stability issues exist and concepts to overcome these challenges must be investigated. The mechanics of particles became a very active area of research with own conferences, journals, and a lively research community and progress is fast.
Particle simulations are always time consuming and require a lot of resources and care. In order to reduce computation times, parallel computation is advisable and efficient approaches are required.

Plenary Lecture 7

Date 23.03.2018 11:00–12:00
Room Audimax
Chair Daniel Jean Rixen (Mechanical Engineering, Technical University of Munich)

Why do turbulent flows have an increased state of symmetry? Physical meaning and its implications

Martin Oberlack (*Mechanical Engineering, TU Darmstadt*)

It was A. Einstein in his seminal work on special relativity in which he contemplated the symmetry principle as the axiomatic foundation of physics in general that confines the admissible laws of motion. For classical mechanics this is Galilean invariance, which is also admitted by the elementary equations of fluid motion - the Navier-Stokes equations. Interesting enough, all complete statistical turbulence theories, though uniquely derived from Navier-Stokes equations, admit more invariance properties, i.e. symmetries, which go beyond the Galilean group. It was recently shown that two of these so-called statistical symmetries mirror key properties of turbulence, i.e. intermittency and non-gaussianity. The recent discovery of statistical symmetries has

important consequences for our understanding and derivation of turbulent scaling laws. Beside the classical logarithmic law of the wall, which is now understood to be a symmetry induced invariant solution of the underlying statistical equation of turbulence based on the new statistical symmetries, this finding will be exemplarily revealed employing examples of wall-bounded and free turbulent shear flows. Most important, these scaling laws not only describe the mean velocity but also higher order moments. Finally, symmetries and statistical symmetries have important implications for turbulence models. Since the 70th of the last century, essentially all turbulence models, both RANS and SGS models for LES, did comply with Galilean invariance. Interestingly, for a minor part, turbulence models have already been implicitly equipped with statistical symmetries, as they comply with the log-law. Still, symmetry based turbulence modelling is still at its infancy.

Plenary Lecture 8

Date 23.03.2018 12:00–13:00
Room Audimax
Chair Marco Cicalese (M7, Technische Universität München)

Onsager reciprocity, gradient flows, and large deviations

Mark Peletier (*Technische Universiteit Eindhoven*)

The second law states that in a thermodynamically consistent system the 'entropy' is a Lyapunov function, a function which is monotonic along solutions of the corresponding differential equations. When the system can be written as a gradient flow of the entropy, then this statement is strengthened: not only is this functional monotonic, but it *drives* the dissipative part of the evolution in a precise way, mediated by a 'friction operator'.
In this lecture I will go one step further. Onsager already pointed out how symmetry properties of linear friction operators arise through an upscaling procedure from a microscopic-reversibility property of the underlying system. Fluctuations figure centrally in his argument, but at that time their theory was not well developed, and more could not be said.
However, recently we have found that the connection between microscopic reversibility and macroscopic 'symmetry' properties is not at all limited to the close-to-equilibrium, linear-friction-operator context of Onsager's. I will describe how the large-deviation theory of fluctuations allows one to make a much more general statement, where microscopic reversibility is one-to-one coupled to 'symmetry' at the macroscopic level - provided one generalizes the concept of symmetry in an appropriate way.

Minisymposia

MS1 | Adaptive control with performance guarantees

Date 20.03.2018 14:00–16:00
Room 0601
Organiser Thomas Berger (*Fachbereich Mathematik, Universität Hamburg*)
Stephan Trenn (*Jan C. Willems Center for Systems and Control, University of Groningen*)

On the history of funnel control

Achim Ilchmann (*Institut für Mathematik, Technische Universität*) 14:00–14:20

Adaptive control without any identification of the systems parameters was introduced in the early 1980s. It started with the standard high-gain control $u = -ky, \dot{k} = y^2$, and became more practical when the λ-tracker was introduced 1994. These control strategies are feasible for large system classes with stable zero dynamics and known relative degree. However, they all share the shortcoming that the gain increases monotonically and transient behaviour is not addressed. Funnel control resolved theses shortcoming while preserving the simplicity of the controller. This was introduced in 2002, and generalized for various system classes, various applications. A recent breakthrough is the extension to a funnel precompensator to achieve (simple) funnel control for systems of higher relative degree.

Prescribed Performance Adaptive Control of Uncertain Nonlinear Systems: State-of-the-art and Open Issues

George Rovithakis (*ELKE A.P.TH.*) 14:20–14:40

Performance in adaptive control designs for uncertain nonlinear systems, whose uncertainty is not purely parametric, was traditionally restricted to enforcing, besides stability, desirable behavior at steady-state. In the literature, rigorous proofs have been provided guaranteeing tracking error convergence to residual sets, whose size depends on design parameters and some bounded though unknown terms. Therefore, even controllable, steady-state accuracy was impossible to be a priori selected by any systematic procedure. Furthermore, transient performance such as maximum overshoot and convergence rate, was difficult to be established analytically even for known systems. The problem was approached via minimizing certain performance indices, which unfortunately were connected only indirectly with the actual system response. Hence, even though performance improvement is anticipated, no connection to a priori specified trajectory oriented metrics could be achieved. For classes of nonlinear systems Funnel Control has been proposed to provide solution. However, the problem remained largely unsolved for the case of adaptive closed-loop uncertain systems. To fill in the gap, the Prescribed Performance Adaptive Control (PPAC) methodology was presented. This work is a review on PPAC, highlighting on its main advantages and discussing on probably the most important open issues.

Funnel control for nonlinear systems with higher relative degree

Timo Reis (*Mathematik, Universität Hamburg*), Thomas Berger (*Fachbereich Mathematik, Universität Hamburg*), Lê Huy Hoàng (*Fachbereich Mathematik, Universität Hamburg*) 14:40–15:00

We consider tracking control for nonlinear multi-input, multi-output systems which have arbitrary strict relative degree and input-to-state stable internal dynamics. For a given sufficiently

smooth reference signal, our aim is to design a controller which achieves that the tracking error evolves within a prespecified performance funnel around the reference signal. To this end, we introduce a new controller which involves the first $r-1$ derivatives of the tracking error, where r is the strict relative degree of the system. We further present some simulations where our funnel controller is applied to some mechanical multibody systems.

Non-identifier based adaptive control with internal models for mechatronic energy systems

Christoph M. Hackl (*Munich School of Engineering / Control of renewable energy systems, Munich School of Engineering*) 15:00–15:20

This talks discusses non-identifier based (high-gain) adaptive control with internal models and its applications to the control of mechatronic energy systems such as industrial servo-systems, wind turbine systems, electrical machines and rigid-revolute joint robots. In mechatronics, the engineer often has only rough knowledge of the considered system – sometimes only its structure is obvious. Due to parameter uncertainties, nonlinearities and unknown disturbances (e.g. dynamic friction & time varying loads), model-based control strategies might reach their limits without time-consuming system identification or parameter estimation. The presented non-identifier based adaptive controllers in conjunction with internal models are easy to implement, compensate for disturbances and are inherently robust to parameter uncertainties and nonlinearities, and tolerate noise. Moreover, the presented controllers guarantee reference tracking with „transient accuracy" (i.e. the tracking error will evolve within an a priori defined region) and will eventually achieve asymptotic tracking.

Funnel Flight Controller for a Simulation Model and a Divert and Attitude Control System

Norman Hopfe (*Bayern-Chemie GmbH*) 15:20–16:00

Abstract – The mission of a ballistic missile defense weapon system is to defend against short and medium range missiles at significant distances from the intended target and at low and high altitudes. Contrary to conventional ground-to-air interceptor systems that are only accelerated by a rocket motor, an integrated Divert and Attitude Control System (DACS) provides a continuous thrust profile and increases the performance of the overall missile system that depends on the flight conditions.
The DACS provides a quick reaction system which positions the missile (which accelerates the agility) and/or its kill-vehicle to intercept the target. The DACS provides then therefore two kinds of propulsions – namely a) one for the attitude control (ACS) and b) the other for missile and/or kill-vehicle maneuvering as divert control system (DCS).
In general, a DACS can be regarded as a small scale rocket engine with the capability of providing thrust at certain points of the operational activity which is usually realized by a set of circumferentially mounted "mini" motors which can be triggered individually while the missile performs a rotational movement along its longitudinal axis or by a continuous burning (solid propellant) motor which feeds a throttleable Cartesian nozzle configuration.
The advantage of such a system is that it provides a continuous operation capability. The thrust direction can be controlled by a simultaneous modification of the ACS and DCS nozzle throats, usually realized by a hot gas valve system consisting of so called pintles which can be shifted (either pairwise coupled or individually controlled) backwards and forth to increase or reduce the respective nozzle throat area.
Modeling has become an important tool for predicting the behavior and the design of dynamical systems resulting in a reduced need for numerous and often expensive testing. Especially

if the system under investigation cannot be tested completely under accessible test conditions on ground, the development of reliable simulation tools is mandatory for its design. The simulation of in-flight performance has been an important area throughout the history of missile development.
Within this paper, the development of an advanced simulation tool is presented which is able to predict the behavior of a so called DACS which is used to adjust the attitude and position of a missile to agility requirements commanded by the onboard guidance, navigation and control device. Here the focus is laid on the internal dynamics and control of such nozzle pintle actuator system.
For the current investigation a DACS is simulated which consists of a gas generator that produces a hot gas which is led into a pair of throttleable nozzles. The nozzles are aligned along a straight line and throttled by a coupled pintle system. The pintles connected via a metallic rod are shifted backwards and forth to change the respective nozzle throats such that with closing one throat the other will be opened. The rod is connected via a lever with an actuator.
Such a configuration allows very fast thrust modifications by side thrust change and due to this a very fast position change of the missile depending of the location of the ACS and DCS with respect to the missile's center of gravity.
This paper comprises the simulation model and application for such a DACS containing brief descriptions of the flight control algorithms and a mathematical simulation model. It investigates the performance prediction for the DACS.
For all models a funnel controller method is used as an automatic control tool. It is shown how the funnel controller is used in a simulation and a test facility trial aiming at a fast thrust variation for a maneuver track.
The theoretical funnel control and experimental results of a laboratory rotatory mechanical system from [SIAM2013] are combined and extended to speed funnel control with nonlinear disturbances and elastic deformation without active damping where only thrust measurement is available. The extended funnel control concept is applied to this highly reactive DACS and guarantees extremely fast thrust tracking with a required transient accuracy in the low millisecond range to achieve maximum performance. The knowledge of all system parameters, the nonlinear mass flow link and the actuator interaction is not required.
Finally, the operational potential of such a system is discussed by an analysis of the DACS performance along hypothetical thrust profiles by simulation and simplified test facility trials.
Keywords - Funnel control, Attitude Control System, Divert Control System, nonlinear systems, transient behavior, solid propellant, gelled propellant, simulation model, propellant burnback, Matlab

MS2 | Computational interdisciplinary modeling

Date	20.03.2018	14:00–16:00
Room	0602	
Organiser	Alexander Ostermann (*Department of Mathematics, University of Innsbruck*)	

On computational interdisciplinary modeling for reliability assessment of high-speed train – bridge interaction

Christoph Adam (*Unit of Applied Mechanics, University of Innsbruck*), Benjamin Hirzinger (*Unit of Applied Mechanics, University of Innsbruck*), Michael Oberguggenberger (*Unit of Engineering Mathematics, University of Innsbruck*), Patrick Salcher (*Unit of Applied Mechanics, University of Innsbruck*) 14:00–14:20

The current world-wide expansion of the rail network for high-speed trains comes along with the construction of bridges with longer spans crossed by trains with higher speeds and larger capacities. In a stochastic approach, where uncertainties in the bridge-train interaction system are explicitly accounted for, the serviceability limit-state (SLS) and the ultimate limit-state (ULS) are assessed more realistically. Large bridge deck acceleration may lead to ballast instability and to derailment, and thus, it is often the limiting factor in dynamic railway bridge design. The limit state function becomes multi-dimensional and is of high complexity. Full reliability assessment of the interacting bridge-train system is conducted in an interdisciplinary approach, bringing together the disciplines of structural mechanics, engineering mathematics, and high performance computing. A realistic numerical vehicle-bridge interaction model is created, taking into account rail irregularities. Distributions for random parameters such as material properties, geometry, environmental impact, etc., are defined. Assessment of failure with small probabilities requires the application of elaborated methods such as subset simulation or line-sampling with small estimator variances. The efficiency of these methods with respect to application of the uncertain bridge-train interaction problem is evaluated.

BLieDF: Lie group time integration for constrained mechanical systems with large rotations

Martin Arnold (*Institute of Mathematics, Martin Luther University Halle-Wittenberg*), Stefan Hante (*Institute of Mathematics, Martin Luther University Halle-Wittenberg*), Victoria Wieloch (*Institute of Mathematics, Martin Luther University Halle-Wittenberg*) 14:20–14:40

Highly-flexible slender structures like cables, pipes and hoses are modelled conveniently in nonlinear configuration spaces with Lie group structure that allow the parametrization of (large) rotations free of singularities. In his plenary lecture at the 83rd Annual GAMM conference [1], O. Brüls (Liège) presented a 2nd order Newmark type Lie group integrator that avoids frequent re-parametrizations of the configuration space by a *Lie algebra approach* [2] that substitutes the classical update of configuration variables in the (*nonlinear*) Lie group by an update of configuration increments in a *linear* space.
In the present paper, we combine this Lie algebra approach with BDF which are the time integration methods of choice in most industrial multibody system simulation packages. For $k \leq 3$, the k-step BLieDF integrators achieve their classical order $p = k$ by a Lie group specific

correction term that may be evaluated efficiently. For constrained systems, BLieDF discretizes the stabilized index-2 formulation of the equations of motion.
The benefits of BLieDF are illustrated by numerical test results for a geometrically exact Cosserat beam model that uses quaternions to parametrize the rotational degrees of freedom of the beam centerline.

[1] O. Brüls: *Lie group formulations and integration methods in flexible multibody dynamics.* - 83rd Annual GAMM conference, March 2012, Darmstadt.

[2] M. Arnold, A. Cardona, O. Brüls: *A Lie algebra approach to Lie group time integration of constrained systems.* In: P. Betsch (ed.): Structure-Preserving Integrators in Nonlinear Structural Dynamics and Flexible Multibody Dynamics, vol. 565 of CISM Courses and Lectures, pp. 91-158. Springer. - 2016.

Modeling bone ultrastructure: mechanics - chemistry - biology - physics

Christian Hellmich (*TU Wien, Vienna University of Technology*), Claire Morin (*Ecole des Mines de Saint Etienne*), Ales Kurfürst (*TU Wien*) 14:40–15:00

Micromechanical representation of bone ultrastructure as a composite of aligned mineralized collagen fibrils embedded in a porous polycrystalline matrix has allowed for successfully predicting the (poro/visco-)elastic and strength properties of bone tissues throughout the entire vertebrate animal kingdom, based on the "universal" mechanical properties of the material's elementary components: molecular collagen, hydroxyapatite, and water-type fluids. We here check whether the explanatory power of this schematic representation might extend beyond the realm of mechanics; namely, towards electrodynamics and X-ray physics. Therefore, we consider the previously reported identity of the extracollageneous mineral concentration in the fibrillar and extrafibrillar, as well as in the gap and the overlap compartments of bone ultrastructure, and insert the corresponding electron densities into Fourier transform-type solutions of the Maxwell equations specificied for a Small Angle X-ray Scattering setting. The aforementioned mineral distribution, as well as random fluctuations of fibrils, both within their transverse plane around a hexagonal lattice and in form of axial shifts, turn out to be the key for successfully predicting experimentally observed X-ray diffraction patterns. This marks a new level of quantitative, "mathematized" understanding of the organization of bone ultrastructure.

Numerical algorithms for plasma physics

Lukas Einkemmer (*University of Tuebingen*) 15:00–15:20

The description of plasmas is important in many fields of science and engineering. A better understanding of these systems has implications from studying coronal mass ejections to enabling magnetic confinement fusion. Numerical simulations are playing an increasingly important role in this quest. In this talk, we will consider examples of research on improved numerical methods that have resulted in computer codes with significantly reduced computational requirements that are able to more faithfully model the physics under consideration.
First, we consider the simulation of a Tokamak in the context of a fluid model. Already in 1966, Arakawa proposed a finite difference approximation that conserves vorticity, kinetic energy, and enstrophy. This numerical method was not appreciated because it does not generalize to three dimensions. In magnetized plasmas, however, the dynamics parallel and perpendicular to the magnetic field can be separated, resulting in quasi two-dimensional turbulent fluid-like structures. Here we show how to extend Arakawa's method to a discontinuous Galerkin scheme of arbitrary order that still conserves all three invariants. The computer code FELTOR has

been developed based on this numerical scheme and can simulate three-dimensional plasmas on arbitrary structured grids
A further numerical challenge encountered in plasma physics are kinetic models. These models are posed in an up to six-dimensional phase space and are thus extremely challenging from a computational point of view. In this context, we will discuss recent research on both the development of more efficient algorithms as well as their implementation on state of the art computer systems.

On the stability of leap-frog type methods

Marlis Hochbruck (*Mathematics, KIT - Karlsruhe Institute of Technology*), Andreas Sturm (*KIT - Karlsruhe Institute of Technology*) 15:20–15:40

In this talk we discuss the stability of leap-frog type methods. The standard test problem to study the stability is the unforced harmonic oscillator with a fixed frequency. It is well known that the leap-frog method is stable (in the sense that the approximation remains bounded uniformly w.r.t. the simulation time) if the product of the frequency with the time step size is strictly smaller than two. Modifications of the leap-frog method which weaken this strong step size restriction have been recently proposed in the literature. However, these schemes lose the stability property of the leap-frog method.
In this talk we present a general stability result for such time integration methods and show how to construct stable variants of the leap-frog method allowing for larger time step sizes. Numerical results show the superior stability and convergence properties of these new methods compared to recent schemes.
This is work is supported by DFG CRC 1173.

Towards better patient care based on computational interdisciplinary modeling

Wolfgang A. Wall (*Institute for Computational Mechanics, TU München*), Christian Roth (*Institute for Computational Mechanics, TU München*), Lena Yoshihara (*Institute for Computational Mechanics, TU München*) 15:40–16:00

In this talk we try to demonstrate the potential of computational interdisciplinary modeling (CIM) along with a very challenging but also very promising application, that also has a high relevance for society. The idea is to use computational biomedical engineering not just for some nice scientific studies but really push it towards clinical relevance. As case example we will use intensive care patients with lung injury or neonates that both need artificial ventilation. For better protective ventilation strategies a better understanding of the human respiratory system is needed. We will show how interdisciplinary modeling can help to not only better understand the lung but also predict it's behavior. And we will further show how CIM can be used to model special imaging techniques that are essential for validation. Crucial ingredients for success of such complex modeling tasks are a deep understanding of the underlying physical (and biological) processes, modeling that relies on a sound and advanced mathematical basis and the according proficiency in computer science.

MS3 | Experimental mechanics

Date	20.03.2018	14:00–16:00
Room	0606	
Organiser	Stefan Diebels (*Chair of Applied Mechanics, Saarland University*)	
	Stefan Hartmann (*Clausthal University of Technology*)	

Characterization and modeling of long-fiber reinforced polymers

Malte Schemmann (*Institute of Engineering Mechanics, Karlsruhe Institute of Technology (KIT)*), Loredana Kehrer (*Institute of Engineering Mechanics, Chair for Continuum Mechanics, Karlsruhe Institute of Technology (KIT)*), Juliane Lang (*Institute of Engineering Mechanics, Chair for Continuum Mechanics, Karlsruhe Institute of Technology (KIT)*), Thomas Böhlke (*Institute of Engineering Mechanics, Chair for Continuum Mechanics, Karlsruhe Institute of Technology (KIT)*) 14:00–14:20

The first part of this talk covers the characterization of discontinuous fiber reinforced polymers by means of dynamic mechanical analysis (DMA) [1]. DMA is applied to both material systems, neat and discontinuous fiber reinforced thermoset samples, also known as sheet molding compounds (SMCs). The thermoviscoelastic material behavior is investigated and the nonlinear temperature and frequency dependency is discussed in detail. The second part of this talk covers the characterization and prediction of anisotropic damage in SMC. The goals are the characterization of the anisotropy of damage evolution (by stiffness degradation) and the damage behavior in biaxial stress states. A key challenge is the design of an appropriate specimen geometry. Typical geometries fail in the arms before a sufficiently high stress is reached in the observing area of interest. This talk describes two possibilities to reinforce the cruciform specimen's arms [2]. The experimental results validate a two-scale anisotropic damage model. This mean field damage model captures matrix damage and fiber-matrix-debonding. Based on the fiber orientation distribution and a Weibull probability distribution of the interface strength, the damage evolution on the microscale is determined. The macroscopic behavior yields from a homogenization by means of the Mori-Tanaka scheme.

[1] Kostka, P., Holeczek, K., Höhne, R., Filippatos, A., Modler, N., 2016. Extension and application of dynamic mechanical analysis for the estimation of spatial distribution of material properties. Polymer Testing 52, 184–191.

[2] Smits, A., Van Hemelrijck, D., Philippidis, T.P., Cardon, A., 2006. Design of a cruciform specimen for biaxial testing of fibre reinforced composite laminates. Composites Science and Technology, 66 (7–8), 964-975

Recent experimental methods to characterise polymer ageing

Michael Johlitz (*Institute of Mechanics, Universität der Bundeswehr München*) 14:20–14:40

Polymers and polymer components are highly important in industrial applications such as bearings, seals, bonds and coatings. Since these components are used in various areas of engineering, it is obvious that they are exposed to different environmental influences such as mechanical stresses, temperature profiles and chemical or biological substances. Therefore, their properties change over time leading to limited operating times. Representative examples are the high-cycle fatigue as a result of the exposure of polymer components to mechanical load collectives, the

physical ageing of lacquer coatings or the thermooxidative ageing of elastomeric bearings in ships and automobiles. In order to estimate the lifetime of the above mentioned polymers in relation to their field of application, there is a great interest to develop new simulation methods and software tools that are able to consider complex long-term processes in the framework of multiphase continuum mechanics. These models incorporate a number of material parameters which have to be stratergically identified through experimental studies. This is the point where the proposed contribution attaches. At first, the state of the art is presented in relation to the various ageing phenomena and highlighted by scientific data. Several challenges from the areas of mechanical fatigue, physical and chemical ageing are pointed out and discussed. In a next part of the presentation, the experimental equipment which is necessary for ageing and durability studies is introduced and explained. This includes both standard mechanical experiments as well as caloric and chemical analyses. According to that, comprehensive experimental investigations performed at our institute are provided and discussed. The contribution is closed by a summary and various outlooks to future trends and objectives.

Bioreactor development for regenerative tissues of the locomotor system

Marcus Stoffel (*Institute of General Mechanics, RWTH Aachen*), Gözde Dursun (*Institute of General Mechanics, RWTH Aachen*), Julia Nachtsheim (*Institute of General Mechanics, RWTH Aachen*), Nadine Fuhrmann-Nelles (*Institute of General Mechanics, RWTH Aachen*), Bernd Markert (*Institute of General Mechanics, RWTH Aachen*) 14:40–15:00

In order to identify the interaction between mechanical stimuli and changes in mechanical properties of living biological tissues, experimental set-ups such as bioreactor systems are necessary. From the viewpoint of medical science these in-vitro experiments become more and more important, since new types of implants are proposed for replacing ill or injured human tissues. Furthermore, for the purpose of experimental validation, bioreactors allow a possibility for verifying numerical simulations predicting growth and remodeling processes in biological materials. Due to the fact, that the evolution of mechanical properties of soft tissues, such as cartilage or tendons, depend on the loading history, bioreactors with complex and preferably physiological movements were developed in recent years. This includes an online-monitoring system of the cultivated biological material. In the present study, developed bioreactors are presented, focusing on the remodeling in cellular and acellular biological tissues. In the case of acellular materials the cell migration problem plays a dominant role. Finally, the experimentally observed evolution processes of the material are going to be included in a continuum mechanical model.

Investigations in the field of material mechanics using strain gages

Thomas Lehmann (*Chair of Solid Mechanics, Chemnitz University of Technology*), Martin Stockmann (*Chair of Solid Mechanics, Chemnitz University of Technology*), Jörn Ihlemann (*Chair of Solid Mechanics, Chemnitz University of Technology*) 15:00–15:20

In this contribution, investigations of the stress-strain behavior of different metals using strain gage technique are presented. The measurement of strains using strain gages provides high measuring accuracy. In case of large deformations, the nonlinearity of the resistance-strain-relation, including elastic and plastic strain of the gage grid material, has to be considered. Moreover, for the detection of large deformations, high-elongation strain gages and special bonding adhesives are used. Furthermore, at larger resistance changes the nonlinearity of the Wheatstone bridge has to be taken into account.
As an example, the stress-strain behavior of the steel 50CrV4 with three different process states in the small deformation range during tensile tests is demonstrated. The differences of the resulting

stress-strain curves of the material in the different process states are analyzed. Additionally, specimens of the aluminum alloy EN AW-2024 are investigated in a large deformation range using tensile tests. Therein, the strain transmission enabled by the bonding is in the special focus. Furthermore, results of the large deformation tests are compared to the strain measurement using Digital Image Correlation.

Harmonic experiments: Powerfull tools for the characterization of porous materials

Holger Steeb (*Continuum Mechanics, Institute of Applied Mechanics, University of Stuttgart*) 15:20–15:40

Hydro-mechanical characterization of porous materials saturated with an inherent viscous pore fluid based on (coupled) experiments is well established and various testing devices like e.g. low- and high-pressure triaxial cells for geomaterials and porous rocks have been developed in recent decades. Similar testing devices have been developed for the determination of effective transport and storage properties, like Darcy's permeability and/or storage capacity. Most of the related testing devices are based on quasi-static boundary conditions and, therefore, the experimentally-obtained parameters characterize the DC behavior of the material. Beside quasi-static tests, dynamic characterization methods, like e.g. resonant column bars or the forced oscillation method for probing (stiff) rock-like materials have been developed for the characterization of AC properties but applications to porous materials are rather rare. Especially the frequency range above 100 Hz is not investigated with the mentioned dynamical hydro-mechanical testing tools.
In the present study, we are aiming for a discussion of the forced oscillation method [1] for probing the effective visco-elastic properties of porous rocks in the frequency range up to 1 kHz as well as a forced oscillation method for determining the effective (dynamic) permeability.

[1] Pimienta, L., J. Fortin and Y. Guéguen [2015]. Experimental study of Young's modulus dispersion and attenuation in fully saturated sandstones. *Geophysics* **80**(5), L57-L72.

From Experiment to Material Parameter Identification

Stefan Hartmann (*Institute of Applied Mechanics, Clausthal University of Technology*), Rose Rogin Gilbert (*Institute of Applied Mechanics, Clausthal University of Technology*) 15:40–16:00

There are only a few experiments yielding homogeneous deformations, and, accordingly, specified stress states. Thus, the constitutive models can be evaluated directly, so that material parameters can be identified by the resulting system of algebraic equations, ordinary differential equations, or differential-algebraic equations. In all other cases, inhomogeneous deformations are obtained, which holds, particularly, also for biaxial tensile tests. In that case, the entire boundary-value problem has to be solved, where we draw on finite elements. In this presentation the general formulation of material parameter identification is discussed, where in the case of constitutive models of evolutionary-type, the sensitivity analysis is connected to *simultaneous sensitivity equations*, which can be shown to be equivalent to *internal numerical differentiation* for the same time-integration scheme to solve the differential-algebraic equations – resulting from the spatial discretization in finite elements. The consequence of displacement and/or force control for digital image correlation data is discussed as well. Particular, practical examples are formulated.

MS4 | High-performance computing for continuum mechanical problems

Date	20.03.2018	14:00–16:00
Room	1601	
Organiser	Matthias Bolten (*Mathematik, Bergische Universität Wuppertal*) Andrea Walther (*Mathematics and its Applications, Paderborn University*)	

FE2TI – Combining Computational Scale Bridging and Domain Decomposition Methods for Dual-Phase Steel

Axel Klawonn (*Mathematical Institute, University of Cologne*), Oliver Rheinbach (*Institute of Numerical Mathematics and Optimization, TU Freiberg*), Martin Lanser (*Mathematisches Institut, University of Cologne*), Matthias Uran (*Mathematisches Institut, University of Cologne*) 14:00–14:20

The computational simulation of modern high-strength steel materials with micro structure is still a challenge. As a computational homogenization approach we consider the FE^2 method combined with efficient parallel domain decomposition methods of FETI-DP type. In this approach, in each Gauss integration point of the macroscopic problem, a microscopic problem on a representative volume element (RVE) is solved. The microscopic problems are only coupled through the macroscopic level and can be solved all in parallel. Each of these microscopic problems itself will be solved using a parallel FETI-DP domain decomposition method. This approach is implemented in PETSc and uses efficient solver packages including BoomerAMG, MUMPS, and UMFPACK, resulting in the parallel computational homogenization software FE2TI. We present weak scalability results obtained on JUQUEEN (FZ Jülich, 458, 752 BG/Q cores) and Mira (Argonne National Laboraroty, 786, 432 BG/Q cores).

A Computational Two-Scale Model for the Simulation Dual-Phase Steels under Cyclic Loading

Ashutosh Gandhi (*Institut für Computational Engineering, Ruhr-Universitaet Bochum*), Daniel Balzani (*Chair of Continuum Mechanics, Ruhr-Universität Bochum*), Lisa Scheunemann (*Institut für Mechanik, Universität Duisburg-Essen*), Dominik Brands (*Institut für Mechanik, Universität Duisburg-Essen*), Jörg Schröder (*Institute of Mechanics, Department of Civil Engineering, University Duisburg-Essen*) 14:20–14:40

Dual-Phase (DP) steels exhibit excellent macroscopic properties such as high strength, ductility and energy absorption. However, the increase of strength also results in a large springback behavior which should be considered for an optimal production process design. Thus, accurate modeling of springback during forming applications is important. The macroscopic behavior of DP steels is closely tied to the phenomena taking place on the microstructural level. The presence of kinematic hardening and graded properties in ferrite together with complex interactions of the different phases at the microscale have a large influence on the macroscopic springback response. Therefore, a micro-macro scale bridging approach is applied wherein statistically similar representative volume elements (SSRVEs) are considered to capture the DP-steel microstructure, c.f. [1],[2]. This ensures effective modeling of the microstructure while significantly reducing the complexity of the microstructural morphology and thus reducing the computing time. A mixed hardening model, see [4], along with the initial volumetric strain approach, see [3], enables incorporating the kinematic hardening as well as graded properties in the microstructure. Multiscale

calculations of cyclic tests show the performance of the model by measuring the Bauschinger factor and the attained stress levels during deformation.

[1] Balzani, D., Scheunemann, L., Brands, D., Schröder, J., "Construction of two- and three-dimensional statistically similar RVEs for coupled micro-macro simulations", *Comp. Mech.*, 54(5),pp. 1296-1284, 2014.

[2] Balzani, D., Scheunemann, L., Brands, D., Schröder, J., "Construction of two- and three-dimensional statistically similar RVEs for coupled micro-macro simulations", *Comp. Mech.*, 55, pp. 861-871, 2015.

[3] Brands, D., Balzani, D., Scheunemann, L., Schröder, J., Richter, H., Raabe, D., "Computational modeling of dual-phase steels based on representative three dimensional microstructures obtained from EBSD data", *Arch. Appl. Mech.*, 86, pp. 575-598, 2016.

[4] Simo, J.C., "Algorithms for static and dynamic multiplicative plasticity that preserve the classical return mapping schemes of the infinitesimal theory", *Comput. Methods in Appl. Mech. Eng.*, 99, pp. 61-112, 1992.

Trailing Edge Noise Mitigation by Analysis and Optimization of Porosity Parameters

Wolfgang Schröder (*Aerodynamisches Institut, RWTH Aachen University*), 14:40–15:00
Nicolas Gauger (*Chair for Scientific Computing, TU Kaiserslautern*)

The impact of various porous surfaces on trailing-edge noise is analysed by a coupled large-eddy simulation/computational aeroacoustics method. The Darcy drag induced by the porous structures directly influences the acoustic attenuation by reducing the flow acceleration near the trailing edge. The porous surface prescribed by porosity and permeability is extremely effective to reduce the tonal and the broadband noise at zero angle-of-attack up to 11dB OASPL. To circumvent the computational cost of evaluating design sensitivities of geometries with large numbers of design variables, a highly efficient adjoint-based method has been used to optimize the porosity parameters, which is able to compute the entire design gradient vector at a cost comparable to that of the primal simulation. The adjoint solver developed based on algorithmic differentiation (AD) features favorable accuracy and stability properties that makes it highly attractive to optimization problems involving unsteady phenomena such as turbulence induced noise.

Trailing Edge Noise Mitigation by Analysis and Optimization of Porosity Parameters, Part 2

Wolfgang Schröder (*Aerodynamisches Institut, RWTH Aachen University*), 15:00–15:20
Nicolas Gauger (*Chair for Scientific Computing, TU Kaiserslautern*)

The impact of various porous surfaces on trailing-edge noise is analysed by a coupled large-eddy simulation/computational aeroacoustics method. The Darcy drag induced by the porous structures directly influences the acoustic attenuation by reducing the flow acceleration near the trailing edge. The porous surface prescribed by porosity and permeability is extremely effective to reduce the tonal and the broadband noise at zero angle-of-attack up to 11dB OASPL. To circumvent the computational cost of evaluating design sensitivities of geometries with large numbers of design variables, a highly efficient adjoint-based method has been used to optimize the porosity parameters, which is able to compute the entire design gradient vector at a cost

comparable to that of the primal simulation. The adjoint solver developed based on algorithmic differentiation (AD) features favorable accuracy and stability properties that makes it highly attractive to optimization problems involving unsteady phenomena such as turbulence induced noise.

Numerical simulation techniques for fluids with complex rheology with special application to rubber polymers

Stefan Turek (*Mathematik, TU Dortmund*), Jochen Kroll (*TA Instruments*) 15:20–15:40

In the lecture we present numerical simulation techniques for incompressible fluids showing complex rheological behaviour, often with 'extreme' changes of the viscosity which may vary significantly by several orders of magnitude, for instance due to non-isothermal behavior and pressure, resp., shear dependency as well as due to viscoelastic effects with broad relaxation spectra. We discuss special discretization and solver techniques in which case the coupling between the velocity, pressure and additional variables for the stresses, which leads to restrictions for the choice of the FEM approximation spaces, and the (often) hyperbolic nature of the problem are handled with special Finite Element techniques including stabilization methods. The resulting linearized systems inside of outer Newton-type solvers are (special) nonsymmetric saddle point problems which can be solved via geometrical multigrid approaches such that the combination with appropriate High-Performance-Computing techniques leads to very powerful - w.r.t. numerical as well as computational efficieny - simulation tools based on our inhouse CFD software FEATFLOW-PRO. The presented methodology is illustrated and analyzed numerically in the context of industrial applications for several nonlinear flow models.The pros and cons of existing approaches are evaluated, particularly we present new modeling aspects for describing the multiscale behaviour of rubber polymers. Further we discuss the corresponding numerical and computational challenges which are currently under progress to be realized in FEATFLOW-PRO as a simulation tool for such kind of flow problems.

Numerical simulation techniques for fluids with complex rheology with special application to rubber polymers, Part 2

Jochen Kroll (*TA Instruments*), Stefan Turek (*Mathematik, TU Dortmund*) 15:40–16:00

In the lecture we present numerical simulation techniques for incompressible fluids showing complex rheological behaviour, often with 'extreme' changes of the viscosity which may vary significantly by several orders of magnitude, for instance due to non-isothermal behavior and pressure, resp., shear dependency as well as due to viscoelastic effects with broad relaxation spectra. We discuss special discretization and solver techniques in which case the coupling between the velocity, pressure and additional variables for the stresses, which leads to restrictions for the choice of the FEM approximation spaces, and the (often) hyperbolic nature of the problem are handled with special Finite Element techniques including stabilization methods. The resulting linearized systems inside of outer Newton-type solvers are (special) nonsymmetric saddle point problems which can be solved via geometrical multigrid approaches such that the combination with appropriate High-Performance-Computing techniques leads to very powerful - w.r.t. numerical as well as computational efficieny - simulation tools based on our inhouse CFD software FEATFLOW-PRO. The presented methodology is illustrated and analyzed numerically in the context of industrial applications for several nonlinear flow models.The pros and cons of existing approaches are evaluated, particularly we present new modeling aspects for describing the multiscale behaviour of rubber polymers. Further we discuss the corresponding numerical and computational challenges which are currently under progress to be realized in FEATFLOW-PRO as a simulation tool for such kind of flow problems.

MS5 | PDE constrained optimization under uncertainty

Date 20.03.2018 14:00–16:00
Room 2750
Organiser Martin Stoll (*TU Chemnitz*)

Taylor Approximation of PDE-Constrained Optimization Under Uncertainty: Application to Turbulent Jet Flow

Peng Chen (*Institute for Computational Engineering and Sciences, The University of Texas at Austin*), Umberto Villa (*The University of Texas at Austin*), Omar Ghattas (*The University of Texas at Austin*) 14:00–14:20

In this talk, we present a scalable method based on Taylor approximation for PDE-constrained optimal control problems under high-dimensional uncertainty. The computational complexity of the method does not depend on the nominal but only on the intrinsic dimension of the uncertain parameter, thus the curse of dimensionality is broken for intrinsically low-dimensional problems. Further Monte Carlo correction for the Taylor approximation is proposed, which leads to an unbiased evaluation of the statistical moments in the objective function and achieves reduction of variance by several orders of magnitude compared to a Monte Carlo approximation. We apply our method for a turbulence model with infinite-dimensional random viscosity and demonstrate the scalability up to 1 million parameter dimensions.

Model Order Reduction Techniques with A Posteriori Error Control for Robust Nonlinear PDE Constrained Optimization

Stefan Ulbrich (*Department of Mathematics, Technische Universität Darmstadt*), Oliver Lass (*Mathematics, Technische Universität Darmstadt*) 14:20–14:40

We consider a nonlinear optimization problem governed by partial differential equations (PDE) with uncertain parameters. It is addressed by a robust worst case formulation. The resulting optimization problem is of bi-level structure and is difficult to treat numerically. We propose an approximate robust formulation that employs linear and quadratic approximations. To speed up the computation, reduced order models based on proper orthogonal decomposition (POD) in combination with a posteriori error estimators are developed. The proposed strategy is then applied to the shape optimization of a synchronous electrical machine under uncertainty. Numerical results are presented to validate the presented approach.

Krylov Space Solver for Optimal Control

Christian Kirches (*Mathematical Optimization, TU Braunschweig*), Felix Lenders (*Interdisciplinary Center for Scientific Computing, Heidelberg University*) 14:40–15:00

We focus on nonlinear programming for control problems and discuss a sequential linear equality constrained quadratic programming (SLEQP) method for discretized control problems with trust region globalization.
The quadratic trust region subproblems are solved using a Krylov subspace method that can be formulated in function space without the need to obtain a discretization and builds on Goulds generalized Lanczos trust region method.
We provide examples from PDE-constrained optimization to demonstrate mesh-independent convergence behaviour of the proposed method and discuss the applicability and effectiveness of the method in online optimization problems arising in nonlinear model predictive control.

Certified Reduced Basis Methods for Variational Data Assimilation

Sebastien Boyaval (*Université Paris Est*), Martin Grepl (*RWTH Aachen University*), Mark Kärcher (*RWTH Aachen University*), Nicole Nellesen (*RWTH Aachen University*), Karen Veroy-Grepl (*AICES, RWTH Aachen University*) 15:00–15:20

In this talk, we present a certified RB approach to variational data assimilation. Several works have explored the use of reduced order models as surrogates in a variational data assimilation setting. We consider here the case in which the behavior of the system is modelled by a parametrised PDE where certain model inputs (e.g., model parameters, or in the time-dependent case, the initial condition) are unknown, and where the model itself may be imperfect. We consider (i) the standard strong-constraint approach, which uses the given observational data to estimate the unknown model inputs, and (ii) the weak-constraint formulation, which additionally provides an estimate for the model error, and thus can deal with imperfect models. Since the model error is a distributed function, the variational data assimilation formulation generally leads to a large-scale optimization problem that must be solved for every given parameter instance. We introduce RB spaces for the state, adjoint, model error, and in the parabolic case, the initial condition. We then build upon recent results on RB methods for optimal control problems to derive a posteriori error estimates for RB approximations to solutions of the variational data assimilation problem. Numerical tests are conducted to verify the validity of the proposed approach.

Low-rank techniques for computing posterior covariance matrices in Bayesian inverse problems

Peter Benner (*Computational Methods in Systems and Control Theory, Max Planck Institute for Dynamics of Complex Technical Systems*), Martin Stoll (*TU Chemnitz*), Yue Qiu (*Max Planck Institute for Dynamics of Complex Technical Systems*) 15:20–15:40

We consider the problem of estimating the uncertainty in statistical inverse problems using Bayesian inference. When the probability density of the noise and the prior are Gaussian, the solution of such a statistical inverse problem is also Gaussian. Therefore, the underlying solution is characterized by the mean and covariance matrix of the posterior probability density. However, the covariance matrix of the posterior probability density is full and large. Hence, the computation of such a matrix is impossible for large dimensional parameter spaces. It is shown that for many ill-posed problems, the Hessian matrix of the data misfit part has low numerical rank and it is therefore possible to perform a low-rank approach to approximate the posterior covariance matrix. For such a low-rank approximation, one needs to solve a forward partial differential equation (PDE) and the adjoint PDE in both space and time. This in turn gives $\mathcal{O}(n_x n_t)$ complexity for both, computation and storage, where n_x is the dimension of the spatial domain and n_t is the dimension of the time domain. Such computations and storage demand are infeasible for large problems. To overcome this obstacle, we develop a new approach that utilizes a recently developed low-rank in time algorithm together with the low-rank Hessian method. We reduce both the computational complexity and storage requirement from $\mathcal{O}(n_x n_t)$ to $\mathcal{O}(n_x + n_t)$. We use numerical experiments to illustrate the advantages of our approach.

Uncertainty quantification for inverse problems

Claudia Schillings (*University of Mannheim*), Andrew Stuart (*Caltech*), Simon Weissmann (*Universität Mannheim*) 15:40–16:00

Many applications require the design or optimal control of a complex process governed by partial differential equations. Due to limited knowledge or uncertainty in input parameters, boundary and initial conditions, the treatment and minimization of uncertainties is indispensable in order to increase the confidence in numerical simulations and to ensure a robust performance and reliability of the computed designs / controls in a real-world setting. In this talk, we will focus on the identification of parameters through observations of the response of the system - the inverse problem. In cases, where the model evaluations are prohibitively expensive, ad hoc methods such as the Ensemble Kalman Filter (EnKF) for inverse problems are widely and successfully used by practitioners in order to approximate the solution of the inverse problem. We will discuss an analysis of the EnKF based on the continuous time scaling limits, which allows to derive estimates on the long-time behaviour of the EnKF and, hence, provides insights into the convergence properties of the algorithm. Results from various numerical experiments supporting the theoretical findings will be presented.

Young Researcher's Minisymposia

YR1 | Isogeometric methods

Date 19.03.2018 16:30–18:30
Room N1070
Organiser Wolfgang Dornisch (*Lehrstuhl für Technische Mechanik, Technische Universität Kaiserslautern*)
Stefanie Elgeti (*Chair for Computational Analysis of Technical Systems (CATS), RWTH Aachen University*)

Intrinsically locking-free formulations for isogeometric beam, plate and shell analysis

Bastian Oesterle (*Institut für Baustatik und Baudynamik, Universität Stuttgart*), Simon Bieber (*Institut für Baustatik und Baudynamik, Universität Stuttgart*), Renate Sachse (*Institut für Baustatik und Baudynamik, Universität Stuttgart*), Ekkehard Ramm (*Institut für Baustatik und Baudynamik, Universität Stuttgart*), Manfred Bischoff (*Institut für Baustatik und Baudynamik, Universität Stuttgart*) 16:30–16:50

Isogeometric Analysis (IGA) [1] opened up a broad field of new concepts and applications in computational mechanics. Some key properties are smooth function spaces (e.g. B-splines, NURBS) and higher inter-element continuity. In earlier contributions within the group of authors [2, 3], transverse shear locking has been successfully removed for isogeometric beam, plate and shell elements by means of hierarchic concepts, which benefit from the higher inter-element continuity of NURBS. We want to emphasize that these finite elements rely on a primal (purely displacement based) formulation, whereas transverse shear locking is avoided intrinsically, i.e. on the level of theory rather than discretization.
Recent investigations [4] concern the construction of a novel mixed concept utilizing displacement-like variables only, thus called Mixed Displacement (MD) concept. It is a unified concept to treat all geometrical locking effects. Strong relations between hierarchic displacements, strain gaps from the DSG method [5] and the novel mixed displacement variables can be identified.
In this contribution we will present a class of formulations for beams, plates and shells avoiding locking, independent of the utilized discretization scheme. In particular, we will confirm this statement by several numerical tests using different smooth ansatz spaces, e.g. NURBS or meshless maximum entropy approximants. Furthermore, some applications to different solution schemes will be studied, i.e. weak form Galerkin-type solution and collocation based on the corresponding Euler-Lagrange equations of the boundary value problem. In all numerical studies the quality of both stress resultants and displacements will be investigated.

[1] T.J.R Hughes, J.A. Cottrell, and Y. Bazilevs. Isogeometric analysis: CAD, finite elements, NURBS, exact geometry, and mesh refinement. Computer Methods in Applied Mechanics and Engineering, 194, 4135-4195, 2005.

[2] R. Echter, B. Oesterle, M. Bischoff. A hierarchic family of isogeometric shell finite elements. Computer Methods in Applied Mechanics and Engineering, 254, 170-180, 2013.

[3] B. Oesterle, E. Ramm, M. Bischoff. A shear deformable, rotation-free isogeometric shell formulation. Computer Methods in Applied Mechanics and Engineering, 307, 235-255, 2016.

[4] S. Bieber, B. Oesterle, E. Ramm, M. Bischoff, A variational method to avoid locking -

independent of the discretization. International Journal for Numerical Methods in Engineering, submitted.

[5] K.-U. Bletzinger, M. Bischoff, E. Ramm, A unified approach for shear-locking-free triangular and rectangular shell finite elements. Computers and Structures, 75(3), 321-334, 2000.

Mixed isogeometric collocation methods

Simone Morganti (*University of Pavia*), Ferdinando Auricchio (*University of Pavia*), Carlo Callari (*University of Molise*), Laura De Lorenzis (*Technical University of Braunschweig*), John Andrew Evans (*University of Colorado Boulder*), Thomas JR Hughes (*University of Texas at Austin*), Alessandro Reali (*University of Pavia*) 16:50–17:10

Isogeometric Analysis (IGA) is a recent analysis framework aiming at bridging the gap between Computational Mechanics and Computer Aided Design (CAD). In addition to clear advantages in terms of geometry representation capabilities, the use of functions typically used by CAD systems (e.g., NURBS) leads to superior results with respect to standard finite elements on a per degree-of-freedom basis, thanks to their high regularity properties. In the framework of NURBS-based IGA, collocation methods have been recently introduced as an efficient and promising alternative to standard isogeometric Galerkin approaches, characterized by a high accuracy-to-computational-cost ratio. In this work, we study the approximation of incompressible elastic problems via isogeometric collocation. In particular, we introduce and discuss several mixed formulations and we present a number of numerical tests showing the behavior of the proposed methods. Moreover, we initiate the study of deformable fluid-saturated porous media. The combination of the superior accuracy and smoothness of spline basis functions with the low computational cost and simplicity of collocation techniques seems to constitute an optimal basis for accurately modeling complex and computationally demanding time-dependent problems expressed in mixed form, like those arising in the context of poroelastic media. In particular, we will focus on the one-dimensional application of the Biot model and present a mixed u-p formulation leading to very encouraging results.

Isogeometric Boundary Element Methods

Jürgen Dölz (*Graduate School CE & TEMF, Technische Universität Darmstadt*), Helmut Harbrecht (*Mathematik und Informatik, Universität Basel*), Stefan Kurz (*Graduate School CE & TEMF, Technische Universität Darmstadt*), Sebastian Schöps (*Graduate School CE & TEMF, Technische Universität Darmstadt*), Felix Wolf (*Graduate School CE & TEMF, Technische Universität Darmstadt*) 17:10–17:30

We will introduce the concept of boundary element methods and explain how they can be formulated within the framework of isogeometric analysis for different problems. Boundary element methods reformulate certain problems, where we will consider Laplace, Helmholtz, or Maxwell problems as examples, in terms of integral equations on the boundary of a given domain. The induced problem requires the approximation of a density on the boundary; which must be investigated in so-called trace spaces, i.e., spaces induced by restricting the corresponding volumetric spaces to the boundary in a limit sense. However, the induced norms on the boundary are non-local, which poses certain problems: The convergence of boundary methods on locally nonsmooth domains can be impaired globally. This behaviour will be explained and investigated, both numerically and analytically. Moreover, since in industrial applications geometries of interest are seldom smooth, we will discuss the utilisation of higher order methods on such problems. This will be done through a set of numerical experiments, where we compare both isogeometric and classical higher-order methods.

Acknowledgement: The work of Jürgen Dölz is supported by the Swiss National Science Foundation (SNSF) through the project H-Matrix Techniques and Uncertainty Quantification in Electromagnetism. The work of Felix Wolf is supported by DFG Grants SCHO1562/3-1 and KU1553/4-1, the Excellence Initiative of the German Federal and State Governments and the Graduate School of Computational Engineering at TU Darmstadt.

Isogeometric Analysis with Trimmed CAD Models

Benjamin Marussig (*Technische Universität Graz*) 17:30–17:50

The treatment of trimmed CAD models is a key challenge regarding the interaction of CAD and numerical simulations. These models are ubiquitous in current CAD since trimming procedures provide the basis for fundamental geometric operations such as surface-to-surface intersections. There are two essential problems: (i) trimming is primarily a visualization technique and (ii) it cannot be performed exactly. In other words, the related concepts are not designed for analysis purposes and lead to approximation errors within CAD models. The latter results in gaps and overlaps between the objects' surfaces. These inaccuracies are well-hidden from users, but can yield severe problems in isogeometric simulations, mesh generation, and other applications that receive CAD data [1].
The direct application of trimmed CAD models to an isogeometric analysis is presented. It is demonstrated that these models can lead to ill-conditioned system matrices. This issue is resolved by combining so-called extended B-splines [2] with a local refinement procedure [3]. The proposed approach modifies the spline basis in the vicinity of trimmed areas and can be applied Galerkin and collocation methods. The numerical examples are carried out by an isogeometric boundary element method.
This research is supported by the Austrian Science Fund (FWF): J3884-N32.

[1] Marussig and Hughes. A review of trimming in isogeometric analysis: Challenges, data exchange and simulation aspects. *ARCME* (2017).

[2] Höllig and Reif. Nonuniform web-splines. *CAGD* (2003).

[3] Giannelli, Jüttler, and Speleers. THB-splines: The truncated basis for hierarchical splines. *CAGD* (2012).

Nitsche's method for isogeometric thermo-mechanical contact problems

Alexander Seitz (*Institute for Computational Mechanics, Technical University of Munich*), Wolfgang A. Wall (*Institute for Computational Mechanics, Technical University of Munich*), Alexander Popp (*Institute for Mathematics and Computer-Based Simulation, Bundeswehr University Munich*) 17:50–18:10

This talk presents the application of Nitsche's method to finite deformation thermo-mechanical contact problems in the framework of isogeometric analysis. The isogeometric concept thereby proves to be beneficial in two ways: for once, contact mechanics relies on an accurate and, at best, smooth surface representation, which can be achieved using NURBS basis functions. The second advantage is related to Nitsche's method itself, which requires a consistent contact traction vector derived from the stress state of the underlying bulk discretization. In case of classical finite elements, this stress is discontinuous across element boundaries, thus resulting in a discontinuous approximation of the contact traction. Due to the higher inter-element continuity of NURBS basis functions, the contact traction becomes continuous in isogeometric analysis. In the present contribution, Nitsche's method will be applied to various constraints at the contact

interface, namely the non-penetration condition in normal direction, Coulomb's law of friction in tangential direction of the mechanical problem as well as heat conductivity and frictional heating introduced in the thermal field. Numerical examples demonstrate the optimal convergence rates achieved from the variationally consistent treatment of all interface conditions.

Weak imposition of constraints for multipatch membrane structures in transient geometrically nonlinear isogeometric analysis

Andreas Apostolatos (*Chair of Structural Analysis, Technical University of Munich*), Roland Wüchner (*Lehrstuhl für Statik, Technical University of Munich*), Kai-Uwe Bletzinger (*Lehrstuhl für Statik, Technical University of Munich*) 18:10–18:30

Membranes have been extensively used for the design of architectural and general structural models due to their low cost and high load capacity behaviour. Traditionally such models were discretized using the classical low order *Finite Element Method* (FEM) which typically results in a compromised description of the geometry. However the accurate geometry description of those structures is essential as for instance bifurcation points in geometrically nonlinear analysis may or may not be accurately predicted when the geometry description of the model is not accurate enough. In this contribution, the form-finding analysis using the *Updated Reference Strategy* (URS) and the geometrically nonlinear transient analysis of membranes is extended to multipatch *Isogeometric Analysis* (IGA) using *Non-Uniform Rational B-Splines* (NURBS). As typical in IGA for real CAD geometries, multiple patches with non-matching parametrizations are considered and therefore the continuity of the solution field and the application of weak Dirichlet boundary conditions need to be addressed. Thus, four different constraint enforcement methods are elaborated and compared, namely, the *Penalty*, the *Lagrange Multipliers*, the *augmented Lagrange Multipliers* and a *Nitsche*-type method. For the latter method, a solution dependent stabilization approach is employed in order to render the Nitsche-type method coercive. All methods are elaborated and systematically compared in both, form-finding analysis, whenever necessary, and subsequently in geometrically nonlinear transient analysis. The results suggest that the Nitsche-type method is advantageous for these kinds of problems as no parameter or discretization other than the isogeometric discretization of each patch needs to be specified prior to the analysis.

YR2 | Mechanics of porous cellular materials

Date	19.03.2018	16:30–18:30
Room	N1080	
Organiser	Anne Jung (*Saarland University*) Ameya Rege (*Department of Continuum Mechanics, RWTH Aachen University*)	

In-situ and ex-situ micromechanical testing of open-cell metal foams

Anne Jung (*Saarland University*), Jutta Luksch (*Technische Mechanik, Universität des Saarlandes*), Thomas Bleistein (*Technische Mechanik, Universität des Saarlandes*) 16:30–16:50

Metal foams are cellular materials with structural features resembling to lightweight load-bearing materials such as bones. Their high stiffness-to-weight-ratio coupled with their long flat stress-strain response make them ideal candidates as energy absorbers. Their macroscopic properties are strongly influenced by both the mechanical behaviour of single pores at the mesoscopic level and the struts and their structure at the microscopic length-scale based on a strong structure-property relationship. Whereas macroscopic mechanical characterisation is widespread, micromechanical characterisation and assessment of parameters on single struts is very limited. Micromechanical characterisation of individual struts is very challenging but an emerging field of research. The present contribution deals with the mechanical characterisation of open-cell foams on the meso and micro scale. In-situ and ex-situ micro compression and micro tensile tests respectively were conducted on individual pores as well as individual struts. X-ray computed tomography (CT) and a photogrammetric method were used to create 3D finite element models of the pores as well as the struts in order to perform numerical simulations. Furthermore, in-situ X-ray CT micro tensile tests and ex-situ micro tensile tests were conducted on individual struts. There is a large scattering in the micro material parameters deduced from individual strut. X-ray CT scans during micro tensile testing and ex-situ micro tensile tests performed on struts, where the local microstructure (blowholes, pores, cracks and intermetallic inclusions) was previously determined in CT scans, were performed. The scattering in the material parameters is largely connected to the occurring defects in the microstructure of individual struts.

Multiscale characterisation and simulation of open cell metal foams

Thomas Bleistein (*Lehrstuhl für Technische Mechanik, Universität des Saarlandes*), Anne Jung (*Lehrstuhl für Technische Mechanik, Universität des Saarlandes*), Stefan Diebels (*Lehrstuhl für Technische Mechanik, Universität des Saarlandes*) 16:50–17:10

The complex microstructure of open cell metal foams results in beneficial global material properties, like a good weight to force ratio, which make this special group of cellular materials interesting for several applications. Open cell metal foams are suitable for lightweight applications as well as for energy management systems.
The dependency of the entire samples mechanical behaviour on its microstructure induces the demand of experiments and simulations on different scales. Therefore, the characterisation is split into three different parts, which concern the micro-, meso- and the macroscale. All levels deal with different structures of the foam. The microscale deals with individual struts, the mesoscale with individual pores and the macroscale treats the whole sample. Hence, a couple of experiments are necessary to specify the material properties of open cell aluminium foams. On

the macroscopic level several tests with different load cases, such as pure torsion, pure tension or compression and the superposition of these loading conditions, are needed to obtain the yield surface for the different types of foams. The material parameters on the microscopic level can be identified by micro tensile tests and inverse calculations using a 3D model of the strut. The deviation of the simulation results and the experimental data is minimised by an optimisation. Thus, the used material parameters in the simulations are changed, until the numerical results match the experiments.
In this contribution the focus is the characterisation of open cell metal foams on different hierarchical levels.

Modeling and Simulation of the Coating Process on Open Porous Metal Foams

Christine Grill (*Lehrstuhl für Technische Mechanik, Universität des Saarlandes*), Anne Jung (*Lehrstuhl für Technische Mechanik, Universität des Saarlandes*), Stefan Diebels (*Lehrstuhl für Technische Mechanik, Universität des Saarlandes*) 17:10–17:30

Due to an increasing demand of energy and raw materials, resources should be used efficiently. Therefore, multifunctional materials and lighter constructions are needed, which can endure higher payloads. Cellular materials like metal foams are bionic materials consisting of nodes and struts. By a coating of the foam structure, the material properties per unit mass can be optimised. The metallic coating is done by electrodeposition. In consequence of the mass transport limitation inside the foam, there is an inhomogeneous coating thickness. To get a homogeneous coating thickness, in this project the factors influencing the electrochemical coating process are studied and simulated based on a coupled material model.
The electrodeposition process can be described by an ion source at the anode, the mass transport from anode to cathode and an ion sink at the cathode. The Forchheimer-extended Darcy equation is used to model the velocity distribution in the foam. The mass transport and the deposition process are characterised by the continuity equation with convection, diffusion, migration and a sink term.
In this project the factors influencing the coating thickness are investigated by numerical simulation to provide a homogeneous coating thickness. A material model coupling mass transport with electrodeposition is developed. A finite difference approach was used to simulate the velocity and the ion concentration distribution inside the foam. A one-sided coupling of the Darcy equation with the continuity equation is already considered. Different velocities, diffusion constants and linear deposition rates are studied by the simulation.

Multi-scale modeling of polysaccharide and protein based aerogels

Ameya Rege (*Department of Continuum Mechanics, RWTH Aachen University*), Mikhail Itskov (*Department of Continuum Mechanics, RWTH Aachen University*) 17:30–17:50

Polysaccharide and protein based aerogels are a class of highly porous organic aerogels, widely used in the biomedical industry. These aerogels are characterized by a cellular morphology and their macroscopic mechanical behavior is based on the mechanics of their cell wall fibrils. In our study, two models are presented. The compression model is based on the bending and compression of the cell wall fibrils [1]. Large deformations are accounted for by using the extended Euler-Bernoulli beam theory [2]. On the other hand, the tension model is based on the bending and stretching of the cell wall fibrils [3]. Under tension, aerogels only undergo small deformations. Accordingly, their behavior is captured using the standard Euler Bernoulli beam theory. The damage and failure mechanisms are based on the critical stresses generated in the cell wall fibrils. The network of microcells is defined using the pore size distribution data obtained via the Barrett-Joyner-Halenda (BJH) model. The model predictions are validated against experimental data.

This microcell based modeling idea is also extended to capture the effect of wetting on their mechanical response. Due to wetting, the water-filled pores provide impedance to the bending deformation of the cell walls. This resistance to deformation is modeled by Winkler-type of elastic foundation for the cell walls. The so resulting stiffness of the foundation is then correlated to the water content. A constitutive model is thus proposed, and its results are validated against experimental data.

[1] Rege A., Schestakow M., Karadagli I., Ratke L., and Itskov M. (2016) Micromechanical modelling of cellulose aerogels from molten salt hydrates. Soft Matter 12, 7079-7088.

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Homogenization of cellular solids for magneto-elastic properties.

Raghvendra Pratap Singh (*Applied Physics, Micromechanics Lab, University of Groningen*) 17:50–18:10

Smart magnetostrictive materials transform magnetic energy into mechanical energy and can be used as actuators. In magnetic shape memory alloy (MSMA) larger strains can be obtained, compared to conventional Joule-based magnetostrictive (JMS) materials, due to magnetic field-induced crystallographic changes. However, the strains obtained by MSMAs are still very small, due to the mismatch in crystal orientation between neighboring grains. Two recent developments have led to a profound increase in strains which enhanced the potential of magnetostrictive actuators considerably. First, the introduction of porosity has been shown to alleviate the constraints imposed by the mismatch between grains, leading to much larger strains in MSMA materials [1]. Similarly, bonded metal fibre networks have been demonstrated to generate appreciable strains with modest magnetic fields [2]. Second, polymeric materials containing magnetic nanoparticles have a much larger magneto-mechanical compliance than the conventional metallic systems and thus generate much larger strains, especially in low-dimensional configurations as beams and shells [3]. These two recent developments open the door for new applications, by exploiting the large magnetocompliance of highly-porous magnetic actuators.
Starting from a continuum formulation, we have recently developed a methodology to estimate the deflection and demagnetization field for a slender object in a uniform external magnetic field. We want to extend our developed model to simulate 2D regular hexagonal lattices and general 3D cellular solids. To do so, we will develop a homogenization method for the magneto-elastic properties of cellular solids.

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Simulation of PCM-Saturated Porous Solid Matrix for Thermal Energy Storage using the Phase-Field Method

Abdel Hassan Sweidan (*Institute of General Mechanics, RWTH Aachen University*), Yousef Heider (*Institute of General Mechanics, RWTH Aachen University*), Bernd Markert (*Institute of General Mechanics, RWTH Aachen University*) 18:10–18:30

In the underlying research project, a latent heat storage medium using a PCM-saturated highly conductive porous metal matrix is being studied. High porosity cellular metal foams are believed to be a promising material for enhancing the heat transfer performance of the PCMs due to their high surface area to volume ratio, ultra-light weight and relatively high thermal conductivity [1-2]. The heat transfer between the solid material and the PCM as well as the flow of the liquid PCM in the voids is modeled based on the volume-averaging method (macroscopic approach), taking into consideration the effect of natural convection and thermal expansion. The system is modeled using the finite element method, where the phase-field method (PFM) is employed to account for the phase change process. The PFM relies on the specification of the free energy density function and employs a phase-field variable that defines the states of the material (solid or liquid) [3], where it is considered a reliable method to simulate phase change problems on the macro scale.

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[2] Y. Zhao, C. Y. Zhao, Z. G. Xu, and H. J. Xu. Modeling metal foam enhanced phase change heat transfer in thermal energy storage by using phase field method. International Journal of Heat and Mass Transfer (2016) 170–181.

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YR3 | Non-standard mixed finite element schemes for solid mechanics

Date	19.03.2018	16:30–18:30
Room	N1179	
Organiser	Fleurianne Bertrand (*Fakultät für Mathematik, Universität Duisburg-Essen*) Friederike Hellwig (*Institut für Mathematik, Humboldt-Universität zu Berlin*)	

Supercloseness of a Least-Squares Finite Element Method for Elasticity

Fleurianne Bertrand (*Fakultät für Mathematik, Universität Duisburg-Essen*) 16:30–16:50

Least-squares FEM are an attractive class of methods for the numerical solution of partial differential equations, as the idea minimizing the L^2 residuals in the partial differential equations combines the advantages of the mixed FEM with the production of symmetric and positive definite discrete systems and an inherent a posteriori error indicator. The related physical equations in the context of linear elasticity are the equilibrium equation and the constitutive equation. To preserve the symmetry of the stress, a modified weak form obtained by introducing the vorticity in $L^2(\Omega)$. The new least-squares functional is shown to be elliptic and continuous in the $H(div,\Omega)^d \times H^1(\Omega)^d \times L^2(\Omega)$ norm, which leads to the optimal error estimates for its finite element subspaces. Due to the strong connection of the stress approximation to that obtained from a mixed formulation based on the Hellinger-Reissner principle, the error associated with momentum balance is proved (similarly to (2)) to be of higher order than the overall error for the least-squares approach. This implies that the favorable conservation properties of the dual-based mixed methods and the inherent error control of the least squares method can be combined.

(1) Z. Cai, G. Starke, *Least squares methods for linear elasticity.* SIAM J.Numer.Anal. (2004) 42:826-842

(2) J. Brandts, Y. Chen and J. Yang *A note on least-squares mixed finite elements in relation to standard and mixed finite elements.* IMA J.Numer.Anal. (2006) 26:779-789.

A Mixed finite element discretization for plate problems

Mira Schedensack (*Institut für Analysis und Numerik, Universität Münster*) 16:50–17:10

For fourth-order problems as they arise in plate theory, standard conforming finite element methods require ansatz spaces with high regularity. This leads to complicated ansatz functions and complex implementations in finite element programs. This talk will introduce a new mixed formulation based on a Helmholtz-type decomposition that reformulates the fourth-order problem as a second-order problem. This new formulation can then be discretized with standard Lagrange ansatz functions. This enables the disretization with lowest-order ansatz functions as well as the discretization with higher polynomials. This talk will also introduce a posteriori error estimators and will show some numerical results.

Phase-Field Modeling of Fracture in Variably Saturated Porous Media

Tuanny Cajuhi (*TU Braunschweig*), Lorenzo Sanavia (*University of Padova*), Laura De Lorenzis (*TU Braunschweig*) 17:10–17:30

Porous media consist of a solid skeleton and pores filled with fluids, e.g. air and water. Complex mechanisms of flow and transport take place within the pore network and can lead to deformation of the solid skeleton and eventually to fracture phenomena [1]. Phase-field modeling of fracture has recently emerged as an alternative to conventional approaches such as remeshing, extended finite element methods or cohesive zone modeling. The phase-field framework can be considered a special type of gradient damage modeling approach, where a diffusive approximation of the crack is taken into account and the continuous phase-field parameter is used to describe the material integrity. The essential advantages are the possibility to describe arbitrarily complicated fracture patterns such as nucleation, branching and merging, without ad-hoc criteria on a fixed mesh, through the solution of partial differential equations derived from variational principles [2, 3, 4, 5]. Phase-field modeling of fracture in porous media has been addressed in some recent publications [6, 7], which however have only focused on the fully saturated case. Objective of this contribution is to describe fracture in partially saturated porous media using a phase-field approach [8]. In this study, the material is described by its linear-elastic properties. The overall balance of linear momentum, the continuity equation and the phase-field evolution equation constitute a nonlinear coupled and time-dependent system of equations, which needs to be discretized and linearized. We formulate the coupled non-linear system of partial differential equations governing the problem with displacements, capillary pressure and crack phase-field as unknowns. The spatial discretization is carried out with finite elements of appropriate order for the different unknowns. We discuss its solution and present some relevant examples related to soils and cement-based materials.

[1] L. Simoni, B.A. Schrefler, Multi field simulation of fracture. *Advances in Applied Mechanics*, 2014.

[2] B. Bourdin, G.A. Francfort, J-J. Marigo, Numerical experiments in revisited brittle fracture. *Journal of the Mechanics and Physics of Solids*, **48**, 797-826, 2000.

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[5] M. Ambati, T. Gerasimov, L. De Lorenzis, A review on phase-field models of brittle fracture and a new fast hybrid formulation. *Computational Mechanics* **55**, 383-405, 2014.

[6] A. Mikelić, M.F. Wheeler, T. Wick, A phase-field method for propagating fluid-filled fractures coupled to a surrounding porous medium. *SIAM Multiscale Modeling and Simulation* **13(1)**, 367-398, 2014.

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[8] T. Cajuhi, L. Sanavia , L. De Lorenzis Phase-field modeling of fracture in variably saturated porous media. *Journal of the Computational Mechanics*, in print, 2017.

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Numerical Simulation of Crack Propagation in an anisotropic medium

Carola Bilgen (*Maschinenbau, Universität Siegen*), Paul Hennig (*Technische Universität Dresden*), Markus Kästner (*Technische Universität Dresden*), Kerstin Weinberg (*Universität Siegen*) 17:30–17:50

Phase-field methods have been proven to address the main challenges in fracture mechanics – the identification of crack initiation and the simulation of the unknown crack paths – in an elegant way. The approach has therefore become very popular recently. Our contribution sets the focus on different ways to capture anisotropy in the phase-field model.
In order to deal with the tension-compression anisotropy in fracture problems, a suitable operator split has to be deduced to take only the tensile deformations, which lead to crack growth, into account. In general, the strain energy function can be written in terms of principal stretches or principal invariants. A comparison of different anisotropic splits is demonstrated in the context of both, finite and linearized strains. Furthermore, energetic and stress based fracture criterions are considered and checked against each other in more detail.
Additionally, material anisotropy is examined within the phase-field approach. Basis of this ansatz is an operator-scaling anisotropic random field to consider the microstructure of the material implicitly, proposed by [1], which is applied here on the fracture phase-field method. The models are studied within a series of suitable numerical examples.

[1] D. Anders, A. Hoffmann, H.-P. Scheffler and K. Weinberg. Application of operator-scaling anisotropic random fields to binary mixtures. *Philosophical Magazine*, 91, No. 29, 3766–3792, 2011.

A discontinuous skeletal method for Bingham fluids

Karol Cascavita (*Université Paris-Est, CERMICS (ENPC) and INRIA Paris*), Jérémy Bleyer (*NAVIER, UMR 8205, École des Ponts, IFSTTAR, CNRS, UPE.*), Xavier Chateau (*NAVIER, UMR 8205, École des Ponts, IFSTTAR, CNRS, UPE.*), Alexandre Ern (*Université Paris-Est, CERMICS (ENPC) and INRIA Paris.*) 17:50–18:10

Keywords: *Discontinuous Skeletal methods, Viscoplastic flows, Augmented Lagrangian methods*

This work is motivated by the growing interest in the simulation of yield stress fluids for civil engineering materials, blood, foams, etc. To this aim, we propose a Discontinuous Skeletal (DiSk) method for the antiplane Bingham model, inspired by the Hybrid-High Order method introduced in [1] for linear elasticity. In particular, we focus on the lowest order case, where discrete velocity unknowns are constant polynomials: one per cell and one per face, and the cells unknowns are eliminated by static condensation. The main advantages are local conservativity and the possibility to use general meshes. We consider the Augmented Lagrangian method to solve the variational inequalities resulting from the discrete Bingham problem. We introduce constant Lagrange multipliers for the velocity gradient in each cell and for its jumps at each face. In comparison to Finite Element Methods, such as the use of Taylor-Hood elements [2], a crucial advantage of DiSk methods is that polytopal meshes are supported. We can exploit their use in performing local mesh adaptation, either locally refining around liquid-solid interfaces or coarsening in the solid regions. Numerical results are presented for circular and square domains and for different Bingham numbers. We show local adaptation can be exploited and the method is shown to capture regions of sharp transition between solid- and fluid-like regimes.

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[2] P. Saramito and N. Roquet. An adaptive finite element method for viscoplastic fluid flows in pipes. *Comput. Meth. Appl. Mech. Eng.*, Vol. **190**, pp 5391 -5412, 2001.

Optimal Convergence Rates in dPG for Elasticity

Friederike Hellwig (*Institut für Mathematik, Humboldt-Universität zu Berlin*), 18:10–18:30
Carsten Carstensen (*Institut für Mathematik, Humboldt-Universität zu Berlin*)

The discontinuous Petrov-Galerkin methodology enjoys a built-in a posteriori error control in some computable residual term plus data approximation terms. This talk establishes an alternative error estimator, which is globally equivalent, but allows for the proof of the axioms of adaptivity and so guarantees optimal convergence rates of the associated adaptive algorithm. The talk exemplifies the analysis for the Poisson model problem $-\Delta u = f$ with a right-hand side f in $L^2(\Omega)$ in the polyhedral domain Ω simultaneously for the four lowest-order discontinuous Petrov-Galerkin schemes. Those and a low-order ultraweak scheme for linear elasticity are rewritten in terms of the first-order nonconforming Crouzeix-Raviart functions $CR^1_0(\mathcal{T})$ and its conforming subspace $S^1_0(\mathcal{T})$, with respect to a shape-regular triangulation $\mathcal{T}$ into simplices, some projection $Q : L^2(\Omega) \to L^2(\Omega)$ and a parameter α.
For solutions $(v_{CR}, u_C) \in CR^1_0(\mathcal{T}) \times S^1_0(\mathcal{T})$ to this reduced mixed system, the novel error estimator $\eta(T)$ consists of the expected volume contributions $|T|^{1/n} \, \|f - \alpha Q v_{CR}\|_{L^2(T)}$ and the jump terms of the piecewise gradient of v_{CR} across the sides of any simplex $T \in \mathcal{T}$. The estimator exclusively involves the variable v_{CR} and seemingly ignores the conforming contribution u_C, but surprisingly also controls the error term $u - u_C$. The optimal convergence rates rely on standard arguments for stability and reduction, while the discrete reliability involves an additional term $h_0 \, \eta(\widehat{\mathcal{T}})$ for an admissible refinement $\widehat{\mathcal{T}}$ of $\mathcal{T}$; this eventually enforces the additional condition of a sufficiently small initial mesh-size h_0 for optimal convergence rates.

YR4 | Optimal design and control of multibody systems

Date	19.03.2018	16:30–18:30
Room	N1189	
Organiser	Karin Nachbagauer (*University of Applied Sciences Upper Austria, Campus Wels*) Alexander Held (*Hamburg University of Technology*)	

Design and Optimization of Large-Deformation Compliant Mechanisms

Alexander Humer (*Institut of Technical Mechanics, Johannes Kepler University Linz*) 16:30–16:50

As compared to conventional mechanisms, compliant mechanisms exploit flexible deformation rather than rigid body motion of its components. The key advantage of jointless structures lies in the absence of relative motion between the links. Besides the reduction in parts required to perform a task, compliant mechanisms typically show little friction, if any, and do not require lubrication to minimize wear. On the downside, design and synthesis of compliant mechanisms becomes more involved than with rigid-body linkages. In particular, optimization of compliant mechanisms relying on (sub-)structures subjected to large flexible deformation is a challenging task, in which several, possibly conflicting aspects need to be considered. First and foremost, kinematic analysis of compliant mechanisms usually requires geometric non-linear to be accounted for. Further, limitations in actuation forces and torques impose constraints on the design. Depending on the application, the performance of compliant mechanisms may crucially depend on the natural frequencies and their change over the range of operation. In view of the diverse aspects, we typically have to deal with multi-objective optimization problems in comparatively high-dimensional parameter spaces. In the present paper, we outline our approach for the design of compliant mechanisms based on flexible multibody systems and evolutionary optimization.

Large-Scale Gradient Computation in Flexible Multibody Systems

Ali Moghadasi (*Mechanik und Meerestechnik, Hamburg University of Technology*), Alexander Held (*Hamburg University of Technology*), Robert Seifried (*Hamburg University of Technology*) 16:50–17:10

In the analysis and optimization of flexible multibody systems, the gradient computation is often a necessary step. Considering a gradient-based optimization of a flexible multibody system, the sensitivity of an objective function with respect to the design variables is required. The gradient computation is based on the complete time-dependent solution of the flexible multibody system, and is a computationally expensive step. Therefore, in many of the previous works on optimization of multibody systems, only low dimensional optimization problems have been considered. For systems where the number of design variables is high, for instance, in topology optimization, the computational cost becomes unfeasible in the sense of time and resources. As a result, the size of dynamic topology optimization problems has been strongly limited. This work addresses the efficient and fast gradient computation for systems with a high number of design variables. In this framework, first the automatic detection and elimination of negligibly small derivation terms are introduced, which increases the computational efficiency without deteriorating the accuracy of gradients. Second, the parallelization of the gradient computation is discussed. Both approaches are tested on the application example of a flexible 3D slider-crank mechanism which is optimized using a gradient-based topology optimization method. With the parallelization and the introduced elimination of negligible terms in the gradients, it is shown

that the gradient computation can be carried out in a feasible time with respect to more than 100000 design variables.

Constrained Structural Optimization of Dynamic Mechanical Systems

Alexander Held (*Institute of Mechanics and Ocean Engineering, Hamburg University of Technology*), Thomas Kohlsche (*Institute of Modelling and Computation, Hamburg University of Technology*) 17:10–17:30

The method of flexible multibody systems is a well-established way to model and analyze mechanical systems, whose components undergo both large rigid-body motions and deformations. The simulation models can be used not only to determine the dynamic loads on the components but also in simulation-based optimization. For instance, in structural optimization, the objective is often to find an optimal lightweight design of the components which shows no undesired vibrations or deformations under the dynamical loads. Considering the full dynamic system in the optimization, a large, nonlinear, and continuous optimization problem must be solved. It has been shown, that gradient-based optimization algorithms in combination with a dual method are an efficient way to tackle these optimization problems, as long as the number of constraints remains small. Stress and deformation constraints, however, have to be satisfied at each point of the body and, for dynamic systems, also at each time point. Therefore this talk aims to present two different aggregation strategies to consider time- and space-dependent constraints in the optimization of flexible multibody systems. On the one hand, an equivalent integral formulation is used to transform a set of inequality constraints into one equality constraint. On the other hand, a conservative approximation from all inequality constraints is derived using the Kreisselmeier-Steinhauser function. Both approaches are tested by means of a flexible slider-crank mechanism, whose piston rod is optimized using topology optimization.

Optimization based muscle wrapping in biomechanical multibody simulations

Johann Penner (*Chair of Applied Dynamics, University of Erlangen-Nuremberg*), Sigrid Leyendecker (*Chair of Applied Dynamics, University of Erlangen-Nuremberg*) 17:30–17:50

Biomechanical simulation based on multibody systems representing the skeleton and actuation by Hill-type muscle models is established as a major tool for investigating human motion. In addition to the activation level, typically, muscle models depend on the muscle length, contraction velocity and a force direction depending on the dynamics of the skeleton motion. In particular, the muscle force direction is influenced by the muscle path. The anatomical structure of the human body commonly forces muscles to wrap around obstacles such as bones and neighboring tissue, thus most muscle paths cannot be represented adequately as straight lines. Assuming that the muscles are always under tension, their path is often modelled as a locally length minimizing curve between their origin and insertion points [1].
This work is based on a mechanical analogue to find the shortest path on general smooth surfaces, using a discrete variational principle. In this context, the geodesic path is reinterpreted as the force-free motion of a particle in n dimensions, under holonomic constraints. The muscle path is then a G1-continuous combination of geodesics on adjacent obstacle surfaces. It can be described as a shortest path boundary value problem with G1-continuous transitions [1, 2, 3].
Using also discrete variational calculus to describe the dynamics [4] yields the advantage of a unified treatment for the complete musculoskeletal system. The resulting discrete Euler-Lagrange equations are a coupled equation system that can be solved for the skeleton and muscle path simultaneously. This is of particular importance in optimal control simulations, where inner optimizations for the muscle paths lead to very expensive computational costs and need to be

avoided. In the given form, the formulation avoids such nested loops and is well suitable to be used in an optimal control framework based on a direct discretization technique for mechanical systems, known as DMOCC (Discrete mechanics and optimal control for constrained systems [5]).

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Parameter Identification in Multibody Systems in Frequency Domain using Adjoint Fourier Coefficients

Karin Nachbagauer (*University of Applied Sciences Upper Austria, Campus Wels*), Stefan Oberpeilsteiner (*University of Applied Science Upper Austria, Campus Wels*), Thomas Lauß (*University of Applied Science Upper Austria, Campus Wels*), Wolfgang Steiner (*University of Applied Science Upper Austria, Campus Wels*)

17:50–18:10

The field of optimal design of multibody systems often includes an inverse problem to solve, as e.g. the parameter identification in an engineering multibody application. The inverse problem could be defined as an optimization task described by minimizing a cost function. The gradient of this cost function can be computed very efficiently also in complex multibody systems when incorporating the adjoint method.
In case of the identification of parameters in oscillating multibody systems, a combination of a Fourier analysis and the adjoint method is a promising approach. In most cases of the classical adjoint method in time-domain, the results lead to some kind of best-fit solution which means that high frequency components with low amplitudes are not considered. However, the identification of parameters which influence the system at particular frequencies or frequency ranges is an important issue. The basic idea is to compute the Fourier coefficients for the relevant oscillations and include the according amplitudes in the cost function. Now, spectral data from a test bench can be used to identify the amplitude response.
In order to reduce computational effort, the cost function is rewritten here from the classical Lagrange form to Mayer form leading to constant adjoint Fourier coefficients. This powerful combination of the Fourier analyses and the adjoint method for the computation of the cost function in Mayer form is presented here.

Identification of a nonlinear spring and damper characteristics of a motorcycle suspension using test ride data

Thomas Lauß (*Josef Ressel Zentrum für innovative Mehrkörperdynamik, University of Applied Sciences Upper Austria*), Dominik Sterl (*University of Applied Sciences Upper Austria*), Stefan Oberpeilsteiner (*University of Applied Sciences Upper Austria*), Wolfgang Steiner (*University of Applied Sciences Upper Austria*)

18:10–18:30

During test rides of motorcycles modifications are made to the suspension. In order to quantify this changes, the nonlinear spring and damper characteristics must be determined. However, it is not always possible to perform measurements of the suspension on a test bench. Hence, a parameter identification after a test run, formulated as an optimization task, seems to be an auspicious approach. For this purpose, a cost function is defined, which is minimized by considering the dynamics of the system. The strength of the contribution is the efficient gradient computation using the adjoint variable approach. In order to approximate the nonlinear spring and damper characteristic cubic splines are used. The values of the spline functions at specified grid points are adjusted such that the deviation between simulation and measurement is minimal. As an example we consider the rear suspension of a KTM motorcycle with given measured data from a test ride. The nonlinear spring and damper characteristics are described by cubic splines with nine parameters to identify in total. After a number of iterations, the cost function cannot be further reduced, and the optimal set of parameters leads to acceptable accordance of the measured and simulated displacements in the chosen time interval.

YR5 | Variational aspects of multiscale modelling in materials science

Date	19.03.2018	16:30–18:30
Room	N1190	
Organiser	Elisa Davoli (*Universität Wien*)	
	Manuel Friedrich (*Universität Wien*)	

Optimal Design for mixtures of ferromagnetic interactions

Leonard Kreutz (*Mathematics, University of Vienna*), Andrea Braides (*Mathematics, Tor Vergata University of Rome*) 16:30–16:50

We present a general framework for the optimal design of surface energies on networks. We give sharp bounds for the homogenization of discrete systems describing mixtures of ferromagnetic interactions by constructing optimal microgeometries, and we show that there holds a localization principle which allows to reduce to the periodic setting in the general non-periodic case. Furthermore we discuss the issue of crystallinity of the homogenized energy densities of spin systems in the periodic setting. This is joint work, in progress, with Andrea Braides and Antonin Chambolle.

Free energies on stochastic lattices

Marco Cicalese (*TU Munich*), Antoine Gloria (*Université Pierre et Marie Curie Paris VI*), Matthias Ruf (*Université libre de Bruxelles*) 16:50–17:10

We study the asymptotic behavior of large volume Gibbs measures associated with discrete Hamiltonians that are defined on deformations of a stationary stochastic lattice. Assuming polynomial growth and finite range interactions for the discrete Hamiltonian, we prove a large deviation principle with a continuum elasticity-type rate functional. We then investigate this functional in the small temperature regime. Under suitable continuity assumptions on the microscopic Hamiltonian, we show that there exists a zero temperature limit that coincides with the Γ-limit of the rescaled discrete Hamiltonians.

Long-range elastic fields induced by crystal defects

Julian Braun (*University of Warwick*) 17:10–17:30

Classically, deformations around crystal defects are approximated with linear elasticity theory. In my talk, I will give precise decay rates on the remaining error far away from the defect core in this approximation and, more importantly, present higher order approximations. This more precise understanding of the far-field of the deformation is not just of analytical interest but also gives rise to greatly improved computational methods by providing very accurate boundary conditions.

Gradient estimates for homogenization of nonlinear elasticity under small loads

Mathias Schäffner (*Institute of scientific computing, TU Dresden*), Stefan Neukamm (*TU Dresden*) 17:30–17:50

We consider a nonlinear elastic composite with a periodic micro-structure described by the non-convex integral functional

$$I_\varepsilon(u) = \int_\Omega W\left(\frac{x}{\varepsilon}, \nabla u(x)\right) - f(x) \cdot u(x)\, dx.$$

As it is well-known, under suitable growth conditions, I_ε Γ-converges to a functional with a homogenized energy density $W_{\text{hom}}(F)$, which is given by an *infinite-cell formula*. Under appropriate assumptions on W (e.g. frame indifference, minimality at identity, non-degeneracy and smoothness in a neighborhood close to the set of rotations) and on the microstructure (e.g. matrix material and a finite number of smooth but possibly touching inclusions), we show that in a neighbourhood of rotations the homogenized stored energy function W_{hom} is characterized by a *single-cell homogenization formula*. For this, we combine the construction of a matching convex lower bound and Lipschitz-estimates for sufficiently small solutions of nonlinear elliptic systems with piecewise smooth coefficients that depend on the shape and the size of the surfaces of discontinuity but are independent of the distance between these surfaces.
Moreover, for small and well-prepared data, we establish existence and uniform Lipschitz estimates for minimizers of I_ε and establish a quantitative two-scale expansion.

Asymptotic rigidity for layered materials and its applications in elastoplasticity

Fabian Christowiak (*Fakultät für Mathematik, Universität Regensburg*), Carolin Kreisbeck (*Department of Mathematics, Universiteit Utrecht*) 17:50–18:10

In elastic composite materials, the stiffness of single components can be a decisive factor for the overall material response. Focusing ourselves on the case of fine bilayered structures we study the effective macroscopic behavior as the layer thickness tends towards zero in a variational setting. In particular, our interest lies in the question of optimal scaling relations between the thickness and the stiffness of the layers.
Since common rigidity results such as Reshetnyak's theorem - a generalization of the Liouville theorem, which says that every local isometry of a domain corresponds to a rigid body motion - only apply to connected sets, our layered geometry calls for a new type of asymptotic rigidity lemma. For sufficiently stiff layers, this result states that macroscopically the only locally volume preserving deformations are globally rotated shear deformations in layer direction. The optimality of the scaling is shown by suitable bending constructions.
This result is key to determine explicitly the homogenized Γ-limits for models of bilayered materials, as we demonstrate on two models in nonlinear elasticity and in finite crystal plasticity. In particular, we illustrate how asymptotic ridigity leads to an essentially one-dimensional character of the problem that allows to overcome the issue of localization.

A density result in GSBD^p with applications to the approximation od brittle fracture energies

Antonin Chambolle (*Ecole polytechnique-CMAP*), Vito Crismale (*CMAP, École Polytechnique*) 18:10–18:30

The space $GSBD$ and its subspaces $GSBD^p$, with $p > 1$, have been introduced in 2012 by Dal Maso as the most general spaces of displacements for brittle fracture models in small-strain assumption. More precisely, $GSBD^p$ is the natural domain for the so-called 'Griffith energy with p-growth in the bulk', and every function in $GSBD^p$ represent a displacement whose corresponding deformation is p-integrable. With Antonin Chambolle we have recently proven that every u in $GSBD^p$ is approximated, in the sense of 'Griffith energy with p-growth in the bulk', by functions whose jump sets are smooth and which are smooth outside their jump set. The result holds for any $p > 1$ and under general assumptions on the 'reference configuration' Ω, that can be a n- dimensional set with finite perimeter, for n generic. As an application we prove the Γ-convergence approximation à la Ambrosio-Tortorelli of brittle fracture energies with Dirichlet boundary conditions by suitable phase-field energies.

DFG Priority Programmes

DFG-PP1748 | Reliable simulation techniques in solid mechanics. Development of non-standard discretization methods, mechanical and mathematical analysis

Date 20.03.2018 14:00–16:00
Room N1070
Organiser Jörg Schröder (*Universität Duisburg-Essen*)

Similarities between the discontinuous Galerkin approach and reduced integration methods

Stefanie Reese (*Institute of Applied Mechanics, RWTH Aachen University*), Hamid Reza Bayat (*RWTH Aachen University*), Stephan Wulfinghoff (*RWTH Aachen University*) 14:00–14:20

Discontinuous Galerkin methods and the methods of reduced integration with hourglass stabilization have a different origin. Whereas the discontinuous Galerkin idea was first introduced to solve hyperbolic PDEs, the reduced integration technology started out from the observation of the locking problem in the limit of incompressibility - in the context of elliptic PDEs. Today, the “discontinuous Galerkin" and the “reduced integration” communities are still disjunct from each other although it has already been recognized that discontinuous Galerkin methods can be also used to circumvent locking phenomena in elasticity (see e.g. [1,2])
The idea of the present contribution is to find a direct equivalence between a method of discontinuous Galerkin (see [3,4]) and reduced integration with hourglass stabilization [5,6]. The transfer between the two methods is carried out in the context of finite elasticity. Thus arbitrarily large deformations can be applied. It is easily seen that also inelastic material behaviour with large deformations could be cast into the new concept. The main advantage is that the choice of the “free” parameter θ in Nitsche’s method is no longer unclear but uniquely determined by the connection to the hourglass stabilization. Further important in this context is the replacement of the scalar parameter θ by a symmetric 2 x 2 matrix (if two-dimensional problems are considered which is here the case).
The result of the derivation is a very strong finite element technology which shows very good convergence behaviour - not only in the limit of incompressibility but also for bending of thin structures.

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[2] Y. Shen and A. J. Lew. A locking-free and optimally convergent discontinuous-Galerkin-based extended finite element method for cracked nearly incompressible solids, *Computer Methods in Applied Mechanics and Engineering*, 273: 119-142, 2014.

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Mesh adaptivity for variational phase-field fracture problems

Thomas Wick (*Institut für Angewandte Mathematik, Leibniz Universität Hannover*) 14:20–14:40

In this presentation, we consider phase-field fracture propagation in solid mechanics. The main purpose is the development of robust and efficient schemes for local mesh adaptivity. Using phase-field fracture, a smoothed indicator function determines the crack location and is characterized through a model regularization parameter. In addition, modeling assumes that the fracture can never heal, which is imposed through a temporal constraint, leading to a variational inequality system. The present work focuses now on the interplay of the model regularization parameter and the spatial mesh size parameter and consequences on spatial mesh adaptivity. First, this is accomplished for propagating fractures in terms of a predictor-corrector scheme. Second, goal functionals are evaluated for stationary settings by emloying a partition-of-unity dual-weighted residual estimator. Our developments are substantiated with several numerical tests and are the basis for future extensions towards quasi-stationary and time-dependent cases as well as different solid models.

Modelling of Ductile Fracture by a Phase Field Approach

Ralf Müller (*Institute of Applied Mechanics, University of Kaiserslautern*), Timo Noll (*Institute of Applied Mechanics, University of Kaiserslautern*), Charlotte Kuhn (*Computational Mechanics, University of Kaiserslautern*) 14:40–15:00

A phase field model for ductile fracture with linear isotropic hardening is proposed. In phase field models a scalar valued order parameter describing the state of material in terms of fracture on a fixed finite element mesh constitutes a fundamental advantage compared to conventional fracture models where cracks are described by sharp surfaces and remeshing techniques are necessary to adapt the mesh to new crack topologies.
The model is based on an energy functional with an elastic energy contribution, a plastic dissipation potential and a Griffith type fracture energy. The coupling between crack field and displacement fields, which serve as independent variables, is established by a degradation function reducing the stiffness of the material and the plastic contribution of the energy density in broken material. This type of coupling allows for the application of an unaltered radial return algorithm, to compute the plastic update on the element level. Furthermore, a monolithic iterative solution scheme is feasible to solve the global system of differential equations formed by the transient approximation of the quasi-static evolution equation of the fracture field and the mechanical field equations.
In a 1D analysis the choice of the degradation function and the meaning of the fracture resistance, a model parameter stemming from the underlying brittle fracture model, are investigated in context of ductile fracture e.g. regarding the fracture strain. To which extend the findings of the 1D analysis can be transferred to the 3D case is investigated in numerical examples.

Analysis and simulation for a phase-field fracture model at finite strains based on modified invariants

Marita Thomas (*WIAS Berlin*), Carola Bilgen (*University of Siegen*), Kerstin Weinberg (*University of Siegen*) 15:00–15:20

Phase-field models have already been proven to predict complex fracture patterns in two and three dimensions for brittle fracture at small strains. Here, we discuss a model for phase-field fracture at finite deformations in more detail: We here present a phase-field model at finite strains, which takes into account the anisotropy of damage by applying an anisotropic split and the modified invariants of the right Cauchy-Green strain tensor. We introduce a suitable weak notion of solution that also allows for a spatial and temporal discretization of the model. In this framework we study the existence of solutions and we show that the time-discrete solutions converge in a weak sense to a solution of the time-continuous formulation of the model. Numerical examples in two and three space dimensions are presented.

A novel Hellinger-Reissner type Mixed Finite Element for Elasticity

Nils Viebahn (*Institute of Mechanics, Department of Civil Engineering, University of Duisburg-Essen*), Karl Steeger (*Vertex Antennentechnik GmbH*), Jörg Schröder (*Institute of Mechanics, Department of Civil Engineering, University of Duisburg-Essen*) 15:20–15:40

Locking is a well known problem of the primal finite element method in the framework of elasticity [1]. The mixed finite element method is a promising approach to circumvent volume locking. Unfortunately the construction of stable finite elements with exact symmetric stresses can only be realized with high polynomial order interpolation. Weakening the symmetry constrain allows for lower order approaches, e.g. [2]. However, these methods need additional degrees of freedom in order to enforce stress symmetry in a weak sense.
In the proposed work, a low order finite element based on a Hellinger-Reissner formulation with weak enforcement of the stress symmetry is presented. The novel element gets along without any additional degrees of freedom beside the displacements and stresses. Therein, lowest order Raviart-Thomas interpolation is utilized for the stresses and a C^0-continuous polynomial interpolation of first order is adopted for the displacements. This combination leads to a very efficient and robust element formulation which will be depicted in a couple of numerical examples.

Acknowledgment

The authors acknowledge support by the Deutsche Forschungsgemeinschaft in the Priority Program 1748 "Novel finite elements - Mixed, Hybrid and Virtual Element formulations at finite strains for 3D applications" (SCHR 570/23-2).

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[2] D.N. Arnold, F. Brezzi, J. Douglas, *PEERS: A New Mixed Finite Element for Plane Elasticity*, Japan J. Appl. Math, vol. **1** (1984), 347-367.

Weakly symmetric stress reconstruction and a posteriori error estimation for elasticity

Fleurianne Bertrand (*Universität Duisburg-Essen*), Bernhard Kober (*Universität Duisburg-Essen*), Marcel Moldenhauer (*Universität Duisburg-Essen*), Gerhard Starke (*Universität Duisburg-Essen*) 15:40–16:00

By following the framework given in [1] and [2] we were able to reconstruct weakly symmetric stresses for the nonconforming P2 finite element method of linear elasticity. We successfully derived an a posteriori error estimator which gave us a completely computable upper bound of the error [3].
We introduce a more general framework of weakly symmetric stress reconstruction and a posteriori error estimation with respect to Taylor-Hood Elements. First we want to show results for linear elasticity in the compressible and incompressible limit.
Afterwards we extend this idea to hyperelastic material models based on [4].

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[3] F. Bertrand, M. Moldenhauer, G. Starke, A posteriori error estimation for planar linear elasticity by stress reconstruction, *in review*, *available at: https://arxiv.org/abs/1703.00436*

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DFG-PP1798 I Compressed sensing in information processing (CoSIP)

Date	20.03.2018	14:00–16:00
Room	N1080	
Organiser	Gitta Kutyniok (*Mathematik, Technische Universität Berlin*) Rudolf Mathar (*Institute for Theoretical Information Technology, RWTH Aachen University*)	

Bilinear Compressed Sensing

Jakob Geppert (*Insittute for Numerical and Applied Mathematics, Georg-August-University of Göttingen*), Peter Jung (*TU Berlin*), Felix Krahmer (*Mathematics, Technische Universität München*), Dominik Stöger (*Mathematics, Technische Universität München*) 14:00–14:40

A number of problems in signal processing are well respresented by a bilinear measurement model. In wireless communication, for example, one can assume that the received signal depends linearly on the transmitted signal and the channel parameters. In this talk we give an overview over recent progress in analyzing recovery from such bilinear measurements from a compressed sensing perspective. That is, our aim is to show that in a generic setup, the problem behaves better than what can be expected in the worst case. More concretely, we discuss near-optimal recovery guarantees for demixing and deconvolution and present an improved initialization analysis for the sparse power factorization algorithm.

The role of compressed sensing in wireless communications

Giuseppe Caire (*EECS, TU Berlin*) 14:40–15:00

In this talk, I will review a number of wireless communication technologies that are expected to form the backbone of the forthcoming 5th generation of wireless networks, and show how compressed sensing or, more in general, compressed sensing-inspired approaches, can lead to very efficient solutions to some important problems related to these technologies. In particular, I will consider massive MIMO with hybrid digital-analog beamforming (with application to mmwave communications), and massive MIMO for frequency-division duplexing systems, where the downlink channel must be explicitly learned by the users via downlink common training and sent back in the form of uplink feedback.

Sparse Recovery using Denoising Autoencoders

Martin Klaus Rohbeck (*Institute for Theoretical Information Technology, RWTH Aachen*), Arash Behboodi (*RWTH Aachen University*), Rudolf Mathar (*Institute for Theoretical Information Technology, RWTH Aachen University*) 15:00–15:20

During recent years, deep learning architectures offered significant performance improvements compared to other machine learning and signal processing methods in tasks like pattern recognition and natural language processing. However it is not clear whether they can perform equally well in other signal processing tasks. In this work, we apply neural network architectures in the context of compressed sensing theory with the main goal of providing further insights to the success of deep learning architectures, particularly when they are applied to a problem with a well know theoretical background. It is investigated whether neural networks are capable of approximating the compressed sensing decoder, namely ℓ_1 minimization, and even improving it

by adapting to a dataset with additional implicit structure. Denoising autoencoders with their encoder-decoder structure are used for sparse recovery problem. The effect of gradient-based training is additionally investigated on the sensing matrix with different initialization methods and different training methods. Using this parallel to compressed sensing theory, theoretical insights are provided for the neural network design.

l1-Analysis Minimization and Generalized (Co-)Sparsity: When Does Recovery Succeed?

Maximilian März (*Mathematik, Technische Universität Berlin*), Martin Genzel (*Mathematik, Technische Universität Berlin*), Gitta Kutyniok (*Mathematik, Technische Universität Berlin*) 15:20–15:40

This talk addresses the problem of signal estimation from undersampled sub-Gaussian measurements under the assumption of a cosparse model. Based on generalized notions of sparsity, we derive novel recovery guarantees for the ℓ_1-analysis basis pursuit, enabling accurate predictions of its sample complexity. The corresponding bounds on the number of required measurements do explicitly depend on the Gram matrix of the analysis operator and therefore particularly account for its mutual coherence structure. Our findings defy conventional wisdom which promotes the sparsity of analysis coefficients as the crucial quantity to study. In fact, this common paradigm seems to break down in many situations of practical interest, for instance, when applying a redundant (multilevel) frame as analysis prior. By a series of numerical experiments, we demonstrate that, in contrast, our theoretical sampling-rate bounds reliably capture the true recovery performance of various examples, such as redundant Haar wavelets systems, total variation, or random frames. Due to a novel localization argument, it turns out that the presented framework naturally extends to stable recovery, allowing us to incorporate compressible coefficient sequences as well.

Trade-offs in Compressed Sensing with Multi-Bit Quantization

Lars Palzer (*Institute for Communications Engineering, Technische Universität München*), Johannes Maly (*Mathematics, Technische Universität München*), Gerhard Kramer (*Institute for Communications Engineering, Technische Universität München*) 15:40–16:00

Consider the problem of efficiently recovering an unknown high-dimensional signal $x \in R^n$ from few linear measurements $y = Ax \in R^m$ where $A \in R^{mxn}$ defines the measurement process and $m \ll n$. This problem is ill-posed in general, and the theory of compressed sensing states that a solution becomes feasible for $m \gtrsim s \cdot ln(n/s)$ by considering s-sparse signals, i.e., $|\{x_i \neq 0\}| <= s$. In contrast, practical systems work digitally and the measurements have only finite precision, yielding a new quantized model $y = q(Ax)$, where q is inherently discontinuous, e.g., $q(z) = sign(z)$. It is known that approximation from sign measurements with only one bit per measurement is asymptotically possible in the same regime with $m \gtrsim s \cdot ln(n/s)$. However, approximation from these extremely quantized measurements comes at the price of significant approximation errors. This work investigates the trade-off between approximation errors and measurement rates when varying the quantization depth from the extreme of one bit per measurement to very fine quantization. The numerical results show that the optimal choice of bit-level changes depending on the overall quantization rate, or on the desired average distortion.

DFG-PP1886 | Polymorphic uncertainty modelling for the numerical design of structures

Date 20.03.2018 14:00–16:00
Room N1179
Organiser Michael Kaliske (*Institute for Structural Analysis, TU Dresden*)

Polymorphic uncertainty quantification for stability analysis of fluid saturated soil and earth structures

Carla Henning (*Institute of Mechanics and Structural Analysys in Aerospace Engineering, University of Stuttgart*), Tim Ricken (*University of Stuttgart*) 14:00–14:20

Nowadays, numerical simulations enable the description of mechanical problems in many application fields, e. g. in soil or solid mechanics. During the process of physical and computational modelling, a lot of theoretical model approaches and geometrical approximations are sources of errors. These can be distinguished into aleatoric (e. g. model parameters) and epistemic (e. g. numerical approximation) uncertainties. In order to get access to a risk assessment, these uncertainties and errors must be captured and quantified. To describe the strongly coupled solid-fluid response behavior, the theory of porous media (TPM) will be used. In order to capture the impacts of different uncertainties on computational results, two promising approaches of analytical and stochastic sensitivity analysis will enhance the deterministic structural analysis. A simple consolidation problem already provided a high sensitivity in the computational results towards variation of material parameters and initial values. The variational sensitivities are used as a tool for optimization procedures and capture the impact of different parameters as continuous functions. An advantage is the accurate approximation of the solution space and the efficient computation time, a disadvantage lies in the analytical derivation and algorithmic implementation. In the probabilistic sensitivity analysis from the field of statistics, the expense only increases proportionally to the problems dimension. The overall objective is to figure out the respective strengths of both accesses to develop more efficient methods and tools for the reliable and economic sizing of earth structures in the long-run.

Fuzzy uncertainty in forward dynamics simulation using variational integrators

Markus Eisentraudt (*Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Sigrid Leyendecker (*Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*) 14:20–14:40

In engineering applications, dynamic investigations are usually carried out with precisely defined input parameters, like inertia quantities, initial conditions on state and velocity level or geometric quantities. Here, the sharply defined input parameters are mapped by a deterministic mapping onto a precisely defined output. In practice, these parameters can only be determined with limited accuracy. To consider this epistemic uncertainty, parameters can be modeled as fuzzy quantities, which were introduced by Zadeh [6]. Hereby, the deterministic mapping has to be transformed into a fuzzy mapping, which maps the fuzzy input onto a fuzzy output. The transition from deterministic to fuzzy mappings is based on the extension principle of fuzzy-set theory, which is described in detail in [3, 1]. Because of numerical difficulties in the direct implementation of the extension principle [3], α-discretisation is usually used instead, which is based on the work of Nguyen [5]. Nevertheless, the numerical realisation of fuzzy mappings in forward dynamics requires high computational effort, which is strongly correlated with the number of fuzzy parameters and the number of time-steps.

Therefore, a new approach for the numerical consideration of fuzzy parameters in forward dynamics is presented in this contribution, which aims to achieve a lower numerical complexity than available methods. The response of the system, which can be represented by a fuzzy function, is determined on the basis of α-discretisation together with α-level optimisation [4, 3]. The shown methods focus on an efficient implementation of α-level optimisation with combinations of local optimisations, optimality tests and forward dynamics steps. The tests for first order optimality conditions, which are also known as Karush-Kuhn-Tucker conditions, are used to reduce the number of optimisations and hence the numerical effort. The system is simulated using forced discrete Euler-Lagrange equations, which are based on a variational principle [2]. The underlying variational integrators exhibit conservation properties on energy and momentum level. Further, a possibility is demonstrated, which allows the reduction of the number of optimisation variables and eliminates equality constraints. Performance and characteristics of the developed methods is demonstrated by means of a linear and a nonlinear dynamical system.

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Polymorphic uncertainty modeling for optimization of timber structures

F. Niklas Schietzold (*Institute for Structural Analysis, Technische Universität Dresden*), Michael Kaliske (*Institute for Structural Analysis, Technische Universität Dresden*), Wolfgang Graf (*Institute for Structural Analysis, Technische Universität Dresden*)

14:40–15:00

The uncertainty characteristics of wood are mainly affected by natural variation. Out of this, the traditional approach of stochastic variables can be expanded to a polymorphic uncertainty model. Therefore, e.g. fuzzy probability based randomness is used in such a way, that stochastic variables are equipped with fuzzy variables in parameterization concerning the distribution functions. So the coupling of both aleatoric and epistemic uncertainty is involved in the uncertainty analysis. The FEM is applied as a basic solution of particular load situations and focused timber structures. This is based on a local-orthotropic evaluation of material properties on each integration point with respect to a specified location of the tree trunk axis.
In this contribution, an approach to polymorphic uncertainty modeling for timber structures is introduced. Models representing the spatial variation and interdependencies of material parameters are necessary. For this purpose on the one hand interactions between fuzzy variables, on the other hand correlations among stochastic variables are considered. Random fields are utilized to capture spatially varying material properties in context with the discretization of FE, and approaches to both spatially and structurally depending correlations are presented for these. The prearrangements are aiming on an optimization in design of timber structures, provided that polymorphic uncertain design, as well as a priori parameters are considered. The tools for

uncertainty analysis and the basic FEM solution are embedded in an automated optimization processing, whereas they are preferably parallelized, incorporating methods for reducing the numerical effort. The features are shown in examples.

Optimization Approaches for Durable Reinforced Concrete Structures considering Interval and Stochastic Parameter Uncertainty

Steffen Freitag (*Institute for Structural Mechanics, Ruhr-Universität Bochum*), Philipp Edler (*Institute for Structural Mechanics, Ruhr-Universität Bochum*), Katharina Kremer (*Institute for Structural Mechanics, Ruhr-Universität Bochum*), Michael Hofmann (*Institute for Structural Mechanics, Ruhr-Universität Bochum*), Günther Meschke (*Institute for Structural Mechanics, Ruhr-Universität Bochum*) 15:00–15:20

The durability of reinforced concrete (RC) structures is dominated by steel reinforcement corrosion and uncertain service loads, which have to be considered in the lifetime oriented design of RC structures. The transport of corrosive substances into the structure is considerably influenced by load induced cracking. The crack width therefore is a major controlling factor for the lifetime of RC structures. To improve the design for durability, finite element models in combination with optimization approaches for polymorphic uncertain data are presented. Here, the crack width at the reinforcement layer is used as the optimization objective to be minimized. The structural reliability is treated as a constraint of the optimization task in terms of the accepted failure probability. The reinforcement layout (number and diameter of reinforcement bars) and the concrete cover are chosen as design parameters. Whereas the number and diameter of the reinforcement bars are discrete deterministic design parameters, the concrete cover is modeled as an interval design parameter, with a midpoint to be optimized and a given radius to take construction imprecision into account. The loading and the concrete material parameters (Young's modulus and strength) are considered as stochastic a priori parameters within the optimization. A particle swarm optimization (PSO) approach in combination with an artificial neural network surrogate model is applied to solve the optimization problem. Within the optimization, the uncertain structural response is computed by a combination of Monte-Carlo simulations and optimization-based interval analysis to consider the stochastic and interval parameters, respectively. A representative application is presented to demonstrate the performance of the proposed approach.

A Method to Quantify Material Parameter Uncertainties Resulting from Microstructure Variation based on Artificial Microstructures

Niklas Miska (*Chair of Continuum Mechanics, Ruhr-Universität Bochum*), Daniel Balzani (*Chair of Continuum Mechanics, Ruhr-Universität Bochum*) 15:20–15:40

The design of engineering constructions made of micro-heterogeneous materials depends on an accurate description of the material response. This is in many cases governed by the material's microstructure morphology, which may statistically vary significantly with its location in the individual component or from component to component. In this paper, a numerical method is proposed to quantify uncertainties of the resulting macroscopic material response as a result of variations in the material's microstructure. The approach is based on repeatedly simulating microscopic boundary value problems using the finite element method and homogenizing the microscopic mechanical fields to identify the resulting macroscopic material properties. In each of these numerical calculations a varying microstructure is considered such that over all, the statistics of the considered morphologies is as similar as possible to the variations in the real materials. For that purpose the concept of statistically similar representative volume elements

(SSRVEs) [1] is extended, where originally, artificial microstructures were constructed by solving a minimization principle to match a given real microstructure morphology in a statistical sense as closely as possible. Instead of just constructing the best possible artificial microstructure, now a set of statistically similar volume elements is constructed which matches the variation of morphology statistics. To quantify the resulting uncertainties of material properties efficiently, a Multi-Level Monte-Carlo approach is used. The method is exemplarily applied to advanced high strength steels.

[1] D. Balzani, L. Scheunemann, D. Brands, and J. Schröder. Construction of two- and three-dimensional statistically similar RVEs for coupled micro-macro simulations. Computational Mechanics, 54(5):1269–1284, 2014.

Hierarchical uncertainty quantification of probabilistic elastoplastic models

Bojana Rosic (*TU Braunschweig, Institute of Scientific Computing*), 15:40–16:00
Hermann G. Matthies (*TU Braunschweig, Institute of Scientific Computing*)

Concrete and human bone tissue are typical examples of materials which exhibit randomness in the mechanical response due to an uncertain heterogeneous micro-structure. In order to develop an appropriate probabilistic macro-scale mathematical description, the essential step is to address the material as well as possible other sources of uncertainties (e.g. excitations, change in geometry etc.) in the model. By extending already existing deterministic models derived from Helmholtz free energy and the dissipation functions characterising ductile or quasi-brittle behaviour, the goal of this talk is to identify and quantify uncertainty in the system response. For this purpose a hierarchical Bayesian probabilistic setting is considered in which the imprecise modeller's a priori knowledge about the model parameters and the available set of data obtained by experiments are taken into account when identifying the corresponding probability distribution functions of unknown parameters. Identification in the form of Bayesian inverse problems - in particular when experiments are performed repeatedly - requires an efficient solution and representation of possibly high dimensional probabilistic forward problems, i.e. the estimation of the measurement prediction given prior assumption. An emergent idea is to propagate parameter uncertainties through the model in a Galerkin manner in which the solution of the corresponding differential equations is represented by a set of stochastic basis polynomials, the cardinality of which grows exponentially. To allow an efficient solution of high-dimensional problems this talk will present the new low-rank Galerkin schemes combined with Bayesian machine learning approaches.

DFG-PP1897 | Calm, smooth and smart - novel approaches for influencing vibrations by means of deliberately introduced dissipation

Date	20.03.2018	14:00–16:00
Room	N1189	
Organiser	Peter Eberhard (*Institute of Engineering and Computational Mechanics, University of Stuttgart*)	

Limitation of an adjustable two degree-of-freedom damper system for directional damping

Aditya Suryadi Tan (*Mechanical Engineering, Ilmenau University of Technology*), Martin Dahlmann (*Ilmenau University of Technology*), Thomas Sattel (*Ilmenau University of Technology*) 14:00–14:20

For a better and more flexible damping, a smart damper is required. Such damper should be able to adjust the damping magnitude and damping direction independently. In this work, two degree-of-freedom damping with two fixed orthogonal damping directions is investigated. The damping magnitude can be adjusted independently for each damping direction. This kind of adjustment can be realized through the implementation of field responsive fluid, such as electro- or magnetorheological fluid. In order to describe the behavior of the damping system, investigations were conducted for several combinations of damping magnitude and velocity directions. It is shown that fully independent damping adjustment is only possible to be realized along the fixed orthogonal damping directions. Therefore, it is not possible to control the direction of the damping independently with only two damping elements. It can be concluded, that the possibility to influence the damping direction is found to be still challenging.

Decoupling Coupled Structural-Acoustic Systems: Investigation of Structural Acoustic Damping Mechanisms.

Suhaib Koji Baydoun (*Chair of Vibroacoustics of Vehicles and Machines, Technische Universität München*), Steffen Marburg (*Chair of Vibroacoustics of Vehicles and Machines, Technische Universität München*) 14:20–14:40

In the context of the present project within the DFG priority program 1897 “Calm, Smooth and Smart“, dissipation of kinetic energy of vibrating structures into the acoustic far field is studied. This phenomenon can be understood as radiation damping and is particularly relevant for weakly damped lightweight structures, musical instruments and underwater applications. The physical coupling between the fluid carrying the sound pressure waves and the dynamic behavior of the structure is hardly amenable to analytical solutions. Moreover, experimental damping determination necessitates reference measurements inside vacuum chambers to deduce the effect of radiation damping and is therefore accompanied by an excessive effort.
In this paper, the coupled equations of time-harmonic elastodynamics and acoustics are addressed by means of finite and boundary element methods respectively and solved monolithically. The loss factor, which quantifies the extent of radiation damping, is determined by relating radiated sound power to structure-inherent power. Radiation damping of simple geometrical configurations, such as flat panels and hollow spheres, is systematically investigated. However, the analyses of coupled structural-acoustic systems require a high computational effort due to the frequency-dependency of sound radiation. Therefore, this project will involve the derivation of numerical formulations, which enable the consideration of radiation damping in decoupled structural simulations. First steps towards efficient decoupling comprise forming the Schur complement and approximating

the resulting damping matrices. The presented results enable researchers to better understand the effect of acoustic radiation damping and to estimate its relevance for future research.

Model and Parameter Study of a Shape-Adaptable Beam for Vibration Control

Alexander Nowak (*Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Kai Willner (*Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Alexander Hasse (*Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*) 14:40–15:00

Shape adaptation is an effective approach for vibration damping. In this context, a numerical model of a slender, shape-adaptable beam is introduced. The beam is essentially an arrangement of compliant ribs which are interconnected by a hull structure. The compliant ribs are characterized by at least two desired deformations modes with a low modal stiffness, whereas the remaining modes are considerably stiffer. By actively exciting the first desired deformation mode, the cross-sectional stiffness of the beam can be altered between a low and a high stiffness state and therefore, the vibration behavior of the beam can be influenced.
In detail, this paper presents a surrogate model of the compliant ribs which easily allows for modifying the stiffness properties of the ribs by a low number of parameters. The surrogate model is integrated in the FE-modelled hull structure in order to simulate the 3D behavior of the entire structure. The influence of shape adaptation on the dynamic behavior of the free vibrating beam as well as for excited oscillation is examined. Especially, modal energies and their transfer between the modes due to the shape adaptation are considered. In addition, we are conducting a study on the parameters of the surrogate model in order to gain a deeper insight into the complex interrelationships of vibration reduction through shape adaptation.

Experimental and numerical characterization of fiber-metal-elastomer laminates by using dynamic-mechanical analysis regarding its damping behavior

Vincent Sessner (*Institut for Applied Materials, Karlsruhe Institute of Technology - KIT*), Wilfried Liebig (*Karlsruhe Institute of Technology - KIT*), Luise Kärger (*Institute of Vehicle System Technology, Karlsruhe Institute of Technology - KIT*), Kay André Weidenmann (*Institute for Applied Materials, Karlsruhe Institute of Technology - KIT*) 15:00–15:20

Hybrid Carbon fiber-Metal-Elastomer Laminates (HyCEML) consist of alternating layers of carbon fiber reinforced plastics, elastomer layers and aluminum sheets. These laminates offer great potential for a lightweight structural material with adjustable damping properties. The material damping is strongly influenced by the viscoelastic properties of the elastomer layers which damps by the principle of constrained layer damping when the laminate is vibrated. In this study the material damping is experimentally characterized by three point bending dynamic-mechanical analysis. In this regard, HyCEML specimens were tested on different frequencies and temperatures. The loss factor, storage- and loss modulus were measured to characterize the damping over the temperature and frequency range. Time-temperature superposition was applied to determine the damping characteristics at higher and lower frequencies. The experimental results were compared to numerical studies on the basis of a characterization of the single constituents. Detailed multi-layer finite element (FE) models are generated offering high flexibility in terms of type and number of finite elements especially in the direction of laminate thickness. By using the multi-layer FE-models, parametric studies are carried out to investigate the damping behavior for varying constellations, e.g. laminate lay-up and thickness of the elastomer. For this purpose, existing material models are used to investigate the influence of each component on the system's damping behavior. It could be shown, that even small changes in thickness and stiffness of the elastomer affect significantly to the damping behavior of the laminate. The authors would like to thank the DFG for supporting the project as a part of the priority program SPP 1897.

Numerical investigations of polymer-based fibre-reinforced structures with fluidically actuated Compressible Constrained Layer Damping

Klaudiusz Holeczek (*Institute of Lightweight Engineering and Polymer Technology (ILK), Technische Universität Dresden*), Tomasz Schlieter (*Institute of Computational Mechanics and Engineering, Silesian University of Technology*), Tom Ehrig (*Institute of Lightweight Engineering and Polymer Technology, Technische Universität Dresden*), Pawel Kostka (*Institute of Lightweight Engineering and Polymer Technology (ILK), Technische Universität Dresden*) 15:20–15:40

Lightweight-focused design often leads to a problematic vibration susceptibility of designed components. To reduce potential environmental and health risks, excessive vibrations have to be mitigated preferably through lightweight-compatible solutions. The presented studies aim at the establishment of almost weight-neutral solutions for adaptive tuning of the dynamic behaviour of lightweight components.
The proposed unique actuating principle is based on structural cavities generating evanescent deformations when supplied with fluidic medium. These cavities encapsulate compressible, viscoelastic elements which combined with the surrounding layers operate according to an extended principle of Constrained Layer Damping. The evanescent morphing is used to deliberately alter the geometrical and material properties of the viscoelastic elements through compression in order to achieve a damping capacity adaptation.
The analysed Compressible Constrained Layer Damping (CCLD) structure is configured as a three layered beam consisting of the load-bearing structure as well as constraining and compressible viscoelastic layer. The main studies were conducted using a developed finite-element model. Herein, the geometrical, material and load property range has been parametrised so that generalised conclusions about the CCLD dynamic behaviour could be drawn. The deformation kinematics of the CCLD under combined loads resulting from static tension and flexural vibrations has been analysed. Furthermore, the assessment of the dynamic behaviour adaptation potential of different compressible viscoelastic materials was carried out. The goal of this study was on the one hand to determine a feasible initial configuration of the CCLD for its successful application and on the other hand the assessment of its damping efficiency.

Mesoscale Simulation of Shape Memory Alloy Film Damping

Shahabeddin Ahmadi (*Microstructure Technology, KIT - Karlsruhe Institute of Technology*), Kiran Jacob (*Microstructure Technology, KIT - Karlsruhe Institute of Technology*), Frank Wendler (*Materials Simulation, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Manfred Kohl (*Microstructure Technology, KIT - Karlsruhe Institute of Technology*) 15:40–16:00

The vibration-damping performance of pseudoelastic shape memory alloy (SMA) film devices is investigated under non-isothermal conditions on a mesoscopic (micrometer) scale and correlated with the performance on the macro (device) scale. SMA materials are predestined for damping of vibration and shock impacts due to their high work density. Until now, however, they have mainly been exploited in large-scale applications like the protection of buildings against seismic activity. Here, we investigate the passive damping performance of TiNi thin-film-based bridge structures which is of special interest, e.g., for vibration damping of portable electronic devices or handheld cameras. The investigation is based on a thermodynamics-based Gibbs free energy model that includes a martensite-austenite interface free energy term using formulations from a phase-field model [1]. The dynamics of an external spring-mass system is represented by a differential equation and coupled to the finite element domain as a boundary condition. Macroscopic

as well as local material properties are determined experimentally. Regarding to this approach, it is possible to describe the nonlinear vibration characteristics and to optimize damping capacity for the cases of free and forced vibration conditions.

[1] F. Wendler, H. Ossmer, C. Chluba, E. Quandt, M. Kohl, Mesoscale simulation of elastocaloric cooling in SMA films, Acta Materialia, 136, 105-117 (2017)

DFG-PP1962 | Non-smooth and complementary-based distributed parameter systems: simulation and hierachical optimization

Date 20.03.2018 14:00–16:00
Room N1190
Organiser Michael Hintermüller (*WIAS Berlin*)

Recent Advances in Non-smooth and Complementarity-based Distributed Parameter Systems

Michael Hintermüller (*WIAS Berlin*) 14:00–14:20

The first part of the talk highlights some recent activities of the SPP 1962. In a second part, a brief report on research progress in the optimal control of classes of variational inequalities with applications in multiphase flows and the motion of droplets is presented.

Towards Semi-Smooth Newton Methods for VI Constrained Shape Optimization Problems

Kathrin Welker (*FB IV - Mathematik, Universität Trier*), Volker Schulz (*Universität Trier*) 14:20–14:40

Shape optimization problems arise frequently in technological processes which are modelled in the form of partial differential equations (PDEs). Recently, efficient algorithms in terms of shape spaces and the resulting framework from infinite dimensional Riemannian geometry has been developed to solve PDE constrained shape optimization problems. Some PDEs arise from simplified variational inequalities (VIs). Thus, it is a natural question to ask how we can optimize shape optimization problems constrained by VIs. In this talk, VI constrained shape optimization problems are treated from an analytical and numerical point of view in order to formulate approaches aiming at semi-smooth Newton methods on shape vector bundles. It is not a very far step from the optimization approaches on shape spaces for PDE constrained problems to semi-smooth Newton methods. However, VI constrained shape optimization problems are very challenging because of the necessity to operate in inherently non-linear and non-convex shape spaces. In classical VIs, there is no explicit dependence on the domain, which adds an unavoidable source of non-linearity and non-convexity due to the non-linear and non-convex nature of shape spaces.

Directional differentiability for elliptic QVIs of obstacle type

Amal Alphonse (*Weierstraß-Institut*), Carlos Rautenberg (*WIAS Berlin*), Michael Hintermüller (*WIAS Berlin*) 14:40–15:00

Quasi-variational inequalities (QVIs) are generalisations of variational inequalities where the associated constraint set is no longer explicitly given but in fact depends on the solution of the inequality itself. This adds to the nonsmooth and nonlinear nature of the problem and represents a major obstacle for the sensitivity analysis. In this talk, we present some results on the directional differentiability of the mapping that takes the source term of a QVI onto the solution. We characterise the directional derivative as the limit of a monotonic sequence of directional derivatives associated to specific variational inequalities.

Optimal Control of Static Contact in Finite Strain Elasticity

Matthias Stoecklein (*Department of Mathematics, University of Bayreuth*), Anton Schiela (*University of Bayreuth*) 15:00–15:20

Nonlinear elastic problems usually appear in modeling the deformations of nonlinear materials in classical mechanics. These deformations can be described as minimizers of an respective energy functional. Solving such problems is already a highly challenging task owing to the nonlinearity and nonconvexity of elastic energy functionals. Extending this to contact problems and an optimal control approach results in a nonsmooth, nonconvex, nonlinear and constrained optimization problem. To address these kinds of problems we have to apply suitable regularization and optimization methods in function space.
The talk will therefore deal with the theoretical foundations of static contact problems in nonlinear elasticity and corresponding optimal control problems. The focus here will lie on theoretical results we have achieved so far such as existence theory and convergence results for the regularized problem. Also, a short discussion about suitable algorithms to solve such problems numerically will be given.

Optimisation via successive piecewise linearisation: Towards infinite dimensional problems

Andrea Walther (*Universität Paderborn*), Olga Ebel (*Institut für Mathematik, Universität Paderborn*), Stephan Schmidt (*Universität Würzburg*) 15:20–15:40

For finite dimensional problems that are unconstrained and piecewise smooth the optimization based on successive piecewise linearisation is well analysed yielding for example linear or even quadratic convergence under reasonable assumptions on the function to be optimised. The inner loop of this optimization approach minimizes a piecewise linear function with a proximal term. In this talk we discuss the extension of this loop to infinite dimensions preparing the field for the optimization of optimal control problems that are constrained with nonsmooth partial differential equations.

Set-Oriented Multiobjective Optimal Control of PDEs using Certified ROMs

Dennis Beermann (*Universität Konstanz*), Michael Dellnitz (*Universität Paderborn*), Sebastian Peitz (*Universität Paderborn*), Stefan Volkwein (*Mathematics and Statistics, University of Konstanz*) 15:40–16:00

In this talk we combine a global subdivision algorithm for multiobjective optimization problems with a-posteriori error estimates for reduced-order models (ROMs) based on Proper Orthogonal Decomposition (POD) in order to efficiently solve multiobjective optimization problems governed by partial differential equations. A-posteriori error estimates for parabolic differential equations are developed in such a way that the errors in the conflicting objectives can be estimated individually. The resulting algorithm constructs a library of locally valid ROMs online using a Greedy search. Using this approach, the number of evaluations of the full-order model can be reduced by a factor of more than 1000.

DFG-PP2013 I Property improvements of components by metal forming induced residual stresses

Date	20.03.2018	14:00–16:00
Room	N1090	
Organiser	Wolfram Volk (*Chair of Metal Forming and Casting, Technical University of Munich*)	

Targeted Use of Forming Induced Internal Stresses in Metal Components

Wolfram Volk (*Technical University of Munich, Chair of Metal Forming and Casting*) 14:00–14:20

The increased demand for lightweight constructions in industrial productions requires the design, manufacture, and use of application oriented components. Forming manufacturing processes have many advantages over machining processes. Not only are the material utilization and productivity optimized, but also the fiber orientation is adapted to the specific task. This results in increased mechanical characteristics and dynamic strength of formed metal components. However, internal stresses greatly influence the performance of components manufactured by forming procedures. The state of initial stress is mainly responsible for component failure during the manufacturing process as well as during the use of the component afterwards. For this reason, internal stresses are currently considered as a highly unfavorable characteristic, which has a negative impact on a component's feasibility. Efficient models and experimental testing equipment for operational stability already showed promising results for the potential usefulness of internal stresses. Therefore, the objective of the priority program is to regulate and control internal stresses by utilizing forming technologies in order to achieve a positive impact on relevant characteristics of components manufactured by forming processes.

Comments on Strain-Gradient Plasticity

Paul Steinmann (*FAU Erlangen-Nürnberg; University of Glasgow*), Philipp Landkammer (*FAU Erlangen-Nürnberg*), Andrew McBride (*University of Glasgow*), B. Daya Reddy (*University of Cape Town*) 14:20–14:40

We focus on aspects of geometrically linear strain-gradient plasticity [1]. Motivated by the presence of dislocation densities, gradient effects are accounted for either through their inclusion in the free energy or in an extension of the flow law, i.e. via energetic and dissipative models. Here, we will ana-lyse features of dissipative models. We review the global nature of the flow relation formulated in terms of a dissipation potential. This result addresses the apparent dilemma that presents itself when considering the flow law in its local form where the micro-stresses are undetermined in the elastic region and thus making it impossible to decide whether yield has occurred. We remove the dilemma through a global approach to the flow law. Determining the corresponding global yield func-tion and normality relation is complex; only an upper bound for the yield function is obtained. The expression for the yield function as a supremum of a quantity involving the dissipation potential makes it possible to understand the presence of an elastic gap in the case of problems in which non-proportional loading occurs through a change in micro-boundary conditions.

[1] C. Carstensen, F. Ebobisse, A.T. McBride, B.D. Reddy, P. Steinmann,
Some properties of the dissipative model of strain-gradient plasticity,
Philosophical Magazine, http://dx.doi.org/10.1080/14786435.2016.1274836, 2017

On the analysis of microstructural residual stresses in hot bulk forming parts under specific cooling

Dominik Brands (*Institut für Mechanik, Universität Duisburg-Essen*), Rainer Niekamp (*Institut für Mechanik, Universität Duisburg-Essen*), Christoph Kock (*Institut für Umformtechnik und Umformmaschinen, Leibniz Universität Hannover*), Alexander Chugreev (*Institut für Umformtechnik und Umformmaschinen, Leibniz Universität Hannover*), Bernd-Arno Behrens (*Institut für Umformtechnik und Umformmaschinen, Leibniz Universität Hannover*), Jörg Schröder (*Institut für Mechanik, Universität Duisburg-Essen*)

14:40–15:00

Nowadays, the primary focus to treat the residual stresses in metallic components produced by forming is by their prevention or minimization in order to improve the durability as well as manufacturability. In contrast, the central aspect of the DFG priority programme 2013 is the application of residual stresses for improvement of properties e.g. the operational strength in the field of forming technology.
The aim of this project is to investigate the various influences on distribution and stability of the residual stress development in thermo-mechanically processed components by means of controlled cooling in both the experiment as well as the numerical investigations. In the long term, the goal is to optimize the forming process in such a way that a targeted use for improvement of the component's behavior becomes possible. A precise representation of the residual stresses, their development in numerical simulation as well as their interpretation in experimental results requires a profound knowledge of the thermal, mechanical as well as metallurgical properties of the used material. The numerical modeling of the residual stresses requires a multiscale view because of their classification into first, second and third 3rd type. A macroscopic, phenomenological description in the framework of the Finite Element Methods (FEM), see [1], taking into account the thermo-mechanical and metallurgical properties will be used for the representation of the residual stresses of the first kind whereas, the phase-field theory, see [2] and the FEM, see [3] will be used to model the microstructural residual stresses of second and third type. The microstructural transformation will be simulated by means of a phase-field model and representative volume elements will be created, which are to be used for the subsequent FEM simulations on the microscale.
In this contribution initial results on the microstructural analysis as well as on experimental evaluations of the considered material will be presented.

[1] B.-A. Behrens and P. Olle. Consideration of transformation-induced stresses in the simulation of press hardening. *Proceeding of International Plasticity*, 2008.

[2] I. Steinbach. Phase-field models in materials science. *Modelling and Simulation in Materials Science and Engineering*, **17**(7):073001, 2009.

[3] D. Brands, D. Balzani, L. Scheunemann, J. Schröder, H. Richter and D. Raabe. Computational modeling of dual-phase steels based on representative three-dimensional microstructures obtained from EBSD data. *Archive of Applied Mechanics*, **86**:575–598, 2016.

Influence of residual stresses on fatigue crack initiation and propagation – experiments and phase-field modeling

Markus Kästner (*Mechanical Sciences and Engineering, Institute of Solid Mechanics, TU Dresden*), Martha Seiler (*TU Dresden*), David Kühne (*TU Dresden*), Franz Ellmer (*TU Dresden*), Peter Hantschke (*TU Dresden*), Christina Guilleaume (*TU Dresden*), Alexander Brosius (*TU Dresden*) 15:00–15:20

Residual stresses are inherently generated during the production of materials, semi-finished products or components. Until now, only the reduction of harmful residual stresses was in the focus of scientific investigations. Instead, we are aiming on the controlled adjustment of residual stresses which requires a fundamental understanding of material-process-property relationships.
Following an overview of the project within the Priority Programme 2013, first results regarding the characterization of the cyclic material behaviour as well as an experimental proof of the improved durability of notched specimens produced by cold forming are presented. In order to understand the positive effects of hardening and residual stresses on the fatigue strength, the experimental analysis is combined with numerical simulation techniques. This is first accomplished on the macro scale using damage models for the description of crack initiation and the further development of phase-field models for fatigue crack propagation. We generalise the phase-field model for brittle fracture to cyclic loadings in terms of a fracture toughness that decreases with the accumulated damage modelled in terms of the Miner rule. That is, novel computational methods are combined with classical concepts of structural durability analysis which allow for an efficient treatment of a large number of load cycles. In this way, both – fatigue crack propagation as well as static brittle fracture – are accommodated by the phase-field model. Initial numerical studies on the effect of a reduction of the fracture toughness as well as regarding the influence of different cyclic degradation functions are presented. This numerical approach is validated by a comparison with empirical methods of fatigue analysis. For a deeper understanding of the effects of residual stresses, future work will focus on the separation of the influences of the various changes in the material induced during the forming process, e.g. residual stresses, surface hardness, and material hardening.

Deformation induced residual stresses in duplex steel: Micromechanical modeling and comparison with experimental data

Thomas Böhlke (*Institute of Engineering Mechanics, Chair for Continuum Mechanics, Karlsruhe Institute of Technology (KIT)*), Hannes Erdle (*Karlsruhe Institute of Technology (KIT)*), Jens Gibmeier (*Karlsruhe Institute of Technology (KIT)*), Nicola Simon (*Karlsruhe Institute of Technology (KIT)*), Samuel Pulvermacher (*Karlsruhe Institute of Technology (KIT)*) 15:20–15:40

In the talk, we discuss the micromechanical modeling of deformation induced residual stresses based on an approach that combines a classical mean field theory [1] with the principle of maximum entropy [2]. The mean field theory is used to estimate on the grain level the total strain, the plastic strain and the eigenstrain based on macroscopic stress, strain and stiffness data. In addition, the maximum entropy estimate is applied to derive an explicit formula for the covariance of stress within the phases. The advantage of the combination of both methods - in comparison to full-field approaches - is the computation time, which allows for an application of the model approach at the integration point level of finite elements. The aforementioned methods are applied to a duplex steel, which consists of a ferritic and an austenitic phase both with the same volume fraction. The predicted residual stresses are compared to experimental data from bending experiments for which loading stresses as well as the residual stresses that

remain subsequent to unloading from elastic-plastic bending have been determined by neutron diffraction in both phases over the thickness, i.e. the bending height of the specimen.

[1] P.P. Castañeda, P. Suquet, Nonlinear Composites, Adv. Appl. Mech. 34 (1997) 171–302

[2] W.S. Kreher, Statistical Theory of Microplasticity of Two-Phase Composites, in: A. Pineau, A. Zaoui (Eds.), IUTAM Symp. Micromechanics Plast. Damage Multiph. Mater., Springer Netherlands, Dordrecht (1996) 363–370.

Simulation of incremental sheet forming processes: current status and challenges

Markus Bambach (*Chair for Mechanical Design and Manufacturing, BTU Cottbus-Senftenberg*) 15:40–16:00

Incremental sheet forming (ISF) processes comprise a class of processes which use generic tooling instead of dedicated dies. They are used primarily for the production of small batches and individualized products. ISF processes are characterized by a local action of the forming tool(s), which are moved relative to the sheet metal using CNC machines or industrial robots. The local plastic deformation under the action of the tool(s) leads to a number of challenges for finite element modelling. In order to simulate such processes efficiently and accurately, re-meshing or domain decomposition methods techniques, robust contact algorithms and material models for cyclic elasto-plastic loading are needed. In addition, issues such as time discretization, error estimates and uncertainty quantification are important for the simulation of ISF processes. The present contribution reviews the current status of simulation methods for incremental sheet forming processes, with a focus on the prediciton of residual stress. Experimental and numerical results for incremental sheet forming on CNC machines are compared and the influence of time and spatial discretization, numerical settings and materials modeling are discussed.

DFG-PP2020 I Cyclic deterioration of high-performance concrete in an experimental-virtual lab

Date	20.03.2018	14:00–16:00
Room	N1095	
Organiser	Ludger Lohaus (*Institut für Baustoffe, Leibniz Universität Hannover*)	

Micromechanical behavior of high performance concrete under cyclic loading at various moisture and thermal conditions

Stefan Harenberg (*Department of Concrete Structures and Structural E*), Antonio Caggiano (*Institut für Werkstoffe im Bauwesen, TU Darmstadt*), Andreas König (*Institute of Mineralogy, Crystallography and Materials Science, Universität Leipzig*), Albrecht Gilka-Bözow (*Institute of Construction and Building Materials, TU Darmstadt*), Milan Schultz-Cornelius (*.Department of Concrete Structures and Structural Engineering, TU Kaiserslautern*), Sha Yang (*Institute of Construction and Building Materials, TU Darmstadt*), Matthias Pahn (*Department of Concrete Structures and Structural Engineering, TU Kaiserslautern*), Frank Dehn (*Institut für Mineralogie, Kristallographie und Materialwissenschaft, Universität Leipzig*), E.A.B. Koenders (*Institute of Construction and Building Materials, TU Darmstadt*) 14:00–14:40

This paper provides preliminary results of a research study on the fatigue behavior of HighPerformance Concrete (HPC). Results of an experimental campaign, performed at the Department of Concrete Structures and Structural Engineering of the Technical University of Kaiserslautern, is firstly proposed. The heterogeneous meso-structure and material degradation of HPC was studied through cyclic bending-tensile tests. A test set-up were specially developed at the TU-Kaiserslautern to perform such activities. Particularly, different upper stress cycles (namely, cycle reversals) characterized by different force/stress amplitudes or number of reversals, were considered and analyzed. The influence of the edge zone on the stress cycles will be tested on notched and normal specimens. The results are used for composing a so-called "Wöhler curve" of the materials' fatigue behavior and will be presented. Damage progress during loading was monitored by means of a digital image correlation system and where the results were used for improving the measurement accuracy. Based on these results, macroscopic and mesoscale simulations were performed at the TUDarmstadt's Institute of Construction and Building Materials. A meso-mechanical approach for the numerical analysis of HPC specimens subjected to low- and high-cycle fatigue actions will be presented. The possibilities of modelling the materials' fracture response induced by fatigue is taken into account by means of a systematic use of zero-thickness interface elements equipped with a fracture-based model and combined with a continuous damage constitutive law. A "plastic-damage" based model for concrete subjected to cyclic loading is developed combining the concept of fracture-energy theories with a stiffness degradation, representing the key phenomenon occurring in concrete under cyclic responses. The experimental and numerical activities proposed in this paper stem out from the DFG Priority Program 2020 Project "Cyclic Damage Processes in High-Performance Concretes in the Experimental Virtual Lab".

Computational modeling to investigate the influence of the micro-structure and disorder on damage evolution in concrete

Vladislav Gudžulić (*Institute for Structural Mechanics, Ruhr-University Bochum*), Ildar Khisamitov (*Institute for Structural Mechanics, Ruhr-University Bochum*), Jithender J. Timothy (*Institute for Structural Mechanics, Ruhr-University Bochum*), Günther Meschke (*Institute for Structural Mechanics, Ruhr-University Bochum*) 14:40–15:00

Concrete is material with a random disordered microstructure across multiple scales. The effective macroscopic material behavior of concrete is strongly dependent on the material properties and the interactions of the individual constituents at the microscale. Failure of concrete as a quasi-brittle material is generally characterized by distributed micro-crack nucleation that governs strain softening behavior, followed by localization of damage eventually leading to structural failure. The aim of this study is to investigate the influence of micro-structure and initial disorder on damage evolution in a strongly heterogeneous material such as concrete. The principal mechanism of failure is assumed to be governed by a cascade of localized microcracking and re-distribution of stresses [1]. This mechanism is modeled within the scope of this work using a voxel-sized finite element approximation of the disordered micro-structure with a non-uniform distribution of strengths for each material phase. The potential to incorporate material disorder within a variational interface model [2] for fracture will also be discussed. In the presentation, the influence of different disorder distributions on damage evolution and failure is discussed and results of selected numerical experiments are presented.

[1] Timothy, J. J., Iskhakov, T., & Meschke, G. (2017) Transport properties of microcracked porous materials: Micromechanics models and mesoscale simulations. Proceedings of the 7th GACM Colloquium on Computational Mechanics, Stuttgart. DOI: 10.18419/opus-9334

[2] Khisamitov, I. & Meschke, G. (2018) Variational approach to interface element modeling of brittle fracture propagation Computer Methods in Applied Mechanics and Engineering, 328, 452-476

Objective modeling of multixial softening of concrete

Michael Kaliske (*Institute for Structural Analysis, TU Dresden*), Imadeddin Zreid (*ISD, TU Dresden*) 15:00–15:20

Concrete in tension and low confined compression is characterized by strainsoftening behavior, which manifests itself in the form of highly localized cracks or shear bands. Attempting to incorporate this response in standard continuum descriptions leads to unstable and mesh sensitive results. This work presents a coupled plasticity-damage microplane model for concrete regularized by an implicit gradient enhancement. Combining plasticity and damage is necessary to describe the cyclic response of concrete, where plasticity accounts for the permanent deformation and damage for the reduction in the elastic stiffness. The yield surface used is based on a microplane version of the Drucker-Prager yield function supplemented with tension and compression caps with smooth transitions. The damage part contains a split to consider the transition between compression and tension. Regularization of the model is achieved by an over-nonlocal implicit gradient formulation. This type of nonlocal enhancement ensures the continuity of the strains in the localized region by introducing extra degrees of freedom, which represent the nonlocal averages of some local variables. The model is implemented in a 3D finite element code and its capabilities are illustrated by examples dealing with both plain and reinforced concrete.

Analysis of pullout behavior of single steel fibers embedded in high performance concrete using phase-field modeling

Mangesh Pise (*Institute of Mechanics, University of Duisburg-Essen*), Dominik Brands (*Institut für Mechanik, Universität Duisburg-Essen*), Gregor Gebuhr (*Lehrstuhl Werkstoffe im Bauwesen, Bergische Universität Wuppertal*), Jörg Schröder (*Institut für Mechanik, Universität Duisburg-Essen*), Steffen Anders (*Lehrstuhl Werkstoffe im Bauwesen, Bergische Universität Wuppertal*) 15:20–15:40

In the recent decades great research effort has been carried out which result to new innovative concrete types such as high performance concrete (HPC). The availabilitiy of wide varieties of composition make HPCs different from classical concrete types. The dense microstructure of HPCs gives high strength and superior durability compared to normal strength concrete, see [1]. Apart from being used as additional reinforcement, steel fibers are necessary in high strength concretes to provide a sufficient ductility. During fracture the stresses in concrete are transmitted from matrix to the fibers. These fibers restrain the further growth of the crack and contribute to the energy absorption capacity of the concrete, compare [2, 3]. The modeling of fiber-matrix interaction occurring during fiber pullout is necessary to analyze the post-cracking response of HPCs in tension, see [4]. In this contribution, a continuum phase-field model based on the variational formulation is implemented to examine the pullout behavior of a single steel fiber and its influence on the overall material behavior of HPCs. The development of the damage parameter is controlled by an evolution equation, which corresponds to known diffusive phase-field models within a continuum mechanical framework, see [5]. The proposed phase-field model of fracture by [6] is followed. Therein, they used an additive decomposition of the elastic energy so that an energy-release-driven fracture occurs due to tension only. The predictive capability of the above mentioned model is analyzed by simulating a single fiber pullout test and compared against experimental data.

[1] P. C. Aïtcin. High-performance concrete. *Modern concrete technology*, **5**, E & FN spon, London, 1998.

[2] F. Germano, G. Tiberti, and G. Plizzari. Post-peak fatigue performance of steel fiber reinforced concrete under flexure. *Materials and Structures*, **49**:4229-4245, 2016.

[3] J. Zhang. Fatigue Fracture of Fibre Reinforced Concrete – An Experimental and Theoretical Study. *Technische Universität von Dänemark*, Dissertation, 1998.

[4] J. Grünberg, L. Lohaus, C. Ertel and M. Wefer. Mehraxiales mechanisches Ermüdungsmodell von Ultra-Hochfestem Beton. *Beton- und Stahlbetonbau*, **102**:388-398, 2007.

[5] C. Kuhn and R. Müller. A continuum phase field model for fracture. *Engineering fracture mechanics*, **77**:3625-3624, 2010.

[6] C. Miehe, M. Hofacker, and F. Welschinger. A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits. *Computer Methods in Applied Mechanics and Engineering*, **199**:2765-2778, 2010.

Micro-Structure Related Modelling of Ultra-High Performance Fibre Reinforced Concrete (UHPFRC) Subjected to Cyclic Tensile Loading

Svenja Höper (*Institut für Statik, TU Braunschweig*), Ursula Kowalsky (*Institut für Statik, TU Braunschweig*), Dieter Dinkler (*Institut für Statik, TU Braunschweig*) 15:40–16:00

Ultra-high performance concrete with a compressive strength of more than $140 N/mm^2$ reacts very brittle without the addition of fibres. At designing economical and resource-efficient building components as well as performance-optimized materials, the supporting effects of the additional microfibres must be considered. Prospectively, cyclic loading and the fatigue behaviour of high performance materials and slim components will come to the fore. Therefore, the influence of cyclic deterioration on the load bearing capacity of the interface transition zone connecting microfibres and the surrounding concrete surface must be investigated.
As part of the DFG Priority Programme 2020, the damage mechanisms and processes regarding the deterioration of UHPFRC subjected to cyclic tensile loading are explored in an Experimental-Virtual Lab. Using the concepts of elasto-plasticity and continuum damage mechanics, the material models for the components of the composite material UHPFRC are improved and enhanced to be combined on a mesoscale with the help of a non-linear bond model. This bond model is discretized by interface elements with curved surfaces in 3D space and describes the interaction of fibres and concrete in the bond zone in terms of adhesion and friction effects. For validation and verification, single and multiple fibre pull-out tests are simulated in 3D-finite element analyses. These FE-simulations and preliminary findings are supposed to provide the essential basis for future numerical degradation prediction.

Poster Session

Date	21.03.2018	09:30–10:30
Room	Lobby Theresianum (Building 6)	16:00–16:30
Organiser	Dominik Kern (*TU Chemnitz*)	

General Information about GAMM Student Chapters

Dominik Kern (*TU Chemnitz*), Ailyn Stötzner (*TU Chemnitz*), Benjamin Unger (*Institut für Mathematik, TU Berlin*)

In the year 2015 the GAMM board officially introduced student chapters in order to attract prospective scientists. Since then, two student chapters, in Berlin and Chemnitz, were founded and some more are in preparation. Still, existence and concepts of the student chapter are not familiar to many members of GAMM. This poster illustrates the basic idea behind student chapters, which is bringing together mathematicians and engineers at an early stage in scientific and social events. In addition, information about administrative issues, such as constitution and guidelines, are outlined.

Information about GAMM Student Chapter Chemnitz

Ailyn Stötzner (*Mathematik, TU Chemnitz*)

After the GAMM board officially introduced student chapters in 2015, a so called GAMM Student Chapter was immediately founded at the TU Chemnitz. This poster gives an overview about our activities like the organization of scientific and social events.

Optimization in Shape Spaces

Kathrin Welker (*FB IV - Mathematik, Universität Trier*)

Shape optimization problems arise frequently in technological processes which are modelled by partial differential equations or variational inequalities. In many practical circumstances, the shape under investigation is parametrized by finitely many parameters. This allows the application of standard optimization approaches, but limits the space of reachable shapes unnecessarily. The differential-geometric structure of certain shape spaces is investigated and applied to the theory of shape optimization problems. Furthermore, a diffeological structure on a new space of so-called $H^{1/2}$-shapes is defined. The $H^{1/2}$-shapes are a generalization of smooth shapes and arise naturally in shape optimization problems.

High performance optimization algorithms for interface identification problems

Martin Siebenborn (*Universität Hamburg*)

This poster presents optimization approaches for large scale interface identification problems prepared for supercomputers. In many applications, which are modeled by partial differential equations, there is a small number of spatially distributed materials or parameters separated by interfaces. Often these interfaces form complex contours forcing high resolutions in the discretization schemes. The challenge is thus to combine HPC techniques with shape optimization in order to come up with scalable algorithms even for very large problems. This can be achieved by a combination of multigrid strategies and quasi Newton methods. It is also shown how different shape metrics affect the quality of finite element meshes and which are the most suitable ones.

Thermo-Mechanical FE Analysis of a Power Plant Component

Johanna Eisenträger (*Institute of Mechanics, Otto-von-Guericke-Universität Magdeburg*), Konstantin Naumenko (*Institute of Mechanics, Otto-von-Guericke Universität Magdeburg*), Yevgen Kostenko (*Power and Gas Division, Siemens AG*), Holm Altenbach (*Institute of Mechanics, Otto-von-Guericke-Universität Magdeburg*)

Power plant components have to withstand complex thermo-mechanical loads, i.e. frequent start-ups and shut-downs in combination with long holding times at high temperatures induce creep-fatigue loads. Tempered martensitic steels with high chromium content feature high creep strength and corrosion resistance among other properties such that these alloys are often used for power plant components. This poster presents the results of a thermo-mechanical analysis of an idealized steam turbine rotor with an inlet groove. In a first step, a transient heat transfer analysis is performed with the FE code ABAQUS, taking varying steam temperatures and heat transfer coefficients into account. The computed temperature fields, the steam pressure, and the rotational frequency serve as input for the subsequent structural analysis. As constitutive model, a multi-axial phase mixture model is used. The phase mixture model has been calibrated for a 12% Cr heat-resistant martensitic steel, and it comprises a hard and a soft phase, which are connected via an iso-strain approach. The introduction of a backstress and a softening variable allows for the consideration of non-linear kinematic hardening and microstructural softening effects. A user material subroutine is used to implement the model based on implicit time integration. The structural analysis of the rotor provides stress and strain values, which can be used to assess creep and fatigue damage.

A Least Squares Finite Element Method for Coupled Sea Ice and Subsurface flow

Fleurianne Bertrand (*Fakultät für Mathematik, Universität Duisburg-Essen*), Steffen Münzenmaier (*Fakultät für Mathematik, Universität Duisburg-Essen*), Marcel Moldenhauer (*Fakultät für Mathematik, Universität Duisburg-Essen*)

Consequently to a research voyage on the SA Agulhas II, samples of the thin layer of ice covering the Antarctic ocean (sea ice) were collected and analysed along two spatial transects into the marginal ice zone (MIZ). The sea ice displacements and drift movements were recorded. Since longitudinal and transverse stresses and vertical stress gradients can be neglected, the sea ice layer can be modelled with the shallow ice equations. These are widely used for the simulation of ice that moves significantly slower than the surrounding environnement. The flows are coupled along an interface where we enforce continuity of pressure and continuity of flux. These assumptions lead to a nonlinear system of equations which can be treated by a (Gauss-)Newton method. The hyperbolic character of the shallow ice equations has to be treated accordingly. A least squares finite element method, providing an inherent error estimator and a positive definite system, is used for the spatial discretization with continuous piecewise polynomials combined with Raviart-Thomas elements.

H_2-Optimal Structure-Preserving Model Order Reduction

Petar Mlinarić (*Computational Methods in Systems and Control Theory, Max Planck Institute for Dynamics of Complex Technical Systems*), Sara Grundel (*Max Planck Institute for Dynamics of Complex Technical Systems*), Peter Benner (*Computational Methods in Systems and Control Theory, Max Planck Institute for Dynamics of Complex Technical Systems*)

For unstructured linear time-invariant systems, the Two-Sided Iteration Algorithm (TSIA) [2] is a locally $\mathcal{H}_2$-optimal model order reduction (MOR) method. It is based on Gramian-based necessary optimality conditions, the Wilson conditions [1]. We extend this work to structured systems, e.g. second-order systems, parametric systems, time-delay systems, and network systems. Following the derivation of Wilson conditions, we find the necessary $\mathcal{H}_2$-optimality conditions for structure-preserving MOR. For second-order systems in particular, we can find expressions for the reduced matrices. Based on this, we propose an iterative algorithm, analogous to TSIA, for $\mathcal{H}_2$-optimal structure-preserving MOR of second-order systems.

[1] D. A. Wilson. Optimum solution of model-reduction problem. *Proceedings of the Institution of Electrical Engineers*, 117(6):1161–1165, 1970.

[2] Y. Xu and T. Zeng. Optimal $\mathcal{H}_2$ model reduction for large scale MIMO systems via tangential interpolation. *Int. J. Numer. Anal. Model.*, 8(1):174–188, 2011.

Numerically robust and efficient two-scale FE-FFT-based simulations of elasto-viscoplastic polycrystals

Julian Kochmann (*Institute of Applied Mechanics, RWTH Aachen University*), Stephan Wulfinghoff (*Institute of Applied Mechanics, RWTH Aachen University*), Stefanie Reese (*Institute of Applied Mechanics, RWTH Aachen University*), Bob Svendsen (*Institute of Applied Mechanics, RWTH Aachen University*)

The main objective of this work is the development of a two-scale computational approach for the prediction of the local and effective mechanical behavior of polycrystalline materials with elasto-viscoplastic constitutive behavior subjected to isothermal deformations at finite strains. Assuming scale separation, the microstructural deformations are dictated by the kinematics of the macroscopic continuum body. The macroscopic constitutive behavior is in turn determined by the mean response of the point-wise attached microstructure which is represented by a statistically similar periodic unit cell. The algorithmic formulation and numerical solution of the two locally-coupled boundary value problems is based on the FE-FFT method. In particular, this work deals with the derivation of a numerically robust algorithmic formulation for the computation of the overall algorithmic tangent modulus and the development of an efficient solution strategy for two-scale full-field simulations of powerlaw polycrystals with pronounced intrinsic anisotropy. The results of two- and three-dimensional examples indicate that the proposed method is characterized by numerically robust computations for relatively large time increments and high rate sensitivity parameters as well as an accurate representation of micromechanical fields and moderate overall computation times.

Nano-composites with size effects - Fibre-bending stiffness and FE-formulation

Tobias Kaiser (*Mechanical Engineering, Institute of Mechanics, TU Dortmund University*), Andreas Menzel (*Mechanical Engineering, Institute of Mechanics, TU Dortmund University*)

In this work we elaborate a modelling approach for fibre-reinforced (nano-) composites which allows us to endow the fibres with a certain kind of bending resistance. The work is based on the theoretical developments presented in (Int. J. Non. Linear Mech. 42(2007), 355-368) where it is proposed to take into account the gradient of the (spatial) fibre direction field as an additional argument of the Helmholtz free energy function. By doing so, second-order gradients of the placement field enter the constitutive functions, resulting in a higher-gradient continuum – specifically the framework is based on a couple stress theory. Via their dependence on the stress and on the couple stress tensor, the higher-order gradients enter the balance equations which complicates the finite element based solution procedure due to continuity requirements. For this reason, a mixed-type finite element approach is devised for the solution of the resulting system of coupled partial differential equations, see (Comput. Methods in Appl. Mech. Eng. 317(2017), 1037-1067), and a comparison with analytical solutions is carried out for validation purpose, see (Int. J. Non. Linear Mech. 91(2017), 128-139). The modelling approach is then applied to study the deformation behaviour of fibre-reinforced nano-composites. We derive a particular form of the stored energy function which is based on an invariant that can be interpreted as the fibre-curvature, and show that the resulting contributions to the symmetric part of the stress tensor and to the couple stress tensor can be well interpreted (J. Mech. Phys. Solids 107(2017), 411-432).

Blood Damage Estimation for Medical Device Design

Lutz Pauli (*Chair for Computational Analysis of Technical Systems, RWTH Aachen University*), Stefan Haßler (*Chair for Computational Analysis of Technical Systems, RWTH Aachen University*), Marek Behr (*Chair for Computational Analysis of Technical Systems (CATS), RWTH Aachen University*)

Ventricular assist devices (VADs) are used to provide mechanical circulatory support to chronically ill heart disease patients. Even though the devices improved significantly over the last decade, clinical studies still reveal high rates of adverse events associated with the blood damage caused by these devices. To improve the virtual design of VADs and other blood-handling devices, we developed an Eulerian, strain-based hemolysis model for the quantification of mechanical blood damage and the identification of critical regions within the device. In contrast to commonly used stress-based models, our strain-based model estimates the distortion of red blood cells in the flow field, which allows to consider time-dependent and viscoelastic deformation. Comparisons of stress-based and strain-based hemolysis models in a benchmark blood pump show very significant differences. Stress peaks with short exposure time contribute to the overall hemolysis in the stress-based model, whereas regions with increased shear and long exposure time are responsible for damage in the strain-based model [1].

[1] L. Pauli. *Stabilized finite element methods for computational design of blood-handling devices.* PhD thesis, RWTH Aachen University, 2016.

L1-Analysis Minimization and Generalized (Co-)Sparsity: When Does Recovery Succeed?

Martin Grenzel (*Institut für Mathematik, Technische Universität Berlin*), Gitta Kutyniok (*Institut für Mathematik, Sekr. MA 5-4, Technische Universität Berlin*), Maximilian März (*Mathematik, Technische Universität Berlin*)

In this talk, we will investigate the problem of signal estimation from undersampled sub-Gaussian measurements under the assumption of a cosparse model. Based on generalized notions of sparsity, we derive novel recovery guarantees for the ℓ^1-analysis basis pursuit, enabling accurate predictions of its sample complexity. The corresponding bounds on the number of required measurements do explicitly depend on the Gram matrix of the analysis operator and therefore particularly account for its mutual coherence structure. Our findings defy conventional wisdom which promotes the sparsity of analysis coefficients as the crucial quantity to study. In fact, this common paradigm seems to break down in many situations of practical interest, for instance, when applying a redundant (multilevel) frame as analysis prior. By extensive numerical experiments, we demonstrate that, in contrast, our theoretical sampling-rate bounds reliably capture the true recovery performance of various examples, such as redundant Haar wavelets systems, total variation, or random frames. Due to a novel localization argument, it turns out that the presented framework naturally extends to stable recovery, allowing us to incorporate compressible coefficient sequences as well.

Trajectory Tracking by Servo-constraints

Svenja Otto (*Institute of Mechanics and Ocean Engineering, Hamburg University of Technology (TU Hamburg-Harburg)*), Robert Seifried (*Mechanik und Meerestechnik, Hamburg University of Technology*)

For trajectory tracking of multibody systems, a two degree of freedom control structure is an efficient approach. Feedforward control is designed as an inverse model which cancels the model dynamics exactly if there were no modeling errors or disturbances. In order to account for errors, a state feedback path, e.g. LQR is added. In case of underactuated multibody systems, the derivation of an exact inverse model is not straightforward. Here, numerical model inversion is performed based on servo-constraints. Servo-constraints extend the system dynamics to constrain the output on a specified trajectory. This yields a set of differential-algebraic equations (DAEs) with a structure comparable to the equations of motion derived in redundant coordinates. In case of differentially flat systems, the inverse model is purely algebraic. Otherwise, there remains internal dynamics which is not observable from the input-output relationship. Stability of the internal dynamics has to be analyzed before choosing a suitable solving method. Stability analysis is performed in terms of zero-dynamics based on a coordinate transformation adopted from nonlinear control theory. The different configurations of the arising internal dynamics are analyzed for a mass-on-car system. Solving the high index DAE system then yields the open-loop control input. Experimental results are shown for a differentially flat system. Thereby, the index 3 DAEs are solved in real-time. In the experiments, open-loop control is compared to a control structure with an additional state feedback LQR controller.

Hybrid quantum-classical modeling of quantum dot devices

Markus Mittnenzweig (*Weierstraß-Institut für Angewandte Analysis und Stochastik*)

Quantum optics is currently on the leap from the lab to real world applications. To advance the development of novel, electrically driven quantum dot devices, simulation tools are needed, which combine classical device physics with models from cavity quantum electrodynamics. As a step on this route, we connect the well-established fields of semi-classical semiconductor transport theory and the theory of open quantum systems. By coupling the drift-diffusion system with a Markovian quantum master equation (in Lindblad form), we introduce a new hybrid quantum-classical modeling approach, which provides a comprehensive description of quantum dot devices on multiple scales: It enables the calculation of quantum optical figures of merit and the spatially resolved simulation of the current flow in realistic semiconductor device geometries in a unified way. We construct the interface between both theories in such a way, that the resulting hybrid quantum-classical system obeys the fundamental axioms of (non-)equilibrium thermodynamics. We show that our approach guarantees the conservation of charge, the consistency with the thermodynamic equilibrium and the second law of thermodynamics. The approach is demonstrated by numerical simulations of an electrically driven single-photon source in the stationary and transient operation regime. Joint work with Markus Kantner and Thomas Koprucki.

Model reduction for linear systems with low-rank switching

Benjamin Unger (*Institut für Mathematik, TU Berlin*), Philipp Schulze (*Institut für Mathematik, TU Berlin*)

In this poster we present a new strategy for model reduction of linear switched systems. The main idea is to derive an abstract model without switching - called the envelope system - that is able to reproduce the behavior of the switched system if a suitable feedback is supplied. That advantage of this formalism is that one can use standard MOR techniques and derive an error bound for time-domain simulations. Moreover, the envelope system has a physical interpretation that describes the energy generated by switching between different models. If additionally the subsystems of the switched system are port-Hamiltonian systems, that this structure can be preserved in the reduced model. We demonstrate the efficiency of the proposed methodology with numerical examples.

Convection in porous media

Marco De Paoli (*Institute of Fluid Mechanics and Heat Transfer, TU Wien, Vienna University of Technology*), Francesco Zonta (*Institute of Fluid Mechanics and Heat Transfer, TU Wien, Vienna University of Technology*), Alfredo Soldati (*Institute of Fluid Mechanics and Heat Transfer, TU Wien, Vienna University of Technology*)

Convection in porous media has recently gained renovated attention due to the implications it can bear in the frame of carbon dioxide (CO2) sequestration. Liquefied CO2 is injected in deep geological formations, where it dissolves with the surrounding fluid (brine) and remains trapped, diminishing the concentration of CO2 in the atmosphere and thus reducing the greenhouse effect. Inspired by this geophysical problem and with the aid of pseudo-spectral direct numerical simulations, we propose different modeling approaches to predict the evolution of injected carbon dioxide in underground saline formations. The effect of the soil properties is initially considered. Indeed, saline aquifers identified as possible sequestration sites consist of sedimentary rocks, inherently anisotropic. We observed that this feature of the soil has a positive effect on the dissolution dynamics, increasing the dissolution efficiency [1, 2]. The influence of fluids miscibility is then taken into account. Since CO2 in only partially miscible in brine, we developed a robust and thermodynamically-consistent model to describe the interface existing between these fluids. We observed that the deformability of the surface may induce heterogeneities in the flow structure, with important implications on the future injection scenarios.

[1] De Paoli, Marco and Zonta, Francesco and Soldati, Alfredo, *Influence of anisotropic permeability on convection in porous media: Implications for geological CO2 sequestration*, Physics of Fluids, 28(5):056601, 2016.

[2] De Paoli, Marco and Zonta, Francesco and Soldati, Alfredo, *Dissolution in anisotropic porous media: Modelling convection regimes from onset to shutdown*, Physics of Fluids, 29(2):026601, 2017.

Reduced-Order Models based on the Shifted Proper Orthogonal Decomposition

Philipp Schulze (*Institut für Mathematik, TU Berlin*)

Model order reduction (MOR) methods have experienced a great research effort in the past decades and are nowadays used in various applications. Nevertheless, the efficiency of standard MOR techniques reaches its limits when applied to systems whose dynamics are dominated by advection. This is particularly noticeable when the solution reveals high gradients, for example, in case of traveling shock waves. This type of problem occurs in many applications, including aerodynamics and chemical engineering, and thus it is desirable to develop suitable MOR methods for this. Recently, new model reduction techniques have been proposed which are suited for advection-dominated problems. One of them is the shifted proper orthogonal decomposition (sPOD) algorithm which constructs a low-dimensional decomposition of a given snapshot matrix. The decomposition is based on a linear combination of modes shifted in space, where each mode is assigned a time-dependent amplitude as well as a time-dependent shift. In contrast to most of the other approaches, the sPOD algorithm yields decompositions of very low dimension even in case of multiple advection velocities. On this poster, we present a new framework which uses the modes obtained by the sPOD for obtaining a dynamic reduced-order model (ROM). This is

achieved by a nonlinear projection of the full-order model where the unknowns of the nonlinear ROM are the amplitudes and the shifts of the corresponding modes. For the considered numerical examples, the ROM obtained by the new approach exhibits significantly smaller computation times than a classical POD Galerkin ROM with comparable accuracy.

Modeling Uncertainties in Nonlinear Material Properties and Hysteresis

Ulrich Römer (*TU Braunschweig*)

An accurate modeling of ferromagnetic properties is crucial for the design and analysis of electrical machines, magnets, transformers and other devices. The behavior of magnetic materials can be quite complex, featuring strong nonlinearities and even hysteresis. In view of the required accuracy, the information available for given materials is typically unsatisfactory. In these cases, uncertainty quantification may be used to explore the systems' variability in the presence of uncertainties in the material data. This work is concerned with the modeling of uncertainties in nonlinearities and hysteresis properties of materials. In the anhysteretic case, the nonlinearity is represented by a random field with monotonic paths. This is important due to physical reasons, but also as a prerequisite to apply, e.g., the Newton-Raphson method. In the hysteretic case, the Duhem model is considered, where uncertainties are represented via a small number of cross-correlated random fields in a system of ordinary differential equations. Again, physical and mathematical constraints arise which need to be taken into account in a probabilistic setting. For numerical purposes the random fields also need to be discretized, which is achieved here by using the truncated Karhunen-Loève expansion. Eventually, methods for propagating uncertainties, such as the stochastic collocation method can be applied. Numerical examples will be given, which illustrate both the stochastic modeling and the effect of uncertainties on magnetic fields.

Polyconvexity inspired frameworks and structure-preserving integrators for multi-field problems

Marlon Franke (*Institute of Mechanics - Department of Civil Engineering, Geo and Environmental Sciences, Karlsruhe Institute of Technology - KIT*), Alexander Janz (*Institute of Mechanics - Department of Civil Engineering, Geo and Environmental Sciences, Karlsruhe Institute of Technology - KIT*), Mark Schiebl (*Institute of Mechanics (IFM), Karlsruhe Institute of Technology - KIT*), Rogelio Ortigosa (*Swansea University · Zienkiewicz Centre for Computational Engineering*), Peter Betsch (*Institute of Mechanics (IFM), Karlsruhe Institute of Technology - KIT*)

A new approach for the design of energy-momentum (EM) consistent time integrators for nonlinear coupled problems is proposed. Polyconvexity inspired internal or Helmholtz free energy functionals are obtained by using the rediscovered tensor cross product (see [1]) which is basically applied on the cofactor and the Jacobian of the right Cauchy-Green strain tensor and greatly simplifies the algebra (see [2, 1]). On this basis multi-field problems concerning nonlinear thermo-elastodynamics (see [3]) and electro-elastodynamics (see [4]) are considered. For the former a temperature based weak form is employed which facilitates the design of a structure-preserving time-stepping scheme for coupled thermo-elastic problems. For the latter a three-field internal energy-based formulation is applied. In both cases, the polyconvexity-based framework facilitates the design of EM consistent time integrators. In particular algorithmic stress formulas are employed which show a remarkably simple structure when compared to traditional, elaborate projection-based formulas. The spatial discretization relies on finite element interpolations for the unknown fields. Eventually, the superior performance of the proposed formulations is shown in several numerical examples.

[1] Bonet, J., Gil, A.J. and Ortigosa, R., A computational framework for polyconvex large strain elasticity, *Comput. Methods Appl. Mech. Engrg.*, 283:1061–1094, 2015.

[2] Betsch, P., Janz, A. and Hesch, C., A mixed variational framework for the design of energy-momentum schemes relying on polyconvex stored energy functions, *Comput. Methods Appl. Mech. Engrg.*, submitted, 2017.

[3] Franke, M., Janz, A., Schiebl, M. and Betsch, P., An energy-momentum consistent integration scheme using a polyconvexity-based framework for non-linear thermo-elastodynamics, *Int. J. Numer. Meth. Engng.*, submitted, 2017.

[4] Ortigosa, R., Franke, M., Janz, A., Gil, A. and Betsch, P., An energy-momentum integration scheme based on a convex multi-variable framework for non-linear electro-elastodynamics, in preparation, 2017.

Image Processing via Harmonic Analysis - Perceptual Image Quality Assessment, Visual Servoing and Feature Detection

Rafael Reisenhofer (*Universität Bremen*)

Systems of basis functions developed in the field of applied harmonic analysis, such as wavelets, shearlets or α-molecules, yield efficient representations of images and often highlight important features in a signal. The poster gives an overview of successful applications of such function systems in tasks like perceptual image quality assessment, visual servoing and the detection of edges, ridges and blobs.

A polyconvex extension of the Hencky energy

Robert Martin (*University of Duisburg Essen*), Ionel-Dumitrel Ghiba (*Alexandru Ioan Cuza University of Iasi*), Patrizio Neff (*Mathematics, University of Duisburg-Essen*)

Adapting a method introduced by Ball, Muite, Schryvers and Tirry, we construct a polyconvex isotropic energy function $W\colon \mathrm{GL}^+(n) \to \mathbb{R}$ which is equal to the classical Hencky strain energy

$$W_{\mathrm{H}}(F) = \mu \left\|\mathrm{dev}_n \log U\right\|^2 + \frac{\kappa}{2} \left[\mathrm{tr}(\log U)\right]^2 = \mu \left\|\log U\right\|^2 + \frac{\Lambda}{2} \left[\mathrm{tr}(\log U)\right]^2$$

in a neighborhood of the identity matrix; here, $\mathrm{GL}^+(n)$ denotes the set of $n \times n$-matrices with positive determinant, $F \in \mathrm{GL}^+(n)$ denotes the deformation gradient, $U = \sqrt{F^T F}$ is the corresponding stretch tensor, $\log U$ is the principal matrix logarithm of U, tr is the trace operator, $\|X\|$ is the Frobenius matrix norm and $\mathrm{dev}_n X$ is the deviatoric part of $X \in \mathbb{R}^{n\times n}$. The extension can also be chosen to be coercive, in which case Ball's classical theorems for the existence of energy minimizers under appropriate boundary conditions are immediately applicable. We also generalize the approach to energy functions W_{VL} in the so-called Valanis-Landel form

$$W_{\mathrm{VL}}(F) = \sum_{i=1}^{n} w(\lambda_i)$$

with $w\colon (0,\infty) \to \mathbb{R}$, where $\lambda_1, \ldots, \lambda_n$ denote the singular values of F.

Sections

S01 | Multi-body dynamics

Organiser Thomas Berger (*Fachbereich Mathematik, Universität Hamburg*)
Robert Seifried (*Mechanik und Meerestechnik, Hamburg University of Technology*)

S01.01 | Multi-body dynamics

Date 20.03.2018
Room 1601

Error Estimation for the Simulation of Elastic Multibody Systems

Jörg Fehr (*Institute of Engineering and Computational Mechanics, Institute of Engineering and Computational Mechanics, University of Stuttgart*), Dennis Grunert (*Institute of Engineering and Computational Mechanics, University of Stuttgart, Germany*), Bernard Haasdonk (*Institute of Applied Analysis and Numerical Simulation, University of Stuttgart*), Ashish Bhatt (*Institute of Applied Analysis and Numerical Simulation, University of Stuttgart, Germany*) 08:30–09:10

For safety critical simulations, it is essential to know the error introduced by model order reduction (MOR) used to create the surrogate models to decide whether the simulation can be trusted or not. Typically, a-priori error estimates, are used. They deliver upper bounds for the error – independently of the applied excitation. By contrast, the error estimates from the reduced basis community deliver a-posteriori error bounds, which account for the current excitation. These error bounds use the residual between the reduced and original model to derive an error bound. In this work, we apply the error bound to a simple elastic multibody system (EMBS) described in the floating frame of reference formulation (FFRF). MOR is essential for the simulation of elastic bodies in a multibody system framework. Furthermore, the MOR procedure is made in a modular fashion: (i) only the linear second order FE model is reduced; (ii) the nonlinear ODE of one body in FFRF; (iii) multiple reduced elastic bodies assembled into an EMBS. This allows to interchange the reduced components, e.g., in automotive design. Our error estimation strategy follows the same modular approach. We also give details about the non-intrusive implementation which allows adding error estimation to multibody software like Neweul-M^2.
We show the results by applying the error estimator to a two-link flexible manipulator in 2-D and 3-D and performing an sensitivity analysis. Additionally, large performance improvements have been applied to make the computation of the error estimator negligible in comparison to the reduced simulation.

Modal analysis of flexible multibody systems with singular mass and stiffness matrices

Christian Hente (*Institut für Statik und Dynamik, Leibniz Universität Hannover*), Cristian Guillermo Gebhardt (*Institut für Statik und Dynamik, Leibniz Universität Hannover*), Benedikt Hofmeister (*Institut für Statik und Dynamik, Leibniz Universität Hannover*), Raimund Rolfes (*Institut für Statik und Dynamik, Leibniz Universität Hannover*) 09:10–09:30

A complex mechanical system can be described as a combination of individual rigid and/or flexible components and a set of kinematical constraints. The restrictions can be either internal,

which come on the scene in the case of parameterizing the configuration manifold of a system with a number of parameters larger than its intrinsic dimension, e.g. by employing three directors to describe the Lie Group $SO(3)$ (basically for rigid bodies and beams) or by employing a single unit director to describe the two dimensional sphere with unit radius embedded in the three-dimensional Euclidean space, i.e. S_1^2 , (basically for inextensible shells, in which the component of the Green-Lagrange strain tensor E_{33} is set to be zero at every time), or external ones, which come on the scene in the case of constraining bodies by means of joints, connections or supports. The linearized form of the resulting governing equations possesses usually singular mass and stiffness matrices. This fact represents an issue when the calculation of natural frequencies and natural modes for the whole system is needed. The classical modal analysis (solving directly the generalized eigenvalue problem from the stiffness and mass matrices) is no longer applicable. To overcome this difficulty, it is firstly necessary to utilize the linearized constraint equations that complete the missing information at the level of the mass and stiffness matrices and secondly, to redefine the eigenvalue and -vector problem within a suitable framework. In the current work, we set the focus on the development framework for the modal analysis able to deal with singular matrices.

A geometric view on the kinematics of finite dimensional mechanical systems

Tom Winandy (*Institut für Nichtlineare Mechanik, Universität Stuttgart*), Giuseppe Capobianco (*Institut für Nichtlineare Mechanik, Universität Stuttgart*), Simon R. Eugster (*Institut für Nichtlineare Mechanik, Universität Stuttgart*) 09:30–09:50

A configuration/position of a mechanical system with n degrees of freedom can be regarded as a point in an n-dimensional differentiable manifold known as the configuration manifold Q of the mechanical system. In this framework, the choice of a particular set of generalized coordinates $\mathbf{q} \in \mathbb{R}^n$ corresponds to a certain chart ϕ of the manifold Q. The $2n$-dimensional tangent bundle TQ of the configuration manifold Q is the space of positions *and* velocities, i.e. the state-space of the mechanical system. Accordingly, a chart of the tangent bundle corresponds to a particular set of generalized coordinates and velocities. The natural chart of TQ induced by the chart ϕ on Q provides the classical description of the state as $(\mathbf{q}, \dot{\mathbf{q}})$. In this talk, we will present a chart which uses a set of (possibly nonholonomic) velocity parameters $\mathbf{v} \in \mathbb{R}^n$ with $\dot{\mathbf{q}} = \mathbf{B}(\mathbf{q})\,\mathbf{v}$ such that the state of the mechanical system takes the form $(\mathbf{q}, \mathbf{v})$. The geometric insight allows for a unified treatment of finite dimensional mechanical systems which is independent of the choice of a particular set of generalized coordinates and velocities.

Optimal control simulations of two finger grasping

Uday Phutane (*Chair of Applied Dynamics, University of Erlangen-Nuremberg*), Michael Roller (*Fraunhofer ITWM*), Sigrid Leyendecker (*Chair of Applied Dynamics, University of Erlangen-Nuremberg*) 09:50–10:10

Grasping is a basic, though complex human movement performed with the hand through its many degrees of freedom. During grasping, when the hand closes around the object, the multibody system changes from a kinematic tree structure to a closed loop contact problem. To better understand work-related disorders or optimize execution of activities of daily living, an optimal control simulation to perform grasping would be useful.
We simulate the grasping action with a three-dimensional rigid multibody model composed of two fingers (the thumb, described in [1], and the index finger) along with the wrist and the forearm, modelled with the discrete null-space method, see [2]. The model is actuated using joint torques. The grasping movement is composed of a reaching phase (no contact between

the fingers and the object) and a grasping phase (closed contacts). The contact constraints are imposed first using functions to calculate the distance between the finger tips and the object surfaces and then through spherical joints while moving the object. The durations of each phase is determined by the solution of an optimal control problem, as demonstrated in [3]. Thus, the dynamics is described by a hybrid dynamical system with a given switching sequence and unknown switching times. The closed-loop dynamics realized in this work are adopted from [4]. The optimal control problem is solved using the direct transcription method DMOCC (discrete mechanics and optimal control), see [5], leading to a structure preserving approximation. An objective function such as the sum of all joint torques, the sum of joint torque changes or the sum of angular acceleration over the complete time interval is minimized subject to the discrete Euler-Lagrange equations, boundary conditions and path constraints. The dynamics of the object to grasp, for example a box, is also taken into account.

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Dynamical Modeling and LQR Control of a Gyroscopically Stabilized Bicycle

Hubert Gattringer (*Institute of Robotics, Johannes Kepler University Linz*), Andreas Müller (*Johannes Kepler University Linz*), Daniel Wagner (*Johannes Kepler University Linz*), Tobias Mauernboeck (*Johannes Kepler University Linz*)

10:10–10:30

This contribution focuses on the dynamical modeling and control of a self-balancing bicycle. The bicycle is equipped with two flywheels rotating at constant speed mounted with one additional rotational degree of freedom (DOF) in vertical direction. This DOF is actuated by an external motor. Due to the balance of angular momentum, a torque is generated acting in the perpendicular (forward) direction. This gyroscopic effect is exploited for the stabilization of the bicycle. Two cases are distinguished: 1) For the stabilization of the non-moving bicycle an LQ–controller based on a linear model is used. 2) For the moving bicycle, a non-linear dynamic model in terms of non-holonomic velocities is derived and an LQ-controller based on the linearization of the nonlinear system at constant driving speeds is used to stabilize the bicycle. The model reveals the self-stabilization behavior of a bicycle without flywheels. At a speed of approximately 16km/h, the linearized model has only eigenvalues with negative real part and is therefore stable. Experimental as well as simulation results are presented.

S01.02 | Multi-body dynamics

Date 20.03.2018
Room 1601

A new gradient based method for solving time optimal control problems in multibody dynamics

Wolfgang Steiner (*Josef Ressel Zentrum für innovative Mehrkörperdynamik, University of Applied Sciences Upper Austria*), Thomas Lauß (*Josef Ressel Center for Advanced Multibody Dynamics, University of Applied Sciences Upper Austria*), Stefan Oberpeilsteiner (*Josef Ressel Center for Advanced Multibody Dynamics, University of Applied Sciences Upper Austria*), Karin Nachbagauer (*Josef Ressel Center for Advanced Multibody Dynamics, University of Applied Sciences Upper Austria*) 16:30–16:50

During the last years, our research group developed several approaches for solving optimal control problems in multibody dynamics based on the computation of the gradient of the underlying cost function J to be minimized. The optimizing controls of the system could be obtained very efficiently by solving the set of adjoint equations associated to a multibody system, if the time interval, for which J is defined, is fixed. A more challenging situation arises, if the final time is variable or represents the cost function itself as it is the case for time optimal control problems. Among the class of time optimal control problems we consider the case, where the final time is defined by a scalar terminal condition $\phi(q) = 0$ for the generalized coordinates q. For example, this problem type has to be solved if the controls of a racing car should be computed such that the lap time on a racing circuit is minimized. Here, the terminal condition is satisfied, when the car crosses the finish line. We show, how the adjoint gradient method can be applied to such problems. Moreover, we demonstrate that the gradient of J with respect to the position of the switching points of a bang bang control can also be obtained in this way.

A structur-preserving numerical method for the dynamic optimization of flexible mechanical systems

Simeon Schneider (*Institut für Mechanik, Karlsruher Institute of Technology (KIT)*), Peter Betsch (*Institut für Mechanik, Karlsruher Institute of Technology (KIT)*) 16:50–17:10

Structure-preserving numerical methods often exhibit excellent numerical stability, robustness and qualitative behavior. Because of these qualities, a lot of effort has been put into the design of structure-preserving methods over the last decades. In nonlinear structural dynamics energy-momentum (EM) methods and energy dissipating variants thereof have been of primary concern. EM integrators are capable of conserving the total energy if the underlaying mechanical system is conservative. If the mechanical system has symmetry, EM integrators conserve the corresponding momentum map.
Although there exist many alternative numerical methods for the solution of optimal control problems, little attention has been paid to structure-preservation on the level of the optimal control problem. It is well-known that the Hamiltonian of autonomous optimal control problems is conserved along an optimal path. In addition to that, the optimal control problem inherits symmetries from the underlying mechanical system. These symmetries lead to associated generalized momentum maps, which are preserved on the level of the optimal control problem.
In the talk we will present a structure-preserving approach to optimal control of mechanical

systems. The proposed method does respect the symmetries on the level of both, the mechanical system and the optimal control problem. In addition to that, the proposed method is capable of conserving the Hamiltonian of the optimal control problem.

Staggered grid discretizations on Lie groups with applications in beam and shell theory

Stefan Hante (*Institute of Mathematics, Martin Luther University, Halle (Saale)*), Martin Arnold (*Institute of Mathematics, Martin Luther University, Halle (Saale)*) 17:10–17:30

We will discuss staggered grid space discretizations for micropolar Cosserat models with nonlinear configuration spaces, that possess Lie group structure. The discretization scheme is applied at the level of variational principle, has second order truncation error and uses a staggered grid, where the spatial derivatives are discretized inbetween the discretization points of the material configuration. This approach leads us to the semi-discretized equations of motion, that may be interpreted as the equations of motion of a multi-body system, where the bodies are coupled by nonlinear springs.
Furthermore we will present numericals results for Cosserat beams and micropolar shells, where we have applied a Lie group generalized-α time integration method to the space-discrete equations of motion. The test results show reasonable behaviour for models with a small number of degrees of freedom. Second order convergence in space is observed numerically.

Two-dimensional contact problems revisited – explicit analytical solutions for contact detection with straight and circular counterparts

Ulrich Römer (*Institute of Engineering Mechanics, Karlsruhe Institute of Technology - KIT*), Alexander Fidlin (*Institute of Engineering Mechanics, Karlsruhe Institute of Technology - KIT*), Wolfgang Seemann (*Insitute of Engineering Mechanics, Karlsruhe Institute of Technology - KIT*) 17:30–17:50

Models with unilateral contacts require contact detection as initial step of any analytical or numerical investigation. The potential contact points on two counterparts are all points on the boundaries with antiparallel normal vectors. Analytical solutions for the contact detection problem are not available for complex shapes – surprisingly, an explicit analytical solution for the contact detection problem of two ellipses was published as late as 2007 (Zheng and Palffy-Muhoray).
Explicit solutions for the contact detection problem offer several advantages: the numerical evaluation requires less computation time and is more accurate than iterative solutions. This means that the computational effort is known a priori – a prerequisite for real-time applications like hardware-in-the-loop test benches. Furthermore, explicit solutions may allow for the elimination of redundant degrees of freedom. If a complete reduction to minimal coordinates is possible, the dynamics can be formulated as a set of ordinary differential equations (ODEs) instead of differential algebraic equations (DAEs).
So far, no explicit solutions are known when the shape of both counterparty is arbitrary. However, we will present explicit solutions for the two-dimensional contact detection problem where only one boundary is a straight line or a circle, and the shape of its counterpart is almost arbitrary. The only prerequisite is uniqueness of the contact point. The performance of our approach will be demonstrated with several examples which include model for foot-ground-interaction and the contact between a camshaft and a roller tappet.

Ski vibrations caused by random slope roughness: A multi-body simulation study

Robert Eberle (*Unit of Engineering Mathematics, University of Innsbruck*), Peter Kaps (*University of Innsbruck*), Michael Oberguggenberger (*University of Innsbruck*) 17:50–18:10

In World Cup alpine ski racing, research interests focus on improving athlete performance and avoiding injuries. Especially vibrations of the skis have an influence in both fields and should not be neglected. Ski vibrations are caused by random riplets and disturbances of the slope. However, suitable choices of materials allow one to reduce those vibrations. Parameter optimization can be performed by costly and extensive experiments. Alternatively, computer simulations are helpful tools to investigate the influences of several material parameters on ski vibrations. We have developed a planar multi-body simulation model of a skier, which allows the investigation of transversal vibration of unedged skis during schussing over uneven ski slopes. Torsional vibrations are little during schussing for which they are not taken into account at the moment. The skis are modelled as dynamic Euler-Bernoulli beams and are incorporated as flexible beams into the multi-body skier model. The interaction between skis and snow is incorporated by a Kelvin-Voigt constitutive equation for the snow penetration force. The random roughness of the slope is modelled by random fields. These are generated based on real data obtained from measuring a public ski slope surface with a high resolution laser scanner. The data contain various tracks from skis and the typical riplets of prepared ski slopes. A sequence of runs over random slope surfaces is performed by the Monte Carlo simulation method and the ski vibrations are analysed. The presented simulation model allows one to find optimal material parameters to reduce ski vibrations during schussing.

S01.03 | Multi-body dynamics

Date 21.03.2018
Room 1601

A nonlinear Timoshenko beam formulation for modeling a tendon-driven compliant neck mechanism

Simon R. Eugster (*Institut für Nichtlineare Mechanik, Universität Stuttgart*), Bastian Deutschmann (*Institute of Robotics and Mechatronics, DLR*) 08:30–08:50

In this talk, we discuss the mechanical behavior of a tendon-driven compliant neck mechanism which is used to move the head of a humanoid robot. The neck is realized as a silicone block mounted onto the robot's torso. At the top end of the silicone block a polyamide plate interconnects the compliant neck with the head. At the very same plate tendons are attached whose actuation cause the soft and flexible block to deform thereby inducing a motion of the robot head. For workspace design, feedforward and feedback control of the head's trajectory, a mechanical model is required which appropriately describes the entire system. We present a dynamic model of the neck-head system in which the silicone block and the head are modeled as a nonlinear Timoshenko beam and a rigid body, respectively. The tendon actuations are included as external configuration-dependent forces. Within the Timoshenko beam formulation, a nonlinear constitutive law is suggested to describe the measured stiffening effect in compression of the silicone block. The system is modeled within the variational framework of the virtual work principle by determining the corresponding virtual work contributions of all considered mechanical effects. The discretization of the beam's infinite dimensional kinematics in the corresponding virtual

work contributions automatically generates nonlinear beam finite elements whose interactions with the rest of the system is already guaranteed. The resulting finite dimensional system can then be used to solve for static equilibrium configurations or to analyze the dynamic behavior of the neck-head system.

Co-Simulation of Electro-Mechanical Actuators for Circuit Breakers

Thorsten Schindler (*ABB AG*), Christian Simonidis (*ABB AG*) 08:50–09:10

At the ABB Corporate Research Center, innovative actuators for circuit breakers are investigated to meet the requirements of the future power grid. The development of circuit breakers involves multi-physical problems, e.g. electro-mechanical or arc-physical forces that arise from the electrical contacts to be separated or closed depending on the status of the power grid. The mechanical regime includes the actuator and the linkage between interruption chamber and actuator. Deformational behavior, large rigid body motion, frictional effects, impacts, fatigue and tolerances are topics under consideration. Therefore different co-simulation coupling strategies have been studied and applied depending on the respective investigation purpose. Built-in co-simulation interfaces e.g. to couple MSC Adams and Ansys Maxwell as well as a parallel co-simulation framework based on a general middleware with communication via TCP/IP are used. The latter uses a fast and explicit algorithm based on force-displacement coupling and has been developed in cooperation with the University of Darmstadt. This contribution mainly focuses on actuators, in particular, drives that are based on electro-mechanical principles and discusses amongst others a linear actuator on the basis of the Thomson coil and a recloser. Thereby, MSC Adams is used for the mechanical simulation and Comsol for the electro-magnetic simulation.

Layout of a Driver-in-the-Loop Simulator for Validation of Human Body Models

Fabian Kempter (*Institute of Engineering and Computational Mechanics, University of Stuttgart*), Jörg Fehr (*Institute of Engineering and Computational Mechanics, University of Stuttgart*) 09:10–09:30

In the field of crash simulation, advanced human body models (HBMs) with muscle representation become more and more important because of their ability to emulate the behaviour of real human occupants more accurately than dummy models. To get experimental validation data for these models concerning muscle activation and time-variant stiffness properties, we built up a low-cost Driver-in-the-Loop (DiL) simulator. Driver kinematics and muscle activation are tracked by computer stereo vision and electromyography (EMG). For improved driver immersion, kinematic feedback is provided by a 6-DOF motion platform, a force-feedback wheel and a bassshaker at the back of the driving seat. The DiL-simulation is based on a Simulink model, generated by the software package PreScan, with included mathematical models of vehicles, sensors, drivers, etc. The vehicle states, available in the generated Simulink model, are used to activate the motion platform via UDP-protocol. Due to the physical limitations of the platform, the so-called Motion Cueing Algorithms (MCA) are necessary to emulate real driving sensation by providing motion cues which minimize required translational platform movements. Vibrations in real driving conditions, like those induced by engine and road roughness, can be emulated by activating the bass-shaker at the back of the seat. Velocity dependent steering torques are ensured by the forced feedback steering wheel. Furthermore, functionalities of driver assistance systems, like lane change assistants, can be imitated. The presented setup allows investigations of driver behavior in Pre-Crash scenarios, with and without interaction of driver assistance systems, in a safe environment.

S01.04 | Multi-body dynamics

Date 21.03.2018
Room 1601

Teaching Vision-based Control for Autonomous Driving with LEGO Mindstorms EV3, Raspberry Pi and Simulink

Svenja Otto (*Institute of Mechanics and Ocean Engineering, Hamburg University of Technology (TU Hamburg-Harburg)*), Alexander Schmitt (*Hamburg University of Technology (TU Hamburg-Harburg)*), Daniel-André Dücker (*Hamburg University of Technology (TU Hamburg-Harburg)*), Robert Seifried (*Hamburg University of Technology (TU Hamburg-Harburg)*) 14:00–14:20

Autonomous driving is currently a major topic in vehicle system dynamics. However, in most engineering curricula, this is only partly addressed. In this talk, a hands-on approach to teach basic concepts in autonomous driving is presented.
LEGO Mindstorms is a popular platform to teach beginner-level robotics. The programming of the robots can for example be done in a block-based software provided by LEGO or several open-source projects, e.g. *leJOS*. However, the LEGO software is limited to simple programs and the Java syntax is difficult for beginner-level students. Moreover, LEGO Mindstorms lacks a suitable camera and powerful hardware to process images in real-time.
We expand LEGO Mindstorms by adding a webcam for vision control and a Raspberry Pi for image processing. The programs are written in Simulink, because it provides a suitable abstraction level. Thus, the students are able to focus on high-level functionalities instead of programming syntax.
Goals of the class are threefold: First, we want to teach main robotics concepts. Secondly, the students shall learn about the challenges of software development in a team. Thirdly, they get a high-level understanding of the key elements of autonomous driving. During the first part of class, simple mechanical and image processing principles are taught in short presentations and hands-on sessions. During the second part, the students are divided into groups and work on their own projects such as line following, traffic sign recognition and others. In the future, these concepts are transformed into a course dedicated to more sophisticated vehicle control tasks.

A task space admittance control algorithm for safe human robot interaction

Dominik Kaserer (*Institute of Robotics, Johannes Kepler University Linz*), Hubert Gattringer (*Institute of Robotics, Johannes Kepler University Linz*), Andreas Müller (*Intititue of Robotics, Johannes Kepler University Linz*) 14:20–14:40

A recent development for programming industrial robotic manipulators is the interactive teaching of task motions where a human operator physically guides the end-effector (EE) of a robot. Admittance control schemes are used to this end. Since the operator is in direct contact with the robot, it must be ensured that the velocities of the robot are within a safe range at any time. Thus, in order to guarantee safe operation, position and velocity limits must be respected within the admittance control.
It is shown in this paper how admittance control schemes can be implemented in joint space and in task space. The first implementation immediately allows for limiting joint positions and velocities, but limits on the EE pose and velocity cannot be respected directly. Similarly, the task space implementation allows for directly incorporating limits on the EE motion but not the limits on joint positions and velocities. An admittance control scheme in task space is presented

that is able to simultaneously respect limits on position and velocities in task space and joint space.
The estimation of interaction wrench is crucial for admittance control. Three different methods for obtaining such an estimation are presented. Firstly a six axis force/torque sensor mounted on the robot endeffector is used. The next estimation approach is based on a dynamic manipulator model using the generalized momentum, where the last approach uses a single axis model.
The performance of the algorithm is demonstrated by discussing experimental results obtained using a Comau Racer3 robot.

Influence of friction-induced heating on the dynamic behaviour of rotors supported by journal bearings

Cornelius Irmscher (*Faculty of Mechanical Engineering, Institute for mechanics, Otto-von-Guericke-Universität Magdeburg*), Steffen Nitzschke (*Faculty of Mechanical Engineering, Institute of Mechanics, Otto-von-Guericke-Universität Magdeburg*), Christian Daniel (*Faculty of Mechanical Engineering, Institute of Mechanics, Otto-von-Guericke-Universität Magdeburg*), Elmar Woschke (*Faculty of Mechanical Engineering, Institute of Mechanics, Otto-von-Guericke-Universität Magdeburg*) 14:40–15:00

For the support of high speed rotor systems, e.g. turbochargers, hydrodynamic bearings are commonly used because of their low manufacturing costs and their advantageous thermal behaviour. However, different oil-film-induced instabilities have to be accounted for (fluid whirl and fluid whip [Mus10]), which are strongly dependent on the operating temperature of the system as the oil viscosity can vary significantly with changes in temperature. Usually, temperatures are not considered in detail when the geometry of the hydrodynamic bearing is determined.
In this contribution, a holistic approach for calculating the thermo-hydrodynamic behaviour of a bearing-rotor-system is presented. The hydrodynamic pressure is calculated using the Reynolds-equation and a mass-conserving cavitation algorithm described in [NWSS16]. The resulting pressure field is used to compute the temperatures in the oil film by solving the full three-dimensional energy equation

$$\underbrace{\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial x}+v\frac{\partial T}{\partial y}+w\frac{\partial T}{\partial z}}_{\text{Convective term}}=\underbrace{\frac{\lambda}{\rho\, c_p}\left[\frac{\partial}{\partial x}\left(\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(\frac{\partial T}{\partial z}\right)\right]}_{\text{Conductive term}}+\underbrace{\frac{\eta}{\rho\, c_p}\left[\left(\frac{\partial u}{\partial z}\right)^2+\left(\frac{\partial v}{\partial z}\right)^2\right]}_{\text{Dissipative term}}. \tag{1}$$

Furthermore, conduction is accounted for by including the heat conduction equations for the shaft and the bushing

$$\frac{\partial T}{\partial t}=\frac{\lambda}{\rho c_p}\left(\frac{1}{r^2}\frac{\partial^2 T}{\partial \varphi^2}+\frac{\partial^2 T}{\partial y^2}+\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)\right). \tag{2}$$

All equations are solved iteratively in the time domain to include relevant nonlinear effects and to model the coupling between thermal and mechanical regime correctly. It can be shown, that for high rotational speeds and/or high bearing loads, the stationary orbit of a simple rotor differs considerably from results achieved by isothermal calculations. The simulation model presented in this work will be validated with experimental data of a rotor measured by Glienicke et al., [GEG93]. Improvements in consequence of the increased modeling depth will be pointed out in comparison to simulation results of [Nit16], where an accumulation of friction power was used to estimate effective operating temperatures roughly.
Keywords: thermo-hydrodynamic bearing, high speed rotor dynamics, energy equation

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Mathematical Modeling of the Action of a Medium on a Conical Body

Maxim V. Shamolin (*Institute of Mechanics, Lomonosov Moscow State University*) 15:00–15:20

We consider a mathematical model of a plane-parallel action of a medium on a rigid body whose surface has a part which is a circular cone. We present a complete system of equations of motion under the quasi-stationarity conditions. The dynamical part of equations of motion form an independent system that possesses an independent second-order subsystem on a two-dimensional cylinder.

Consider a plane-parallel motion of a homogeneous rigid body of mass m with the coneshaped front part interacting with a flow of medium under conditions of jet circumfluence of flow-separated circumfluence. For simplicity, we assume that the coordinate y_N of the application point N of the action force of the medium is determined by a single parameter, namely, by the angle of attack α, i.e., the angle between the velocity vector of the point D and the symmetry axis Dx:

$$y_N = R(\alpha). \tag{1}$$

We represent the forces of frontal and side resistance as quadratic functions of the speed of the point D:

$$\mathbf{S}_x = -s(\alpha)v^2\mathbf{e}_x,\ \mathbf{S}_y = -b(\alpha)v^2\mathbf{e}_y,\ |\mathbf{v}_D| = v. \tag{2}$$

Thus, we triple of functions $R(\alpha), s(\alpha)$, and $b(\alpha)$ determines the action of a medium on a rigid body under the quasi-stationarity conditions (see [1, 2]). In this case, the conical shape of the surface of the body and the hypothesis on the quasi-static action of the medium allow one to determine the complete scheme of forces that contains all characteristics of the system. In the sequel, the analysis of systems constructed is performed by well-known methods of qualitative theory and new methods developed especially for systems with variable dissipation (see [2, 3]).

Taking into account the conditions (1) and (2), we can rewrite the dynamical part of equations of motion in the following form:

$$\dot v\cos\alpha - \dot\alpha v\sin\alpha + \Omega v\sin\alpha + \sigma\Omega^2 = -\frac{s(\alpha)}{m}v^2, \tag{3}$$

$$\dot v\sin\alpha + \dot\alpha v\cos\alpha - \Omega v\cos\alpha + \sigma\dot\Omega = -\frac{b(\alpha)}{m}v^2, \tag{4}$$

$$I\dot\Omega = -F(\alpha)s(\alpha)v^2 + \sigma b(\alpha)v^2 - h\Omega v, \tag{5}$$

where I is the central moment of inertia of the body, $\sigma = CD$, C is the center of mass, $F(\alpha) = R(\alpha)s(\alpha)$, and the coefficient $h > 0$ characterizes an additional moment depending on the angular

velocity (see [1, 3]). Note that the the dependence of forces and moments on the angular velocity in such problems is not a priori obvious.
The first two equations are obtained from the theorem on the motion of the center of mass and the third from the theorem on the change of the kinetic moments in the Konig axes. Similar results without side forces were used earlier in [1, 2].
Since the kinetic energy of the body and generalized forces and moments are independent of the location of the body on the plane, the position coordinates in the system are cyclic. This allow one to consider the system of dynamical equations (3)–(5) as an independent system.
To obtain the form of the functions $R(\alpha), s(\alpha)$, and $b(\alpha)$, one need experimental information about properties of jet circumfluence.
In this activity, we obtain an infinite family of phase portraits on the phase cylinder of quasi-velocities corresponding to the presence in the system only of a nonconservative pair of forces.

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Impact Simulations using Reduced Models considering Local and Global Deformation

Robert Seifried (*Mechanik und Meerestechnik, Hamburg University of Technology*), Stephan Tschigg (*Hamburg University of Technology*) 15:20–15:40

During impact bodies are locally deformed in the contract area. These deformations are propagating away from the contact area. While in compact bodies these wave phenomena are negligible, they are essential in impacts involving slender bodies. Thereby, during impact local and global deformations influence the contact process and thus the contact force.
For an efficient impact analysis considering the local and global deformation behavior, reduced models combined with a local contact model can be used. The global dynamic can be approximated using a moderate number of eigenmodes. However, information concerning local deformation at the contact point is missing. Thus, the contact process cannot be captured in detail. One possibility for capturing the local deformation correctly in the contact zone is to add static shape functions to the reduction basis. However, due to the high frequencies introduced by the static shape functions, the numerical stiffness increases which leads to very high computation times.
In this work an efficient contact simulation in such reduced flexible multibody systems is presented. Thereby, the flexible parts in the equations of motion are divided in low and high frequency contributions. Those high frequency parts, introduced by the static shape functions, are only required for capturing the local deformations and have no effects on the low frequency global motion. These high frequency parts are then neglected in the dynamic simulation. The coupling between low and high frequency parts is established by the contact forces. For evaluation, the results will be compared with full nonlinear FE impact simulations.

S02 | Biomechanics

Organiser Sandra Klinge (*Institute of Mechanics, TU Dortmund University*)
Roger A. Sauer (*RWTH Aachen University*)

S02.01 | Biomechanics

Date 20.03.2018
Room 2770

Modelling apoptosis of lung metastases within brain tissue

Patrick Schröder (*Institute of Applied Mechanics (CE), University of Stuttgart*), Arndt Wagner (*Institute of Applied Mechanics (CE), University of Stuttgart*), Daniela Stöhr (*Institute of Cell Biology and Immunology, University of Stuttgart*), Markus Rehm (*Institute of Cell Biology and Immunology, University of Stuttgart*), Antje Jensch (*Institute for Systems Theory and Automatic Control, University of Stuttgart*), Nicole Radde (*Institute for Systems Theory and Automatic Control, University of Stuttgart*), Wolfgang Ehlers (*Institute of Applied Mechanics (CE), University of Stuttgart*) 08:30–08:50

The vascularised lung metastases within brain tissue can be seen as the final step of the metastasation process. A promising treatment can be the infusion of a drug into the interstitial fluid of the brain tissue. Then, the drug is supposed to trigger the cell death of the metastases resulting in a reduction of the cancer cells.
In this contribution, the describing continuum-mechanical model is based on the Theory of Porous Media (TPM). In particular, the constituents are characterised by an elastic solid skeleton (brain cells and metastases) and two immiscible pore liquids (interstitial fluid and blood). Moreover, the interstitial fluid is a real mixture of nutrients, which supply the metastases, and the infused drug. The proliferation and the apoptosis processes are described via mass-production terms.
The governing equations of the model are the overall momentum balance and the adapted mass-balance relations. Therein, the primary variables include the solid deformation, the pressures of the liquids and the concentrations. The coupled system is solved monolithically with the finite-element tool PANDAS. In particular, the discretisation in space uses Taylor-Hood elements and the time discretisation applies an Euler time-integration scheme.
A realistic apoptosis behaviour is achieved by the adaptation of the apoptosis rate using experiments. Therefore, suited experiments observing the behaviour of cancer cells in different drug solutions are evaluated. In the data-driven optimisation, the apoptosis parameters of the continuum-mechanical model are optimised using maximum likelihood estimation.

Efficient numerical simulations of drug delivery in multi-component brain tissue

Arndt Wagner (*Institute of Applied Mechanics, University of Stuttgart*), Davina Fink (*Institute of Applied Mechanics, University of Stuttgart*), Wolfgang Ehlers (*Institute of Applied Mechanics, University of Stuttgart*) 08:50–09:10

In the proposed contribution, we will discuss the problem-specific application of suitable model-reduction techniques to obtain an efficient numerical simulation of therapeutic infusion processes within multi-component brain tissues. For this purpose, a compact summary of the underlying theoretical multi-component brain-tissue model is firstly introduced in the framework of the Theory of Porous Media (TPM). Typically, the straight-forward monolithic solution of the arising

coupled system of equations yields to immense numerical costs. Therefore, the primary aim of this contribution is to apply the method of proper orthogonal decomposition (POD) for a simplified model and the POD in combination with the discrete-empirical-interpolation method (DEIM) for a general nonlinear model in order to reduce the required computation time significantly. In this regard, the required adaptations are derived for both brain-tissue models by customising the POD(-DEIM) such that the different temporal behaviour of the primary variables is represented, while the system's block structure is preserved. Finally, several numerical simulations are discussed in terms of efficiency, accuracy and parameter variations.

Region- and loading-specific finite viscoelasticity of human brain tissue

Silvia Budday (*Department of Mechanical Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Gerhard Sommer (*Institute of Biomechanics, Graz University of Technology*), Gerhard A. Holzapfel (*Institute of Biomechanics, Faculty of Engineering Science and Technology, Graz University of Technology, Norwegian University of Science and Technology Trondheim*), Paul Steinmann (*Chair of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Ellen Kuhl (*Stanford University*) 09:10–09:30

Computational simulations are a powerful tool to understand the mechanical behavior of our brain in health and disease, with the ultimate goal to prevent pathological conditions. Accurate numerical predictions, however, require the development of appropriate constitutive models and, equally importantly, the careful calibration of the corresponding constitutive parameters. This has been exceptionally challenging due to the ultrasoft nature of brain tissue resulting in a distinctly nonlinear, rate-dependent, compression-tension asymmetric, and region-dependent behavior. Previous constitutive models have been deduced from a single loading mode but fail to predict the behavior under arbitrary loading conditions. To overcome this drawback, we performed a combination of cyclic and relaxation experiments under multiple loading modes, simple shear, compression, and tension, on specimens from four different regions of the human brain, the cortex, the basal ganglia, the corona radiata, and the corpus callosum. We developed a large strain, nonlinear, viscoelastic constitutive model and carefully calibrated region-specific material parameters considering all loading modes simultaneously. The model captures time-independent effects such as nonlinearity and compression-tension asymmetry, but also time-dependent effects with substantial pre-conditioning during the first loading cycle, only minor conditioning effects during subsequent cycles, and successive softening when the applied strain is stepwise increased. With close consideration of the underlying microstructure, the viscoelastic material parameters allow us to understand rate-dependent regional trends and seemingly contradictory results in the literature. Our results help to improve the accuracy of human brain simulations during development and disease or to predict outcomes of neurosurgical procedures.

Haemodynamics in an elasto-mechanic model of the human heart

Anna Daub (*Institute of Fluid Mechanics, Karlsruhe Institute of Technology - KIT*), Axel Loewe (*Institute of Biomedical Engineering, Karlsruhe Institute of Technology - KIT*), Bettina Frohnapfel (*Institute of Fluid Mechanics, Karlsruhe Institute of Technology - KIT*) 09:30–09:50

Numerical modelling enables a quantitative evaluation of physiological and patho-physiological relationships within the human heart and the circulatory system. Surgical planning and optimisation of medical equipment using a virtual heart become possible by merging of empirical studies with physical and mathematical knowledge. These goals motivate a multi-physical coupling between electro-physiology, elasto-mechanics, blood flow and the circulatory system.

In a first step a one-way coupling of all four relevant physical domains is considered. Simulation of electro-physiological excitation spread in conjunction with excitation contraction coupling yields the spatio-temporal distribution of cardiac active tension. This, as well as a closed loop model of the circulatory system, drive the continuum mechanics simulation of cardiac deformation and pressure, which in turn serve as a boundary condition for blood flow simulation.
Physiological blood flow dynamics are dominated by the formation of a ring vortex that washes out the ventricles and thereby reduces the risk of thrombogenesis and flow stasis. This process is strongly affected by the heart valves. However, including the three dimensional leaflets and their interaction with the blood flow is computationally expensive. Further, the effort for construction is not negligible. Therefore, a simpler model is implemented as a first step. It comprises of three layers of porous cells that move with the valve plane and time dependently block or open the plane respectively. First results illustrate a high potential of the model to reliably reproduce the physiological vortex formation in the ventricles.

Simulation of cardiac electromechanics of a rat left ventricle

Minh Tuan Duong (*Mechanical Engineering, University of Erlangen-Nuremberg*), David Holz (*Mechanical Engineering, University of Erlangen-Nuremberg*), Theresa Ach (*Mechanical Engineering, University of Erlangen-Nuremberg*), Svea Vanessa Binnewitt (*Pediatric Cardiology, University of Erlangen Nuremberg*), Hedwig Stegmann (*University of Erlangen-Nuremberg*), Sven Dittrich (*University of Erlangen-Nuremberg*), Muhannad Alkassar (*University of Erlangen-Nuremberg*), Sigrid Leyendecker (*University of Erlangen-Nuremberg*)

09:50–10:10

In heart pathology, rat hearts are often preferably employed as surrogates due to their similar structure and function and less ethical problems in comparison to human hearts. In the cardiac electromechanics of a living rat heart, the electrical depolarization wave propagates through the whole heart to trigger mechanical contraction, which is known as excitation-contraction coupling since the electrical activation leads to the mechanical contraction. It is well known that various heart diseases can alter this process to cause heart failure such as electromechanical dyssynchrony. Therefore, developing computational models for rat hearts plays a crucial role since they can provide highly valuable means, which help improve clinical therapies and medical devices with lower costs and reduced time. Furthermore, heart diseases are rising mostly from the left ventricle [1]. Modelling a rat left ventricle (LV) becomes mostly essential for investigating cardiac electromechanical coupling and its disorders. In this study, the modelling of cardiac electromechanics of the left ventricle is thoroughly discussed. With a 3D geometry of a rat LV constructed from MRI images provided by the Pediatric Cardiology in Erlangen, the mechanical properties and fibre orientations of cardiac muscles are then modeled and generated similar to [2]. We employ the FitzHugh-Nagumo and Aliev-Panfilov models for the oscillatory pacemaker and non-oscillatory cardiac muscle cells in the constitutive relations based on the monodomain formulation in which the active stress approach is adopted [3]. The excitation-contraction model is successfully implemented in a finite element setting using implicit Euler time stepping combined with a finite difference method and a Newton iteration algorithm. With the implemented model at hand, several assumed diseased cases of the LV are simulated such as fibrillation. Our results analyse the differences between the healthy and diseased left ventricles, which can be significant findings for improving therapy design and medical devices.

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A coupled thermo-poro-mechanical constitutive model of the breast applied to breast cancer detection

Angela Niedermeyer (*Institute of General Mechancs, RWTH Aachen University*), Songyun Ma (*Institute of General Mechanics, RWTH Aachen University*), Bernd Markert (*Institute of General Mechanics, RWTH Aachen University*) 10:10–10:30

Breast cancer is the most common type of cancer in women worldwide and its incidence is continuously increasing. As early detection significantly improves survival rates, a widely available, harm-free and reliable detection method is desired [1]. Cancerous tissue is known to inhere an increased temperature compared to normal tissues. Recently, diagnostic methods based on infrared thermographic imaging of the skin have shown promising results regarding skin cancer detection [2], whereas the application to breast cancer, which can be located distant from the body surface, has not yet led to satisfying results. The challenge lies in solving the inverse problem and determining the location and intensity of the embedded cancerous heat source from measured infrared radiation of the breast surface. While many research efforts have been devoted to improving image processing for breast cancer detection, the aim of the present work is to develop a computational approach to investigate the relationship between the characteristics of surface temperature distributions and geometrical and thermal characteristics of tumours.
For this purpose, a coupled thermo-mechanical constitutive model of the breast is proposed which accurately describes the interaction between the energy transport and thermomechanical deformations in biological tissues and vessel systems. Porous media theories are well-suited for the detailed modelling of hydrated biological tissue and therefore used in this approach, see [3] among others. In this work, numerical simulations of the breast containing a tumor are conducted to study the correlation between temperature differences of the skin and tumour characteristics. The results demonstrate that the proposed modelling approach can be employed to determine optimal measurement conditions such as surrounding temperature and to evaluate the potentialities of transient measurements.

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S02.02 | Biomechanics

Date 20.03.2018
Room 2770

Homogenisation-based multiscale modelling of skeletal muscle tissue

Christian Bleiler (*Institute of Applied Mechanics, University of Stuttgart*), Pedro Ponte Castañeda (*Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania*), Oliver Röhrle (*Institute of Applied Mechanics, University of Stuttgart*) 16:30–17:10

Skeletal muscle tissue -as well as biological tissue in general- shows a wide variation in its mechanical response for different persons or different muscle types of one single person. It is well known that these distinct mechanical properties are due to variations in the microstructure of the material. For skeletal muscles, especially the arrangement and the stiffness of collagen fibres in the connective tissue define the macroscopic passive stiffness, while the sarcomeres (contractile units) enable an active contractility of the muscles. Moreover, the microstructural arrangement not only influences the stiffness, but also the anisotropy of the material at the macroscale. Continuum-mechanical muscle models based on phenomenological approaches are easy to implement, but lack the ability to take microstructural properties into account in a natural way. Hence, experimental data for every desired muscle type to be modeled is required, but usually not available. Thus, this work presents a homogenisation-based multiscale model for skeletal muscle tissue which enables to include microstructural properties directly into a continuum-mechanical model at the macroscale by using well-founded analytical homogenisation techniques, enhanced by an angular integration model for a comprehensive description of the collageneous network.

The research of viscoelastic mechanical behaviour of human periodontal ligament based on creep and stress-relaxation tests

Bin Wu (*College of Mechanical and Electronic Engineering, Nanjing Forestry University*), Songyun Ma (*Institute of General Mechanics, RWTH Aachen University*), Bin Yan (*Affiliated Hospital of Stomatology, Nanjing Medical University*), Yousef Heider (*Institute of General Mechanics, RWTH Aachen University*), Bernd Markert (*Institute of General Mechanics, RWTH Aachen University*) 17:10–17:30

The mechanical behaviour of the periodontal ligament (PDL) under the correction loadings play an important role in the tooth movement mechanism during orthodontic treatment. The complexity of the fibrous structure of the human periodontal ligament and the limitation of the experimental technology for the small-scale testing lead to an insufficient understanding of the deformation mechanisms and the difficulties in the accurate modelling of the constitutive behaviour. Experimental studies based on animal tests [1-4] have shown that the PDL has nonlinear viscoelastic behaviour. However, there is a large gap between the theoretical descriptions and the experimental observations of the constitutive behaviour of PDL under different loading conditions.
The development of appropriate constitutive model relies on a well-established mechanical testing. The mechanical testing of human PDL is still in the exploratory stage, mainly in static test. Time-dependent tests on Human PDL are not systematically carried out to study its complex deformation behaviour. In this paper, a dynamic thermomechanical analyzer was used to perform creep and stress-relaxation tests on human periodontal ligament samples. Furthermore, a

viscoelastic model with five parameters is employed to correlate the test data. The results show that the stress-strain curves of the four samples under different loadings can be predicted by the used constitutive model. The high correction coefficients above 0.95 for all tests indicate that the five-parameter viscoelastic model is suitable for describing the viscoelastic behaviour of human periodontal ligament.

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Investigating the Role of Meso-scale Structure on the Passive Mechanical Response of Skeletal Muscle Tissues

Ramachandra Kuravi (*Soft Material Systems, Empa - Swiss Federal Laboratories for Materials Science and Technology*), Markus Böl (*Institut für Festköpermechanik, TU Braunschweig*), Alexander Ehret (*Empa - Swiss Federal Laboratories for Materials Science and Technology*)

17:30–17:50

Skeletal muscle, and tendon tissue are highly hierarchical materials with multifarious fibre bundles embedded in sheaths of extracellular matrix manifesting as honeycomb structure like scaffolding [4, 5]. These tissues are typically modeled as transversely isotropic materials with a constitutive form incorporating lumped material properties of their constituents [7, 8]. The often employed assumption of non-contributing muscle and tendon fibres in compression was found wanting by recent observations [1, 2], whereas the meso-scale hierarchy stabilized by collagen sheaths was hypothesized to play a prominent role [2, 3]. This motivates identifying and incorporating the role of this internal hierarchy and structure in modeling to study the peculiar response of these tissues. In this context, multi-scale models capturing these features as well as inter-component interactions could offer a comprehensive framework to analyze these tissues, and finally predict their response.

The present contribution focuses on developing a detailed finite element model for skeletal muscle tissue based on a three-dimensional 'representative' volume element reconstructed from histological sections of unloaded muscle tissue. The perimysium and endomysium sheaths are assumed to consist of layers of collagen tubes, whose disposition in and around fascicles is estimated by drawing an analogy from steady-state heat transfer analyses (cf. [6]). These results are compared with microscopic images of the tissue. Each constituent is then associated with a corresponding material model, properties, and material symmetry. The finite element model thus obtained is used to predict the compression response of muscle tissue, from whence inferences on internal load transfer mechanisms in the tissue can be deduced.

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Modelling voluntary contraction capabilities of vastus lateralis using a motor unit recruitment model

Ekin Altan (*Institute of Applied Mechanics (Civil Engineering), University of Stuttgart*), Leonardo Gizzi (*Institute of Applied Mechanics (CE), Chair of Continuum Mechanics, Continuum Biomechanics and Mechanobiology Research Group, University of Stuttgart*), Oliver Röhrle (*Institute of Applied Mechanics (CE), Chair of Continuum Mechanics, Continuum Biomechanics and Mechanobiology Research Group, University of Stuttgart*) 17:50–18:10

An important feature of skeletal muscles is providing mammals with the ability to move voluntarily. Therefore, the voluntary control of skeletal muscles requires careful investigation. In this work, voluntary control of skeletal muscles is modelled based on a motor-unit recruitment model as suggested by Fuglevand et al. (1993) [2]. The parameters of the recruitment model is altered such that the available information regarding contractile properties of the vastus lateralis (VL) muscle (e.g. see [3]) is included within the model. Being a measure of muscle strength, maximum voluntary contraction (MVC) is reproduced.
Features of motor-unit recruitment behavior (e.g. conduction velocity) can only be measured for a relatively small portion of the whole motor-unit pool known to exist in the vastus lateralis muscle, mainly due to limitations in the tools used for experimental measurements. Previously, Contessa et al. (2011) [1] attempted to reproduce 20 % MVC of the VL. The novel feature of this work lies in its capabilities to speculate on the behavior of individual motor units of vastus lateralis while accounting for the whole motor-unit pool at up to 100% MVC.
Acknowledgement: This study is funded by the German Science Foundation (DFG) within the Cluster of Excellence in Simulation Technology (EXC 310/1) at the University of Stuttgart.

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Fiber-based modeling of muscles in the musculoskeletal system

Michael Gfrerer (*FB Mathematik, TU Kaiserslautern*), Bernd Simeon (*TU Kaiserslautern*) 18:10–18:30

The aim of this contribution is to present a fiber-based modeling approach for the dynamic behavior of muscles within the musculoskeletal system. We represent the skeletal system as a rigid multibody system which is actuated by muscles. For this setting, various models for the muscular force generation with different levels of details can be found in literature. Many models relay on Hill-type force elements incorporating passive and active muscle activities [1]. Such models are computational effective but do not represent the real situation accurately. In contrast to Hill-type models, 3D representations of muscles allow for the inclusion of mass, large deformations, incompressible material behavior, complex geometries, fiber orientations, local activation principles and chemo-electrophysiological aspects [2, 3]. However, such models come along with an increased computational cost and increased modeling complexity.
In the present approach, we model each muscle fiber bundle as a 1D cable with variable cross section undergoing large deformation and strains. We employ a incompressible Neo-Hookean material for the passive behavior and a active stress law found in the literature [2]. We incorporate contact between the fiber bundles with a finite element framework by a penalty method. We apply our framework to conduct a forward simulation of a arm model.

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S02.03 | Biomechanics

Date 21.03.2018
Room 2770

On the phenomenological modelling of potato tissue

Robin Trostorf (*Institute of Solid Mechanics, TU Braunschweig*), Kay Leichsenring (*Institute of solid mechanics, Technische Universität Braunschweig*), Robert Seydewitz (*Institute of solid mechanics, Technische Universität Braunschweig*), Markus Böl (*Institute of solid mechanics, Technische Universität Braunschweig*) 08:30–08:50

The macroscopic stress-strain behavior of potato tuber parenchyma tissue is reflective of its distinct microstructure. A phenomenological constitutive model based on the notion of pseudo-hyperelasticity for different anatomical parts of the potato tuber is presented. The proposed constitutive model expresses the internal stresses in terms of the elastic contribution to the local strains and is controlled by a kinetic memory variable that traces the past strain history. The constitutive parameters are identified based on stress-stretch curves obtained from single-cycle uniaxial compression experiments on samples extracted from the tuber pith, the perimedullary zone, the perimedullary/cortex interface, and the peripheral cortex. The tissue's stress-strain response is characterised by a pronounced and well-reproducible hysteresis. In view of the parenchyma microstructure, the significant reduction in tissue turgidity on unloading may be caused by the eviction of intracellular fluid from parenchyma cells as well as an inelastic cell wall response. To prove the hypothesis, multiple loading and unloading cycles reveal a stable operational range, indicating a partly reversible process. The eviction of intracellular fluid is reversible and assumed to cause the hysteresis for multiple cycles. Besides tissue-level experiments, micromechanical testings at cell level have been realised allowing future investigation in term of multi-scale modelling.

Wobbling masses in human legs: they cost but pay off

Syn Schmitt (*University of Stuttgart*), Daniel Häufle (*University of Tübingen*), Michael Günther (*University of Stuttgart*) 08:50–09:10

Humans seem biomechanically unique in the animal kingdom. Rather than the use of just two straight legs, or even just one as in sleeping birds, it is the amount of muscle mass located in the legs that makes up this human uniqueness. As muscle masses are soft tissue attached to the skeleton they start to "wobble" when the bones are mechanically excited by impacts. That is, they are exposed to visco-elastic forces which induce oscillatory soft tissue movements relative to the bones and come along with energy dissipation. As the latter is expected to scale with the mass portion we asked for absolute numbers: how much energy is dissipated by human wobbling masses after a leg impact? We calculated these numbers in human running by estimating the wobbling mass kinematics from high-speed imaging sequences. The comparison to axial leg work and joint energy balances during ground contact provides a measure of relevance for the irreversible energy loss by leg wobbling masses. We discuss functional explanations for the acquiescence of such a uniquely high amount of wobbling masses in the leg. We also try and explain how they yet pay off although any significant amount of irreversible energy loss like wobbling mass dissipation would seem inefficient and thus expectably avoided as good as possible by nature.

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Lightweight construction with two-dimensional cellular solids in additive manufacturing

Alexander Großmann (*Konstruktiver Leichtbau und Bauweisen, Technische Universität Darmstadt*), Christian Mittelstedt (*Lightweight Construction and Design, Technische Universität Darmstadt*) 09:10–09:30

Cellular structures have served as a role model for lightweight construction for decades. The elastic properties have been investigated by many authors since then. However, the conventional manufacturing possibilities always restricted the design freedom and potential applications for two-dimensional cellular solids. With additive manufacturing, a high degree of manufacturing freedom delivers a wide range of opportunities for applications and structural integration of these structures in order to obtain lightweight structures. This also engenders the need for further investigation of two-dimensional cellular solids. The physical models to assess the elastic properties have not been validated regarding their applicability to additively manufactured structures. To get a high lightweight degree at a given stiffness a construction engineer must be aware of the structure's geometry and the amount of material used in a representative volume element. Even though this can be obtained by simple geometric considerations little research has been conducted on that aspect.

In this work we deliver exact solutions for the so called relative density, which denotes the volume fraction of material used in a representative volume element, which is crucial to assess the lightweight degree. We further derive a new physical model for a representative honeycomb cell to obtain stiffness properties depending only on the geometric parameters. Assuming linear elastic material behaviour Hooke's Law can be used to obtain the stiffness. The corresponding load is given while the deformation can be calculated using the principle of virtual forces. With this contribution we aim to deliver and validate calculation models for both the relative density and elastic properties for additively manufactured two-dimensional cellular solids to enable construction engineers to use cellular solids in additive manufacturing with a maximum lightweight degree.

S02.04 | Biomechanics

Date 21.03.2018
Room 2770

Modelling the active behaviour of striated muscle tissue in continuum mechanics

Thomas Klotz (*Institute of Applied Mechanics, University of Stuttgart*), Christian Bleiler (*Institute of Applied Mechanics, University of Stuttgart*), Oliver Röhrle (*Institute of Applied Mechanics, University of Stuttgart*) 14:00–14:20

Similar to other biological materials striated muscle tissue generates a force in response to an applied deformation. However, in contrast to most other materials, muscle tissue can also actively contract and generate force by converting chemically stored energy into mechanical energy. In continuum mechanics, there exist two approaches to model the active contractile behaviour of striated muscle tissue. One can either add an additional active stress tensor to the standard passive stress tensor, or one can introduce a multiplicative decomposition of the deformation gradient tensor into an active and an elastic component. Both approaches have been successfully applied to model the active properties of muscle tissue and can reproduce muscles' behaviour in response to deformation. While previous comparisons of the different modelling approaches have focused on mathematical aspects like stability, we want to discuss these two modelling approaches with respect to muscle tissues physiological working principles, i.e. the hypotheses of the sliding filament and the cross-bridge theory. We conclude that the active stress approach is in agreement with the major claims of the sliding filament theory and can be considered as a homogenization of Andrew Fielding Huxleys' original myofilament model. However, experimental findings suggest that the simple superposition of active and passive stress contributions might be an oversimplification. Therefore, we propose a new constitutive formalism, using the multiplicative split of the deformation gradient tensor, to describe the coupling between passive and active muscle structures.

A phenomenological approach for modelling force enhancement and depression in skeletal muscle tissue

Robert Seydewitz (*Institute of solid mechanics, Technische Universität Braunschweig*), Tobias Siebert (*Institute of Sport and Motion Science, University of Stuttgart*), Markus Böl (*Institute of solid mechanics, Technische Universität Braunschweig*) 14:20–14:40

Among the different types of soft tissue, muscle is able to contract and to generate active forces. A well-established experimental procedure to obtain active mechanical properties is to measure the force during isometric contraction while the positions of the muscle ends are fixed. Experimental observations revealed, however, that the amount of forces strongly depends on the elongation history. A muscle, which undergoes isometric contraction, isokinetic elongation and again isometric contraction, generates higher active forces than for pure isometric contraction at final length. This force difference is often described as force enhancement. Contrary, considering isokinetic contraction between first and second isometric contraction, forces are lower in comparison to pure isometric contraction. The drop of the active force at same length is designated as force depression. Although, experimental data about history-effects such as force enhancement and depression are available and well documented, the underlying mechanism behind those effects still remains not fully understood. In that sense we present a phenomenological three-dimensional continuum-based approach to simulate the above mentioned history effects. For

the identification of the model parameters experimental data of the Soleus muscle were used. Further, the model was implemented in a finite element framework to analyse stress distribution in the muscle architecture during contraction.

Planar wrapping of "thick" muscle paths with non-constant cross section — comparison of analytical versus numerical methods

Katharina Müller (*University of Duisburg-Essen*), Andres Kecskemethy (*University of Duisburg-Essen*) 14:40–15:00

Within musculoskeletal simulations, muscle paths are usually modelled as thin, massless lines and evaluated regarding their lengths as well as rates of length change to compute muscle forces, moment arms and the resulting body and joint loads. Hereby, curved paths are often modelled as polygon-type lines deflected at via points. However, this approach does not render correct moment arms. In [1], a wrapping algorithm using natural geodesic variations is presented, which is computationally very efficient and produces continuous results for arbitrary smooth surfaces. However, for volumetric muscles, muscle paths currently can be only computed either by FEM or discretized approaches, which are either computationally slow or discontinuous.
In this paper, a new method is proposed for computing resulting continuous paths of the midline of thick muscles with non-constant cross section, assuming (1) no elongation, (2) known constant cross section at each point of the midline, (3) massless muscles, (4) no friction, and (5) a given rigid surface. Hereby, only the planar case is regarded. The method is based on formulating the kinematic (velocity) wrapping condition at the midline and integrating this to obtain the global curves. The approach is tested for a conus-type cross-section profile wrapped around a circle, an ellipse or a lemniscate, showing its computational efficiency as well as its correspondence either with analytic solutions (conus on circle giving a logarithmic spiral) or discretized methods in the literature [2]. Further developments will consist in extending the method to 3D surfaces by combining it with the geodesic method.

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Predicting skeletal muscle force from motor-unit activity using 3D FEM

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Deeper understanding of the neuromuscular (NM) pathway, from the recruitment and firing of motor-units (MUs) to sarcomere contraction and overall muscle force production, can provide valuable insights concerning the underlying mechanisms of healthy and pathological human movement [1]. Typically, such forward biomechanical models of skeletal muscles use a global neural

drive applied over the entire muscle, which simplifies the underlying physiological structure of skeletal muscle. That is, by using a single per-muscle neural drive, both the spatial distribution and activation of individual MUs cannot be taken into account. On the other hand, multi-scale models, which explicitly model muscle fibres (MFs), and therefore MUs, require a very large model setup effort and the subsequent computation time required for their solution limits the use of these models in practice.
The current work aims to bridge this gap by incorporating neural drive into status-quo continuum models of skeletal muscle. The proposed model takes as inputs the individual stimulation trains of the MUs and predicts the resulting local stress response within the MU territory (MUT), which sums to give the overall muscle force production. Since MFs are not explicitly modelled in the current continuum model, the inclusion of MUTs is accomplished by considering MUTs in a distributed sense over the entire muscle rather than in a discrete sense in terms of MFs. The MU-MF innervation distribution is according to an exponential function [2], however, since MFs are not explicitly modelled innervation is transformed in terms of total muscle volume. MUTs are then spatially assigned to the continuum FE model by first, selecting a random MU centre (MUC) and second, assigning the allotted MU volume outwards according to some predefined distribution. The MU activations, derived from the decomposition of HD-sEMG data, are then applied to the spatially distributed MUs in the muscle model and the local stress/strain response is computed. Model data such as geometry, muscle fibre orientation and muscle activation are derived from a single subject, therefore ensuring compatibility between the individual model components.
The current work provides a methodology to integrate motor unit activity with overall force production without the need to explicitly model MFs. While the preclusion of MFs limits the physiological realism of the model, it provides a computationally efficient and easy to set-up model for investigations into the neural drive of skeletal muscles.

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The effect of the collagen fibrils network on the damage behavior of articular cartilage: a computational study

Dongxu Liu (*Institute of General Mechanics, RWTH Aachen University*), Songyun Ma (*Institute of General Mechanics, RWTH Aachen University*), Bernd Markert (*Institute of General Mechanics, RWTH Aachen University*), Marcus Stoffel (*Institute of General Mechanics, RWTH Aachen University*)

15:20–15:40

Human articular cartilage plays a vital role in the function of synovial joints. Osteoarthritis (OA) can cause diarthrodial joint wear and eventually destruction to articular cartilage, which is closely related to the microstructural degradation of articular cartilage. The viscoelastic collagen fibril network is the main structural constituent of articular cartilage and resists most of the straining and swelling pressures [1]. Therefore, it is crucial to understand the relationship between the microscopic features of the complex collagen fibrils network and macroscopic damage behavior of articular cartilage under mechanical loadings. Recently, experimental and numerical studies have been carried out to understand articular damage [2]. However, the effect of the morphology of the fibrils network on the cartilage damage is still not yet well understood.
The aim of this work is to study the damage behavior and the microstructural degradation of articular cartilage by employing a multiscale computation approach. For this purpose, an anisotropic viscoelastic damage model based on the finite strain theory is proposed to describe the

damage process of collagen fibrils [3]. In addition, the inelastic deformation of the non-fibrillar matrix and the debonding of interfaces are incorporated in the micromechanical simulation as well. The stress and damage distribution are investigated to determine the influence of the fiber distribution on the cartilage damage. The computation results reveal that the location and magnitude of the damage in cartilage are strongly dependent on the orientation, distribution and the ratio between the primary and secondary level of the fibril network.

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Development of an internal physiological muscle controller within an open-source Hill-type material model in LS-DYNA

Oleksandr Martynenko (*Biomechanics and Biorobotics, Institute of Sport and Motion Science, University of Stuttgart*), Fabian Kempter (*Institute of Engineering and Computational Mechanics, University of Stuttgart*), Christian Kleinbach (*Institute of Engineering and Computational Mechanics, University of Stuttgart*), Syn Schmitt (*Biomechanics and Biorobotics, Institute of Sport and Motion Science, University of Stuttgart*), Jörg Fehr (*Institute of Engineering and Computational Mechanics, University of Stuttgart*)

15:40–16:00

Further improvement of vehicle safety with the means of only passive systems development has low potentials left, because of the serious limitations on construction material properties and time of action during collision. Thus, the focus is shifted to active safety systems development, which could operate during the so-called pre-crash phase and have less strict limits for action time, interaction with the occupants and type of their intervention functionality/actions. This process rises a new demand for a simulation tool, e.g. Finite Element Human Body Model (FE HBM), the ability to replicate active vehicle occupant behaviour. Such biofidelity improvement could be done through the integration of special active muscle elements to existing HBMs and development of the special muscle activation methods, enabling a realistic kinematic response.
In a previous study [1] an extended four element Hill-type muscle model from [2], enhanced with several major advantages in contrast to existing *MAT_MUSCLE, was integrated into LS-DYNA and publishes as an open-source active muscle user material. Current contribution presents the development of a physiologically inspired muscle controller, which could be subsequently integrated into this material.The controller is based on the internal muscle spindle length as control feedback [3, 4]. As a result, it is possible to control the muscle elements internally without any additional superior controller level or complementary keyword coding in LS-DYNA through the calculation of appropriate muscle activation levels, based on equilibrium point control [3] or reflexive muscle patterns [5]. Validation example with the optimized controller parameters and the short discussion are given.

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S02.05 | Biomechanics

Date 21.03.2018
Room 2770

Computational study of the interaction between degradation of biodegradable magnesium implants and bone remodelling

Songyun Ma (*Institute of General Mechanics, RWTH Aachen University*), 16:30–17:10
Bernd Markert (*Institute of General Mechanics, RWTH Aachen University*)

Biodegradable magnesium implants are increasingly applied to promising fixation devices in the orthopaedic application due to obvious advantages over conventional permanent implants. However, potential risks of environment assisted fatigue failures during their service in human body have not been systematically studied [1], which leads to a limitation of the extensive applications of the magnesium implants. In addition, the influence of the degradation process of magnesium implants on the bone remodelling after surgery is also a critical factor for their applications. Therefore, a modelling approach is required to understand their interactions with the physiological environment and improve the design of biodegradable magnesium implants with respect to the healing efficiency of fractured bones.
In the present work, three-dimensional computer simulations are conducted for a fractured tibia fixed by the bone plate and screws to investigate the service behaviour of magnesium implants and their interaction with the bone healing process. A mechano-regulatory model based on the biphasic stimuli is used to simulate tissue differentiation and bone remodelling of the fractured tibia. A corrosion-fatigue damage model is proposed to describe the complex degradation process of mechanical integrity of magnesium implants under physiological loadings. The simulation results are consistent with the experimental observation. The present modelling approach provides an efficient tool in the design and the performance evaluation of biodegradable magnesium implants.

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Simulation of Load Distribution in the Knee Joint

Jakob Schneck (*Numerical Mathematics, Zuse Institute Berlin (ZIB)*) 17:10–17:30

The movement of the lower extremities can be simulated by a rigid multi body model of the musculoskeletal system with measurement data from gait analysis as input. This allows for the individual identification of the overall contact loads in the joints but provides no information about the force distribution at the contact surface. Such a force distribution can be obtained by representing the joint components coming into contact, i.e. the cartilage, as elastic bodies and combining elastomechanical and rigid body model. Knowledge of the detailed cartilage strain can be helpful for the investigation of potential causes for joint diseases such as osteoarthritis.
In this talk we will present the elastomechanical contact model for the knee joint used by us and the steps towards a coupling with the musculoskeletal model for the lower limb. Suitable numerical methods necessary for the simulation, which have to cope with a partial differential equation, inequality constraints and nonlinear optimization, will also be addressed.

Development of a passive, wearable knee orthosis for the support of sit-to-stand movement with adaptive assistance moment

Jakob Ziegler (*Institute of Robotics, Johannes Kepler University Linz*), Herbert Parzer (*Institute of Robotics, Johannes Kepler University Linz*), Hubert Gattringer (*Institute of Robotics, Johannes Kepler University Linz*), Andreas Müller (*Institute of Robotics, Johannes Kepler University Linz*) 17:30–17:50

With the worldwide population aging along with higher risk of stroke and muscle weakness there recently has been an increasing interest in wearable robotic devices for movement assistance and rehabilitation. The ability to perform a sit-to-stand movement is prerequisite for other activities of daily living like walking and a major factor of functional independence. This work is focused on the development of a wearable knee orthosis that assists people with reduced ability of generating knee extension moment to perform the sit-to-stand movement.
The system consists of a spring mechanism mounted on the thigh segment of the orthosis and a cable connection to the shank segment with a deflector guiding the cable. As the knee flexes while sitting down the spring mechanism is loaded, thus generating a moment that assists standing up again. In order to prevent unintentional knee extension when the person is fully seated and to reduce the load on a potential locking mechanism the generated moment should be minimal in sitting and standing position but maximal in between. Assistance moment modulation is realized with a variable lever arm resulting from the deflector geometry. An optimization of this geometry is done according to a kinematic model of the orthosis and a desired moment progress. Describing the geometry with B-splines reduces the number of optimization parameters, additionally simplifying the formulation of constraints. Furthermore, the 2D coordinates of the deflector surface are composed of two separate splines enabling increased resolution along the geometry path. A first prototype shows promising experimental results.

Simulation of bone ingrowth into bone substitutes on implant level length scale

Ann-Kathrin Krüger (*Institut für Kontinuumsmechanik LUH*), Stefan Julmi (*Institut für Werkstoffkunde LUH*), Christian Klose (*Institut für Werkstoffkunde LUH*), Silke Besdo (*Institut für Kontinuumsmechanik LUH*), Hans Jürgen Maier (*Institut für Werkstoffkunde LUH*), Peter Wriggers (*Institut für Kontinuumsmechanik LUH*) 17:50–18:10

There are different indications for bone substitutes. All have in common that they result in a defect in bone, which cannot be filled autonomously by the body. This gap has to be filled with an appropriate structure and material. Therefore, open-pored structures have been developed and investigated as bone tissue can grow into these structures. It is known that bone changes its density and shape related to external loading. Near to the implant, bone remodelling occurs due to the mechanical perturbation introduced by the implant. Within the implant, formation of new bone occurs. As the length scale of the bone as organ and the pore size of the implant vary significantly, the bone growth has to be modelled on a meso scale. Therefore, in this study, the ingrowing behaviour of bone into bone substitutes is simulated on the implant level length scale. The simulations are based on numerical models for the phenomenological description of stress adaptive bone remodelling on a macro scale, which have been discussed already in the past. After the implantation the implant is filled with blood and tissue. Therefore, the bone ingrowth was modelled as a remodelling process from blood to bone, since no new material has to be build up at the bone surface. The state of bone during the ingrowth process is represented by the material density. With the implemented model, the bone ingrowth into an open-pored structure can be simulated using finite element method.

A finite element formulation for adhesive contact between bone and implant

Katharina Immel (*Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University*), Roger A. Sauer (*Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University*), Guillaume Haiat (*Laboratoire de Modélisation et de Simulation MultiEchelle, UMR CNRS 8208, Université Paris-Est*) 18:10–18:30

In this work, a new three-dimensional finite element formulation with isogeometrically enriched elements for adhesive contact between bone and implant is presented. This model is based on a cohesive zone model and combines sliding friction, adhesion and debonding for solid-solid interfaces of deformable bodies. This formulation is applied to investigate stability of cementless bone implants. Therefore, pull-out and mode III cleavage tests on osseointegrated coin-shaped titanium implants are modeled. For the material properties of bone a nonlinear Neo-Hookean material formulation is used, with parameters accounting for material properties of newly formed and mature bone based on measurements in [1, 3]. The results are compared with data from in-vitro experiments [2].

Keywords: adhesive contact, friction, bone, implant, debonding, finite element method, isogeometric analysis.

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S02.06 | Biomechanics

Date 22.03.2018
Room 2770

Remarks on Fluid-Structure-Interaction in Patient-Specific Arterial Geometries with regard to the Transmural Stress Distribution

Simon Fausten (*Institut für Mechanik, Universität Duisburg-Essen*), Daniel Balzani (*Institute of Mechanics and Continuum Mechanics, Ruhr University Bochum*), Alexander Heinlein (*Mathematical Institute, University of Cologne*), Axel Klawonn (*Mathematical Institute, University of Cologne*), Oliver Rheinbach (*Institute of Numerical Mathematics and Optimization, TU Freiberg*), Jörg Schröder (*Institute of Mechanics, University of Duisburg-Essen*) 08:30–08:50

Fluid-Structure-Interaction (FSI) is a research field with a broad variety of applications. Here, we focus on the field of hemomechanics, in detail the simulation of patient-specific arteries, where the interaction of the blood flow and the vessel wall is of special interest. Based on pervious research, cf. [1], our existing framework for FSI-simulations is extended towards patient-specific arterial geometries. The inflow and outflow boundary conditions for the fluid, which are based on [5], as well as the boundary conditions for the structure are enhanced and adjusted to the chosen patient-specific geometry. In detail, an inflow profile for arbitrary shaped cross-sections, a modified absorbing boundary condition and an additional layer of perivascular tissues surrounding the structure will be considered. Furthermore, the vessel wall is discretized considering multiple components, i.e. plaque, media and adventitia. The geometry and material parameters are adopted from [3]. Finally, a more realistic fiber orientation for the collagen fibers is considered, see [4]. Here, the collagen fibers are reoriented according to the direction of the first and second principal stresses in an iterative procedure. In order to deal with the increasing complexity of the boundary value problem massive parallel computing and a novel two-level overlapping Schwarz method are applied, cf. [2]. The numerical simulations are performed, using the Open-Source project LifeV, in particular a code which has been developed by and in cooperation with the group of Prof. Quarteroni from the EPF Lausanne.

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Towards the generation of dry patient-specific human aortic valve models from medical imaging data

Sergio Morales (*Institute of Applied Mechanics, University of Stuttgart*), Oliver Röhrle (*Institute of Applied Mechanics, University of Stuttgart*) 08:50–09:10

Considering the geometry of the human aortic valve as one of the key factors influencing directly on its function, deformation and performance, we focus on the generation of 3-D Finite Element models of these valves under healthy and diseased conditions. The latter with the specific aim of investigating the cause-effect factors linking the aortic valve's extracellular matrix (ECM) destructive remodelling processes with explicit ventricular diseases.
Patient-specific geometries are extracted from medical imaging data (MRI, 3D-TEE and CT) to replicate the particularities of the human aortic valve's geometry. To this end, intensity dependent and independent edge detection methods are implemented on the sets of available image data to extract the valvular geometry components of interest. Paralelly, the effectiveness of each implemented geometry extraction method is analized and compared to each other towards the development of a reliable and automated geometry model generation algorithm.
Besides from the extracted geometries, the 3-D Finite Element model proposed is constructed with suitable constitutive models fitted to experimental data as well as to data from literature, along with case-specific boundary conditions which are applied to the models to reproduce the bending and tensile stretches suffered by the cusps along the heart cycle. The overall aim of this project is to use modelling to determine for a range of ventricular and aortic pressure loading patterns the resulting stress and strains distributions within the aortic cusps. The data generated from these models as well the dynamics of the valves observed in medical imaging data, give us significant information to study the development of calcific aortic valve disease from initial alterations in the tissue to end-stage calcification.

Simulation of angioplasty using isogeometric shell elements

Farshad Roohbakhshan (*Aachen Institute for Advanced Study in Computational Engineering Science (AICES)*), Roger A. Sauer (*Aachen Institute for Advanced Study in Computational Engineering Science (AICES)*) 09:10–09:30

The typical treatment for the opening of obstructed arteries or veins is balloon angioplasty. Several computational studies based on finite element analysis (e.g. Gasser and Holzapfel, 2007) have been performed to optimize angioplasty parameters, among which the most important ones are the internal pressure, location and mechanical properties of the balloon. Most numerical simulations of angioplasty use 3D solid elements to model artery walls. However, as shown in the presented work, in many circumstances shell elements, which are computationally less expensive, are sufficiently accurate to describe and analyze the walls of arteries and veins.

Here, the isogeometric shell formulation of Roohbakhshan and Sauer (2016,2017) is used to model arteries. The new formulation allows for the modeling of laminated composite shells constructed from different materials, like the adventitia, media and intima layers of an artery. The new shell formulation is based on the Kirchhoff–Love hypothesis and both the artery and balloon are discretized by NURBS-based finite elements. Furthermore, the numerical results are compared with those obtained by using 3D solid elements. The comparison shows very good agreement.

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A combined framework for multiplicative growth and remodeling in arterial walls

Anna Zahn (*Ruhr-Universität Bochum*), Daniel Balzani (*Ruhr-Universität Bochum*) 09:30–09:50

As a living biological medium, arterial tissue is able to adapt to changes in its mechanobiological environment by means of growth and remodeling processes, which improve the load-bearing capacities. These adaptation processes are closely related to the generation of residual stresses, which exist in externally unloaded arteries and which have thus to be included in numerical simulations, see e. g. the numerical approaches in [1, 6]. In the context of constitutive material modeling, which considers the tissue as an isotropic matrix material with two families of embedded fibers, growth can be incorporated by an increase of the tissue volume and remodeling can be accounted for by a reorientation of the fiber directions.
The growth model is based on a multiplicative decomposition of the deformation gradient into an elastic and a growth part as e. g. in [3, 5]. In order to account for the anisotropy of the growth mechanism, the growth part itself is decomposed into up to three individual parts, where each part is formulated in dependence on the direction of a principal stress. By specifying the form of the individual growth tensors, different isotropic and anisotropic growth formulations can be realized.
It is assumed that the target fiber directions are aligned symmetrically with respect to the directions of the tensile principal stresses as described in [4]. The reorientation towards these directions can either be treated incrementally [2] or by defining an evolution equation for the angle between the existing and the target fiber vector. Comparing both approaches, the second one proves to be more stable and efficient.
Since the whole framework is formulated in terms of general local quantities, namely the principal stress state at the integration point, it is in principle applicable to arbitrary arterial geometries.

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A Multiscale and Multiphase Model for the Description of Paracetamol-induced Hepatotoxicity Using the Example of the Human Liver

Lena Lambers (*Institute of Mechanics, Structural Analysis, and Dynamics, University of Stuttgart*), Navina Waschinsky (*Chair of Mechanics, Structural Analysis, and Dynamics, TU Dortmund University*), Tim Ricken (*Institute of Mechanics, Structural Analysis, and Dynamics, University of Stuttgart*) 09:50–10:10

The liver is the most important organ related to metabolism processes in human beings. A central task of the human liver is the detoxification of toxic metabolites since excessive amounts of several medications can cause damages in the liver structure which can lead up to acute liver failure.
One example for a medicine which can cause hepatotoxicity is analgesic Paracetamol (Acetaminophen). The toxic metabolites of the Paracetamol are normally depleted by conjunction with the internal Glutathione. If the concentration of hepatic Glutathione is exhausted, the Glutathione are no longer capable of binding the molecules and the reactive metabolites react with cellular proteins causing liver necrosis.
The now developed model is an extension of a previous published work, where a multicomponent, poro-elastic multiphasic and multiscale function-perfusion approach has been presented, cf. [2],[3],[4].
In addition, the depletion of toxic medicines causing cell damage through an acute overdose is supplemented using the example of Paracetamol . Furthermore the kinetic relations of the Paracetamol and the internal metabolite Glutathione are appended.
The human liver consists of liver lobules, which contain small cells, called hepatocytes, where the metabolism takes place. Therefore, the toxic metabolites, just like other nutrients and substances, are initiated in the liver with an anisotropic blood flow via the sinusoids (slender capillaries sited between the periportal field and the central vein). As the structure of the liver lobules is extremely complex, we use a multicomponent mixture theory based on the Theory of Porous Media (TPM), see [1]. Applying the TPM, the allocation of the sinusoids as well as the complex distribution of the hepatocytes can be homogenized.
The computational model consists of a tetra-phasic component body, composed of a porous solid structure φ^{S}, fat tissue with the ability of growth φ^{FL}, a liquid phase representing the blood φ^{L} and a solid phase φ^{N}, which characterizes the damaged necrotic cells. The phases present a carrier phase φ^{α}, also called solvent, and solutes $\varphi^{\alpha\beta}$, representing microscopic components, that are solved in the solvent and consist of the nutrients responsible for the metabolism in the liver. To calculate the processes and describe the production, utilization and storage of the metabolites, an embedded set of coupled ordinary differential equations (ODE) is used.

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S02.07 | Biomechanics

Date 22.03.2018
Room 2770

A computational study of the multiaxial fatigue behaviour of a posterior dynamic stabilisation device

Agnes Beckmann (*IAM, Institut für Allgemeine Mechanik, RWTH Aachen*), Songyun Ma (*RWTH Aachen*), Marcus Stoffel (*RWTH Aachen*), Bernd Markert (*RWTH Aachen*) 14:00–14:20

Polyether ether ketone (PEEK) has been increasingly employed as a commercial biomaterial for orthopedic, trauma, and spinal implants due to its excellent biocompatibility and mechanical properties. Compared with titanium-based metallic implants, its similar stiffness to bone leads to more physiological load distributions, which minimise the risk of stress shielding and the reduction of bone mineral density. Many PEEK implants are designed for long term lifespan and inevitably subjected to complex dynamic loadings during daily activities. Therefore, it is of importance to understand the fatigue behaviour of PEEK under multiaxial and non-propotional loading conditions.
The aim of this study is to predict the fatigue failure of a posterior dynamic stabilisation device (PDSD) based on a 3D finite element (FE) simulation. To this end, a 3D FE model of a PDSD, which showed fatigue failure in an on-going clinical study, was adopted from a former study [1]. The PDSD was included in a modified FE model of the lumbar spine. The local stress of the PDSD under complex loadings is computed with an incremental cyclic plasticity model and a multiaxial notch-correction approach. The fatigue life of the PDSD was estimated by a multiaxial fatigue criterion based on the critical plane concept. The computational results were validated by comparing to experimental results of the instrumented spine from a former in vitro study.

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Personalized orthopedic trauma surgery by patient-specific simulations of bone-implant-systems

Michael Roland (*Chair of Applied Mechanics, Saarland University*), Thorsten Tjardes (*Klinik für Unfallchirurgie, Orthopädie und Sporttraumatologie Köln-Merheim, Universität Witten/Herdecke*), Bertil Bouillon (*Klinik für Unfallchirurgie, Orthopädie und Sporttraumatologie Köln-Merheim, Universität Witten/Herdecke*), Stefan Diebels (*Chair of Applied Mechanics, Saarland University*) 14:20–14:40

Today fractures of the long bones, like the tibia or the femur, are treated surgically. This means that implants are used that allow early post operative weight bearing and physiotherapy of the injured limb. However, the implants currently used in orthopedic trauma surgery do not account for individual specificities of the patient and of the fracture. A personalized approach to fracture therapy necessitates the integration of techniques from mechanics and computer science. In order to implement a workflow applicable in everyday clinical routine, relevant concepts have to be merged. The starting point are the routinely acquired computed tomography image stacks or standard sets of X-ray images. In an image processing step, the images are segmented and the

material properties are assigned based on the data given by a calibration phantom included in the CT images. This data structure is passed to a meshing procedure, resulting in a hexahedral as well as a tetrahedral mesh of the bone-implant-system. The models are equipped with appropriate realistic boundary conditions given by the OrthoLoad database, scaled via patient-specific meta data and passed to a finite element simulation. The simulation is seperated in a preparing step, generating additional aspects for the biomechanical simulation, like the formation of the callus structure and a biomechanical step, simulating the stresses and strains arising in the implant and the interfragmentary move as the key quantity in bone healing. The simulation part is looped in order to optimize the implant design with respect to predefined tasks given by the clinicians.

Optimal Hip Implant Positioning

Marian Moldenhauer (*Computational Medicine, Zuse Institute Berlin (ZIB)*), Martin Weiser (*Numerical Mathematics – Computational Medicine, Zuse Institute Berlin (ZIB)*), Stefan Zachow (*Visual Data Analysis – Computational Medicine, Zuse Institute Berlin (ZIB)*) 14:40–15:00

In an aging society where the number of joint replacements rise, it is important to also increase the longevity of implants. In particular hip implants have a life-time of at most 15 years which derives from factors that are affected by the positioning of the implant during the surgery. Current joint replacement 2D software tools fail to take into account the patients' natural range of motion as well as stress distribution in the 3D joint induced by different daily motions. We consider with the optimization of the hip joint implant positioning. Mechanical loading is derived from in vivo measured data (orthoload.com). A quasistatic approach to contact mechanics allows to formulate loading as density in the force-momentum domain which can be adapted to patient characteristics. For the calculation of the objective function, we combine Monte Carlo integration of highly nonlinear terms with a Kriging surrogate model for smooth contributions. The sampling points are drawn by importance sampling for the loading density. The change of grid topologies due to the repositioning of the implant introduces artificial objective discontinuities. We us special line search based on approximate gradient continuity across such points.

Structural classification of confocal microscopy images using machine learning

Pouyan Asgharzadeh (*Continuum Biomechanics and Mechanobiology, Institute of Applied Mechanics, University of Stuttgart*), Annette I Birkhold (*Advanced Therapies, Siemens Healthcare GmbH*), Bugra Özdemir (*Faculty of Biology, Chair of Plant Biotechnology, Albert-Ludwigs-University of Freiburg*), Ralf Reski (*Faculty of Biology, Chair of Plant Biotechnology, Albert-Ludwigs-University of Freiburg*), Oliver Röhrle (*Continuum Biomechanics and Mechanobiology, Institute of Applied Mechanics, University of Stuttgart*) 15:00–15:20

State-of-the-art imaging techniques allow to resolve structural details of protein networks [1]. Manual analysis of these features is limited, laborious, time-consuming, and error prone. Here we, present an automated method to classify subfamilies of the same protein network despite various similarities in structural features by exploiting a 3D convolutional neural network (CNN). A total of 20 3D confocal microscopy images of two isoforms of filamentous temperature sensitive Z (FtsZ) protein networks (FtsZ1-2 and FtsZ2-1; $n = 10$/group) of chloroplasts of living cells (*Physcomitrella patens*) were analyzed (voxel size $21\,nm$ x $21\,nm$ x $240\,nm$). Images are segmented using an semi-automatic iterative approach. From that data, a volume model and a spatial graph are created [2] and 25 features representing the shape and substructures are determined. A convolutional neural network (CNN) consisting of 8 convolutional layers was created and trained with the extracted features for automatic classification of the isoforms.

The trained model was evaluated by a train/test split of the data reaching approximately 80% classification accuracy.
The reached accuracy is comparable to recent classification networks applied to microscopic data [3]. The developed classification CNN has the potential to identify pathological changes occurring in other filamentous protein networks such as cytoskeleton. However, further research is necessary to determine the extension of this algorithm for further applications.

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[2] Asgharzadeh et al. *PAMM* 16.1 (2016), 69–70.
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Mathematical models of bio-inspired rotatable sensors with elasticities for object scanning

Lukas Merker (*Department of Mechanical Engineering, Technische Universität Ilmenau*), Joachim Steigenberger (*Technische Universität Ilmenau*), Carsten Behn (*Department of Mechanical Engineering, Technische Universität Ilmenau*) 15:20–15:40

Rats and mice use some special tactile hairs in their snout region for a non-visual exploration of their environment. These hairs, known as mystacial macro-vibrissae, are each embedded in their own elastic support, called follicle-sinus complex. This consists of several mechanoreceptors converting tactile information into neural impulses for the CNS. Using their vibrissae, rats and mice are capable of detecting distances to objects, object contours and surface textures. Due to this outstanding ability vibrissae frequently serve as a paradigm for technical tactile sensors. In this paper, we present a model for object shape scanning and contour reconstruction. Here, we especially focus on the important property "elasticity" of the follicle-sinus complex, which has rarely been taken into account for object scanning in literature. We set up models for three different elastic supports. Based on solutions of the arising boundary- and initial-value problems, we simulate the scanning process, investigate the related support reactions during a single rotational quasi-static sweep of a straight vibrissa along a strictly convex object contour and reconstruct its shape. In doing this, we investigate the influence of the different elasticities of the model on the scanning and reconstruction procedure.

Determination of Gait Parameters in Real-World Environment Using Low-Cost Inertial Sensors

Marion Mundt (*Institute of General Mechanics, RWTH Aachen University*), Wolf Thomsen (*Institute of General Mechanics, RWTH Aachen University*), Franz Bamer (*Institute of General Mechanics, RWTH Aachen University*), Bernd Markert (*Institute of General Mechanics, RWTH Aachen University*) 15:40–16:00

Over the course of the last decade, the amount of wearable sensors, especially inertial measurement units (IMUs), used for gait analysis has been rising. They can address the issues of time efficiency and limited measuring volume of existing systems by detecting spatiotemporal gait parameters such as stride time, stride length and cadence [1, 2]. The amount of higher cost commercial systems including analysis tools is also continuously increasing [3]. These systems have the advantage of being easy to use but, in turn, do not allow for fine-tuning with respect to the current research goal and, therefore, may not be suitable for the population that has to be analysed.
To overcome this problem, a sensor network is built based on four low-cost IMUs (TinyCircuits, Akron, OH, USA) with an associated microcontroller (Atmel ATmega328P) and a WIFI-board

(Atmel ATWINC1500). An Android application is developed to collect the data on a smartphone. The data analysis is undertaken offline using MATLAB®. The stride segmentation is based on the algorithm proposed in [4]. Using a time warping algorithm, it is possible to define steps based on a patient specific template. Thereby, also strides of impaired gait can be identified. Additionally, idle time is excluded automatically from further analysis.
The sensor network and algorithm will be validated in an experimental set up using an instrumented treadmill (Zebris Rehawalk), which can be considered the gold standard for the determination of spatiotemporal parameters.

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S02.08 | Biomechanics

Date 22.03.2018
Room 2770

Thin film models for an active gel

Barbara Wagner (*Weierstraß-Institut für Angewandte Analysis und Stochastik*), Georgy Kitavtsev (*School of Mathematics, University of Bristol*), Andreas Münch (*Mathematical Institute, University of Oxford*) 17:30–17:50

In this talk we present a free-boundary problem for an active liquid crystal based on the Beris-Edwards theory that uses a tensorial order parameter and includes active contributions to the stress tensor to analyse the rich defect structure observed in applications such as the Adenosinetriphosphate (ATP) driven motion of a thin film of an actin filament network. The small aspect ratio of the film geometry allows for an asymptotic approximation of the free-boundary problem in the limit of weak elasticity of the network and strong active terms. The new thin film model captures the defect dynamics in the bulk as well as wall defects and thus presents a significant extension of previous models based on the Leslie-Erickson-Parodi theory. Analytic expression are derived that reveal the interplay of anchoring conditions, film thickness and active terms and their control of transitions of flow structure.

Vibrational analysis of hydrogels for novel applications in Tissue Engineering

Sascha Schwarz (*Technical University of Munich, Chair of Applied Mechanics*), Stefan König (*Polytec GmbH*), Jan Winter (*Munich University of Applied Sciences*), Alfred Fuchsberger (*Munich University of Applied Sciences*), Stefanie Sudhop (*Munich University of Applied Sciences*), Hauke Clausen-Schaumann (*Munich University of Applied Sciences*), Daniel Jean Rixen (*Technical University of Munich, Chair of Applied Mechanics*) 17:50–18:10

Laser Doppler vibrometry (LDV) enables a contactless, non-destructive vibrational analysis of surfaces and is mainly applied in structural dynamics (e.g. automotive industry). The aim of this study is the transfer of this measurement method into the field of Tissue Engineering by applying it to hydrogels which can be used as call-laden biomaterials. By the integration of the LDV into this emerging scientific field, a huge variety of novel applications are enabled, since the mechanical properties of tissues and therefore of the hydrogel, which is used as potential tissue substitute, are crucial for a proper functionality. Preliminary results are showing the feasibility regarding the contactless characterization of transparent hydrogel samples via LDV. Furthermore, changes in the stiffness of hydrogels samples are detectable. One future application is the integration into the bioprinting process for analyzing and if necessary adjusting the mechanical properties of hydrogels during the printing process. This novel workflow allows for the production of tissue equivalents possessing a mechanical anisotropy and hard/soft transitions, which also can be found in the human body regarding tissues such as bone, cartilage and tendon.

S02.09 | Biomechanics

Date 23.03.2018
Room 2770

Investigation of Tenocyte Migration Behavior by Application of Mechanobiological Concepts

Gözde Dursun (*Institute of General Mechanics (IAM), RWTH Aachen University*), Dilmin Ürek-Yavas (*Institute of General Mechanics (IAM), RWTH Aachen University*), Mersedeh Tohidnezhad (*Institute of Anatomy and Cell Biology, RWTH Aachen University*), Bernd Markert (*Institute of General Mechanics (IAM), RWTH Aachen University*), Marcus Stoffel (*Institute of General Mechanics (IAM), RWTH Aachen University*) 08:30–08:50

Chronic or acute tendon injuries are common clinical problems. Healing of tendon tissue requires tenocytes migration from intact regions of the injured tendon to the repair site, followed by cell proliferation and synthesis of the extracellular matrix [1]. The enhancement of tenocyte migration and proliferation could improve the effectiveness of cell-based therapies in tendon healing. Since tendon tissue is subjected to mechanical loading, our study aims to investigate the mechanobiological response of tendon cells using of a custom-made tensile bioreactor. Mechanical stretching is an important regulator in functional tendon tissue engineering and increases the organization and strength of engineered tissues while inducing beneficial cell responses [2]. It has been already observed that mechanical stretching induces the regulation processes of tendon cells, such as collagen synthesis and repair activity. Nonetheless, little is known about the effects of uniaxial stretching on tenocyte migration behavior [3] [4]. Therefore, our main focus in this study is to examine and enhance the migration behavior of tenocytes by application of uniaxial mechanical stretch. Uniaxial stretching will be applied to tenocyte-seeded collagen membranes,

which are considered to be a promising candidate for tendon engineering because of its biological properties. Understanding of tenocytes cellular mechanisms will improve our knowledge about tendon healing and provide new approaches for specific treatments.

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Investigation of worm-like chain models for collagen molecules

Markus Hillgärtner (*Dept. of Continuum Mechanics, RWTH Aachen University*), Kevin Linka (*Dept. of Continuum Mechanics, RWTH Aachen University*), Mikhail Itskov (*Dept. of Continuum Mechanics, RWTH Aachen University*) 08:50–09:10

Collagen is the main structural protein in various biological tissues and of high interest for microstructural multi-scale models due to its load bearing functionality. The worm-like chain (WLC) model [3] with its approximation [4] is a widely used approach for the modeling of DNA, which has a helical structure similar to tropocollagen. However, the classical WLC is suitable only for the entropic deformation regime of collagen. By modeling the extension behavior, it fails to give accurate predictions when the helical structure of the molecule starts twisting under higher loads.
The twistable worm-like chain [2] and its special case referred to as the extensible worm-like chain [5] aim to include the mechanical coupling between bond stretching and twist of the helix using a twist-stretch coupling term, leading to more accurate predictions in the energetic regime. This contribution discusses different variations and coupling terms describing the molecular behavior behind the transition state between the entropic and energetic regime. Experimental data of the literature [1] are used to make a quantitative comparison of the discussed models and their applicability.

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Viscoelasticity of cross-linked actin network embedded in cytosol

Tillmann Wiegold (*Institute of Mechanics, TU Dortmund University*), Sandra Klinge (*Institute of Mechanics, TU Dortmund University*), Serhat Aygün (*Institute of Mechanics, TU Dortmund University*), Robert P. Gilbert (*Department of Mathematical Sciences, University of Delaware*), Gerhard A. Holzapfel (*Institute of Biomechanics, Graz University of Technology*) 09:10–09:30

A eukaryotic cell is a complex system including various components with the different structure and role. The current presentation deals with the microscopic and macroscopic simulation of a cell if two of its components are considered: cytosol and actin network embedded in it. At microscopic level, the actin is modeled by the Holzapfel-Ogden model, including an extension for viscous effects. The Holzapfel-Ogden model provides a relationship between the stretch of a single polymer chain and applied tension force. This relationship includes the influence of the physical length of a single chain, its end-to-end distance and the stretch modulus. The viscous effects, occurring through deviatoric changes, are modeled corresponding to a spring and a dashpot of the generalized Maxwell model. The cytosol is modeled by a large strain viscous model from the FEAP program. At macroscopic level, the multiscale finite element method is applied to simulate the effective behavior of cell cytoplasm. This method has been intensively used because it is suitable for simulating nonlinear heterogeneous materials with the zero-ratio of the characteristic lengths of scales. The presentation includes various examples typical of testing viscous material behavior such as tension tests with holding phases and tension tests with the sudden decrease/remove of the load. The influence of the fiber orientation on the effective behavior is also studied.

Influence of hemorheology on nanoparticle transport in vessel bifurcations

Mahrokh Bavandi (*Chair of Fluid Mechanics, University of Kassel*), Olaf Wünsch (*Chair of Fluid Mechanics, University of Kassel*) 09:30–09:50

Magnetic Drug Targeting (MDT) is a novel area in biomedicine[1]. In this method, nanoparticles are coated with drugs and injected into the blood vessels. These particles are then directed to a desired location by using an external magnetic field[2]. This prevents the unnecessary side effect of drugs to the healthy tissue of the patient's body[3].
Numerical simulations are a helpful tool in the design of MDT applications. Investigating the influence of various conditions on the particles paths is always the key objective. This study focuses on the effect of the hemorheology under the absence of a magnetic field on the particles paths. A bifurcation vessel is simulated for steady state and pulsating flows.
The Carreau-Yasuda model is used to characterize the shear properties of the blood-nanoparticles mixture. Particle concentration is modelled by a convection-diffusion equation. The method is implemented in OpenFOAM.

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Chondrocyte migration in an acellular tissue-engineered cartilage substitute

Julia Nachtsheim (*Institute of General Mechanics, RWTH Aachen University*), Gözde Dursun (*Institute of General Mechanics, RWTH Aachen University*), Bernd Markert (*Institute of General Mechanics, RWTH Aachen*), Marcus Stoffel (*Institute of General Mechanics, RWTH Aachen University*)

09:50–10:10

Focal cartilage defects are a major cause for the development of osteoarthritis, often affecting patients at young age. Since at present there is no therapy available which stops or inverses the progredience of cartilage depletion, small defects require medical treatment at an early stage to preserve the joint function [1,2]. A new therapeutic approach is the implantation of a cell-free collagen type I (COL1) based scaffold, which fills in the defect zone. The COL1 scaffold is highly biocompatible and possesses comparable structure and mechanical properties as the extracellular collagen matrix of native cartilage. In vivo, the acellular implant serves as an autogenerate, allowing for chondrocyte migration and tendious remodelling processes. First clinical studies have revealed good clinical results [3,4]. Still, fundamental therapeutic questions are yet to be answered.
In this study we focus on chondrocyte migration into and inside a cell-free collagen type I based matrix as it is pivotal for subsequent remodelling processes and for the therapeutic success. Therefore, we have developed an in vitro model to study the migration inside scaffolds of varying COL1 concentrations, microstructures and mechanical properties. In addition to this, an in-house developed bioreactor system is used to analyse the impact of mechanical stimuli. After a cultivation period of 21 days, the chondrocyte distribution inside the matrix is examined using optical sectioning microscopy. Subsequently, the obtained experimental results will be used to identify a numerical description of chondrocyte migration.

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Bridging protein rigidity theory and normal modes using kino-geometric analysis

Dominik Budday (*Mechanical Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Sigrid Leyendecker (*Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Henry van den Bedem (*SLAC National Accelerator Laboratory, Stanford University*)

10:10–10:30

About twenty years ago, two distinct coarse-grained approaches to study conformational flexibility of macromolecules were born: rigidity analysis using the pebble-game and elastic network models (ENM). Since then, they have provided tremendous insight into the dynamics of molecular mechanisms and function. However, the topological nature of the pebble game and its strong dependence on a network of non-covalent constraints have limited its applicability and comparability to dynamic, normal mode approaches like ENM. Here, we present an alternative, geometric approach which eliminates these drawbacks. Our analysis of the underlying rigidity matrix, the constraint Jacobian **J**, brings together topological rigidity and ENM, providing an orthonormal basis for the full spectrum of collective motions. It allows to directly compare and contrast motion modes obtained from both traditional approaches. Non-covalent constraints, like hydrogen bonds, encode a hierarchy of protein motions, ranked by increasing singular values. This hierarchy predicts energetic perturbations associated with each mode. The spectrum of singular values yields a fold-specific footprint, differentiating stiffer alpha-helical from beta-sheet proteins. Interestingly, detecting these differences requires normal mode analysis; they go undetected in simplified ENM. Collectivity of protein motions, measured by Shannon entropy, is significantly lower for motions obtained by topological rigidity theory versus normal mode approaches, and generally higher for beta over alpha folds. Overall, these results indicate that hydrogen bond networks have evolved with different protein folds to tailor structural dynamics and thus, fold-related function, with broad implications for protein engineering and drug design.

S03 | Damage and fracture mechanics

Organiser Björn Kiefer (*Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg*)
Christian Linder (*Stanford University*)

S03.01 | Damage and fracture mechanics

Date 20.03.2018
Room 2760

A mixed extended finite element formulation for the simulation of cracks in nearly incompressible materials

Stefan Löhnert (*Institute of Mechanics and Shell Structures, Technical University Dresden, Germany*) 08:30–09:10

The efficient and accurate simulation of nearly incompressible materials such as rubber using lower order finite elements can be achieved using mixed methods such as the well known Q1P0 element formulation [1]. During the last years the eXtended Finite Element Method (XFEM) [2] has shown to be an excellent method for the simulation of cracks and their propagation. Even though the enrichment functions lead to an increased flexibility of the deformation in the vicinity of the crack front and along the crack surface, XFEM simulations based on lower order extended Lagrange finite element formulations may still show locking behaviour for nearly incompressible materials. In this contribution an extension of the XFEM using a mixed formulation similar to the Q1P0 element is presented. Elements that are completely intersected by the crack as well as crack front elements require special treatment due to the discontinuity of the displacement as well as the pressure field. By means of several fracture mechanics examples it is shown that this mixed extended finite element formulation leads to significantly better convergence rates compared to standard lower order extended finite elements.

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A Virtual Element Method for Crack Propagation

Ali Hussein (*Leibniz Universität Hannover, Institut für Kontinuumsmechanik*), Peter Wriggers (*Leibniz Universität Hannover, Institut für Kontinuumsmechanik*), Blaž Hudobivnik (*Leibniz Universität Hannover, Institut für Kontinuumsmechanik*) 09:10–09:30

The finite element method (FEM) has proven itself to be a strong numerical method for solving various engineering problems. When it comes to the modelling of moving discontinuities as in the case of crack propagation, the application of the method is limited. This limitation can be handled by using various remeshing techniques at the vicinity of the crack tip, which usually

leads to very large time-consuming and the need for high-performance computing. Furthermore, the results can be mesh-dependent and difficult to validate.
In this contribution crack propagation within brittle materials is presented by means of a novel technique, the virtual element method (VEM). The method, which is introduced in [1], can be seen as a generalisation of the classical finite element method. In comparison to FEM, VEM allows usage of arbitrary polygonal (2D) and polyhedral (3D) elements due to its applicability beyond the isoparametric concept. In addition to usage of arbitrary number of nodes in the elements, it is easily possible to add extra nodes to existing elements during the computation without the need to change the element formulation. Such a method can be extremely useful for simulation of crack propagation problems. Further information about the implementation of the method used in this contribution can be found in the work of Wriggers et al. [2].
Once a crack has been initiated, the direction of growth can be predicted using different propagation criteria; the maximum circumferential stress criterion (MCSC), the maximum strain energy release rate criterion and the minimal strain energy density criterion. In this work, MCSC introduced by Erdogan and Sih [3], is considered. To determine the MCSC, the stress intensity factors for the mixed-mode loading conditions are calculated. The stress intensity factors are numerically obtained by using the interaction integral, which accurately calculates these factors. When the direction of crack growth is known, there are two possibilities to allow the crack to propagate: either between, or within the elements. The first one can be accomplished by the classical finite element method. The second case represents the new idea in this work. By means of the virtual element method we can split the crack tip element in the direction of the crack propagation to lead the crack within the element to propagate.
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Mesh bias for the eigenerosion approach

Aurel Qinami (*Institute of Structural Analysis, Technische Universität Dresden (TUD)*), Michael Kaliske (*Institute for Structural Analysis, Institute for Structural Analysis*) 09:30–09:50

In fracture problems, having the right crack path is a necessary condition for producing reliable results. On the other hand, a discretized continuum is unable to represent a random crack path perfectly. Thus, challenges lie ahead on the accuracy of the numerical representation of this crack.
Albeit the eigenfracture scheme is well established in the recent years (e.g. [1, 2]), different simulation results have shown some dependencies of the crack path on the mesh orientation, particularly when dealing with unstructured meshes. The core of this work is to investigate how the mesh bias is influenced by the binary approach of the eigenerosion scheme and to what extent does the regularization of the method avoids this effect. To achieve that, for different meshes, the crack path deviation is studied by comparing the shortest path on the mesh between two elements and their Euclidean distance, following a similar framework presented in [3]. The quality of the mesh is then determined by the value of this deviation. In a further step, it is examined how the regularization of the eigenfracture approach, represented by the concept of the neighboring elements, effects the mesh bias. Meshes which do not exhibit any preferential direction are considered to be isotropic and they produce the most accurate results.

Investigating the bounds of the eigenerosion scheme related to meshing and the introduction of possible improvements, contribute on avoiding mesh induced anisotropy and further consolidate the approach.

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Investigation of the laminate free-edge effect by means of the scaled boundary finite element method

Sebastian Dölling (*Fachgebiet Strukturmechanik, TU Darmstadt*), Sascha Hell (*Fachgebiet Strukturmechanik, TU Darmstadt*), Wilfried Becker (*Fachgebiet Strukturmechanik, TU Darmstadt*) 09:50–10:10

Free edges of laminate structures composed of fibre-reinforced plies induce highly localised interlaminar, theoretically infinite stresses due to the layer-wise discontinuous strongly anisotropic stiffness properties. As a consequence, the so called free-edge effect, first investigated by Pipes and Pagano [1], may lead to a premature sudden failure by formation of delamination cracks between layers. In practice the assessment of local interlaminar stress fields regarding delamination onset is crucial in order to predict the effective strength of laminates. Due to the singular character of the stress fields and the abscence of a pre-existing crack, neither classical failure criteria nor purely energy based fracture mechanics methods allow for predicting delamination onset. In order to tackle this problem, Leguillon [2] proposed a coupled stress and energy criterion within the framework of the finite fracture mechanics (FFM). For predicting shear delamination onset in angle-ply laminates, Martin et al. [3] used the FFM approach where the stress distribution near the free edge is determined using a numerical finite element model.
In the present study, delamination onset at a free edge in symmetric laminates based on the Pipes and Pagano model (generalized plane strain) is investigated using FFM. For that purpose, the required singular stress field near the laminate edge is obtained by the scaled boundary finite element method (SBFEM) in order to significantly decrease the numerical effort compared to classical finite element method. The SBFEM, first introduced by Song and Wolf [4], reduces the spatial dimension of the problem by one and is a useful method to treat stress singularities. In 2D, the boundary is discretized by one-dimensional finite elements whereas the inner domain is considered analytically. Therefore the system of partial differential equations of linear elasticity theory is transformed by a separation of variables approach for displacements yielding a system of differential equations of Cauchy-Euler type which can be solved by standard methods. In order to assess the reliability of the obtained SBFEM results a comparison to a finite element model is presented.

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[2] D. Leguillon. Strength or toughness? A criterion for crack onset at a notch. *European Journal of Mechanics-A/Soilds*, 21(1):61–72, 2002.

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Convergence properties of the enriched Scaled Boundary Finite Element Method in fracture mechanics

Sophia Bremm (*Fachgebiet Strukturmechanik, TU Darmstadt*), Sascha Hell (*Fachgebiet Strukturmechanik, TU Darmstadt*), Wilfried Becker (*Fachgebiet Strukturmechanik, TU Darmstadt*) 10:10–10:30

The Finite Element Method (FEM) has established itself as an efficient numerical solution method for elliptic boundary value problems in various physical problems and is also applicable within solid mechanics. For smooth domains, the standard FEM yields the desired optimal rates of convergence. Fracture mechanics is a branch of solid mechanics which is concerned with the treatment of cracks, corners and notches and the resulting singularities. In this case, the smoothness condition which is required for the standard finite element error estimations is violated. This leads to low rates of convergence which are independent of the polynomial degree of the used trial functions. As a consequence, in order to regain full rates of convergence, an appropriate adaptation and a skilful choice of test and trial space of the FEM is necessary.

The Scaled Boundary FEM (SBFEM) makes use of a separation of variables approach [1]. Hence, only the boundary has to be discretised, while the solution inside the domain is considered analytically. This has turned out to be an appropriate method for the treatment of two dimensional crack problems, when the singularity is located entirely within the considered domain. However, in 3D there are singularities still present where the crack front meets the discretised boundary. Then, the SBFEM suffers from the same drawbacks as the standard FEM. In order to dispel this inconvenience, an extension of the trial space with asymptotic crack tip displacement solutions (enrichment, for standard FEM see [2, 3]) is considered. In the present work, improved rates of convergence resulting from an enrichment are discussed. The enriched SBFEM [4] is applied to a cubical domain with a crack penetrating the discretised boundary. This model problem serves for verifying and quantifying the expected rates of convergence aforementioned.

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S03.02 | Damage and fracture mechanics

Date 20.03.2018
Room 2760

Phase-field description of brittle fracture in plates and shells

Josef Kiendl (*Norwegian University of Science and Technology*), Davide Proserpio (*Norwegian University of Science and Technology*), Laura De Lorenzis (*TU Braunschweig*), Marreddy Ambati (*TU Braunschweig*) 16:30–16:50

Phase-field modeling of brittle fracture is a promising modern approach that enables a unified description of complicated failure processes, including crack initiation, propagation, branching, and merging, as well as its efficient numerical treatment [1]. In this work, we apply the phase-field fracture approach to shell structures, describing both the structure and the phase field by surface models. For avoiding fracture in compression, we split of the deformation tensor in tension and compression terms as proposed in [1]. We show that this requires special attention in structural models like plates and shells, where bending deformation typically induces both tension and compression at opposite sides of the structure. We propose a new approach [2], which allows for a varying degradation through the thickness while the phase field is represented as a single two-dimensional field on the shell's middle surface. The numerical implementation is based on isogeometric analysis with a rotation-free Kirchhoff-Love shell formulation for structural analysis. We extended the NURBS-based implementation to locally refinable LR-NURBS enabling local and adaptive mesh refinement, which is a crucial aspect for computational efficiency considering that the phase-field approach requires very fine mesh resolution locally in the cracked areas.

[1] C. Miehe, M. Hofacker, F. Welschinger. A phase field model for rate-independent crack propagation: robust algorithmic implementation based on operator splits. CMAME (2010).

[2] J. Kiendl, M. Ambati, L. De Lorenzis, H. Gomez, A. Reali. Phase-field description of brittle fracture in plates and shells. CMAME (2016).

Phase-Field Modelling of Fracture in Heterogeneous Materials

Arne Claus Hansen-Dörr (*Institute of Solid Mechanics, TU Dresden*), Markus Kästner (*TU Dresden*), Maik Gude (*TU Dresden*), Robert Böhm (*TU Dresden*) 16:50–17:10

Different from a discrete crack representation, phase-field models solve an additional scalar field problem representing the regularised crack topology. The additional field is coupled to the mechanical boundary value problem. Cumbersome topological updates of the analysis mesh are avoided. Phase-field models for brittle fracture [1] allow for the proper modelling of crack initiation and propagation.
In this contribution, we apply a phase-field model to simulate fracture processes in heterogeneous materials. The local material structure is modelled in a diffuse manner, e.g. by a local reduction of the fracture toughness. In order to obtain a physically meaningful crack propagation, the interaction between the length scales of the diffuse microstructure and the regularised crack are studied. We employ a local correction of the fracture toughness assigned to the interface domain. The developed method is verified in several numerical benchmark problems and applied to simulate fracture processes in heterogeneous and porous materials. As a particular application, outgassing processes as they occur due to chemical transformations during pyrolysis of carbon fibres, are considered.

[1] C. Miehe, M. Hofacker, F. Welschinger, A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits, Computer Methods in Applied Mechanics and Engineering 199 (45-48) (2010) 2765–2778.

A phase-field model for the description of fatigue phenomena

Marreddy Ambati (*Institut für Angewandte Mechanik, Technische Universität Braunschweig*), Pietro Carrara (*Institut für Angewandte Mechanik, Technische Universität Braunschweig*), Roberto Alessi (*Dip. Matematica, Università Roma La Sapienza, Italy*), Stefano Vidoli (*Dip. Ingegneria Strutturale e Geotecnica, Università Roma La Sapienza, Italy*), Laura De Lorenzis (*Institut für Angewandte Mechanik, Technische Universität Braunschweig*) 17:10–17:30

Fatigue is a key phenomenon in mechanics, and is responsible for more than 75% of structural failures. Despite the significance of the problem, most existing fatigue theories are based on empirical laws that lack of generality and predictive capabilities. Hence, the development of mathematically sound and reliable fatigue models is still an open issue.
Recently, Alessi et al. [1] proposed a new variational fatigue phase-field model where the formulation relies on the introduction of a suitable internal (strain) history variable. The basic idea of the model is to let the fracture energy decrease as the accumulated strain measure increases, which is obtained by introducing a dissipation potential which explicitly depends on the strain history. Here the analysis is limited to a simple case, namely: one-dimensional, linear elasticity, brittle material behavior and symmetric response in tension and compression.
In this work, we extend this model to higher dimensions including the unsymmetric response in tension and compression for the evolution of both phase-field and internal strain variable. The tension-compression splits proposed by Amor et al. [2] and Miehe et al. [3] are adopted. To show the predictive capability of the proposed model, classical benchmark problems, such as single edge tension/shear test and compact tension (CT) specimen for cyclic loadings are investigated. The effects of load amplitude and fatigue material parameters on the fatigue life are studied. Also, for the CT specimen, the curve relating the fatigue crack growth rate ($\frac{\Delta a}{\Delta N}$) vs. the stress intensity factor (ΔK) are numerically obtained. It is shown that the model is able to describe all three typical fatigue fracture regimes, namely the elastic, the stable fatigue crack propagation and the final abrupt fracture stages.

[1] R. Alessi, S. Vidoli, L. De Lorenzis, Variational approach to fatigue phenomena with a phase-field model: the one-dimensional case, *submitted* (2017).

[2] H. Amor, J.J Marigo, C. Maurini, Regularized formulation of the variational brittle fracture with unilateral contact: Numerical experiments, Journal of the Mechanics and Physics of Solids 57 (2009) 1209-1229.

[3] C. Miehe, F. Welschinger, M. Hofacker, Thermodynamically consistent phase-field models of fracture: variational principles and multi-field FE implementations, International Journal of Numerical Methods in Engineering 83 (2010) 1273-1311.

Phase field modeling of brittle fracture in materials with anisotropic fracture resistance

Christoph Schreiber (*Institute of Applied Mechanics, University of Kaiserslautern*), Charlotte Kuhn (*Computational Mechanics, University of Kaiserslautern*), Ralf Müller (*Institute of Applied Mechanics, University of Kaiserslautern*) 17:30–17:50

A directional fracture resistance significantly effects the propagation direction of a crack exposed to a certain load state. This kind of anisotropy is often caused by manufacturing processes like rolling or extruding and therefore occurs in thin walled metallic structures like tubes or plates. Concerning the prediction of crack paths this anisotropic behavior has to be considered within approaches for crack growth simulations.

For the simulation of a crack path, phase field modeling of fracture is one approach, that provides several benefits and was recently applied to quasi static brittle fracture. Within a phase field fracture model, the evolution of the crack field is governed by the nature of the total energy as sum of elastic and crack surface energies. No additional criterion to estimate the propagation direction has to be utilized like within conventional crack prediction methods, especially in case of an anisotropic fracture resistance. The modification of an isotropic phase field fracture model is based on an enhancement of the non-local component of the surface energy part. As consequence of the coupling in the evolution equation, effects on the crack field's evolution, caused by a modification of the non-local term of the crack functional, are complex and complicate a parameterization with regard to the anisotropic material behavior.

In order to gain more insight into its behavior several aspects of the modified phase field model are discussed. Furthermore, results of crack path simulations are presented to show the accuracy of the proposed model, also with respect to experimental findings.

Restrictions in phase field modeling of brittle fracture

Michael Strobl (*Institute of Mechanics, Karlsruhe Institute of Technology - KIT*), Thomas Seelig (*Karlsruhe Institute of Technology - KIT*) 17:50–18:10

Phase field approaches to fracture have steadily gained popularity to compute complex crack patterns. The smooth approximation of cracks without explicit description of the crack surface and gradual degradation of material stiffness are key features of the method, which is said to result in mesh independent solutions.

This contribution is concerned with restrictions and open issues in phase field approaches to brittle fracture. The underlying conceptually simple techniques like isotropic stiffness degradation and the corresponding isotropic phase field evolution severely restrict the scope of application. Hence, basic concepts from continuum damage mechanics like tension-compression splits have been adapted and are widely established. But, with the exception of a few special cases, common splits violate the specific conditions at cracks like traction free crack surfaces. Instead, fracturing of brittle solids is a highly anisotropic process. Therefore, at least some additional constitutive assumptions have to be taken into account to obtain physically reasonable results.

The suitable choice of the internal length parameter is another important and controversial issue. It is introduced as a regularization parameter and can be interpreted as a material parameter at the same time, which determines the tensile strength. Especially in the case of crack initiation, the internal length parameter plays a crucial role and has to fulfill additional requirements.

One of our main focus is the simulation of *indentation fracture* by using the phase field approach. In this specific task, which constitutes a non-standard problem of fracture mechanics, the proper treatment of each aforementioned issue is essential. Numerical results are discussed for various modifications of the phase field model and its capabilities are illustrated by comparison with other numerical techniques and experimental results.

Phase-field modeling of fracture based on a nonsmooth multigrid solution scheme

Daniel Kienle (*Institute of Applied Mechanics, University of Stuttgart*), Carsten Gräser (*Fachbereich Mathematik und Informatik, Freie Universität Berlin*), Oliver Sander (*Institute of Numerical Mathematics, Technische Universität Dresden*), Marc-André Keip (*Institute of Applied Mechanics, University of Stuttgart*) 18:10–18:30

In the last decades the phase-field approach to fracture [1, 2, 3] has gained wide popularity due to its advantages such as straight-forward modeling of complex crack patterns and crack branching while using standard multi-field finite-element discretizations.
Phase-field models of fracture are formulated in terms of a biconvex minimization problem for which a standard monolithic Newton-Raphson scheme usually fails to converge. However, a solution could still be found by using operator-splitting methods [2] or predictor-corrector schemes [4]. Such methods come at the cost of high computational efforts. Furthermore, models incorporating the thermodynamically consistent local irreversibility of the damage phase field lead to a nonsmooth minimization problem [2].
To improve the numerical treatment and to reduce the computational costs originating from the biconvexity and the nonsmoothness of the energy functional, we employ a nonsmooth multigrid method that can solve such problems roughly in the time of one equivalent linear problem [5]. We will show that the proposed solution scheme yields the same results as classical solution schemes [2]. Furthermore, we will analyze the computational speed by means of classical benchmark problems of brittle fracture.

[1] G. A. Francfort and J.-J. Marigo. *Revisiting brittle fracture as an energy minimization problem*, Journal of the Mechanics and Physics of Solids, 46:1319–1342, 1998.

[2] C. Miehe, M. Hofacker and F. Welschinger. *A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits*, Computer Methods in Applied Mechanics and Engineering, 199:2765–2778, 2010.

[3] C. Kuhn and R. Müller. *A continuum phase field model for fracture*, Engineering Fracture Mechanics, 18:3625–3634, 2010.

[4] T. Gerasimov and L. De Lorenzis. *A line search assisted monolithic approach for phase-field computing of brittle fracture*, Computer Methods in Applied Mechanics and Engineering, 312:276–303, 2016.

[5] C. Gräser and O. Sander. *Truncated Nonsmooth Newton Multigrid Methods for Block-Separable Minimization Problems*, arXiv: 1709.04992, 2017.

S03.03 | Damage and fracture mechanics

Date 21.03.2018
Room 2760

Fault diagnosis using Probability of Detection (POD)-based sensor/information fusion for vibration-based analysis of elastic structures

Daniel Adofo Ameyaw (*Mechanical Engineering, Universität Duisburg-Essen*), Sandra Rothe (*Mechanical Engineering, Universität Duisburg-Essen*), Dirk Söffker (*Mechanical Engineering, Universität Duisburg-Essen*) 08:30–08:50

The Probability-of-Detection (POD) measure quantifies the performance of a measurement device to nondestructive testing (NDT) taking into account statistical variability. The time and cost involved has given rise to Model-Assisted POD (MAPOD) to improve the effectiveness of POD models with little or no specimen testing. Similar criteria regarding capabilities of FDI (Fault Detection and Isolation) or diagnostic approaches applied to vibration-based analysis are currently not in existence. This results from complexity of the dynamical behavior in relation to faults and sensors position (observability). In this contribution the complexity of POD-based analysis applied to fault detection of elastic mechanical structures is examined. Based on experimental results of mechanical modifications on an elastic beam, the POD of different FDI-procedures are examined. Different sensor types are used for eigenfrequency analysis and depending on the modes considered it can be shown why this classical approach often does not lead to satisfying results. To improve the detection quality, suitable assumptions in combination with a new method are applied to eigenfrequency-based analysis as detection task.

Crack detection and parameter identification in finite and semi- infinite plane structures based on remote strain fields and the distributed dislocation technique

Ramdane Boukellif (*Mechanical Engineering, University of Kassel*), Andreas Ricoeur (*University of Kassel*) 08:50–09:10

Engineering structures are in general exposed to cyclic or stochastic mechanical loading. Exhibiting incipient cracks, particularly light-weight shell and plate structures suffer from fatigue crack growth, limiting the life time of the structure and supplying the risk of a fatal failure. Due to the uncertainty of loading boundary conditions and the geometrical complexity of many engineering structures, numerical predictions of fatigue crack growth rates and residual strength are not reliable. Most experimental monitoring techniques, nowadays, are based on the principle of wave scattering at the free surfaces of cracks. Many of them are working well, supplying information about the position of cracks. One disadvantage is, that those methods do not provide any information on the loading of the crack tip. In this work, the development of a concept for the detection of cracks in finite and semi- infinite plate structures under mixed mode loading conditions is presented. The concept is based on the measurement of remote strain fields by using strain gauges and the application of the distributed dislocation technique. As an approach, different from the FEM, cracks are modelled with a collection of discrete dislocations. Within a continuum mechanics framework, these dislocations are no lattice defects but displacement discontinuities describing the local crack opening displacement. Thus, it is not necessary to discretize the domain around the crack, considerably saving computation time and data, which is crucial for an efficient solution of the inverse problem. Solving the inverse problem, e.g. with a genetic algorithm or an adaptive simulated annealing, this allows the identification of external

loading, crack position parameters, such as length, location or angles and the calculation of stress intensity factors for straight and even for curved cracks. Experiments are performed using pre-cracked plates under tensile load.

New biaxially loaded specimens for the material parameter identification of ductile damage

Steffen Gerke (*Institut für Mechanik und Statik, Universität der Bundeswehr München*), Marco Schmidt (*Universität der Bundeswehr München*), Michael Brünig (*Universität der Bundeswehr München*) 09:10–09:30

The damage behavior of ductile sheet metals depends on the stress state, i.e. the stress intensity, the stress triaxiality and the Lode parameter. The different deterioration processes like void growth, nucleation and coalescence or the formation of micro-shear-cracks [1, 3] lead to final failure of the material. These mechanisms are reflected in the phenomenological continuum damage model presented by Brünig et al. [2, 3]. Unfortunately the identification of the parameters appearing in the constitutive equations and their stress-state-dependence is a big challenge and can not be realized by one-dimensional experiments only. Three-dimensional unit cell model calculations [4] could give a first estimate of these parameters while an experimental validation is still pending. Consequently, additional experimental data is needed which can be obtained by newly proposed biaxial experiments.
The presentation focuses on new biaxial experiments and discusses restrictions for their development with special focus on ductile damage. Two new geometries (H- and X02-specimen [5]) are presented and experimental results are given in detail. Accompanying numerical simulations indicate the stress state of the fractured regions. Both geometries indicate good applicability while advantages and disadvantages are pointed out. Furthermore, it is discussed how the experimental data can be linked back to the identification of the material parameters.

[1] Y. Bao and T. Wierzbicki. On the fracture locus in the equivalent strain and stress triaxiality space. *International Journal of Mechanical Sciences*, 46:81–98, 2004.

[2] M. Brünig. An anisotropic ductile damage model based on irreversible thermodynamics. *International Journal of Plasticity*, 19:1679–1713, 2003.

[3] M. Brünig, O. Chyra, D. Albrecht, L. Driemeier, and M. Alves. A ductile damage criterion at various stress triaxialities. *International Journal of Plasticity*, 24:1731–1755, 2008.

[4] M. Brünig, S. Gerke, and V. Hagenbrock. Stress-state-dependence of damage strain rate tensors caused by growth and coalescence of micro-defects. *International Journal of Plasticity*, 63:49 – 63, 2014.

[5] S. Gerke, P. Adulyasak, and M. Brünig. New biaxially loaded specimens for the analysis of damage and fracture in sheet metals. *International Journal of Solids and Structures*, 110:209 – 218, 2017.

S03.04 | Damage and fracture mechanics

Date 21.03.2018
Room 2760

A material point regularization of a damage model with gradient-enhancement

Stephan Schwarz (*Institute of Mechanics of Materials, Ruhr-Universität Bochum*), Philipp Junker (*Institute of Mechanics of Materials, Ruhr-Universität Bochum*), Klaus Hackl (*Institute of Mechanics of Materials, Ruhr-Universität Bochum*) 14:00–14:20

Damage models, which are characterized by softening effects, suffer from ill-posed boundary value problems which result in mesh-dependent finite-element results. Regularization strategies counteract these problems by taking into account the non-local behavior such as realized by the gradient-enhanced formulation presented in [1]. Regularization there was achieved by introducing a non-local field function which couples the local damage parameter to a non-local level, in which the gradient of the field function can be penalized. Two variational equations are resulting at the expense of numerical effort but, however, mesh-independent finite-element results are provided. Based on this, we present a novel approach to regularization of damage processes within the material point level. To this end, the mentioned regularization approach based on gradient-enhancement [1] is modified and applied to the material point level. For this reason, it is not required to introduce a global field function, whereby not only the structure of the model is improved but also the numerical effort is drastically reduced. The complete regularization takes place within the material points by introducing a discretization of each material point on which the same procedure, as mentioned before, is implemented. Our novel approach to regularization already provides mesh-independent results on the material point level and therefore also for the finite-element level above.
The descretization of each material point corresponds to a separation of scales which is why macroscopic and microscopic quantities and energies are introduced and can be transferred by homogenization techniques. The Hamilton principle at the microscopic level provides the Helmholtz equation for the microscopic field function and the evolution equation for the internal variable, the damage parameter. Once we have presented the discretization and governing equations, some numerical examples are presented in order to show the functionality and efficiency of the new damage model.

[1] B. Dimitrijevic, K. Hackl. A method for gradient enhancement of continuum damage models. *Tech. Mech., 28(1):43-52* (2008)

A numerically robust gradient-extended anisotropic damage model

Marek Fassin (*Institut für Angewandte Mechanik, RWTH Aachen*), Robert Eggersmann (*Institut für Angewandte Mechanik, RWTH Aachen*), Stephan Wulfinghoff (*Institut für Angewandte Mechanik, RWTH Aachen*), Stefanie Reese (*Institut für Angewandte Mechanik, RWTH Aachen*) 14:20–14:40

For the presented model, which is based on a damage tensor of second order, the elastic part of the free energy is constructed in such a way that the damage growth criterion, cf. Wulfinghoff et al. [1], is satisfied. This criterion ensures that during a damage process the stiffness of the material decreases in any direction, or to be more precise that the stiffness does not increase

in any direction during a damage process. Numerical robustness is achieved by using a dissipation potential leading to two penalty terms. Mesh objectivity is achieved by a certain gradient extension, called the micromorphic approach according to the work of Forest [2]. It introduces an internal length which incorporates the effect of the microstructure of the material. For the local counterpart of the additionally introduced micromorphic damage variable the accumulated damage is chosen. The whole formulation is tested with several numerical examples. Among other things, numerical robustness as well as the occurrence of diffuse damage are demonstrated.

[1] *Wulfinghoff, S., Fassin, M. and Reese, S., "A Damage Growth Criterion for Anisotropic Damage Models Motivated from Micromechanics", International Journal of Solids and Structures (2017).*

[2] *Forest, S., "Micromorphic approach for gradient elasticity, viscoplasticity, and damage", Journal of Engineering Mechanics,* **135***(3), 117–131 (2009).*

An efficient FE-implementation of implicit gradient-enhanced damage models

Andreas Seupel (*Institute of Mechanics and Fluid Dynamics, Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg*), Geralf Hütter (*Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg*), Meinhard Kuna (*Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg*)

14:40–15:00

We present a strategy which allows to implement a fully coupled, gradient-enhanced damage law into commercial FEM-codes with little effort. This enables a robust simulation of practical engineering problems avoiding spurious mesh dependency due to damage influence. The method is applied to a model for shear dominated, ductile damage of metals, which is used by engineers and often available in its local formulation within FEM-programs; e. g., ABAQUS. The model consists of a damage initiation criterion, followed by a damage evolution law which is coupled to the elastic-plastic constitutive equations. Convergence studies show the applicability of the implementation for 2D and 3D boundary value problems. Crack growth simulations of a benchmark problem show reasonable results compared to similar approaches from literature.

A flexible two-surface gradient-extended damage-plasticity model

Tim Brepols (*Institute of Applied Mechanics, RWTH Aachen University*), Stephan Wulfinghoff (*Institute of Applied Mechanics, RWTH Aachen University*), Stefanie Reese (*Institute of Applied Mechanics, RWTH Aachen University*)

15:00–15:20

In this study, a gradient-extended damage-plasticity model is presented which is based on a 'two-surface' approach. The latter means that damage and plasticity are treated as truly distinct dissipative mechanisms by taking into account independent damage and yield criteria as well as corresponding sets of loading/unloading conditions (see e. g. [1]). Therefore, the model is especially flexible and adaptable to various situations in which the considered material's behavior is either (quasi-)brittle-like, ductile-like or possibly anything in between. The damage variable is gradient-extended (based on an approach by [2]) in order to cure the well-known mesh dependence problem which is otherwise present in finite element simulations involving classical 'local' damage models. Both theoretical and numerical aspects of the model are discussed as well as several structural benchmark tests which illustrate the model's behavior and mesh regularization properties in finite element simulations.

[1] T. Brepols, S. Wulfinghoff, and S. Reese, "Gradient-extended two-surface damage-plasticity: Micromorphic formulation and numerical aspects", Int. J. Plast. **97**, 64-106 (2017)

[2] S. Forest, "Micromorphic Approach for Gradient Elasticity, Viscoplasticity, and Damage", J. Eng. Mech. **135**, 117-131 (2017)

On the rate-dependent regularization for damage modeling

Kai Langenfeld (*Institute of Mechanics, TU Dortmund*), Philipp Junker (*Lehrstuhl für Mechanik, Ruhr-Universität Bochum*), Jörn Mosler (*Institute of Mechanics, TU Dortmund*) 15:20–15:40

Modeling softening behavior often results in ill-posed boundary value problems. This, in turn, results in pathological mesh dependent computations as far as the finite-element-method is concerned. A common approach to regularize such behavior is to include gradients of the internal variables into the underlying model. This is usually associated with high numerical effort, due to the coupling of local variables to their non-local counterparts. An alternative approach is presented in [1], in which the dissipation potential is extended by a quadratic term, such that the evolution of the internal variable becomes rate-dependent. This local regularization will be applied in a relaxation-based damage model [see also [2]]. On the basis of this model the mathematical explanation for mesh-independent finite-element results is examined. Furthermore the model will be compared to an established fracture energy concept [3]. This comparison shows that the rate dependent model cannot capture a constant fracture energy - contradicting experimental observations.

[1] P. Junker, S. Schwarz, J. Makowski, K. Hackl A relaxation-based approach to damage modeling, Continuum Mechanics and Thermodynamics 29 (2017) 291-310
[2] J. Mosler, O. Shchyglo, H.M. Hojjat A novel homogenization method for phase field approaches based on partial rank-one relaxation 68 (2014) 251-266
[3] L.M. Kachanov Introduction to Continuum Damage Mechanics, Springer (1986)

An anisotropic continuum damage model for concrete based on irreversible thermodynamics

Alexander Michalski (*Universität der Bundeswehr München, Institut für Mechanik und Statik*), Michael Brünig (*Institut für Mechanik und Statik*) 15:40–16:00

The presentation deals with an anisotropic continuum damage model for plain concrete. The thermodynamically consistent model is based on kinematic description of damage tensors [1, 2] and provides an efficient macroscopic approach suitable for boundary-value problems with nonlinear behavior. Based on the Helmholtz free energy function an elastic constitutive equation affected by internal variables describing damage is introduced to model deterioration of elastic material properties. The initiation and continuation of damage is governed by a damage surface which allows consideration of the different behavior of brittle materials under tension and compression. Thereby the irreversible deformations and volume increase are depicted by a damage strain tensor. Different branches of damage criteria are taken into consideration corresponding to different stress-state-dependent damage mechanisms acting on the micro- and meso-scales like nucleation, growth and coalescence of micro-cracking. This phenomenological approach is justified both in 2-D on available data from different literature e.g. [3, 4] and in 3-D on a series of experiments with corresponding numerical simulations.
A set of compression and tension tests on cylindrically shaped specimens with corresponding numerical simulations have been performed to validate the proposed anisotropic continuum damage

model. Thereby digital image correlation technique has been used to analyze formation of strain fields on surface area of the specimen under different loading conditions especially compressive loadings.

[1] *Brünig, M., "An anisotropic ductile damage model based on irreversible thermodynamics," International Journal of Plasticity,* **19**, *1679-1713 (2003).*

[2] *Brünig, M., Michalski, A., "A stress-state-dependent continuum damage model for concrete based on irreversible thermodynamics," International Journal of Plasticity,* **90**, *31-43 (2017).*

[3] *Karsan, I., Jirsa, J., "Behavior of concrete under compressive laodings," Journal of Engineering Mechanics,* **95**, *2535-2563 (1969).*

[4] *Kupfer, H., Hilsdorf, H., Rüsch, H., "Behavior of concrete under biaxial stresses," ACI Journal,* **66**, *656-666 (1969).*

S03.05 | Damage and fracture mechanics

Date 21.03.2018
Room 2760

Critical Pore Clusters in Brittle Materials: A Data Science Approach

Thomas Hochrainer (*Institut für Festigkeitslehre, Technische Universität Graz*), 16:30–17:10
Phil Daro Krummrich (*BIME, Universität Bremen*)

Fracture in porous brittle materials with random pore structures is often assumed to be linked to so-called clusters of pores. But in the literature there is no consensus on the definition of clusters. Most available definitions of clusters are based on purely geometrical criteria, considering short paths between a few pores or identifying regions of (markedly) higher-than-average porosity. However, mechanical criteria for the identification of a cluster are usually not considered.
We suggest to derive a mechanical cluster definition for specific loading cases from evaluating a large number of finite-element simulations. By evaluating local failure criteria, we identify the most probable failure location in a brittle material with randomly generated pore structure. From many simulations we extract the average pore structure surrounding the most probable failure locations. We find that the average pore structures around the critical location are loading case dependent and strongly depend on porosity and (average) pore radius. For instance, for 40% porosity with a fixed pore radius we find correlations of the failure location with about five neighboring pores, located in a distance of at most five pore radii from the failure location. We demonstrate that the average pore surroundings of the failure location yield a mechanical cluster definition, which may be used to predict critical pore cluster locations in according microstructures under the same loading.

The effect of the medium-range configuration on the atomistic fracture behaviour of amorphous silica

Firaz Ebrahem (*Institute of General Mechanics, RWTH Aachen University*), 17:10–17:30
Franz Bamer (*Institute of General Mechanics, RWTH Aachen University*),
Bernd Markert (*Institute of General Mechanics, RWTH Aachen University*)

In this work, we use molecular dynamics (MD) simulations for the investigation of fracture in amorphous silica. Several inter-atomic configurations of silica glass at room temperature are generated by the use of a two-body and three-body interaction potential considering different quenching rates [1, 2]. Subsequently, tensile loadings are subjected to the atomistic sample boxes in order to analyse the influence of the medium-range configuration on the fracture initiation.

[1] Vashishta, P., Kalia, R.K., Rino, J.P., Ebbsjö, I.: *Interaction potential for SiO_2: A molecular-dynamics study of structural correlations*, Vol. 41 of Physical Review B. American Physical Society, pp.12197-12209 (1990).

[2] Chowdhury, S.C., Haque, B.Z., Gillespie, J.W.: *Molecular dynamics simulations of the structure and mechanical properties of silica glass using ReaxFF*, Vol. 51 of Journal of Materials Science. Springer, pp.10139-10159 (2016).

Lattice Boltzmann method applied to antiplane shear loading of a stationary crack

Thomas Reinirkens (*Institute of Applied Mechanics, Technische Universität Kaiserslautern*), Ralf Müller (*Institute of Applied Mechanics, Technische Universität Kaiserslautern*), Charlotte Kuhn (*Computational Mechanics, Technische Universität Kaiserslautern*)

17:30–17:50

In this work, the dynamic behavior of linear elastic solids under antiplane shear deformation is studied by the lattice Boltzmann method. The governing set of partial differential equations reduces to a scalar wave equation for the out of plane displacement in a two dimensional domain. We use the approach developed by Guangwu in 2006 [1] as starting point to solve this problem numerically. In the beginning a short repetition of the approach is given with a focus on the boundary conditions. Special attention is given to the boundary condition of a stationary crack. The numerical performance of the lattice boltzmann scheme is tested for a stationary crack which can be compared to an analytical solution. Guangwu's examples are just for one and two dimensional models without cracks. Furthermore the performance of the lattice Boltzmann simulations are compared to classical FEM computations. Finally the stability with respect to the relaxation parameter is studied.

[1] Y. Guangwu. A lattice boltzmann equation for waves. J. Comput. Phys., 161(1):61–69, 2000.

Configurational forces in fracture mechanics: A comprehensive concept of crack initiation and growth

Paul Judt (*Engineering Mechanics / Continuum Mechanics, University of Kassel*), Andreas Ricoeur (*University of Kassel*)

17:50–18:10

In engineering structures cracks typically initiate at stress raisers such as holes and notches. In terms of a fracture mechanical assessment, it is important to identify the position x_k, the angle φ_c and the length Δa_c of initiating cracks. Classically a stress based criterion is applied to obtain the position of crack initiation. Recently, the finite fracture mechanics approach [1] was presented, combining a stress and energy based criterion to obtain the position and initiation length of cracks. In this approach, the energy states of the uncracked and the cracked specimens are compared, providing the reduction of the elastic potential $\Delta\Pi$ due to crack initiation. In general, the global solution $\Delta\Pi(x_k, \varphi, \Delta a)$ is required for accurately predicting new cracks.
In this paper, the material or configurational forces [2] at stress raisers are investigated with respect to the initiation of cracks. The material forces are strongly related to path-independent

integrals, e.g. the J-integral [3] as crack driving quantity or loading quantity at notches [4]. A new criterion based on configurational forces is suggested, efficiently providing all data of the onset of cracks at stress concentrators. Different boundary value problems with notches and holes of arbitrary shape are solved by FE calculations and the initiation and shape of crack paths are predicted in connection with an intelligent remeshing algorithm [5]. Experiments of crack initiation and growth at aluminum foil specimens are carried out and compared with the numerical results.

[1] D. Leguillon, Stress or toughness? A criterion for crack onset at a notch. European Journal of Mechanics A/Solids, 21:61–72, 2002.

[2] R. Mueller, G.A. Maugin, On material forces and finite element discretizations. Computational Mechanics, 29:52–60, 2002.

[3] J.R. Rice, A path independent integral and the approximate analysis of strain concentration by notches and cracks. Journal of Applied Mechanics, 35(2):379–386, 1968.

[4] P. Lazzarin, P. Livieri, R. Zambardi, A J-integral-based approach to predict the fatigue strength of components weakened by sharp V-shaped notches. International Journal of Computer Applications in Technology, 15(4/5):202–210, 2002.

[5] P.O. Judt, A. Ricoeur, Accurate loading analyses of curved cracks under mixed-mode conditions applying the J-integral. International Journal of Fracture, 182: 53–66, 2013.

An energy based peridynamic state-based failure criterion

Christian Willberg (*Structural Mechanics, German Aerospace Center*), Martin Rädel (*German Aerospace Center*)

18:10–18:30

The simulation of the structural behavior and particularly damage response is a key instrument for the development of lightweight structures as required in aerospace engineering or wind rotor blade development. The prediction of damage initiation and propagation in structural elements is a challenging task, even for state-of-the-art numerical procedures, such as the finite element method. The peridynamic theory presents a promising approach for these requirements. It is a non-local theory which takes long-range forces between material points into account. Utilizing the state-based formulation arbitrary materials can be modeled and analyzed. Proper failure criteria are needed for this formulation. The majority of publications use the so-called critical stretch model. Therein, a bond between two points breaks when its stretch exceeds a critical value. However, this model reaches its limits when convergence is considered. In this paper a mode-dependent energy based failure criterion has been developed. The criterion has been implemented in the peridynamic code Peridigm. In the scope of this publication, the fundamental theory of the failure criterion as well as the implementation in a massively parallel peridynamics code are explained. Based on these implementations, studies regarding the effect of probabilistic material properties to the crack initiation position are shown.

S03.06 | Damage and fracture mechanics

Date 22.03.2018
Room 2760

Diffusive fluid-driven brittle fracture in saturated porous media

Yousef Heider (*Institut für Allgemeine Mechanik (IAM), RWTH Aachen University*), Bernd Markert (*Institute of General Mechanics (IAM), RWTH Aachen University*) 08:30–08:50

Hydraulic fracturing of porous materials is an important subject in various engineering applications, especially in the energy sector such as enhanced geothermal systems (EGS). In EGS, high-pressure water is injected into deep rock layers with low permeability in order to enhance the rock's permeability, which leads to improve the system's efficiency and helps to produce electricity with lower prices. Hydraulic fracturing using pressurised liquids with chemical additives is also used in petroleum engineering to extract shale gas. In similar fashion, the developed numerical models can be applied to simulate phenomena like intervertebral disc herniation in biomechanics.
The aim in this research work is to develop a numerical model of fracturing in saturated heterogeneous porous media. To this end, the phase-field modelling (PFM) scheme together with the continuum mechanical Theory of Porous Media are applied. The proposed modelling framework accounts for the crack nucleation and propagation, deformation of the solid matrix and the different types of fluid flow in the porous domain and the crack, see [1, 2, 3] for details and references. The proposed treatment within the TPM assumes a steady-state behaviour (quasi-static) and neglects all thermal and chemical effects as well as any mass exchange between the constituents. Special focus is on the description of the interface between the porous domain and the free flow in the crack. To reveal the ability of the proposed modelling strategy in capturing the basic features of hydraulic fracture, numerical examples using the finite element method will be presented and compared with experimental data.

[1] Markert, B., Heider, Y.:*Coupled Multi-Field Continuum Methods for Porous Media Fracture, in: Recent Trends in Computational Engineering - CE2014*, Vol. 105 of Lecture Notes in Computational Science and Engineering. Springer International Publishing, pp.167–180 (2015).

[2] Heider, Y., Markert, B.: *A phase-field modeling approach of hydraulic fracture in saturated porous media*, Mech. Res. Commun., 80 (2017) 38-46.

[3] Heider, Y., Markert, B.: *Modelling of hydraulic fracturing and fluid flow change in saturated porous domains*, PAMM, (2017).

Heuristic pressure profiles in hydraulic fracturing

Markus Schätzer (*Institute of Structural Analysis, Graz University of Technology*), Thomas-Peter Fries (*Institute of Structural Analysis, Graz University of Technology*) 08:50–09:10

In hydraulic fracturing, a fluid is pumped into the rock until fractures are generated, stimulating the flow in a reservoir. The pressure exerted by the fracking fluid onto the surrounding rock is typically obtained from a non-linear coupled model known as the Reynolds equation. However, this leads to a complex behaviour, in particular at the crack tip/front (toughness or viscous regimes). For simple crack geometries, the resulting pressure distributions are given in

a dimensionless form according to different propagation regimes, see, for example, in [1]. Our aim is to replace the Reynolds equation by predefined pressure distributions which characterise the behaviour of these known profiles. This approach offers a simple and robust procedure for dealing with arbitrarily curved three dimensional crack geometries.
For the mapping of the dimensionless pressure distribution onto the physical crack surface of the structure, a dimensionless distance function (DDF) is required which describes the relative distance of a point between the injection point and the crack front. In this contribution, the computation of the DDF in the context of the extended finite element method (XFEM) and a hybrid explicit-implicit crack description [2] is discussed. The DDF is obtained by solving the Laplace-Beltrami operator on the explicit representation of the manifold, i.e., the surface mesh, where distances are evaluated along streamlines which represent the fluid flow of the fracking fluid within the fracture.

[1] Adachi, J.I.; Detournay, K.: Self-similar solution of a plane-strain fracture driven by a power-law fluid. *Int. J. Numer. Anal. Methods Geomech.*, **26**(6), 579-604, 2002.

[2] Fries, T.P.; Baydoun, M.: Crack propagation with the extended finite element method and a hybrid explicit-implicit crack description. *Int. J. Numer. Meth. Engng.*, **89**, 1527-1558, 2012.

A multi-physics approach to investigate the influence of hydrogen on short fatigue crack propagation

Volker Schippl (*Maschinenbau, Universität Siegen*), Sven Brück (*Maschinenbau, Universität Siegen*), Hans-Jürgen Christ (*Maschinenbau, Universität Siegen*), Claus-Peter Fritzen (*Maschinenbau, Universität Siegen*)

09:10–09:30

Hydrogen leads to a macroscopic embrittlement and under cyclic loading to increasing crack growth rate and a shorter fatigue life of mechanically loaded components. To address this problem, a better understanding of the hydrogen damaging mechanism is needed.
As the short crack propagation could dominate the whole fatigue life, a two-dimensional model is presented to simulate short crack propagation to get a better understanding of the fundamental mechanisms leading to failure. The simulation results are compared with experimental observations on the crack growth behavior in pre-charged specimens of a metastable austenitic stainless steel. The model includes intergranular and transgranular crack growth and considers the plastic deformation along shear bands. The hydrogen concentration in the microstructure is calculated and the amount of the local hydrogen at the crack tip changes the crack growth mechanism.
This multi-physics problem is addressed by using a sequential staggered BEM & FEM approach. At first, stresses and displacements are calculated by using a boundary element method. Based on the calculated hydrostatic stress field, the redistribution of hydrogen is determined using a finite element method.
With this approach, it could be found that hydrogen leads to an increasing part of the irreversible plastic deformation at the crack tip which results in increasing crack growth rates and thus to shorter lifetime.

Micromechanical simulation of ferroelectric domain processes at crack tips

Sergii Kozinov (*Institute of Mechanics and Fluiddynamics, TU Bergakademie Freiberg*), Meinhard Kuna (*TU Bergakademie Freiberg*)

09:30–09:50

Piezo/ferroelectric ceramics, widely used in microelectromechanical systems (MEMS) and smart structures, are very brittle and crack prone. Preliminary failure of such devices can lead to

catastrophic consequences and is due to high electromechanical field concentrations near crack-like defects or electrodes. In the current numerical simulations the micromechanical ferroelectric model implemented as user routine for the finite element code Abaqus is used to study ferroelectric domain processes, including domain switching at the crack tip. For this purpose a finite element model of the compact tension specimen (CT-specimen) made of a soft tetragonal lead zirconate titanate ceramic is employed. The results of our numerical simulations demonstrate good agreement with measurements of domain orientation distribution done by a high-energy synchrotron X-ray transmission at CT in-situ experiments. Domain switching patterns around the crack front under mechanical loading of the CT-specimen are displayed as a function of the in-plane position for a set of different azimuth angles. The relationship between the stress field and the domain orientation is also investigated. Some fracture mechanics quantities such as electromechanical J-integral and configurational forces are subsequently derived. As a result of the simulations, the preferred domain orientations in the specimen (which depend on the position around the crack tip) are found and thoroughly investigated.

Micromechanical Modeling of a Generator Stator Electrical Insulation System

Thank Thank Nguyen (*Institut für Angewandte Mechanik, RWTH Aachen*), Stephan Wulfinghoff (*Institut für Angewandte Mechanik, RWTH Aachen*), Stefanie Reese (*Institut für Angewandte Mechanik, RWTH Aachen*) 09:50–10:10

Due to the renewable energy act fossil power plants are exposed to a new load ramp with a frequent start up and shut down process. Consequently the current applied technologies for the insulation System reaches their limits. Therefore the origin of the failure in the woven composite (glass fiber and epoxy resin) with insulation has to be detected numerically. In order to obtain a comprehensive understanding of the the microstructural influence on the properties of the composite, simulations will be carried out. Within these simulations, various parameters are systematically varied. The aim of the project is to get an optimal parameter combination to meet the requirements.
A unit cell with three components (woven fiber, epoxy resin and insulation) is created. To obtain the influence parameters for damage initiation and growth (fatigue) of the current composite material it is necessary extend the so far elastic model with methods of damage and/or fracture mechanics.

A Damage Mechanics based Cohesive Zone Model for Delamination and Failure Behaviour of Coatings at High-Temperature

Joachim Nordmann (*Otto-von-Guericke Universität Magdeburg*), Konstantin Naumenko (*Otto-von-Guericke Universität Magdeburg*), Holm Altenbach (*Otto-von-Guericke Universität Magdeburg*) 10:10–10:30

A Cohesive Zone Model (CZM) is derived within the framework of continuum thermodynamics for pure Mode I opening. The model is physically motivated what is in contrast to the usual phenomenological definition of a CZM and the separation is additive decomposed into elastic and inelastic parts. For the evolution of inelastic separation a power law in combination with a damage law is used to consider tertiary creep, additionally. Thereby, the damage evolution is related to energy release rate and inelastic opening rate. Further on, an additional equation is added to the CZM, thus, that no contact problem must be solved in the compression case and the numerical effort can be reduced.

S03.07 | Damage and fracture mechanics

Date 22.03.2018
Room 2760

Fatigue Reliability Analysis and Design for Structural Components in Quasi-One-Shot Device

Min Chen (*Industrial Design, Xi'an Jiaotong-Liverpool University*), Xiaofei Yao (*State Key Laboratory of Electrical Insulation and Power Equipment, Xi'an Jiaotong University*), Bin Wu (*Institute of General Mechanics, RWTH Aachen University*), Yousef Heider (*Institute of General Mechanics, RWTH Aachen University*), Derrick Tate (*Xi'an Jiaotong-Liverpool University*), Zhiyuan Liu (*Xi'an Jiaotong University*) 14:20–14:40

High-voltage vacuum circuit breakers are designed to protect and control the electrical power transmission networks. If they fails to be activated once they are needed, it might lead to extensive damage of the whole system and cause enormous economical losts. Like the automobile air bags, they belong to the class of "one-shot" devices, which are found in a stand-by readiness state for a long time. The traditional reliability design methods consider the MTBF (mean time between failures) or MTTF (mean time to failure) to measure the reliability of structures with normal failure distribution, which is not appropriate for circuit-breakers. In this paper, a general approach that comprises of PoF (Physics of Failure) and RF (Reliability of Physics) is proposed to study the root cause of the failure behavior and to evaluate the fatigue life of the critical structural components in the spring-type operating mechanism of the circuit breakers. Moreover, the fatigue sensitivity and limit load are also discussed for a design reference. An interlocking component is used as a validation example, which shows a good match of the experimental testing and the numerical simulation.

A rate-dependent damage model for prediction of high-speed cracks

Sahir Butt (*Institute of structural mechanics, Ruhr-Universität Bochum*), Günther Meschke (*Institute of structural mechanics, Ruhr-Universität Bochum*) 14:40–15:00

Experiments [1] have shown that the energy release rate in high-speed dynamic fracture processes strongly depends on the the macro crack propagation velocity. This dependence is due to the fact that the rate of the fracture surface creation is proportional to the energy flux into the crack. A crack propagating at high-speed can create an order of magnitude larger fracture surface in form of micro-branches than a low-speed crack [2]. To this end, a rate dependent damage model, which is based on the physics of micro-branching, is presented and incorporated into peridynamic continuum theory. Numerical simulations are carried out on a plexiglas (PMMA) plate to show that the proposed model is capable of reproducing the physical phenomena observed in experiments.

[1] Sharon, E., Gross, S. P. & Fineberg, J. (1996) Energy dissipation in dynamic fracture. Physical review letters, 76, 12.

[2] Fineberg, J. & Bouchbinder, E. (2015) Recent developments in dynamic fracture: some perspectives. International Journal of Fracture, 196, 1-2.

A Continuous-Discontinuous Approach for 3D Dynamic Fracture

Mahmoud Pezeshki (*Mechanical Engineering, Institute of Continuum Mechanics, Leibniz Universität Hannover*), Stefan Löhnert (*Civil Engineering, Institute of Mechanics and Shell Structures, Technical University Dresden, Germany*), Peter Wriggers (*Mechanical Engineering, Institute of Continuum Mechanics, Leibniz Universität Hannover*) 15:00–15:20

A continuous-discontinuous approach to fracture is utilized to model dynamic crack propagation in 3D media. The continuum-based models require highly refined mesh resolutions for a sharp representation of the crack while this can be achieved by combining these models with discrete models such as the eXtended Finite Element Method (XFEM) [1]. This provides an acceptable accuracy at a significantly lower computational cost.

Here a gradient-enhanced damage model is used to model the material degradation in front of the discrete crack [2]. Using this model resolves mesh dependency problem of the local damage models and avoids energy dissipation in a narrow band. When the damage reaches its maximum value, a discrete crack is introduced within the damage band. Unlike cohesive methods, XFEM needs an additional approach to find the crack propagation direction. Adopting a gradient-enhanced damage model give us the possibility to find the propagation direction based on the damage values. To this end a strategy based on the maximum damage value is utilized. The Level Set Method is used to represent the crack geometry and to track the crack growth. To avoid solving additional equations for the level set field a simple and efficient geometrical level set update approach is used. The nodal level sets are updated locally around the current crack fronts [3]. Finally, to prove efficiency and robustness of this method some numerical examples are provided.

[1] T. Belytschko, T. Black. Elastic crack growth in finite elements with minimal remeshing, International Journal for Numerical Methods in Engineering, 45(5), 601-620, 1999.

[2] R.H.J. Peerlings, R. de Borst, W.A.M. Brekelmans, J.H.P. de Vree. Gradient enhanced damage for quasi brittle materials. International Journal for Numerical Methods in Engineering, 39, 3391-3403, 1996.

[3] S. Loehnert, D.S. Mueller-Hoeppe, P. Wriggers. 3D corrected XFEM approach and extension to finite deformation theory. International Journal for Numerical Methods in Engineering, 86, 431-452, 2011.

Modelling of nonlinear damage accumulation for the lifetime prediction of adhesively bonded joints

Ulrich Kroll (*Department of Mechanical Engineering, Institute of Mechanics, University of Kassel*), Anton Matzenmiller (*Department of Mechanical Engineering, Institute of Mechanics, University of Kassel*) 15:20–15:40

The adhesive joint in the bonded component suffers creep and fatigue damage caused by sustained mechanical loading with constant or variable amplitudes during service up to the rupture time, where the lifetime is attained. Besides mean stress and multiaxiality of the loading, the chronological order of the loading values leading to nonlinear damage accumulation must be considered for the lifetime prediction of the bonding layer. For this purpose, a damage model is presented, which is based on the theory of continuum damage mechanics. The model consists

of a creep and fatigue damage part, which both capture the influence of the mean stress on the lifetime. Multiaxiality of the loading is taken into account by an equivalent stress, which is adapted for ductile adhesives. The damage approach contains parameters, which are determined by means of rupture times from creep and constant amplitude fatigue tests. Nonlinear fatigue damage accumulation is considered by a term in the fatigue damage part. In the case of pure fatigue damage, this term influences the lifetime prediction by the model for variable amplitude loadings, while the prediction for constant amplitude loadings is unaffected. Several approaches for the consideration of nonlinear fatigue damage accumulation can be applied through the term. These approaches may imply parameters, which are identified by means of tests with so called two-level loadings or indirect measurement of damage evolution in constant amplitude fatigue tests until rupture. Numerical examples are presented in order to investigate the validity of the proposed model.

A continuum damage based approach for cavitation and shear failure of hyperelastic adhesives for finite element applications

Alexander Nelson (*Mechanical Engineering, University of Kassel*), Anton Matzenmiller (*Mechanical Engineering, University of Kassel*) 15:40–16:00

Ship- and rail-vehicle building as well as automotive industry use rubber-like adhesives for glazing and joining of structural components. These adhesives are suitable to compensate relative deformations of adherends due to their ability to withstand large elastic deformations. Depending on the particular loading, the adhesive layer exhibits distinct amounts of isochoric and volumetric deformations. The volumetric deformations decisively effect the occuring failure mechanism. The objective of this contribution is to develop and validate a material model for the failure prediction of adhesively joined, large structures under quasi-static loading. To this end, data of uniaxial tensile tests, thick adherend shear tests and buttjoint specimens with different adhesive layer thicknesses are evaluated and the findings are used for a phenomenologically based constitutive apporach. The Mooney-Rivlin-model is applied to describe the hyperelastic response. The failure is modelled with a continuum damage based approach, which takes into account cavitation and shear failure. The damage functions are energy based. All introduced model parameters are physically sound and are identified using the data of the aforementioned tests. Finally, computations of component-like specimens are performed and the results are compared to according test data to validate the model.

S03.08 | Damage and fracture mechanics

Date 22.03.2018
Room 0601

Damage and failure mechanisms of ductile metals in biaxial experiments with non-proportional loading paths

Moritz Zistl (*Institut für Mechanik und Statik, Universität der Bundeswehr München*), Steffen Gerke (*Universität der Bundeswehr München*), Michael Brünig (*Universität der Bundeswehr München*) 17:30–17:50

The presentation deals with the effects of non-proportionally loaded biaxial specimens on damage and failure mechanisms of ductile materials. A continuum damage model with thermodynamically consistent anisotropic damage and failure mechanics is discussed. Its kinematics are based on the introduction of damaged and fictitious undamaged configurations [1]. This leads to a damage affected elastic material law based on free energy functions. An experimental series of biaxially

loaded specimens and a numerical comparison of different failure mechanisms is displayed. With the use of the digital image correlation (DIC) technique the development of the strain fields can be used to validate the corresponding numerical simulations. It is well known that plastic flow, damage and failure depend on stress intensity, stress triaxiality and the Lode parameter [2]. New cruciform specimens [3] are used in biaxial experiments and its applicability to obtain a variety of different stress states is shown. In former research activities the loading paths and therefore the stress states have been kept constant. In the presented research the loading is applied sequentially and thus the loading ratio and the stress-state-dependent processes change during the experiment. Based on the examination of the fracture surfaces under a scanning electron microscope (SEM) the different topologies are a clear indication that different micro-level mechanisms are present and distinct from proportional experiments. Differences between the non-proportional and proportional experiments indicate path-dependent damage behavior.

[1] M. Brünig, An anisotropic ductile damage model based on irreversible thermodynamics. *International Journal of Plasticity*, Vol. **19**, 1679–1713, 2003.

[2] Y. Bao and T. Wierzbicki, On the fracture locus in the equivalent strain and stress triaxiality space. *International Journal of Mechanical Sciences*, Vol. **46**, 81–98, 2004.

[3] S. Gerke, P. Adulyasak and M. Brünig, New biaxially loaded specimens for the analysis of damage and fracture in sheet metals. *International Journal of Solids and Structures*, Vol. **110**, 209–218, 2017.

Numerical and experimental analyzes of the effect of negative stress triaxialities on ductile damage and failure

Marco Schmidt (*Universität der Bundeswehr München*), Steffen Gerke (*Universität der Bundeswehr München*), Michael Brünig (*Universität der Bundeswehr München*)

17:50–18:10

The presentation deals with an anisotropic continuum damage and fracture model for ductile materials and discusses the effects of negative stress triaxialities. A kinematic definition of damage tensors is fundamental for the thermodynamically consistent anisotropic damage and fracture model [1]. It includes fictitious undamaged and damaged configurations where free energy functions are defined. A yield condition and a non-associated flow rule are used to characterize the plastic behavior of ductile materials. In a similar way, a stress-dependent damage criterion based on a series of experiments and corresponding numerical simulations is proposed [2]. Furthermore, a damage rule takes into account different damage mechanisms like growth of voids, formation of micro-shear-cracks and their combination which depends on stress intensity, stress triaxiality and Lode parameter.

To validate the proposed phenomenological approach for negative stress triaxialities a series of shear-compression experiments and corresponding numerical simulations have been performed. The displacement and strain fields of the critical regions of the biaxially loaded specimens have been analyzed with a digital image correlation technique. In addition, the fracture surfaces have been examined by a scanning electron microscopy to investigate the microscopic failure mechanisms. Within this context, the existence of a critical value of negative stress triaxiality [3] is discussed below which fracture never occurs for ductile materials and a Lode-parameter-dependent cut-off value of stress triaxiality is proposed.

[1] M. Brünig. An anisotropic ductile damage model based on reversible thermodynamics. *International Journal of Plasticity*, Vol. **19**, 1679–1713, 2003.

[2] M. Brünig, D. Brenner and S. Gerke. Stress state dependence of ductile damage and fracture behaviour: Experiments and numerical simulations. *Engineering Fracture Mechanics*, Vol. **141**, 152–169, 2015.

[3] Y. Bao and T. Wierzbicki. On the cut-off value of negative triaxiality for fracture. *Engineering Fracture Mechanics*, Vol.**72**, 1049–1069, 2005.

Detection of the real concrete mesostructure with CT scan for the numerical implementation

Pietro Carrara (*Institute of Applied Mechanics, TU Braunschweig*), Roland Kruse (*Institute of Applied Mechanics, TU Braunschweig*), Laura De Lorenzis (*Institute of Applied Mechanics, TU Braunschweig*) 18:10–18:30

Concrete is a composite material whose structure at the mesoscale, i.e. at a scale where the cementitious matrix, aggregates and pores are separately identified, plays a significant role. Hence, knowledge on the concrete degradation processes can be gained by explicitly accounting its heterogeneous structure into numerical simulations. To this end, in the past few years the use of a computed tomography (CT) has become a very attractive option. However, the identification of the various phases, i.e. the segmentation process, is not trivial especially because the limited contrast between cementitious matrix and aggregates due to similar composition. Also, since the dimension of the inclusions in concrete spans many orders of magnitude, a threshold length above which the heterogeneities are explicitly modeled is needed. This work explores the possibility to add contrast enhancers powders into the concrete mixes to allow an easier segmentation and mesh generation. This allows to adopt high fidelity geometries of the concrete mesostructure into numerical simulations. Characterization tests, such as semi-adiabatic calorimetry, ultrasonic and compression tests, are performed in order to ensure that the concrete mix is not appreciably affected by the presence of the enhancers. The results of both normal and modified concretes are compared to demonstrate the validity of the method.

S03.09 | Damage and fracture mechanics

Date 23.03.2018
Room 2760

Modeling of matrix damage and fiber-matrix interface debonding in sheet molding compound

Johannes Görthofer (*Institute of Engineering Mechanics, Karlsruhe Institute of Technology (KIT)*), Malte Schemmann (*Institute of Engineering Mechanics, Karlsruhe Institute of Technology (KIT)*), Thomas Seelig (*Institute of Mechanics, Departement of Civil Engineering, Geo and Enviromental Sciences, Karlsruhe Institute of Technology (KIT)*), Andrew Hrymak (*Departement of Chemical and Biochemical Engineering, Western University (UWO)*), Thomas Böhlke (*Karlsruhe Institute of Technology (KIT)*) 08:30–08:50

Sheet molding compounds (SMC) possess a comparably high mass-specific strength and stiffness. Therefore, their deployment in mass-reduction strategies in the automotive and aerospace sector is of great interest. In order to apply SMCs as structural components, an understanding of their behavior under uniaxial and multiaxial loading is crucial. To correctly predict the macroscopic behavior of SMC, a corresponding model should take the microstructure into account. The different characteristics of the constituents as well as their interaction need to be depicted.

The SMC considered in the present work consists of a thermoset matrix reinforced with long (≈ 25mm) glass fibers, and typically features a heterogeneous and anisotropic fiber orientation distribution (FOD).
A mean field anisotropic damage model based on the FOD, is presented. It captures the dominant damage mechanisms in a Mori-Tanaka homogenization framework. Matrix damage is modeled as a phase-averaged isotropic stiffness degradation. Since in the considered temperature range, the thermoset matrix is brittle, a maximum stress criterion is applied. The interface stress state is represented by a direction-dependent equivalent stress which governs the interface damage. Hereby, the inhomogeneous stress distribution (including normal and shear stresses) on the interface is taken into account. A Weibull distribution for the interface strength is assumed. Hence, interface debonding is modeled by an evolving fraction of load-carrying fibers which results in an overall anisotropic material behavior.
The model is validated by means of uniaxial and biaxial tensile tests with different fiber volume content. The simulation results are within a satisfactory accurate range compared to the experimental results.

A comprehensive model of material removal mechanism in lapping process by single-grain scratch test

Driss Fares (*Maschinenbau und Verfahrenstechnik, Technische Universität Kaiserslautern*), Kristin de Payrebrune (*TU-Kaiserslautern*) 08:50–09:10

Lapping is a final manufacturing process of loose, geometrically undefined grains mixed in a liquid.
During machining, the workpiece is pressed onto a rotating lapping disk. Loose lapping grains mixed with a liquid are introduced in the gap between the workpiece and the lapping disk. Due to the rotation of the lapping disk, the lapping grains move in a completely disordered manner, which leads to material removal, which leads to a very high surface quality of the workpiece. The unpredictable kinematics of grains and the strongly varying local contact conditions, makes the lapping process very complex. The Institute of Applied Structural Mechanics conducts experimental investigations and simulations to better understand the process. The goal is to develop an overall model of the grinding process, with which process estimations can be made.
The kinematics of the lapping grains play a decisive role for material removal. In order to determine correlations between the local material removal and the grain geometry, and kinematics, an FEM simulation model is developed for single-grain scratch tests. At first, of a geometrically simple and fixed grain, the direction of movement, the relative velocity to the workpiece and the penetration pressure will be varied and the material removal mechanism investigated. In future, scratch simulations with more complex grain geometries and irregular movements will be carried out. The latter is currently being investigated by discrete element simulations.

Modelling and Simulation of Metal Cutting Processes by use of the stabilized Optimal Transportation Meshfree Method

Dengpeng Huang (*Instituts für Kontinuumsmechanik, Leibniz Universität Hannover*), Christian Weißenfels (*Institute of Continuum Mechanics, Leibniz Universität Hannover*), Peter Wriggers (*Leibniz Universität Hannover*) 09:10–09:30

In metal machining processes, very complex loading conditions exist during the chip formation process, where the material is removed continuously from the work-piece. It is still an important challenge to give an accurate prediction of cutting force, chip morphology and temperature by numerical modeling approach. The difficulties lie in constitutively predicting the response and ductile failure of metallic materials under highly dynamic loadings, as well as numerically dealing with the topology change due to large plastic deformation and fracture in cutting zones.

In this work, the chip formation process is simulated by use of the stabilized Optimal Transportation Meshfree (OTM) method [1]. A modified Johnson-Cook hardening law within the hyperelasto-plasticity framework is used to account for the strain hardening, the strain rate hardening and the thermal softening [2]. Due to the shear strain localization and high temperature in the cutting zone, an improved ductile damage model is applied. The plastic dissipation-induced temperature rise is evaluated by considering that a certain amount of the plastic work rate is converted into heat. The material-point erosion approach is applied to simulate the ductile fracture as well in the present work.
Combined with the above constitutive model and the improved ductile failure criteria, the stabilized OTM method has shown a good convergence for simulation of chip formation in metal cutting process. The cutting force and the temperature at different cutting speeds and cutting depths have been calculated and compared with experimental results in the literature.

[1] C. Weißenfels and P. Wriggers, Stabilization algorithm for the optimal transportation meshfree approximation scheme. Comput. Methods Appl. Mech. Eng., 2017.

[2] G. R. Johnson, and W. H. Cook, Fracture characteristics of three metals subjected to various strains, strain rates, temperatures and pressures. Eng. Fract. Mech., Vol. 21, pp. 31-48, 1985.

A new material approach towards shear cutting of fiber reinforced plastics

Lukas Poggenpohl (*Institut für Angewandte Mechanik, RWTH Aachen University*), Stephan Wulfinghoff (*Institut für Angewandte Mechanik, RWTH Aachen*), Stefanie Reese (*Institut für Angewandte Mechanik, RWTH Aachen*) 09:30–09:50

The aim of this project is to develop and validate a new material model to simulate the material behavior of carbon fiber reinforced plastics during shear cutting. Here, the focus lies on the initiation and evolution of damage in the cutting plane. A geometrically nonlinear elastic-brittle material model with non local damage variables will be used. Experimental data suggest to distinguish between damage of the matrix and damage of the fibers. Therefore, a material model will be shown, where two scalar damage variables are used. The material model will be fitted and tested on experimental data.

An Anisotropic Damage-Mode Based Constitutive Model for Fibre-Reinforced Polymer Composites

Madhukar Chatiri (*CADFEM International GmbH*), Anton Matzenmiller (*Institute of Mechanics, University of Kassel*) 09:50–10:10

This contribution presents a three dimensional constitutive model for anisotropic damage to describe the onset and propagation of ply failure mechanisms in unidirectional fibre reinforced laminated composites. The primary objective of the work focuses on the three dimensional relationship between damage of the material and the effective elastic properties for the purpose of stress analysis of composite structures. A homogenized continuum is adopted for the constitutive theory of anisotropic damage and elasticity. Damage initiation criteria are based on Puck failure criterion for first ply failure and orientation of the fracture plane. Progressive micro crack propagation is based on the idea of continuum damage evolution. Internal variables are introduced to describe the evolution of the damage state under loading and as a subsequence the degradation of the material stiffness. Emphasis is placed on a suitable coupling among the equations for the rates of the damage variables with respect to the different damage modes. The model is validated using several component tests performed on unidirectional specimens as well as multidirectional laminates. A good correlation between experimental observations and numerical predictions is obtained

The Influence of Interface Bonding Models on Propagating Matrix Cracks

Johannes Scheel (*University of Kassel*), Andreas Ricoeur (*University of Kassel*) 10:10–10:30

If any kind of inclusion is embedded in an otherwise homogeneous matrix, the prediction of crack paths becomes a challenging task due to the inhomogeneous state of stress and complex bonding and interface properties. The interface can either be perfect or imperfect having a crucial impact on propagating matrix cracks. In particular the latter case intrinsically leads to defect interaction thus requiring closer investigation [1]. Finally, the matrix crack path and the failure of the structure depend on proper modeling of the interfaces, where cohesive zones are a frequently used approach. The influence of different models on the crack tip loading and resulting crack paths is investigated just as their thermodynamical consistency. Incremental crack extensions constitute the matrix crack growth, requiring a continuous modification of the geometry. An intelligent re-meshing procedure is applied, where the loading history cannot be neglected due to the presence of dissipative processes at imperfect interfaces. The crack tip loading is calculated numerically with the J-integral, where remote integration contours are used [2,3]. In order to appropriately incorporate the cohesive zones, the J-integral has to be reformulated.

[1] J. Scheel, A. Ricoeur; *Procedia Structural Integrity* 2017; 5: 255-262.

[2] P. Judt, A. Ricoeur; *International Journal of Fracture* 2013; 182: 53-66.

[3] P. Judt, A. Ricoeur, G. Linek; *Engineering Fracture Mechanics* 2015; 138: 33-48.

S04 | Structural mechanics

Organiser Christoph Adam (*University of Innsbruck*)
Johannes Gerstmayr (*Institute for Mechatronics, University of Innsbruck*)

S04.01 | Structural mechanics

Date 20.03.2018
Room 0602

Homogenized material properties for cross-laminated timber

Thomas Furtmüller (*University of Innsbruck*), Christoph Adam (*University of Innsbruck*), Benjamin Giger (*University of Innsbruck*) 08:30–08:50

In this contribution material properties for large-scale Finite Element (FE) analyses of point-supported cross-laminated timber (CLT) slabs are derived by means of numerical homogenization. In the first step, material properties of the constituents of the considered CLT elements are determined. Quasi-static three point bending tests are performed for three configurations and FE simulations of these tests are employed in an optimization procedure to derive both orthotropic elastic material parameters and parameters of Hill's yield function for the spruce wood boards. Parametric studies reveal significant material properties as well as parameters that cannot be identified satisfactorily by means of uniaxial bending tests. In the second step, a numerical homogenization scheme is employed in order to derive the elastic stiffness matrix of a generalized shell section representing the CLT floor. To this end, a repeating unit cell is defined, where macroscopic homogeneous strains and curvatures can be implemented by means of nodal displacements and corresponding macroscopic shell normal forces and bending moments can be computed from the nodal reaction forces. To verify the homogenization procedure, modal analysis is conducted for a ficticious point-supported CLT slab with dimension of approximately 10x10 m. A computationally very expensive solid element model is compared to a shell model with generalized shell stiffness as computed by the homogenization scheme. The shell element model provides an excellent approximation of the resonant frequencies and the mode shapes, requiring only a fraction of the computational expense of the solid element model. Homogenization is extended to inelastic deformation of the unit cell simulations. An approximate failure surface is derived and implemented as postprocessing variable. As a verification of the failure surface, an ultimate load analysis is performed for the solid element model. Plastic zones are in good agreement with the predictions obtained by the postprocessing variable in a corresponding shell element model.

Efficient analysis of stress concentrations in laminated composite structures with geometric discontinuities

Jan Eike Schnabel (*Institute of Materials Research, Materials Mechanics (Geb. 59), Helmholtz-Zentrum Geesthacht*), Christian Mittelstedt (*FB Maschinenbau, FG Konstruktiver Leichtbau und Bauweisen, Technische Universität Darmstadt*) 08:50–09:10

This paper discusses analysis method for displacements, strains and stresses in a laminated composite plate under tensile load that is reinforced by a doubler. The analysis works in two parts. First, a global solution based on Classical Laminated Plate Theory (CLPT) is introduced. In the second step, a local model is presented that includes the three-dimensional nature of the

stress state in the vicinity of the plate-doubler junction. This local solution uses a discretization of the physical layers into a certain number of mathematical layers which leads to a quadratic eigenvalue problem that requires numerical treatment. Hence, the analysis approach is of a semi-analytical nature. The current analysis model delivers excellent results in comparison to finite element computations, this however at only a fraction of the computational time and effort required for the FEM analyses.

Modeling of anisotropic boundary layer effects in plate theory

Patrick Schneider (*Mechanical Engineering, KLuB / Technische Universität Darmstadt*), Reinhold Kienzler (*Department of Production Engineering, bime / University of Bremen*) 09:10–09:30

In the talk, the modeling of a Reissner-type plate theory for elastic, monoclinic material is presented. The basic theory is derived using the a-priori-assumption free uniform-approximation approach, which is based upon series expansions of the displacement field and a structured truncation of the elastic potential that gives rise to hierarchies of approximating theories. An a-priori estimate for the approximation error shows that higher-order theories have indeed a higher rate of convergence with respect to the relative thickness of the plate. Using a pseudo-reduction approach the number of PDEs to be solved is reduced significantly. The resulting first-order theory is the classical monoclinic plate theory, whereas, the second order theory is not determined uniquely by the approach. Uniqueness is achieved by introduction of an orthogonal decomposition of higher-order gradients of the in-plane displacement. The final second-order theory coincides with the Reissner-Mindlin theory for the special case of isotropic material.

A modified plate model for an efficient analytical treatment of stress concentrations at notches

Julian Felger (*Strukturmechanik, Technische Universität Darmstadt*), Marvin Schmidt (*Technische Universität Darmstadt*), Wilfried Becker (*Strukturmechanik, Technische Universität Darmstadt*) 09:30–09:50

Since the use of lightweight design concepts attains increasing attention, a detailed analysis of stress concentrations, for instance at holes or sharp notches, is necessary. While stress raisers in the plane extensional case have been investigated exhaustively in literature using analytical methods [3], the treatment of out-of plane or bending load cases still poses challenges. On the one hand, the well established classical Kirchhoff-Love plate theory is no longer adequate in the presence of stress concentrations associated to notches with an characteristic length in the same order as the plate's thickness [4]. On the other hand, the well suited Reisser-Mindlin plate theory yields a system of partial differential equations impeding an analytical solution on complex domains.

In the present work, a modified plate model is proposed lying in between the established Kirchhoff-Love and Reissner-Mindlin plate theories. The proposed model includes the effect of transverse shear deformation and enables the formulation of three physically sound boundary conditions crucial for an adequate description of the local stress field near boundaries. The resulting system of partial differential equations can be solved using a complex potential approach which allows for tackling geometries such as sharp or rounded notches. Using the proposed model, the singular stress field in the vicinity of a sharp notch is obtained explicitly and the influence of the notch opening-angle on the singular behaviour is investigated. It is shown that the resulting bending moments and transverse shear forces locally match with asymptotic solutions of Reissner-Mindlin theory [1, 2] and are in very good agreement with numerical results.

[1] J Felger and W Becker. A complex potential method for the asymptotic solution of wedge problems using first-order shear deformation plate theory. *European Journal of Mechanics-A/Solids*, 61:383–392, 2017.

[2] A Rössle and AM Sändig. Corner singularities and regularity results for the Reissner/Mindlin plate model. *Journal of Elasticity*, 103(2):113–135, 2011.

[3] NI Muskhelishvili. Some basic problems of the mathematical theory of elasticity *Nauka, Moscow*, 1966.

[4] SP Timoshenko and S Woinowsky-Krieger. Theory of plates and shells *McGraw-Hill*, 1959.

Nonlinear modeling framework on soft electro-elastic plates accounting for electrostriction

Elisabeth Staudigl (*E325 Institut für Mechanik und Mechatronik, TU Wien, Vienna University of Technology*), Michael Krommer (*Institute of Mechanics and Mechatronics, TU Wien, Vienna University of Technology*), Yury Vetyukov (*Institute of Mechanics and Mechatronics, TU Wien, Vienna University of Technology*) 09:50–10:10

Motivated by nature, actuation devices made of soft electro-active polymers capable of coupled electric and mechanic fields are a current topic of research. Due to their low elastic modulus, their application is prone to thin structures, which motivates the modeling within a structural mechanics framework. In this work, we outline the constitutive modeling of soft actuation devices in this latter framework.
Because of their capability to undergo large strains, the theory necessitates a geometric nonlinear formulation, which at first, is developed for the full set of three dimensional field equations, by incorporating a generalized free energy function composed of a pure mechanical strain energy and a mixed electro-mechanical free energy. The key of the formulation is the electro-mechanical coupling, accounted for by a multiplicative decomposition of the deformation gradient tensor, applied to the case of electrostriction. By applying the Gauss law of electrostatics, the model is further extended to the case of charge driven actuation, which has been reported to prevent pull-in failure [1].
The three dimensional constitutive relations are eventually reduced to the structural level of thin plates by imposing a plane stress condition on the total stress tensor. A non-linear Finite-Element analysis is employed to study the effect of the material nonlinearities as well as the effect of the voltage and charge driven actuation. Comparison to experimental results motivate further investigations on special materials, capable of a pronounced electrostrictive effect to enhance the structural actuation properties.

[1] T. Lu, Ch. Keplinger N. Arnold, S. Bauer, and Z. Suo. Charge localization instability in a highly deformable dielectric elastomer, *Applied Physics Letter*, 104: 022905. 2014.

Kirchhoff-Love shell theory based on Tangential Differential Calculus

Daniel Schöllhammer (*Institute of Structural Analysis, Graz University of Technology*), Thomas-Peter Fries (*Institute of Structural Analysis, Graz University of Technology*) 10:10–10:30

The classical approach of modelling Kirchhoff-Love shells is to introduce a local coordinate system [1]. This concept requires the introduction of co- and contra-variant base vectors and Christoffel symbols, which makes the approach less intuitive and more complex. Yet it is the standard approach to simulate shells for the last decades.

We propose a new formulation of the Kirchhoff-Love shell theory without the explicit introduction of curvilinear coordinates. In particular, we recast the shell equations in the frame of tangential operators using a global Cartesian coordinate system, which leads to a more compact and intuitive implementation. In [2] a rather technical procedure to recast the shell equations is presented. A recent approach in [3] only considers flat shells.

For the numerical simulation, the derived equations are discretized with IGA. The approach is equivalent compared to the classical theory for curved shells. Furthermore, convergence analyses for numerous test cases are performed. The numerical results show that our proposed approach is equivalent to the classical theory, yet from a different viewpoint.

[1] Kiendl, J.; Bletzinger, K.-U.; Linhard, J.; Wüchner, R.: Isogeometric shell analysis with Kirchhoff–Love elements. *Comp. Methods Appl. Mech. Engrg.*, **198**(49), 3902–3914, 2009.

[2] Delfour, M.C.; Zolésio, J.P.: Tangential Differential Equations for Dynamical Thin Shallow Shells. *J. Differential Equations*, **128**, 125–167, 1996.

[3] Hansbo, P.; Larson, M., Continuous/discontinuous finite element modelling of Kirchhoff plate structures in R^3 using tangential differential calculus. *Comput. Mech.*, **60**, 693–702, 2017.

S04.02 | Structural mechanics

Date 20.03.2018
Room 0602

Elastodynamic displacement and stress tracking by eigenstrains: Some novel theorems.

Hans Irschik (*Institut für Technische Mechanik, Johannes Kepler University Linz*)

16:30–17:10

The present paper deals with the linear theory of elastodynamics in the presence of actuating eigenstrains. We deal with the problems of tracking desired displacement or of desired stress fields by eigenstrains. The displacement tracking problem is solved in the framework of the displacement based formulation of elastodynamics, while the stress tracking problem is treated in the stress based formulation. Necessary and sufficient conditions for the existence of these solutions are formulated. Special emphasis is given to mechanics based interpretations. Both solutions are split into two identically enlarged parts, one of them being stress free, the other one being displacement free. From these findings, some new theorems on zero strain tracking and on zero stress tracking are derived. A short account on applications of these theorems to beam-type force-loaded structures is given.

A new holistic approach to the local buckling behavior of open-profile composite laminated beams

Philip Schreiber (*Konstruktiver Leichtbau und Bauweisen, Technische Universität Darmstadt*), Christian Mittelstedt (*Konstruktiver Leichtbau und Bauweisen, Technische Universität Darmstadt*) 17:10–17:30

The present work deals with the local buckling of thin-walled composite-beams with I, Z, C, L and T-cross-sections under axial load. The beam is simply supported at both ends (Euler case II) and the plate behaviour of web and flange is described by the Classical Laminated Plate Theory (CLPT). Furthermore symmetric and orthotropic laminates are considered. In this study the analysis of the buckling load of the complete composite-beam is performed using the Ritz-method. In existing investigations on composite-beams the plates are considered as a separate composite plate. In the present method a new holistic approach of the beam is realised. The individual webs and flanges of the beam are unified by suitable continuity conditions in one system. In order to achieve that, new displacement shape functions for web and flange that fulfill all boundary conditions have been developed. The present closed-form analytical method enables the explicit representation of the buckling load for the entire composite-beam under axial load. The comparison between the present approach and the finite element simulations shows a satisfactory conformity. The present method is highly efficient in terms of computational effort and its practical suitability.

Modelling planar pantographic sheets using a nonlinear Euler-Bernoulli beam element based on B-Spline functions

Giuseppe Capobianco (*Institute for Nonlinear Mechanics, University of Stuttgart*), Simon R. Eugster (*Institute for Nonlinear Mechanics, University of Stuttgart*), Tom Winandy (*Institute for Nonlinear Mechanics, University of Stuttgart*) 17:30–17:50

An undeformed pantographic sheet consists of two orthogonal arrays of straight fibres interconnected by interal pivots. In this paper, we model the fibres of this lattice-shaped sheet as nonlinear Euler-Bernoulli beams. The Euler-Bernoulli assumption, demanding the fibers of the cross sections of the beam to remain orthogonal with respect to its centerline, allows for a formulation using the motion of the centerline only. As one of the strain measures, we choose the material curvature being a function of first and second derivatives of the centerline. Thus, a finite element analysis of such a beam formulation requires at least C^1-continuity for the shape functions. However, even higher continuity will sometimes lead to better convergence behavior. For this reason, we use B-Spline functions for the finite element discretization of the Euler-Bernoulli beam. Among others, some static simulations of the pantographic sheet are shown, where different models for the pivot, i.e. the points of interconnection between the two arrays of fibres, are engaged.

The Validation of Bredt's Formulas by the Method of Asymptotic Splitting

Christian Schmidrathner (*Department of Mechanics and Mechatronics, TU Wien, Vienna University of Technology*) 17:50–18:10

Due to their little weight compared to the stiffness, single- and multi-cell thin-walled beams are widely used in engineering. Very useful tools for their design are the formulas of Bredt. In case

of a cross section with only one cell they read

$$M_T = 2A_m T, \quad \text{with } T = \int \tau dh \approx \tau h \tag{1}$$

$$2A_m \mu \alpha = \oint_{\Gamma_m} \tau ds. \tag{2}$$

In (1) the torque M_T is connected with the shear flow T and the embedded area A_m, surrounded by the middle line Γ_m with the arc coordinate s. The formulas are derived under the engineering assumption of a constant shear stress over the thickness. Shear stresses orthogonal to Γ_m are neglected. Hence the shear flow, defined as the integral of the shear stress τ over the wall thickness h, becomes $T = \tau h$. Eq.(2) describes the twisting rate α, with shear modulus μ.
In the present talk we validate the engineering assumptions by an asymptotic analysis of an arbitrary cross section with variable wall thickness h. We consider the Saint-Venant problem of a linear elastic beam. In the limit of small thicknesses h, represented by a formal small parameter λ, the cross section can be characterized by its middle line and a small dimension orthogonal to it. The strong form of the equations is developed asymptotically to obtain the principal terms of warping function, Prandtl stress function, etc. The determination of the principal terms requires the solvability conditions of the minor terms, which is intrinsic to the procedure of Asymptotic Splitting.
The results are further used to find expressions of the two definitions of the shear center. The analytical results are validated numerically.

On a geometrically exact Euler-Bernoulli beam element

Sascha Maassen (*Institut für Mechanik, Universität Duisburg-Essen*), Càtia da Costa e Silva (*Polytechnic School, University de Sao Paulo*), Paulo Pimenta (*Polytechnic School, University de Sao Paulo*), Jörg Schröder (*Institut für Mechanik, Universität Duisburg-Essen*) 18:10–18:30

In this work, a geometrically exact, fully nonlinear Euler-Bernoulli beam formulation is presented. Herewith a special case of Timoshenko rod models, discussed in various publications such as [2] or [4], is considered. Following the basic assumptions of transversal shear rigidity and plane cross sections, the formulation is based on displacements, their derivatives and a torsional rotation angle, in order to cover finite deformations and rotations. A straight reference configuration is considered, whereas the possibility for initially curved configurations is discussed in [1]. Within the Euler-Bernoulli theory a cross section undergoes ridged body translation and rotation. While the translation is described by the motion of the beam axis only, the rotation is accounted within a rotational field, see e.g.[3]. In the present formulation, the rotational field is parametrized by the rotation tensor based on Rodrigues formula, which yields a simple update scheme as shown in [5], and is the first of its kind for Euler-Bernoulli beam models. Using this parametrization an ansatz is presented, that allows for consistent connection of structural members, even in cases of physical discontinuities. On the element level C^1 continuous Hermite polynomials are used to interpolate the displacements an their derivatives, while a Lagrangian interpolation scheme is chosen for the torsional rotation. Various numerical Benchmark problems are presented to demonstrate the performance of the finite element formulation.

[1] P. Pimenta. Geometrically exact analysis of initially curved rods, Civil-Comp Press(UK) 99–108, 1996.

[2] P. Pimenta, T. Yojo. Geometrically exact analysis of spacial frames. Applied Mechanics Rev, 1993

[3] I. Romero. The interpolation of rotations and its application to finite element models of geometrically exact rods. Computational Mechanics 34 121–133, 2004

[4] F. Gruttmann, R. Sauer, W.Wagner. Theory and numerics of three-dimensional beams with elastoplastic material behaviour. International Journal for numerical Methods in Engineering 48 1675–1702, 2000

[5] P. Pimenta, E.M.B. Campello, P. Wriggers. An exact conserving algorithm for nonlinear dynamics with rotational DOFs and general hyperelasticity. Part 1:Rods. Computational Mechanics 2008

S04.03 | Structural mechanics

Date 21.03.2018
Room 0602

Thermo-viscoelastic fiber-reinforced continua simulated by variational-based higher-order energy-momentum schemes

Michael Groß (*Mechanical engineering, Technische Universität Chemnitz*), Julian Dietzsch (*Mechanical Engineering, Technische Universität Chemnitz*), Matthias Bartelt (*Mechanical Engineering, Technische Universität Chemnitz*) 08:30–08:50

In this presentation, novel higher-order accurate energy-momentum schemes are presented, emanating from a discrete mixed principle of virtual power. These time-stepping schemes are designed for simulating an uni-directional fiber-reinforced material, considered as transversally isotropic nonlinear continua. The matrix material is considered as an isotropic thermo-viscoelastic material and the fibers behave thermo-elastic. Hence, the model takes into account an independent conduction of heat according to Duhamel's law with a transversally isotropic conductivity tensor as well as an independent heat expansion and heat capacity of the matrix and the fibers. The higher-order accurate energy-momentum schemes preserve each balance law of the continuous problem also in the discrete setting, independent of the chosen time step size and the prescribed Neumann and Dirichlet boundary conditions. Therefore, the implemented time step size control with the iteration number as target function does not influence the preservation properties of the time-stepping schemes. The balance laws are also preserved together with different time scales in the mechanical, thermal and viscous time evolution. By calculating each generalized reaction on the boundary, numerical examples verify the energy-momentum consistency of the schemes applied to dynamic simulations of different transient Dirichlet and Neumann boundary conditions.

Time step estimates for explicit dynamics with reciprocal mass matrices

Anton Tkachuk (*Institute for Structural Mechanics, University of Stuttgart*), Anne-Kathrin Schaeuble (*Institute for Structural Mechanics, University of Stuttgart*), Manfred Bischoff (*Institute for Structural Mechanics, University of Stuttgart*) 08:50–09:10

In this contribution, a novel local, node-based time step estimate for reciprocal mass matrices is proposed. Reciprocal mass matrices are sparse matrices used in explicit dynamics that allows computation of nodal acceleration from the total force vector. They can be built algebraically and variationally and aim for higher critical time step or/and accuracy than the lumped mass matrix approximation. Since reciprocal mass matrices are not additive, element-based estimates may

be not conservative and are consequently inadequate. Therefore, the nodal time step estimate for diagonally lumped mass matrices based on Gershgorin's theorem is further developed for application to reciprocal mass matrices. Additionally, simplifications of the proposed time step estimate that improve computational efficiency, especially for contact problems with the penalty method, are discussed. These simplifications use subadditivity and submultiplicativity properties of expressions used in Gershgorin's theorem. Finally, accuracy and efficiency of the proposed estimates are evaluated by numerical examples.

Polyconvexity inspired frameworks and structure-preserving integrators for multi-field problems

Marlon Franke (*Institute of Mechanics, Karlsruhe Institute of Technology, Germany*), Alexander Janz (*Institute of Mechanics, Karlsruhe Institute of Technology, Germany*), Mark Schiebl (*Institute of Mechanics, Karlsruhe Institute of Technology, Germany*), Rogelio Ortigosa (*Swansea University · Zienkiewicz Centre for Computational Engineering*), Peter Betsch (*Institute of Mechanics, Karlsruhe Institute of Technology, Germany*) 09:10–09:30

A new approach for the design of energy-momentum (EM) consistent time integrators for non-linear coupled problems is proposed. Polyconvexity inspired internal or Helmholtz free energy functionals are obtained by using the rediscovered tensor cross product (see [1]) which is basically applied on the cofactor and the Jacobian of the right Cauchy-Green strain tensor and greatly simplifies the algebra (see [2, 1]). On this basis multi-field problems concerning non-linear thermo-elastodynamics (see [3]) and electro-elastodynamics (see [4]) are considered. For the former a temperature based weak form is employed which facilitates the design of a structure-preserving time-stepping scheme for coupled thermo-elastic problems. For the latter a three-field internal energy-based formulation is applied. In both cases, the polyconvexity-based framework facilitates the design of EM consistent time integrators. In particular algorithmic stress formulas are employed which show a remarkably simple structure when compared to traditional, elaborate projection-based formulas. The spatial discretization relies on finite element interpolations for the unknown fields. Eventually, the superior performance of the proposed formulations is shown in several numerical examples.

[1] Bonet, J., Gil, A.J. and Ortigosa, R., A computational framework for polyconvex large strain elasticity, *Comput. Methods Appl. Mech. Engrg.*, 283:1061–1094, 2015.

[2] Betsch, P., Janz, A. and Hesch, C., A mixed variational framework for the design of energy-momentum schemes relying on polyconvex stored energy functions, *Comput. Methods Appl. Mech. Engrg.*, submitted, 2017.

[3] Franke, M., Janz, A., Schiebl, M. and Betsch, P., An energy-momentum consistent integration scheme using a polyconvexity-based framework for non-linear thermo-elastodynamics, *Int. J. Numer. Meth. Engng.*, submitted, 2017.

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S04.04 | Structural mechanics

Date 21.03.2018
Room 0602

Numerical analysis of thin-walled structures based on the scaled boundary finite element method

Milan Wallner (*Universität Duisburg-Essen*), Carolin Birk (*Universität Duisburg-Essen*), Hauke Gravenkamp (*Universität Duisburg-Essen*) 14:00–14:20

Thin-walled structures are currently experiencing an increasing demand due to their efficient load-carrying behaviour. However, the complex statics of shell structures often require numerical analysis. A limitation of FEA using shell elements is the occurrence of locking effects, most noteworthy membrane and shear locking. Membrane locking occurs in curved structures subjected to high bending deformation. Shear locking describes the inability to portray zero transverse shear strains. Approaches to avoid locking have been the subject of research for many years.
In this contribution, the scaled boundary finite element method (SBFEM) is used to analyse shell structures. The semi-discretization process results in a set of ordinary differential equations, which can be solved analytically to obtain the static stiffness matrix. Since locking effects are largely affected by the thickness, discretizing only the mid-surface and handling the solution analytically in the through-thickness direction might decrease locking effects. A similar approach has already been used to develop plate elements, where shear locking could be avoided completely for thin plates.
First studies of axisymmetric shells in the membrane state of stress demonstrate a high correlation to the thin shell theory. The results of classical benchmark problems for shell elements will be presented, including the widely used Scordelis-Lo roof as well as a pinched cylinder subjected to a point load. Both examples are dominated by bending deformations and have been used before to investigate membrane locking. Furthermore, a hemispherical shell with 18° cut-out is analysed.

A finite element formulation in boundary representation for the analysis of nonlinear problems in solid mechanics

Sven Klinkel (*RWTH Aachen University*), Rainer Reichel (*RWTH Aachen University*) 14:20–14:40

The contribution is concerned with a numerical element formulation for the analysis of the nonlinear behavior in solid mechanics. It is based on the so-called scaled boundary finite element method (SB-FEM). The SB-FEM is as a semi-analytical formulation to analyze problems of linear elasticity. The basic idea is to scale the boundary with respect to a scaling center. Hence, the boundary denoted as circumferential direction and the scaling direction span the parameter space. The original SB-FEM approach is based on an analytical ansatz for the displacement response preserving equilibrium in scaling direction. In the present approach, an interpolation in scaling direction is introduced to account for nonlinear problems. Lagrange interpolations with different polynomial order are therefore discussed. The interpolation in circumferential direction is independent of the scaling direction and is defined by independent Lagrange functions. The displacement degrees of freedom are located at the nodes on the boundary and in the interior element domain. The degrees of freedom located in the interior of the domain are eliminated by static condensation, which leads to a polygonal finite element formulation with an arbitrary number of nodes on the boundary. The element formulation allows a priori for Voronoi meshes

and quadtree mesh generation. Numerical examples give rise to the performance of the present approach in comparison to other polygonal element formulations, like the virtual element method (VEM). Some benchmark tests demonstrate the capability of the element formulation and a comparison to standard mixed element formulations is presented.

Adaptive numerical integration of broken finite cells based on moment fitting applied to finite strain problems

Simeon Hubrich (*TU Hamburg (TUHH)*), Alexander Düster (*Numerical Structural Analysis with Application in Ship Technology, TU Hamburg (TUHH)*) 14:40–15:00

The finite cell method (FCM) which is based on the fictitious domain approach and high-order elements provides a fast and simple mesh generation for structures with complex geometry [1]. This simplification in the mesh generation, however, leads to broken cells – which do not conform to the physical boundary – and, thus, standard Gauss quadrature does not perform well anymore. For this reason, commonly, an adaptive integration method based on a spacetree subdivision is used that usually results in a large number of integration points yielding an expensive numerical integration. To this end, in [2, 3] an integration method based on the moment fitting approach was developed which decreases the number of integration points significantly. It was shown that the presented integration method performs well considering linear problems discretized with the FCM. Facing nonlinear problems, however, the moment fitting turned out to be less stable than the adaptive integration.
Due to this reason, we present an adaptive approach which combines the moment fitting with a spacetree subdivision. In doing so, the moment fitting is applied on cell or subcell level for broken cells. To demonstrate the performance, we consider several numerical examples which show that the proposed scheme results in less integration points as compared to the adaptive integration which is commonly used in the FCM. Furthermore, we will investigate the robustness of the new method considering finite strain problems including hyperelasticity as well as elastoplasticity.

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[2] M. Joulaian, S. Hubrich, A. Düster. Numerical integration of discontinuities on arbitrary domains based on moment fitting. Comput. Mech. 57 (2016), 979–999.

[3] S. Hubrich, A. Düster. Numerical integration of discontinuous functions: moment fitting and smart octree. Comput. Mech. 60 (2017), 863–881.

Alternative approach to large deformational contact using VEM

Wilhelm T. Rust (*Institut für Kontinuumsmechanik, Leibniz Universität Hannover*), Peter Wriggers (*Institute of Continuum Mechanics, Leibniz Universität Hannover*) 15:00–15:20

In most classical contact computations nodes are projected on parametrized surfaces where then contact constraints are enforced in tangential and normal direction to differentiate between stick and slip state. As an alternative, contact can be computed without respect to the contact normal by simple coupling of the nodes. The sliding case is then considered afterwards by letting the projected node follow a friction cone defined by normal and tangential tractions. This was applied to node-to-segment contact discretizations in [1]. However these interpolations are dependent on the mesh size and relation.

Now the contact procedure using the Virtual Element Method [2] offers a flexible node-to-node formulation. It is based on freely adding contact nodes to the original mesh [3] and so it easily overcomes differences in mesh size and surface interpolation. In combination with the moving cone description the VEM contact offers a simple formulation for surfaces in sliding contact. Contrary to classical node-to-node contact sliding movement is possible by adjusting the position of the contact nodes in the mesh according to the friction state.

A short introduction to the used virtual elements for large deformations [4] as well as the contact algorithm will be given. Then the talk will focus on the computation of the node adjustment due to the sliding motion and compare the performance to classical contact treatments.

[1] P. Wriggers and A. Haraldsson. A simple formulation for two-dimensional contact problems using a moving friction cone. *Communications in Numerical Methods in Engineering*, 19(04):285-295, 2003.

[2] L. Beirão da Veiga, F. Brezzi, A. Cangiani, G. Manzini, L. D. Marini, and A. Russo. Basic principles of virtual element methods. *Mathematical Models and Methods in Applied Sciences*, 23(01):199–214, 2013.

[3] P. Wriggers, W. Rust, and B. Reddy. A virtual element method for contact. *Computational Mechanics*, 58(6):1039–1050, 2016

[4] P. Wriggers, B.D. Reddy ,W.T. Rust, B. Hudobivnik. Efficient virtual element formulations for compressible and incompressible finite deformations. *Computational Mechanics*, 60:253-268, 2017.

Scaled boundary isogeometric analysis of large deformations in solids

Margarita Chasapi (*Civil Engineering, RWTH Aachen University*), Sven Klinkel (*Civil Engineering, RWTH Aachen University*)
 15:20–15:40

The so-called scaled boundary isogeometric analysis (SB-IGA) combines the advantages of the isogeometric analysis and the scaled boundary finite element method. Here, the parameterization of the solid follows the idea of the scaled boundary finite element method (SB-FEM), where the boundary of the domain is scaled in respect to a specified scaling center inside the domain. According to the isogeometric paradigm (IGA), the NURBS functions that describe the geometry also interpolate the unknown displacement field. Such a combined approach is advantageous for three-dimensional solids, as a radial scaling parameter describes the interior of the solid and only the geometry of the boundary is required for the analysis. This concept fits also the idea of the boundary representation modeling technique, which is the way solids are designed in CAD – namely only by their boundary surfaces. Our contribution introduces the extension of the SB-IGA formulation for geometrical nonlinear 2D problems. The derived formulation concerns a hyperelastic material behavior for large deformations and plane strain conditions for the two-dimensional domain. We solve the boundary value problem with the equation of motion for the quasi-static case by applying the weak form of equilibrium in both radial scaling and circumferential direction of the boundary. Thereafter, the nonlinear deformation behavior requires a linearization and the application of the Newton-Raphson iterative scheme. Finally, we study the performance of this approach on numerical problems of nonlinear elasticity.

Thermomechanical mortar contact problems with hierarchical refined HNURBS for adhesion and anisotropic friction

Melanie Krüger (*Mechanical Engineering, University of Siegen*), Jonathan Schulte (*University of Siegen*), Maik Dittmann (*University of Siegen*), Christian Hesch (*University of Siegen*) 15:40–16:00

In this contribution, we present a novel variational consistent thermomechanical contact formulation [1]. The thermomechanical framework itself rests on the first law of thermodynamics written in terms of an energy balance and the second law of thermodynamics, which provides suitable restrictions on the constitutive law.

The contact formulation involves mechanical and thermal contributions across the interface. This thermomechanical contact interface is although formulated in a thermodynamically consistent way. Taking different contact reactions in normal and tangential direction into account, the Piola-traction vector t on the interface is approximately decomposed. The modeling of contact pressure and adhesion leads to an exponential constitutive model in terms of the normal gap function. Furthermore, the traction in tangential direction is given by the sum of an isotropic and an anisotropic surface vector.

For the spatial discretization we employ hierarchical refined NURBS (B-Splines) and apply a variationally consistent mortar method for the thermomechanical contact interface, see e.g. [2]. In particular, linear Lagrangian shape functions are used for the discrete traction field. The capabilities of this proposed framework are shown within numerous examples.

[1] M. Dittmann, C. Hesch, M. Krüger, F. Schmidt and S. Schuß, Modeling and simulation of thermo-mechanical fracture and contact problems, in preparation.
[2] M. Dittmann, Isogeometric analysis and hierarchical refinement for multi-field contact problems, 2017

S04.05 | Structural mechanics

Date 21.03.2018
Room 0606

Efficient Basis Updating for Parametric Nonlinear Model Order Reduction

Christian H. Meyer (*Faculty of Mechanical Engineering, Technical University of Munich*), Christopher Lerch (*Department of Mechanical Engineering, Technical University of Munich*), Boris Lohmann (*Department of Mechanical Engineering, Technical University of Munich*), Daniel Jean Rixen (*Department of Mechanical Engineering, Technical University of Munich*) 14:00–14:20

Model reduction is one method of choice to speed up the computation of finite element models in structural dynamics. This speed up is highly desired especially in design and optimization applica- tions, where parametric models are considered and the outcoming high-dimensional problems must be solved multiple times.
For systems which undergo large deflections, the equations of motion become nonlinear. In this case model reduction is applied in two steps: First, model order reduction applying a Galerkin projection is done, where a reduction basis is chosen to approximate the displacements as lower-dimensional linear combination of these basis vectors. Second, the nonlinear internal force term is hyperreduced, that speeds up its evaluation, which is essential to reduce computation time.

The first step becomes challenging for parametric systems since the optimal reduction basis strongly depends on the parameter values. One approach is to update the reduction basis and subsequently reduce the system with the updated basis for each new parameter set of interest. However, this approach can be very cost-intensive because in many algorithms for computation of reduction bases the parameter dependent tangential stiffness matrix must be decomposed in full dimension of the non-reduced system.
This contribution shows how basis updating for geometrically nonlinear systems can be accelerated by using iterative solution techniques. An inverse-free preconditioned Krylov subspace method is applied to circumvent the decomposition of the updated tangential stiffness matrix to update the eigenmodes used as basis vectors. Additionally, the modal derivatives used to qualify the basis for nonlinear systems are updated by using a conjugate gradient algorithm.

On the reduced solution of the earthquake-induced multiple seismic pounding problem

Jianye Shi (*Institut für Allgemeine Mechanik (IAM) - RWTH-Aachen*), Franz Bamer (*Institut für Allgemeine Mechanik (IAM) - RWTH-Aachen*), Bernd Markert (*Institut für Allgemeine Mechanik (IAM) - RWTH-Aachen*) 14:20–14:40

Due to the nonlinear contact behavior, earthquake induced pounding problems are computationally demanding. The application of explicit time integration schemes forces the integration time step to be considerably small, therefore, a huge number of computation loops has to be processed to evaluate the whole response function in the time domain.
In this paper, we present a model order reduction strategy based on the Craig-Bampton method [1] that has successfully been applied to nonlinear dynamic problems in earthquake engineering [2,3] and dynamic pounding systems with linear pounding elements [4] and adapt these new strategies to simulations including more realistic contact elements, which include energy dissipation effects. The reduced order computation is performed in a fractional amount of time in comparison to the full solution procedure.

[1] Gruber, F.M., Rixen, D.J.: *Evaluation of Substructure Reduction Techniques with Fixed and Free Interfaces*, Strojniški vestnik, Journal of Mechanical Engineering (2016) 62:7-8 .

[2] Bamer, F., Kazemi, A.A., Bucher, C.: *A new model order reduction strategy adapted to nonlinear problems in earthquake engineering*, Earthquake Engineering and Structural Dynamics (2016) 46:537-559.

[3] Bamer, F., Markert, B.: *An efficient response identification strategy for nonlinear structures subject to non-stationary generated seismic excitations*, Design of Structures and Machines (2017) 45:313-330.

[4] Bamer, F., Shi, J., Markert, B.: *Efficient solution of the multiple seismic pounding problem using hierarchical substructure techniques*, accepted in Computational Mechanics (2017).

Reducing structure-borne noise in thin-walled structures by local thickness variations

Matthias Miksch (*Chair of Structural Mechanics, TU München*), Quirin Aumann (*Lehrstuhl für Baumechanik, TU München*), Gerhard Müller (*TUM Department of Civil, Geo and Environmental Engineering, Chair of Structural Mechanics, TU München*) 14:40–15:00

Thickness variations can modulate the propagation of bending waves in thin-walled structures. A smooth reduction of the thickness results in a decreasing propagation speed and an increasing amplitude of the bending wave. Acoustic black holes (ABH) make use of this modulation to enhance the energy dissipation in the vicinity of these thickness diminution. Using the concept of ABH, no additional mass is needed to reduce structure-borne noise. This concept is therefore suitable for reducing the vibrational energy in lightweight structures, which is vital in aerospace and automotive applications, among others. Locally modifying the thickness of a structure can significantly influence the global energy distribution in the structure. Therefore, this contribution investigates the influence of different local thickness profiles on the global energy distribution. The results deliver insights for the design of such thickness variations in thin-walled structures to improve their vibrational behavior. Several numerical models are evaluated to assess the dependency between the geometric design parameters of the thickness variation and the energy distribution in the structure.

Energy-momentum consistent time integration scheme for non-linear electro–elastodynamics

Alexander Janz (*Institute of Mechanics - Department of Civil Engineering, Geo and Environmental Sciences, Karlsruhe Institute of Technology - KIT*), Peter Betsch (*Institute of Mechanics - Department of Civil Engineering, Geo and Environmental Sciences, Karlsruhe Institute of Technology - KIT*), Marlon Franke (*Institute of Mechanics - Department of Civil Engineering, Geo and Environmental Sciences, Karlsruhe Institute of Technology - KIT*), Rogelio Ortigosa (*Swansea University · Zienkiewicz Centre for Computational Engineering*)

15:00–15:20

The present talk deals with a new approach to the design of energy and momentum (EM) consistent integration schemes in the field of non-linear electro-elastodynamics. The importance of electro-active polymers (EAPs) in different applications such as actors and sensors, soft robotics or artificial muscles requires advanced simulation techniques to prognosticate the behavior of such smart materials. Typically, these materials are described as electro-static but nevertheless the consistent time-integration of the electro-mechanical model plays an important role concerning the numerical stability and accuracy. We present a new approach to the design of energy-momentum consistent algorithms motivated by the structure of polyconvex stored energy functions and tailor-made for the consistent space-time discretization of EAPs. The presented time-integrator is based on the internal energy of the system, which is in accordance with the concept of polyconvexity for nonlinear electro-mechanics [GO16]. Based on a Hu-Washizu-type mixed variational framework with a novel cascade form of kinematic constraints a new algorithmic stress formula is proposed [BJH17]. In addition, the time-discrete weak form of the Gauss's law and Faraday's law along with the concept of partitioned discrete derivatives in the sense of [Gon00], leads to an implicit one-step time integrator which consistently approximates the linear momentum, the angular momentum as well as the total energy. Moreover, the mixed variational framework makes possible a wide variety of alternative finite element formulations. Along with an appropriate combination of the interpolation spaces high performance finite elements can be generated.

[1] A. Gil and R. Ortigosa. A new framework for large strain electromechanics based on convex multi-variable strain energies: Variational formulation and material characterisation. *Comput. Methods Appl. Mech. Engrg.*, Vol. **302**, 293-328, 2016.

[2] P. Betsch, A. Janz and C. Hesch. A Mixed Variational Framework for the Design of Energy-Momentum Schemes Relying on Polyconvex Stroed Energy Functions. *Comput. Methods Appl. Mech. Engrg.*, **submitted**, 2017.

[3] O. Gonzalez. Exact energy and momentum conserving algorithms for general models in nonlinear elasticity. *Comput. Methods Appl. Mech. Engrg.*, Vol. **190**, 1763-1783, 2016

Wave propagation in soft materials

Sam Aghayan (*University of Siegen*), Thomas Reppel (*University of Siegen*), Sören Bieler (*University of Siegen*), Kerstin Weinberg (*University of Siegen*) 15:20–15:40

The investigation of the wave propagation in soft materials is essentially an important task, as it would help to study the effects of shock waves, particularly in the impact. In this study, the effect of induced shock wave on a soft material (at this case brain tissue) is investigated under the impact simulated condition. One of the main causes of damage is the relative motion of the brain with respect to the skull, which results in cavitation phenomena (volumetric damage).
Finite element analysis has been utilized for the numerical investigation. In order to do so, the brain is simulated into a Gelatin base cylinder covered by a PMMA (Polymethylmethacrylat) shell, which is used to conduct the impact simulation in the Hopkinson pressure bar test. the short-time pressure simulation is applied and the model is gone under a pressure by displacement approach. The stress travelling through the model and pressure graphs are extracted from FEA. The other part of the study is related to the experiment, using Split Hopkinson bar for the impact simulation. A cylindrical model of a human head filled with Gelatin is arranged next to the incident bar of the SHPB. The fixed cylindrical model filled with Gelatin would be exposed to an impact of the incident bar (speed of 4m/s). With the use of a high-speed camera, the formation of the cavitations can be observed.

Global and goal-oriented reanalysis in nonlinear structural mechanics

Daniel Materna (*Department of Civil Engineering, Ostwestfalen-Lippe University of Applied Sciences*) 15:40–16:00

Reanalysis methods can be used in order to reduce the overall computational cost in numerical simulation. The main objective is to predict the changes in the state variables or some quantity of interest due to given structural modifications (design changes), e.g. the shape, the topology, material properties etc. Classical applications with successive design steps are for instance structural optimization, reliability analysis or structural damage analysis. In many cases hundreds or even thousands of different design configurations are investigated and the state equation has to be solved for each design step. The repeated structural analysis of large nonlinear problems involve significant computational effort.
In this paper an approach for global and goal-oriented nonlinear reanalysis based on residual increment approximations (RIA) is presented. The method requires only the evaluation of residual vectors, which can be done very fast and efficient. Moreover, the results are improved by using a rational approximation method. The approach is general and can be applied to linear and nonlinear problems with different kind of design modifications. Furthermore, the proposed reanalysis method is easy to implement in existing finite element programs, because no derivatives with respect to the design variables are necessary. The capability of the proposed framework is demonstrated by means of computational examples from nonlinear elasticity.

S04.06 | Structural mechanics

Date 21.03.2018
Room 0602

Gradient-Enhancement of a Rock Model applied to Numerical Simulations of Tunnel Advance

Magdalena Schreter (*Institut für Grundlagen der Technischen Wissenschaften - Arbeitsbereich für Festigkeitslehre und Baustatik, Universität Innsbruck*), Matthias Neuner (*Institut für Grundlagen der Technischen Wissenschaften - Arbeitsbereich für Festigkeitslehre und Baustatik, Universität Innsbruck*), Günter Hofstetter (*Institut für Grundlagen der Technischen Wissenschaften - Arbeitsbereich für Festigkeitslehre und Baustatik, Universität Innsbruck*) 16:30–16:50

Rock is classified as a frictional cohesive material characterized by nonlinear stress-strain relations including softening leading to structural failure. To describe the mechanical behavior of rock comprising the accumulation of irreversible strains, strain hardening, and the degradation of stiffness and strength, an isotropic damage plasticity model for intact rock and rock mass was proposed in [1]. In the context of numerical simulations of tunneling, considering strain softening of rock allows to predict the formation of shear bands emanating from the tunnel surface due to the excavation process, which is crucial for engineers to forecast potentially dangerous situations related to failure. To ensure objective results in the softening regime upon mesh refinement, in the aforementioned rock model the concept of the crack band approach by Bažant and Oh was adopted. As a remedy of known deficiencies related to this regularization approach, the rock model is extended by the over-nonlocal implicit gradient-enhancement proposed in [2]. Accordingly, a nonlocal field of the damage-driving variable, implicitly defined as the solution of a Helmholtz-like partial differential equation, is introduced yielding a fully coupled system of second-order PDEs. In the present contribution, the over-nonlocal gradient enhancement of the rock model is presented and applied together with a time-dependent nonlinear material model for shotcrete [3] to finite element simulations of a deep tunnel constructed by the New Austrian Tunneling Method. Based on this real example, objectivity of the results with respect to the finite element discretization is discussed.

[1] D. Unteregger, B. Fuchs, G. Hofstetter. A damage plasticity model for different types of intact rock, International Journal of Rock Mechanics & Mining Sciences, Vol. 80, 402-411, 2015.

[2] L. H. Poh and S. Swaddiwudhipong. Over-nonlocal gradient enhanced plastic-damage model for concrete. International Journal of Solids and Structures, Vol. 46(25), 4369–4378, 2009.

[3] M. Neuner, P. Gamnitzer, G. Hofstetter. An Extended Damage Plasticity Model for Shotcrete: Formulation and Comparison with Other Shotcrete Models. Materials, Vol. 82, 1–21, 2017.

Harnessing anisotropy to create artificial materials with wave propagation isolation properties

Nikolaos Karathanasopoulos (*MAVT, ETH Zürich*), Hilal Reda (*LEMTA, Université de Lorraine*), Jean-Francois Ganghoffer (*LEMTA, Université de Lorraine*) 16:50–17:10

Artificial materials exhibit mechanical attributes that are typically not encountered in common engineering materials. In the current work, we present a systematic approach to create two-dimensional orthotropic metamaterials with wave propagation isolation characteristics. To that

scope, we employ polygonal-shaped unit cell material architectures of high anisotropy. We compute the anisotropic metamaterial's wave propagation characteristics for all propagating material directions. Thereupon, we identify a material direction of vanishing longitudinal and shear phase velocities. We observe that the vanishing phase velocity direction coincides with the material direction with the weakest normal mechanical modulus. We discuss on the role of Poisson's ratio and shear stiffness on the obtained wave propagation features, deriving overall conclusions on the underlying structural mechanisms.

A macroscopic model on the dynamic behaviour of open cell foams

Stephan Kirchhof (*Institut für Mechanik und Fluiddynamik, TU Bergakademie Freiberg*), Alfons Ams (*Institut für Mechanik und Fluiddynamik, TU Bergakademie Freiberg*) 17:10–17:30

Open cell foams are widely used in engineering which includes an application in areas, where vibration excitations can act on the structures. Therefore dynamical properties as eigenfrequencies and natural modes are of great interest.
We will discuss the description of the dynamic behavior of open cell foams by macroscopic stochastic models. Based on a 3D computed tomography scan of the foam, statistic and spectral analysis has been carried out to determine the parameters of the stochastic model.
Additionally a vibration measurement has been done to provide eigenfrequencies, frequency transfer functions and natural modes of the real foam, which can be compared with the simulation results of the macroscopic model.

Evolution of structures with homogeneous equivalent stress

Ingo Münch (*Institute for Structural Analysis, KIT - Karlsruhe Institute of Technology*) 17:30–17:50

A phase field model is used to evolve structures with almost homogeneous equivalent stress σ_v. The Allen-Cahn equation of the phase field model incorporates the requirements of the objective function $F = \int_{\mathcal{B}} \left(\frac{\sigma_v - \bar{\sigma}_v(\hat{K})}{\bar{\sigma}_v(\hat{K})} \right)^2 \mathrm{d}V$. With $\bar{\sigma}_v(\hat{K})$ we denote an adapted median of the equivalent stress field. Its parameter $\hat{K}$ is the desired filling level of the design region $\mathcal{B}$. In the initial state, $\mathcal{B}$ can be homogeneously filled with material such that no initial topology is required. Since the model presumes no mass conservation, the injection or rejection of material is driven by the derivative of F concerning σ_v. It causes the nucleation of voids within $\mathcal{B}$ such that phase separation appears. The complexity of the evolving structure depends on a penalization factor c_γ for inhomogenous equivalent stress, such that F obtains greater importance compared to other terms of the Allen-Cahn equation. In our contribution we discuss the limits $c_\gamma \to 0$, and $c_\gamma \to \infty$, respectively.
As mentioned above, the objective function bases on an averaged indicator $\bar{\sigma}_v(\hat{K})$, which is found with help of sampling points within $\mathcal{B}$. The data from these points is sorted. Further, the course of $\bar{\sigma}_v(\hat{K})$ is analyzed during the evolution process. With help of 2-D and 3-D examples we discuss the numerical model, some well-known examples from the literature, and the general effect of own weight and traffic load for a bridge-like structure.

Hygro-thermo-chemo-mechanical modelling of shotcrete during tunnel advance

Peter Gamnitzer (*University of Innsbruck*), Magdalena Schreter (*University of Innsbruck*), Günter Hofstetter (*University of Innsbruck*) 17:50–18:10

We present a numerical simulation of tunnelling in an equivalent 2D plane strain model. 3D effects are only considered in an approximate manner. Special attention is paid to the modelling of a shotcrete layer supporting the surrounding rock after excavation. Due to an increasing load caused by further tunnel advance, the shotcrete is loaded in place at a very early age. Hence it is required to accurately model the evolution of its strength and stiffness. This is done using a fully coupled hygro-thermo-chemo-mechanical multi-phase model for the shotcrete [1]. Creep of shotcrete is taken into account using a microprestress-solidification approach [2]. The constitutive model for the shotcrete is calibrated using experimental data obtained from laboratory tests on shotcrete specimens [3]. The setup for the tunnelling simulation is completed assuming an elastic-plastic response for the surrounding rock and the additional steel anchors. The results of this contribution are considered to be a further step towards a more accurate modelling of excavation procedures in conventional drill-and-blast tunnelling.

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[2] Z. Bažant et. al. Microprestress-solidification theory for concrete creep. J Eng Mech (1997) **123**:1188-1201

[3] M. Neuner, P. Gamnitzer, G. Hofstetter. An extended damage plasticity for shotcrete: Formulation and comparison with other shotcrete models. Materials (2017) 10; 82

Numerical models for evaluating the vibro-acoustic properties of acoustic metamaterials based on locally resonant sub-structures

Quirin Aumann (*Lehrstuhl für Baumechanik, TU München*), Matthias Miksch (*Chair of Structural Mechanics, TU München*), Gerhard Müller (*TUM Department of Civil, Geo and Environmental Engineering, Chair of Structural Mechanics, TU München*)

18:10–18:30

While the demand for lightweight structures in aerospace and automotive is on the rise, so are the requirements regarding sound emissions. Materials with a high stiffness-to-mass ratio are often used in this field, but these materials typically have an unfavorable vibrational behavior regarding structure-borne noise. Acoustic meta materials can offer a solution for improving the vibro-acoustic performance of the structure while the stiffness-to-mass ratio remains nearly constant. Such a meta material consists of a pattern of microstructures which are placed on a host structure. The microstructures are often arranged periodically and are capable of modifying the vibrational pattern of the main structure by adding local resonances to the whole structure. Thus they can be used to minimize vibrations of the host structure at distinct frequencies. With the latest advances in additive layer manufacturing, it is possible to create filigree (delicate) microstructures which are directly connected to the main structure, resulting in acoustic meta materials which combine a high stiffness-to-mass ratio with a good vibro-acoustic performance. In automotive or aerospace applications, distinct resonances have a major contribution to the overall acoustic behavior of the structure, so it is of interest to tailor microstructures that generate stop bands at these frequencies. Numerical models, which are suited to simulate the vibration behavior of an acoustic metamaterial are discussed. Different micro-structures and their effect on the host structure are investigated regarding the creation of an anti-resonance at one or more fundamental frequencies of the host structure. It is shown, that the micro-structures have a comparable effect on the main structure as a single tuned mass damper optimized by Den Hartog's criteria.

S04.07 | Structural mechanics

Date 21.03.2018
Room 0606

Implicit forming simulations for "Die-Less-Hydroforming"-structures

Andreas Metzger (*KIT Steel & Lightweight Structures - Research Center for Steel, Timber & Masonry, Karlsruhe Institute of Technology - KIT*), Daniel C. Ruff (*KIT Steel & Lightweight Structures - Research Center for Steel, Timber & Masonry, Karlsruhe Institute of Technology - KIT*), Thomas Ummenhofer (*KIT Steel & Lightweight Structures - Research Center for Steel, Timber & Masonry, Karlsruhe Institute of Technology - KIT*)

16:30–16:50

Within the scope of "Die-Less-Hydroforming" two or more congruent thin metal blanks are positioned each on top of the other and seal-welded at their common edges. Afterwards, the resulting double- or multi-layered seal-welded blank is inflated through a medium under continuous pressure increase whereby it transforms to a spatial structure. Since no external forming tool is used and because of thin metal sheets used, special phenomena like buckling or wrinkling may occur during the forming process. Although this unconventional forming technology was already mentioned in the academic discourse 90 (!) years ago (see [1]), currently many users from different fields of application focus on this special forming technology and manifold applications are arising.
An FEM-forming simulation for "Die-Less-Hydroforming"-structures including some special subjects (e.g. clamping effects) was already presented by the authors recently (cf. [2], [3]). For these FEM-simulations the explicit solver of LS-DYNA was used including the corresponding and well-known but a little bit "dirty" approaches: mass-scaling and time-scaling. By using these both numerical tricks the CPU-time is downsized, on the one hand, by adding a (very high) numerical mass to the real physical mass to increase the critical time step size (according to the Courant-Friedrichs-Lewy-criterion), and on the other hand, by a significant decrease of the simulation time compared to the real process time of the forming process. However these explicit simulations produce very realistic simulation results, which could already be verified by samples from experimental testing.
Nevertheless, the authors intention is to complement the research work by an implicit forming simulation for "Die-Less Hydroforming"-structures by using the implicit LS-DYNA solver. The use of implicit solvers allows omitting the "dirty" approaches, i.e. now the simulation is performed with the real physical mass and quasi-static as during the real process, but this approach will in some cases lead to other numerical problems or to a strong increase of the CPU-time. Consequently, the authors will present some results of an implicit forming simulation for "Die-Less-Hydroforming"-structures including an assessment by comparing the implicit results first with our proven but "dirty" explicit forming simulation results, second with experimental results from inflation tests, and –if possible– third with analytical solutions like Barlow's formula or indeed with the 90 years old analytical approaches of [1].

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Thermally assembled shrink fit with annular inclusion and FGM-hub

Tunc Apatay (*Mechanical Engineering, Gazi University, Faculty of Engineering*), Eray Arslan (*Institute of Mechanics and Mechatronics, Vienna University of Technology*), Werner Mack (*Institute of Mechanics and Mechatronics, Vienna University of Technology*) 16:50–17:10

Shrink fits are an efficient means of connecting a circular inclusion with a hub. Since for given geometrical properties and friction coefficient at the interface the safety against the occurrence of slip depends solely on the interface pressure, the latter should be as large as possible. A way to achieve this is to admit partially plastic behavior, which however is not always acceptable. Moreover, minimizing the weight of the device without loss of performance becomes more and more important. A possibility to comply with the latter objective while also maintaining elastic behavior is the use of a functionally graded material (FGM) for the hub; in particular, the case of radially decreasing density is presumed which may be realized, e.g., by a steel/aluminum FGM. In the present contribution a shrink fit with large axial length of the hub is considered, hence a treatment as a (generalized) plane strain problem is appropriate. It is the aim of the study to investigate the essential features of such shrink fits with hollow inclusion, which behave purely elastically also at rotation. It is shown that significant improvements with respect both to the interface pressure and the weight may be achieved, and special attention is paid also to the thermal assembly. All the results are obtained analytically, and the effects of various degrees of grading and various radii ratios are discussed.

Enhanced Assumed Strain Methods for Implicit Gradient-Enhanced Damage-Plasticity

Matthias Neuner (*Institut für Grundlagen der Technischen Wissenschaften - Arbeitsbereich für Festigkeitslehre und Baustatik, Universität Innsbruck*), Magdalena Schreter (*Institut für Grundlagen der Technischen Wissenschaften - Arbeitsbereich für Festigkeitslehre und Baustatik, Universität Innsbruck*), Günter Hofstetter (*Institut für Grundlagen der Technischen Wissenschaften - Arbeitsbereich für Festigkeitslehre und Baustatik, Universität Innsbruck*) 17:10–17:30

The combination of plasticity theory and continuum damage mechanics facilitates the description of hardening and softening material behavior, accumulation of inelastic strains, and stiffness degradation due to damage. For regularizing softening material behavior in finite element simulations, the enrichment of the constitutive relations by means of a nonlocal counterpart of an internal strain-like thermodynamic state variable, implicitly defined as the solution of a higher order PDE, is a suitable approach in order to obtain mesh-insensitive results [1]. However, for plasticity models assuming dilatant plastic flow, such as commonly employed for cohesive-frictional materials like concrete or rock, spurious locking phenomena due to kinematic constraints can arise in conjunction with low order finite elements. This issue was observed and discussed the first time in [2] for simple linear elastic perfectly plastic material models. As a remedy, specific enhanced assumed strain (EAS) methods to enrich the normal strain rate field were proposed and assessed. The present contribution demonstrates the formulation of these EAS methods combined with the fully coupled displacement-nonlocal damage framework, and shows an application to mode II failure employing a gradient-enhanced damage-plasticity model for concrete.

The insensitivity of the presented approach with respect to the finite element mesh is discussed.

[1] Jirásek M., Rolshoven S. (2009), Localization properties of strain-softening gradient plasticity models. Part II: Theories with gradients of internal variables, Int. J. Solids Struct., 46, (11–12): 2239–2254

[2] De Borst, R. and Groen, A. E. (1995), Some observations on element performance in isochoric and dilatant plastic flow. Int. J. Numer. Meth. Engng., 38: 2887–2906

Finite element formulation of elastoplastic structures by using the symplectic Brezis-Ekeland-Nayroles principle

Nima Shirafkan (*Institut für Allgemeine Mechanik (IAM) - RWTH-Aachen*), An Danh Nguyen (*Institut für Allgemeine Mechanik (IAM) - RWTH-Aachen*), Marcus Stoffel (*Institut für Allgemeine Mechanik (IAM) - RWTH-Aachen*), Bernd Markert (*Institut für Allgemeine Mechanik (IAM) - RWTH-Aachen*) 17:30–17:50

This work presents a finite formulation to study elastoplastic structures by using the symplectic Brezis-Ekeland-Nayroles (BEN) principle. The approach provides a minimum principle for the whole trajectories of dissipative systems including non-smooth dissipation cases, such as collisions, surface friction, viscosity, plasticity, fracture and damage. Here, the evolution can be computed as the limit of the sequence of the space-time. To derive the variational formulation, the Legendre-Fenchel transform is performed to establish the null minimisation problem of the power balance. The formalism is specialized to the small strain plasticity and will be applied to solve some elastoplastic benchmark problems. Some numerical results are presented and compared with the analytical solutions.

[1] Buliga, M., de Saxcé, G.:*A symplectic Brezis-Ekeland-Nayroles principle, Mathematics and Mechanics of Solids,* Mathematics and Mechanics of Solids, 1-15 (2016).

[2] Oueslati, A., Nguyen, A.D, de Saxcé , G.: *A Symplectic Minimum Variational Principle for Dissipative Dynamical Systems,* International conference on Geometric Science of Information, 359-366 (2017).

Mixed Isogeometric Collocation for Elastoplasticity

Frederik Fahrendorf (*TU Braunschweig, Institute of Applied Mechanics*), Simone Morganti (*University of Pavia, Department of Industrial Engineering and Informatics*), Alessandro Reali (*University of Pavia, Department of Civil Engineering and Architecture*), Laura De Lorenzis (*TU Braunschweig, Institute of Applied Mechanics*) 17:50–18:10

Isogeometric analysis is a recently developed framework for the discretization of partial differential equations. The concept is based on smooth basis functions, commonly employed in Computer Aided Design. This particular choice of basis functions leads to an exact description of the geometry in the analysis model. Beyond the original motivation, isogeometric analysis delivers a higher accuracy per degree of freedom compared to conventional C^0 finite element methods as well as several additional advantages. However an efficient numerical implementation is still an issue and one field of attention in current research in IGA. The isogeometric collocation method is a promising alternative to standard Galerkin approaches, as it provides a significant reduction of the computational cost for high-order discretizations. [1]

In this work we investigate a mixed isogeometric collocation method. In the proposed approach, both stress and displacement fields are approximated as primary variables (see e.g. [2] for an analogous Galerkin formulation). The method is applied to examples of elastoplasticity in combination with multi-patch parameterizations. An isotropic / kinematic hardening rule is implemented and the elastoplastic constitutive equations are integrated in time via a classical return-mapping algorithm. Various numerical examples are shown for the aforementioned applications and the results are compared to reference solutions obtained with Galerkin approaches.

[1] D. Schillinger, J.A. Evans, A. Reali, M.A. Scott, T.J.R. Hughes, Isogeometric collocation: Cost comparison with Galerkin methods and extension to adaptive hierarchical NURBS discretizations, *Comput. Methods Appl. Mech. Engrg.*, **267**, 170 - 232, 2013.

[2] R. Bouclier, T. Elguedj, A. Combescure, "Development of a mixed displacement-stress formulation for the analysis of elastoplastic structures under small strains: Application to a locking-free, NURBS-based solid-shell element", *Comput. Methods Appl. Mech. Engrg.*, **295**, 543 - 561, 2015.

S04.08 | Structural mechanics

Date 22.03.2018
Room 0602

Overview of Craig-Bampton Substructuring Approaches for Model Order Reduction of Nonclassically Damped Systems

Fabian M. Gruber (*Department of Mechanical Engineering, Institute of Applied Mechanics, Technical University of Munich*), Daniel Jean Rixen (*Institute of Applied Mechanics, Technical University of Munich*) 08:30–08:50

Dynamic substructuring techniques reduce the size of large models very efficiently. The large model is divided into a number of substructures; each substructure is analyzed and reduced separately and then assembled into a low-order reduced model. Only the substructures' mass and stiffness properties are commonly taken into account for the reduction. Each substructure's reduction basis is thereby constructed exclusively on the properties of the mass matrix and stiffness matrix, but the properties of the damping matrix are usually ignored. Most classical substructuring methods yield great approximation accuracy if the underlying system is damped only slightly or not at all. The most popular approach is a fixed interface method, the Craig-Bampton method, which is based on fixed interface vibration modes and interface constraint modes.
The classical Craig-Bampton method does not consider any damping effects. If damping significantly influences the dynamic behavior of the system, the approximation accuracy can be very poor. There is generally no justification to neglect damping effects. One procedure to handle and decouple arbitrary damped systems is to transform the 2nd order differential equations into twice the number of 1st order differential equations resulting in state-space representation of the system. Solving the corresponding eigenvalue problem allows the damped equations to be decoupled, but complex eigenmodes and eigenvalues occur. Hasselman and Kaplan presented a coupling procedure for damped systems, which employs complex component modes. Beliveau and Soucy proposed another version, which modifies the Craig-Bampton method to include damping by replacing the real fixed-interface normal modes of the 2nd order system with the corresponding complex modes of the 1st order system and they suggest additionally an adaption

of the method of Hasselman and Kaplan. A report of de Kraker gives another description of the Craig-Bampton method using complex normal modes.
We want to present the derivation of all the different Craig-Bampton substructuring methods for viscously damped systems in a comprehensible consistent manner. A detailed comparison between the different formulations will be given. The presented theory and the comparison between the methods will be illustrated on an example.

Parametric model order reduction applied to thin-walled wtructures modified by acoustic black holes

Raúl Rodríguez Sánchez (*Chair of Structural Mechanics, TUM*), Matthias Miksch (*Chair of Structural Mechanics, TU München*), Gerhard Müller (*TUM Department of Civil, Geo and Environmental Engineering, Chair of Structural Mechanics, Technische Universität München*) 08:50–09:10

In thin walled structures a smooth reduction of the thickness results in a decreasing propagation speed and an increasing amplitude of the bending wave. Acoustic black holes (ABH) make use of this modulation to enhance the energy dissipation in the vicinity of the ABH. Modifying a thin walled structure with ABH can significantly influence the energy distribution in the structure. For large systems those investigations become computational expensive. This contribution investigates the influence of the geometric and material parameters that defines the design of an ABH by a parametric Model Order Reduction approach. Several numerical models are evaluated to assess the dependency between the geometric design parameters of the thickness variation and the energy distribution in the structure, the computational time and the quality of the approximation are compared with the solution obtained using the corresponding full-scale FE model.

An Arbitrary Lagrangian-Eulerian Formulation for Cables with Transported Discrete Masses

Johannes Gerstmayr (*Institute for Mechatronics, University of Innsbruck*), Robert Winkler (*Institute of Mechatronics, University of Innsbruck*) 09:10–09:30

The contribution deals with the efficient simulation of rigid bodies transported by moving flexible cables, such as belt drives, cranes, or ropeway systems. In a direct approach to solve such problems, a transient simulation using thin beam elements would lead to high computational costs. Here, a new approach for the transient simulation of ropeway systems is proposed where common numerical tools known from flexible multibody dynamics are adapted. The moving cable is modelled by means of flexible beam elements in an arbitrary Lagrangian-Eulerian manner. That is, the deformational motion of the cable corresponds to the motion of the (Lagrangian) finite element mesh, whereas the overall axial motion is represented by a superimposed Eulerian axial velocity, which enters the formulation as an additional degree of freedom. The gondola cars are modelled by discrete rigid body elements. A special sliding joint formulation is applied to enforce the transportation of the cars along the cable. This approach allows for the application of properly adjusted non-uniform meshes. That is, small element lengths are used to adequately resolve the motion in the vicinity of sheaves (or sheave assemblies) whereas much larger elements are sufficient to reproduce the behavior of the system at the non-supported rope sections. To affirm the computational advantages of the proposed method, a simplified planar laboratory setup of a ropeway system is investigated. A numerical example affirms the computational advantages of the proposed method.

Mixed Eulerian-Lagrangian kinematic description in the statics of a flexible belt with tension and bending hanging on two pulleys

Yury Vetyukov (*Institute of Mechanics and Mechatronics, TU Wien, Vienna University of Technology*), Christian Schmidrathner (*Institute of Mechanics and Mechatronics, TU Wien, Vienna University of Technology*), Evgenii Oborin (*Institute of Technical Mechanics, Johannes Kepler University Linz*), Jakob Scheidl (*Institute of Mechanics and Mechatronics, TU Wien, Vienna University of Technology*), Michael Krommer (*Institute of Mechanics and Mechatronics, TU Wien, Vienna University of Technology*)

09:30–09:50

Established theories of thin-walled structures are available at material (Lagrangian) description. The latter becomes inefficient for axially moving structures with particles move between qualitatively different domains. The mixed Eulerian-Lagrangian formulation features a transformation of variables in the variational equation of virtual work (or minimal potential energy in statics): a material coordinate s becomes a function of a spatial one in the axial direction σ. Transforming the equations, one needs to clearly differentiate between the material variations of mechanical fields at $s = \text{const}$ and their spatial counterparts at a given location $\sigma = \text{const}$. The formulation results in efficient non-material finite element schemes for dynamics and quasistatics of largely deforming axially moving strings, beams and plates.
We consider the statics of a looped belt as a rod hanging in contact with two pulleys. Aiming at the practically relevant case of frictional contact, rotating pulleys and moving belt with weak pre-tension, we first test the kinematic description. We use a compound coordinate system consisting of two regions with polar coordinates and two with cartesian ones and separate the circumferential coordinate σ for the sake of transformation: $s = s(\sigma),\ \nu = \nu(\sigma)$, in which ν is the transverse coordinate. The material particles are free to move across the finite element mesh, which may thus be refined in the contact zones and left coarse in the long free spans. A nonlinear finite element approximation provides the necessary smoothness on the boundaries between the coordinate systems. Numerical experiments demonstrate rapid mesh convergence as well as the correspondence to the analytical results and conventional Lagrangian finite element solutions.

Galerkin-based mixed time finite elements for structural dynamics

Timo Ströhle (*Institute of Mechanics (IFM), Karlsruhe Institute of Technology - KIT*), Peter Betsch (*Institute of Mechanics (IFM), Karlsruhe Institute of Technology - KIT*), Mark Schiebl (*Institute of Mechanics (IFM), Karlsruhe Institute of Technology - KIT*)

09:50–10:10

Numerically stable and accurate time integration methods are important in structural dynamics. We propose such a method based on a mixed variational formulation of the underlying semi-discrete equations of motion. The newly developed scheme relies on a specific combination of the so-called *continuous Galerkin* ($cG(k)$) method and the *discontinuous Galerkin* ($dG(k)$) method. We refer to [1] for an introduction of the original $cG(k)$ and $dG(k)$ methods for ODEs (see also [2]). The mixed approach relies on polynomial approximations of degree k on the level of each time finite element. In particular we make use of hierarchical interpolation polynomials. The present approach is closely related to Hellinger-Reissner type mixed variational formulations for elastodynamics. The mixed method yields implicit time-stepping schemes with order of accuracy equal to $2k$ for the displacements and velocities. In addition to that, the method is capable of conserving the energy in the case of conservative mechanical systems. Numerical examples are presented which highlight the numerical properties of the newly proposed mixed approach.

[1] K. Eriksson, D. Estep, P. Hansbo, and C. Johnson. Computational Differential Equations. *Cambridge University Press*, 1996

[2] P. Betsch, P. Steinmann Inherently energy conserving time finite elements for classical mechanics. *Journal of Computational Physics* **160**, 88-116, 2000

S04.09 | Structural mechanics

Date 22.03.2018
Room 0602

A general framework for the thermodynamically consistent time integration of open nonlinear thermoelastic systems

Mark Schiebl (*Institute of Mechanics, Karlsruhe Institute of Technology*), Peter Betsch (*Institute of Mechanics, Karlsruhe Institute of Technology*) 14:00–14:20

This work deals with the energy-entropy-momentum consistent time integration of open thermoelastic systems. While energy-momentum preserving integrators are well-known for conservative mechanical systems, Romero introduced in [1] the class of thermodynamically consistent (TC) integrators for coupled thermomechanical systems, which further respect symmetries of the underlying coupled system and are therefore capable of conserving associated momentum maps. As mathematical framework for the geometric structure of the non-equilibrium thermodynamics the GENERIC (**G**eneral **E**quation for **N**on-**E**quilibrium **R**eversible-**I**rreversible **C**oupling) framework is used. The GENERIC framework, originally proposed by Grmela and Öttinger for complex fluids [2], expresses the evolution equation as the sum of reversible and irreversible contribution via a Poission and a dissipative bracket.
Since the GENERIC framework does not depend of a specific choice on the thermodynamical state variables [3], we explore the structure of GENERIC framework using the entropy density (see e.g. [4]), the absolute temperature (see e.g. [5]) and further the internal energy density as thermodynamical state variable from which the weak form of the initial boundary value problem can be gained. Applying the notion of a discrete gradient in the sense of Gonzalez [6] leads to a TC integrator.
As boundary conditions rely on the specific choice of the thermodynamical state variable we extend the GENERIC framework to be suitable for open systems following the procedure in [7]. The presentation will indicate keys differences and similarities between the alternative choices of thermodynamical state variables and will include several simulations with different boundary conditions using an energy-based termination criterion.

[1] Ignacio Romero. Thermodynamically consistent time-stepping algorithms for non-linear thermomechanical systems. *International journal for numerical methods in engineering*, 79(6):706–732, 2009.

[2] Miroslav Grmela and Hans Christian Öttinger. Dynamics and thermodynamics of complex fluids. i. development of a general formalism. *Physical Review E*, 56(6):6620, 1997.

[3] Alexander Mielke. Formulation of thermoelastic dissipative material behavior using generic. *Continuum Mechanics and Thermodynamics*, 23(3):233–256, 2011.

[4] Melanie Krüger, Michael Groß and Peter Betsch. An energy-entropy-consistent time stepping scheme for nonlinear thermo-viscoelastic continua. *ZAMM-Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik*, 96(2):141–178, 2016.

[5] Markus Hütter and Bob Svendsen. Thermodynamic model formulation for viscoplastic solids as general equations for non-equilibrium reversible–irreversible coupling. *Continuum Mechanics and Thermodynamics*, 24(3):211–227, 2012.

[6] Oscar Gonzalez. *Design and analysis of conserving integrators for nonlinear Hamiltonian systems with symmetry*. PhD thesis, Stanford University, 1996.

[7] Hans Christian Öttinger. Nonequilibrium thermodynamics for open systems. *Physical Review E*, 73(3):036126, 2006.

On the Treatment of Plastic Deformation in the Particle Finite Element Method

Xialong Ye (*Institut of Applied Mechanics, Technische Universität Kaiserslautern*), Ralf Müller (*Institut of Applied Mechanics, Technische Universität Kaiserslautern*), Christian Sator (*Institut of Applied Mechanics, Technische Universität Kaiserslautern*) 14:20–14:40

The particle finite element method (PFEM) combining the benefits of discrete modeling techniques and approaches based on continuum mechanics provides a convenient tool to deal with the problem of large configurational change, such as metal cutting, in which the nonlinear plasticity plays a key role [1]. In this work we introduce phenomenological plasticity models with the help of a multiplicative decomposition of the deformation gradient and an intermediate local configuration into the PFEM framework. A class of simple integration algorithms are obtained thanks to the notion of the intermediate configuration. Numerical examples including a tensile test as well as cutting simulations are presented to show the performance of the formulation.

[1] M. Sabel, R. Müller, C. Sator [2017], "Simulation of Cutting processes by the Particle Finite Element Method", GAMM-Mitteilung **40**, No.1, 51-70, Wiley

A direct method for dissipative dynamical systems by using the symplectic Brezis-Ekeland-Nayroles principle

An Danh Nguyen (*Institute of General Mechanics, RWTH Aachen University*) 14:40–15:00

We study a direct method for inelastic structures by using the symplectic Brezis-Ekeland-Nayroles variational principle. The principle, which generalises non-smooth motion equations as Hamiltonian inclusions using the concept of symplectic subdifferentials, provides a minimum regulation for the whole trajectories. The null minimisation problem of the power balance will be established and discretised by the use of the orthogonal collocation method to reduce the dynamic optimisation problem to nonlinear programming for the evolution solution directly. The proposed numerical approach is illustrated with elastoplastic problems in small strains. Some numerical results are given and compared with the analytical solutions.

[1] A. Mielke, Variational approaches and methods for dissipative material models with multiple scales, *Analysis and Comptation of Microstructure in Finite Plasticity*, S.Conti and K. Hackl (eds.), Springer Switzerland (2015).

[2] M. Buliga, G. de Saxcé, A symplectic Brezis-Ekeland- Nayroles principle, *Mathematics and Mechanics of Solids*, DOI:10.1177/1081286516629532, **1-15**, (2016).

[3] A. Oueslati, A.D. Nguyen, G. de Saxcé, A Symplectic Minimum Variational Principle for Dissipative Dynamical Systems, *GSI 2017, 3rd conference on Geometric Science of Information*, Mines ParisTech, France, **359-366** (2017).

An elastoplastic intelligent meta-element

Arnd Koeppe (*Institute of General Mechanics (IAM), RWTH Aachen University*), Franz Bamer (*Institute of General Mechanics (IAM), RWTH Aachen University*), Bernd Markert (*Institute of General Mechanics (IAM), RWTH Aachen University*) 15:00–15:20

In recent years, (artificial) neural networks and other computational intelligence methods have leveled the playing field in applications ranging from image processing to natural language recognition and autonomous driving. The predominant computation method in nonlinear solid mechanics, the finite element method, is computationally expensive, if many degrees of freedom are involved.
We propose a new strategy based on *intelligent* elements, computing their time-variant response and stiffness based solely on the information of a reduced set of degrees of freedom. This intelligent element employs a neural network, trainable to the specific geometry and material behavior of a wide range of mechanical problems. The numerical efficiency and accuracy of the strategy is compared to the classical finite element method on an elastoplastic example.

[1] A. Koeppe, F. Bamer, C. A. Hernandez Padilla, and B. Markert. Neural network representation of a phase-field model for brittle fracture. *Proc. Appl. Math. Mech.*, in press, 2017.

[2] A. Koeppe, F. Bamer, and B. Markert. Model reduction and submodelling using neural networks. *Proc. Appl. Math. Mech.*, 16(1):537–538, Oct. 2016.

[3] A. Koeppe, C. A. Hernandez Padilla, M. Voshage, J. H. Schleifenbaum, and B. Markert. Efficient numerical modeling of 3D-printed lattice-cell structures using neural networks. *Manuf. Lett.*, (Special Issue on Industry 4.0 and Smart Manufacturing), under review, 2017.

Soil Modelling - approximation based on NURBS and the Scaled Boundary Finite Element Method

Arturo Méndez Salas (*Chair of Structural Analysis and Dynamics, RWTH Aachen University*), Margarita Chasapi (*Chair of Structural Analysis and Dynamics, RWTH Aachen University*), Sven Klinkel (*Chair of Structural Analysis and Dynamics, RWTH Aachen University*) 15:20–15:40

This paper deals with a numerical soil modelling for time domain analysis. A parametrization method, established on NURBS basis functions is adopted in combination with the principles of the scaled boundary finite element method. The powerful capability of NURBS basis function allows a most stable domain discretization, minimizing the amount of representative degrees of freedom: appropriate attribute by modelling large unbounded domains like soil. The mapping of these degrees of freedom is radially done from the domain boundary to a defined scaling parameter, which is chosen to be conveniently within the domain: *scaling center*. Through this radial scaling, it is possible to discretize the whole domain. Degrees of freedom are finally defined along scaled, but enclosed boundaries; however, regarding to soil modelling, the scaling boundary must be defined for open domains. In this contribution, the scaling boundary is adapted to map an open boundary: consequence of the free surface of the soil. Besides, the

soil is represented using the described methodology for a plane motion scheme solving the initial boundary value problem; therefore, the performance of a narrow-band layer is analysed. A higher degree of NURBS basis functions in scaling direction is defined in order to represent layered soil. The discretized differential equation of motion for the soil is solved using the weak form along the boundary and scaling direction. A set of harmonic excitations are employed over the free surface of the soil. The Rayleigh damping is used in the system and an implicit integration is carried out. To avoid reflections at boundary domain because of wave propagation, an sufficiently extended, and fixed boundary domain is considered. An idealized linear elastic, homogeneous and isotropic material representing the domain is taken into account to evaluate the capabilities of the presented approach. Standard numerical approaches, such as FEM, and analytical solutions are used in order to validate the adopted methodology and compare the results.

S04.10 | Structural mechanics

Date 22.03.2018
Room 0602

An Approach for Stable Time Integration of Dual Craig-Bampton Reduced Systems

Max Gille (*Department of Mechanical Engineering, Institute of Applied Mechanics, Technical University of Munich*), Fabian M. Gruber (*Department of Mechanical Engineering, Institute of Applied Mechanics, Technical University of Munich*), Daniel Jean Rixen (*Department of Mechanical Engineering, Institute of Applied Mechanics, Technical University of Munich*) 17:30–17:50

Time integration using the generalized α-method is demonstrated and investigated for dual Craig-Bampton reduced systems. The dual Craig-Bampton method for the reduction of dynamic systems employs free interface vibration modes, attachment modes and rigid body modes to build the reduction bases of the substructures, but assembles the substructures using interface forces. Thereby, interface incompatibilities associated with the equilibrium residual are allowed between the substructures. Hence, the eigenvalues of the reduced-order model are not guaranteed to be upper bounds for the unreduced system's eigenvalues. The dual Craig-Bampton reduced system will always have as many negative eigenvalues as interface coupling conditions. The reduced system is unstable, rendering a straightforward time integration of the dual Craig-Bampton reduced system impossible.
The feasibility of a reliable time integration of dual Craig-Bampton reduced systems is demonstrated and investigated in detail. The unstable behavior when time-integrating such systems without further modifications is illustrated and a strategy to overcome this instability is suggested: a modal interface reduction during the dual Craig-Bampton reduction process is performed and only interface modes corresponding to the positive eigenvalues are kept. This guarantees the final reduced system to be positive definite. The accuracy using this approach is demonstrated in examples with either different initial conditions or varying external periodic excitations.

The novel discontinuous Petrov-Galerkin Finite Element Method for nearly incompressible material behaviour in solid mechanics

Tobias Steiner (*Leibniz Universität Hannover, Institut für Kontinuumsmechanik*), Peter Wriggers (*Leibniz Universität Hannover, Institut für Kontinuumsmechanik*) 17:50–18:10

Standard finite elements with lower order classical Lagrange polynomial shape functions tend to exhibit the phenomenon of volumetric locking for (nearly) incompressible materials. In this contribution the discontinuous Petrov-Galerkin Finite Element Method (dPG FEM) is introduced

to circumvent this locking effect.
The dPG FEM is a novel mixed method introduced by [1, 2], which was first applied to wave transport problems and the advection-diffusion-equation. The novel discretization scheme was established for linear elasticity [3] and proposed recently as a nonlinear discontinuous Petrov-Galerkin Finite Element Method [4]. There are several possible approaches to obtain a dPG FEM, cf. [5]. In this contribution we focus on the *primal dPG FEM*. To obtain the weak form, the balance of linear momentum is integrated and weighted with a test function as in a standard Galerkin Finite Element formulation. Besides the interpolation of element displacements, the occuring boundary integrals with tractions at the interfaces of neighbouring elements are also evaluated. The resulting system of equations contains two primary unknowns, which are discretized with linear ansatz functions for the displacements, and constant ansatz functions for the tractions at the interfaces. Furthermore, the test function is discretized with discontinuous or *broken* linear Lagrangian functions on the corresponding element leading to the lowest-order primal discontinuous Petrov-Galerkin mixed Finite Element Method.
In the present work the two-dimensional primal discontinuous Petrov-Galerkin Method is presented. The behaviour of this formulation is studied with benchmark simulations in the nearly incompressible case. Furthermore, an extension to a nonlinear Finite Element formulation is suggested.

[1] L. Demkowicz, J. Gopalakrishnan: A class of discontinuous Petrov-Galerkin methods. Part I: the transport equation, *Comput. Methods Appl. Mech. Engrg.* **199**, 1558–1572, 2010.

[2] L. Demkowicz, J. Gopalakrishnan: A class of discontinuous Petrov-Galerkin methods. Part II: Optimal test functions, *Numer. Methods Partial Differential Equations.* **27 (1)**, 80–105, 2011.

[3] F. Hellwig, C. Carstensen: Low-Order Discontinuous Petrov-Galerkin Finite Element Methods for Linear Elasticity, *SIAM J. Numer. Anal.* **54 (6)**, 3388–3410, 2016.

[4] C. Carstensen, P. Bringmann, F. Hellwig, P. Wriggers: Nonlinear discontinuous Petrov-Galerkin methods. *arXiv:1710.00529v1.*

[5] B. Keith, F. Fuentes, L. Demkowicz: The DPG methodology applied to different variational formulations of linear elasticity, *Comput. Methods Appl. Mech. Engrg.* **309**, 579–609, 2016.

Solid-shell formulations based on reduced integration - investigations of anisotropic material behaviour at large deformations

Oliver Barfusz (*RWTH Aachen University*), Stefanie Reese (*RWTH Aachen University*)

18:10–18:30

Some years ago, a family of solid-shell finite elements based on reduced integration [1],[2],[3] was investigated. Many engineering problems with isotropic material behaviour were considered and these elements showed accurate results while beeing more efficient than similar three-dimensional formulations based on full integration. The objective of the present contribution is to extend the analysis to layered structures with anisotropic material behaviour undergoing large deformations. Here, we follow an ansatz which is similar to so called equivalent single layer theories, i.e. we model the inhomogeneous material as a continuum using solely one solid-shell element over the thickness. Therefore, some modifications of the element formulation are needed. First, we introduce an additional mapping procedure which enables both, the usage of a certain quadrature rule within each layer of the composite and the consideration of layers with different thicknesses. Second, we investigate an appropriate hourglass-stabilization which is needed to recover so-called

zero energy modes which might arise from the reduced integration scheme. Considering different benchmark problems from the literature, it will be shown that the new developed ingredients within the solid-shell concept lead to accurate results in terms of the global response of anisotropic structures at large deformations.

[1] S. Reese, International Journal for Numerical Methods in Engineering **69**, pp. 1671–1716, 2007.

[2] M. Schwarze, S. Reese, International Journal for Numerical Methods in Engineering **80**, pp. 1322–1355, 2009.

[3] M. Schwarze, S. Reese, International Journal for Numerical Methods in Engineering **85**, pp. 289–329, 2011.

S05 | Nonlinear oscillations

Organiser Alfons Ams (*Institut für Mechanik und Fluiddynamik, TU Bergakademie Freiberg*)
Dominik Kern (*TU Chemnitz*)

S05.01 | Nonlinear oscillations

Date 21.03.2018
Room 1601

On the impact of superimposed vibrations on the onset of friction-induced oscillations

Simon Kapelke (*Institut für Technische Mechanik, Karlsruher Institut für Technologie*), Wolfgang Seemann (*Institut für Technische Mechanik, Karlsruher Institut für Technologie*) 16:30–16:50

The reduction of effective frictional forces by superimposing vibrations is referred to as vibrational smoothing of dry friction and has been subject of numerous publications. Focussing on the impact of longitudinal vibrations and using simple Coulomb friction modelling, high-frequency vibrations have been shown to change the non-smooth characteristics of dry friction into a viscous-like behaviour. Consequently, providing an appropriate excitation, friction-induced vibrations due to decreasing friction-velocity characteristics or non-conservative coupling can be quenched. Within this contribution, several aspects of the impact of superimposed vibrations on the onset of friction-induced oscillations are discussed. For longitudinal vibrations, the transition from non-smooth to smooth friction characteristics is investigated, showing a complex dynamic behaviour of the corresponding mechanical model. Increasing the excitation intensity, oscillation amplitudes are shown to decrease and yield a bias of the stationary state due to vibrational smoothing. Among longitudinal excitation, also transverse vibrations have been shown to smooth the effective friction-velocity characteristics. However, their influence on friction-induced oscillations has not been discussed so far, such that the impact of superimposed transverse vibrations on decreasing friction-velocity characteristics and non-conservative coupling is investigated. Finally, the effect of extended friction modelling is considered. Using a class of dynamic friction models, the influence of contact compliance on quenching friction-induced vibrations is discussed, showing both quantitative and qualitative effects on the results.

On the operating conditions of the self-adaptive behavior of a sliding mass along a clamped-clamped beam

Noha Aboulfotoh (*Institute of Dynamics and Vibration Research, Leibniz Universität Hannover*), Jens Twiefel (*Leibniz Universität Hannover*), Malte Krack (*Institute of Aircraft Propulsion Systems, University of Stuttgart*), Jörg Wallaschek (*Institute of Dynamics and Vibration Research, Leibniz Universität Hannover*) 16:50–17:10

Systems consisting of a rigid body sliding freely on a vibrating elastic beam have been observed to exhibit a kind of a self-adaptive behavior. The system showed ability to adapt itself to either capture the maximum amplitude or damp the amplitude. The same structure of a sliding mass along a clamped-clamped beam was introduced as a self-damping system in [1] and as a self-resonating system in [2]. Krack et al. [3] introduced a model of an elastic beam with an attached

sliding body, under a harmonic excitation. The model predicted the operating regime of the self-resonating behavior. However, the two behaviors have not been investigated in one study. The operating conditions that differentiate between the self-damping and the self-resonating have not been found out. This experimental study investigates the impact of the operating conditions on the self-adaptive behavior of a sliding-mass-beam system. The influence of the excitation level and the excitation frequency on the behavior is investigated. The investigations include recording videos using a high speed camera and then analyzing the change in the motion of the slider due to the change in the excitation. The frequency behavior at different excitation levels is recorded in two cases: when the mass is fixed without clearance, and when the mass has a slight clearance and achieves a self-adaptive state. The initial position of the sliding mass is varied and its impact on the ability of the mass to slide and achieve the self-adaptive behavior is investigated. In addition, the influence of the excitation level on the velocity of the sliding mass along the beam is investigated. As a conclusion, the operating conditions differentiating between the self-resonating and the self-damping behaviors are presented. The experimental results are briefly compared with a given theoretical model.

[1] Babitsky, V.I. and Veprik, A.M., 1993. Damping of beam forced vibration by a moving washer. Journal of Sound and Vibration, 166(1), pp.77-85.

[2] Miller, L.M., Pillatsch, P., Halvorsen, E., Wright, P.K., Yeatman, E.M. and Holmes, A.S., 2013. Experimental passive self-tuning behavior of a beam resonator with sliding proof mass. Journal of Sound and Vibration, 332(26), pp.7142-7152.

[3] Krack, M., Aboulfotoh, N., Twiefel, J., Wallaschek, J., Bergman, L.A. and Vakakis, A.F., Toward understanding the self-adaptive dynamics of a harmonically forced beam with a sliding mass. Archive of Applied Mechanics, pp.1-22.

A Discrete, Two-Dimensional Frictional Contact Model for Dynamic Contact between Viscoelastic Materials and Rough Counterparts

Frank Schulte (*Faculty of Mechanical Engineering, Chair of Dynamics and Mechatronics, University of Paderborn*), Walter Sextro (*Faculty of Mechanical Engineering, Chair of Dynamics and Mechatronics, University of Paderborn*) 17:10–17:30

Friction between a viscoelastic material and a rough surface occurs in many technical applications, e. g. windshield wiper, rubber gaskets or the tire-road contact. For the investigation of friction phenomena a detailed frictional contact model is necessary. The friction of viscoelastic materials is divided into the two main effects hysteresis friction and adhesion friction. Multiple influence factors on the friction behaviour are known, e. g. material properties of the contact partners, surface pressure, excitation frequency through the counterpart, as well as temperature. Due to the frictional forces a system is significantly influenced in its vibrational properties. For the simulation of the complex friction processes with viscoelastic materials, a two-dimensional friction contact model with the assumption of an isotropic roughness has been developed. The model consists of a rough rigid and a rough viscoelastic layer. The rough rigid layer represents a measured roughness profile. Due to the low stiffness of the viscoelastic material, the counter body can be assumed to be rigid. The viscoelastic layer consists of a number of point-masses with generalised Maxwell-models and represents the viscoelastic material. The normal and tangential contact can be simulated dynamically by this model. Effects such as changing the contact status during the friction process are taken into account. A stiffening of the viscoelastic material and thus a lower real contact surface at higher excitation frequencies or low temperatures can be shown with the model. This is especially important for the calculation of adhesion friction, as it depends directly on the actual contact area.

A comparison of methods for approximating periodic limit cycles in nonlinear systems with joint friction

Jonas Kappauf (*University of Kassel*), Hartmut Hetzler (*University of Kassel*) 17:30–17:50

Hopf-Bifurcations of steady states leading to self-excitation are a common phenomenon in nonlinear dynamical systems. For the analysis of such bifurcation phenomena dissipation is usually modelled as smooth viscous damping. However, real engineering systems usually exhibit a significant amount of frictional damping which especially for small amplitudes is much stronger than the viscous damping.
Due to non-smoothness of the frictional dissipation, methods to approximate solutions should no rely on smoothness of the involved forces: thus, classical methods like averaging (i.e. slowly varying phase and amplitude) or Fourier-Galerkin (Harmonic Balance) are favorable choices. Recently, also the so-calles Energy-Balance has attracted a lot of interest, also in industrial applications.
Within this contribution, classical approaches as well as the Energy Balance shall be compared. In this benchmark three nonlinear systems of low degree of freedom with both smooth nonlinearities and non-smooth joint friction were chosen. Focussing on these systems periodic limit cycles were calculated and a comparison of the methods in terms of parameter variation, accuracy and calculation time is given. Moreover, possibly extensions to the analysis of systems with many DoF shall be discussed.

Analysis of a Lock-up Mass Damper via Averaging Methods of Second Order

Jimmy Aramendiz (*Institut für technische Mechanik, Karlsruher Institut für Technologie - KIT*), Alexander Fidlin (*Karlsruher Institut für Technologie - KIT*) 17:50–18:10

The limiting of oscillations is always a present objective when tuning the parameters of a given system. In Systems with dry friction the nonlinearities are usually regularized or numerically simulated, in order to obtain a set of optimal parameters. However, an analytical solution offers a deeper insight in the dynamics of the system, which simplifies its tuning with respect to the limitation of its oscillations. The objective of this paper is to present an analytical solution which describes the amplitude response of a conservative dual-mass oscillator in which additionally, dry friction connects the masses. In order to address the nonlinearity of the system, an averaging methods of second order is applied in combination with a scaling ansatz. The second order approximation yields matching results with the numerical simulations in the vicinity of the system's resonance, thus the analytical solution can be used to optimize the suppressor's parameters.

Periodic solutions of measure differential inclusions

Manuela Paschkowski (*Institute of Mathematics, Martin Luther University, Halle(Saale)*), Martin Arnold (*Institute of Mathematics, Martin Luther University, Halle(Saale)*) 18:10–18:30

Introduced by Moreau [1], the nonsmooth and set-valued framework of measure differential inclusions allows us to describe mechanical systems with friction and impacts, including accumulation points of discontinuities. Based on this modelling approach, the first part of the talk will cover the analytical study of nonsmooth problems with periodic solutions. We consider a measure valued generalisation of Filippov systems which are the starting point of most approaches dealing

with this topic [2] and are not sufficient in presence of impacts. We present existence theorems for impact oscillator type problems using arguments of convex analysis and degree theory for both cases, the resonance and the nonresonance one.

For Filippov systems a generalisation of the Floquet theory for smooth systems is already well analysed [3]. Inspired by these outcomes, we discuss in the second part of the talk numerical studies of the impact oscillator to illustrate basic aspects of stability analysis. Because solutions of measure differential inclusions are of bounded variation, so in general discontinuous, we use a generalised stability concept, the orbital stability. This approach can handle the fact that solutions with different initial values do commonly not jump at the same time points. The classical stability definition would fail.

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[2] Kunze, M.: Non-smooth dynamical systems. Springer, 2000.

[3] Leine, R.; Nikmeijer, H.: Dynamics and bifurcations of non-smooth mechanical systems. Springer, 2004.

S05.02 | Nonlinear oscillations

Date 22.03.2018
Room 1601

Oscillations of a visco-elastic belt drive

Alois Steindl (*Institute for Mechanics and Mechatronics, TU Wien*) 08:30–08:50

We investigate the loss of stability of the steady configuration of a planar visco-elastic belt drive. The belt is considered as a linearly visco-elastic slender beam with small bending stiffness, which is driven by a steadily rotating drum. Due to the presence of the small damping parameter and the small bending stiffness, the equations of motion are severly singularly perturbed.
By variation of system parameters, like the driving speed, the damping coefficient, the tension force and the radius of the drums, we calculate the steady configuration and its stability limit. We also calculate the direction and stability of the bifurcating solution branches.

Quenched Nonlinear Oscillations

Christian Kuehn (*Mathematics, Technical University of Munich*) 08:50–09:10

Nonlinear oscillators are a key modelling tool in many applications. The influence of annealed noise on nonlinear oscillators has been studied intensively. It can induce effects in nonlinear oscillators not present in the deterministic setting. Yet, there is no theory regarding the quenched noise scenario of random parameters sampled on fixed time intervals, although this situation is often a lot more natural. Here we study a paradigmatic nonlinear oscillator of van-der-Pol/FitzHugh-Nagumo type under quenched noise as a piecewise-deterministic Markov process. There are several interesting effects such as period shifts and new different trapped types of small-amplitude oscillations, which can be captured analytically. Furthermore, we numerically discover quenched resonance and show that it differs significantly from previous finite-noise optimality resonance effects. This demonstrates that quenched oscillators can be viewed as a new building block of nonlinear dynamics.
Details of this work can be found in the paper: "Quenched Nonlinear Oscillations", C. Kuehn, arXiv, 2017

Analysis of the nonlinear chaotic behavior of an inverted flexible pendulum system affected by impulses.

Hartiny Kahar (*Lehrstuhl Steuerung, Regelung und Systemdynamik, Universität Duisburg-Essen*), Dirk Söffker (*Department of Mechanical Engineering, Universität Duisburg-Essen*) 09:10–09:30

In this contribution, the effect of impulses realized by non-perfect feedback to an inverted flexible pendulum system is studied. It is known that impulsive control allows the stabilization and synchronization of chaotic systems using only small control impulses [Osipov 1998]. Using experimental data from chaotic jumping in an inverted flexible pendulum, several techniques of signal processing and time-frequency representation are carried out. These analysis methods are used to observe the changes in nonlinear dynamic properties and time behavior of the system before and during the jumping between equilibrias. The evaluation of the experimentally realized inverted flexible pendulum system for a specific control parameters shows that 'chaotic' jumping behavior between the three equilibrias (with different attractions regions) are depending on the impulses. The results from detailed analysis shows that the jumping is prepared/caused by feedback imperfectness. Considering the time-frequency-based analysis conducted, it can be stated that the (uncontrolled) impulses causing a temporarily disturbance in the energy distribution between the 'modes'/frequency bands the system vibrates with, which finally leads to a new and more stable distribution in energy, followed by related jumping between the equilibrias.

Evaluation of the Reduced Order Models for Thermoelastodynamic Response of Geometrically Nonlinear Finite Element Models

Morteza Karamooz Mahdiabadi (*Department of Mechanical Engineering, Technical University of Munich*), Francesco De Crescenzo (*Industrial engineering, Università degli Studi di Roma "Tor Vergata"*), Daniel Jean Rixen (*Mechanical Engineering, Technical University of Munich*) 09:30–09:50

The development of large finite element (FE) models of structures comprising numerous numbers of degrees of freedom (DOFs) has made dynamic design of such structures prohibitively computationally expensive. Therefore, engineers are more interested in recent years to use reduced order models of large FE models, which have the same accurate dynamic properties (e.g. time response) as the primary models and simultaneously are much more computationally efficient. Model order reduction (MOR) becomes even more crucial for the design of machineries which encounter large deflections (i.e. they are geometric nonlinear) and are under thermal loads (e.g. gas turbine blades) because nonlinear terms in a system generally increase the computational burden drastically.

This work, studies model reduction of geometric nonlinear FE models (coupled with thermal loads). The nonlinear reduced order model (NLROM) of a nonlinear FE model is developed using nonintrusive approaches. The nonintrusive approaches for MOR are based on developing an NLROM without having direct access to the close form equation of the FE model (e.g., when a FE model is built in a commercial FE packages). In this way, the NLROM is constructed using a set of applied forces (displacements) to the FE packages and determining the underlying displacements (forces). These evaluated forces and displacements are then utilized to identify the nonlinear coefficients of the NLROM.

A panel structure subjected to a time-varying temperature field is considered in this study to develop the NLROM with the aforementioned methods and compare the results with the full FE model.

Characterization of brake shims using analytical constrained layer damping theories

Dominik Schmid (*Department of Applied Mechanics, TU Berlin*), Nils Gräbner (*Department of Applied Mechanics, TU Berlin*), Utz von Wagner (*Department of Applied Mechanics, TU Berlin*) 09:50–10:10

Shims in automotive brake systems are applied to suppress brake squeal resulting from self-excited vibrations. These composite structures consist of thin metal plates and elastomer layers having high damping potential. The characterization and subsequent selection of shims is mainly based on a wide range of experimental investigations so far. A significant reduction of measuring efforts and costs can be expected due to a systematic modelling of shims. Approaches from literature for describing surface damping treatments analytically are considered. The applied theory takes the shearing behavior of the viscoelastic core into account which is characterized by the complex shear modulus of the elastomer layer. Sandwich beam theories enable the prediction of natural frequencies and in particular loss factors of bending mode shapes accurately.
In this contribution shims bonded to rectangular steel plates are examined. The main focus is on the determination of geometrical and rheological influencing variables as well as the impact of boundary conditions in detail. Furthermore the patch length, the position and the temperature influence on shims are investigated finding design specifications. A validation on constrained layer structures is carried out to evaluate analytical with experimental results.

Acknowledgement

This work is funded by DFG, WA 1427/27-1, within the PP 1897 “Calm Smooth and Smart - Novel Approaches for Influencing Vibrations by Means of Deliberately Introduced Dissipation“.

S05.03 | Nonlinear oscillations

Date 22.03.2018
Room 1601

Nonlinear dynamics of electrical machines: a kind of electro-mechanical Sommerfeld effect?

Felix Boy (*Institute of Mechanics, University of Kassel*), Hartmut Hetzler (*Institute of Mechanics, University of Kassel*) 14:00–14:40

Electrical machines in modern application, as for example in electric mobility, are operated at high and fast changing rotational speeds. Efficient light weight structures make the system sensitive to lateral rotor oscillations and may cause severe vibrations or machine failure due to electro-mechanical interactions.
To describe these phenomena a computationally fast analytical model is presented and the nonlinear coupling between flux linkages and the rotor motion is analysed. The approach is based on Lagrange-Maxwell equations for both the electrical circuits and the mechanical subsystem. As a key quantity for the systems dynamics, the magnetic co-energy functional is derived using the permeance harmonic method for arbitrary machine winding design. This approach offers the advantage of an energy consistent electro-mechanical interaction model and very low computational effort.
The model is applied to a run-up simulation of a cage induction machine revealing an interesting effect when passing the critical speed: close to it, the lateral rotor vibration strongly modifies

the magnetic flux and electrical currents. This modification may cause a torque break down stopping the machine from accelerating.
This electro-mechanical effect is very similar to the well-known Sommerfeld effect from classical rotordynamics. However, as an important difference, in this case the electrical part of the system instead of mechanical forces causes the loss of drive torque. The new scenario is discussed and relevant parameter influences are outlined within the contribution.

Investigation of the phase space of a centrifugal exciter with two coaxial unbalances

Olga Drozdetskaya (*Institute of Engineering Mechanics, Karlsruhe Institute of Technology*), Alexander Fidlin (*Institute for Engineering Mechanics, Karlsruhe University of Technology*) 14:40–15:00

Unbalance vibration exciters are commonly used for producing linear motion for vibrating machines operating in many industrial processes. In order to reach the operating speed, most of existing exciters should pass through the main resonance, what can lead to an unexpected high level of vibration or even to the capture into the resonance also known as Sommerfeld effect.
The minimal model of a special type of centrifugal exciters with two coaxial unbalances is considered in the present paper. It consists of an unbalanced rotor mounted on a strongly damped oscillatory carrier system and driven by the induction engine of limited power. An additional pendulum unbalance is mounted coaxially on the main rotor. A non-small rotational damping is applied between the rotor and the pendulum unbalance.
The slow dynamics of this system with 3 DOFs can be described with only two first order differential equations. The first equation describes the rotating speed of the main rotor and the second one the phase shift between the unbalances. The objective of the present paper is to analyze possible stationary and periodic solutions of the reduced system in the vicinity of the main resonance of the carrier system. The focus of this analysis is the investigation of the phase space structure and its changes due to variation of the system parameters.

Model reduction of gyroscopic systems in ALE formulation with and without non-linearities

Tim Weidauer (*FAU Erlangen-Nürnberg*), Kai Willner (*FAU Erlangen-Nürnberg*) 15:00–15:20

Rotating systems are subject to gyroscopic influences which alter their dynamic behaviour. The *Arbitrary Lagrangian Eulerian* (ALE) formulation is a popular approach for related models, e.g. for the simulation of tire rolling contact. It allows for decoupling the rotational guiding motion from the relative deformation of the rotating structure. At the same time it complicates contact computations as the relative displacement between two material particles is not tracked naturally by the ALE observer. Model reduction techniques for (non-linear) systems face additional challenges in this context. A variety of these aspects is discussed in this paper, employing common reduction techniques such as *Second Order Modal Truncation* or the *Craig-Bampton method*.

Modeling of Situation-Aware Frictional Energy Dissipation in Refrigerant-Lubricated Gas Foil Bearings

Tim Leister (*Institute of Engineering Mechanics, Karlsruhe Institute of Technology*), Wolfgang Seemann (*Institute of Engineering Mechanics, Karlsruhe Institute of Technology*), Benyebka Bou-Saïd (*Contact and Structure Mechanics Laboratory, National Institute of Applied Sciences of Lyon*) 15:20–15:40

As a benefit of the low-viscosity lubricant film, which separates the rotor journal from the supporting structure, gas foil bearings (GFBs) are characterized by almost wear-free operation with remarkably small damping, making them a key technology in the development of energy-efficient and oil-free turbomachinery. On the other hand, the absence of any major source of energy dissipation, combined with the strongly nonlinear fluid forces, makes the system prone to instability phenomena such as self-excited subsynchronous vibrations. As a countermeasure, the compliant and slightly movable foil structure inside the lubrication gap possesses a situation-aware ability of dissipating some of the excessive energy by means of deliberately introduced dry friction. While stiction between the foil structure and the bearing sleeve is the predominant state in stationary operation with only small unbalances present, contact breakaway and subsequent dissipative sliding occur in response to heavy cyclic loading, thus calming rotor vibrations before their amplitudes become severe. Despite this seemingly simple mechanism, almost none of the computational GFB models found in literature are capable of really capturing the switching nature of stick–slip transitions in dry friction and hence suffer from substantial inaccuracies when assessing the dissipated energy. The presented work addresses this shortcoming by incorporating a dynamic bristle friction law with true stiction into the structural model, which is hereafter coupled to a Reynolds equation for non-ideal compressible gases and to a modified Jeffcott–Laval rotor. Considering the resulting overall model, simulations and stability analyses give novel insights into the nonlinear dynamics of GFBs.

Investigations on elastically deformed journal bearings and their influence on rotor-dynamic systems

Kai Becker (*Institute of Engineering Mechanics, Karlsruhe Institute of Technology - KIT*), Wolfgang Seemann (*Institute of Engineering Mechanics, Karlsruhe Institute of Technology - KIT*) 15:40–16:00

In the context of the improvement of rotor-dynamic systems being supported by journal bearings several different approaches can be found in literature.
Typical realizations are non-cylindrical bearings, like multi-lobe or tilting pad bearings, which proved themselves to have a positive effect on the rotor-dynamic system by means of better stability properties for certain parameter configurations.

The present work focuses on an initially cylindrical journal bearing which is elastically deformed by an appropriate actuation mechanism to establish a 'non-circular' bearing profile. By using just two actuators, different ovally-shaped profiles can be realized, which of course influence the fluid pressure distribution within the bearing. As the rotational symmetry within the bearing is lost (because of the deformation) also other effects such as the rotor's principal load direction come into play, compared to the classical circular profile.
Depending on the elastically deformed bearing, the dynamic behaviour of the attached rotor system can change significantly in the sense of critical revolution speeds and oscillation amplitudes.

The fluid-solid interaction is modelled by means of the Reynolds equation which takes into account the elastic deformation of the corresponding bearing. After approximating the pressure distribution by a combined Galerkin-Finite-Difference-Scheme approach, the resulting equations of motion for an attached Jeffcott rotor are systematically analysed.
The investigations thereby mainly focus on stability thresholds and their dependence on the above mentioned effects.

S05.04 | Nonlinear oscillations

Date 22.03.2018
Room 1601

Approximation of Periodic and Quasi-Periodic Motions of a Rotor-System with Visco-Elastic Seal Support by Using a Multifrequent Fourier-Galerkin-Method

Simon Baeuerle (*Institute for Mechanics - Engineering Dynamics, University of Kassel*), Hartmut Hetzler (*Institute for Mechanics - Engineering Dynamics, University of Kassel*) 17:30–17:50

Quasi-periodic or almost periodic motions can occur in rotor systems, when periodic motions (e.g. induced by rotor unbalance) become unstable. This might happen by self-excitation leading to a Neimark-Sacker bifurcation. Sources of self-excitation are e.g. journal-bearings, aeroelastic coupling or leakage flow through seals. The stability behaviour of rotor systems can also be affected by the elasticity of the structure surrounding the machine like the foundation [1] or the (journal) bearing support [2].
New contact-free rotor-seals use explicitly such elastic properties of the structure as design variables (e.g. HALO Seal [3]). Combining some of the advantages of brush and labyrinth seals, they can adapt their gap to the pressure drop and allow for some rotor movement. Thus, they lower leakages and minimize the risk of rotor-stator contact. Earlier studies showed that these new seal designs can improve the stability behaviour [4].

In the present work, we investigate stable and unstable quasi-periodic motions in a rotor system with a flexible seal. The periodic and quasi-periodic solutions are approximated by using a Fourier-Galerkin method [5].
The system under investigation consists of a balanced Laval-Rotor (Jeffcott-Rotor) and a seal ring, which is visco-elastically supported. The non-linear Muszynska-model [6] accounts for the fluid forces. Depending on parameters, the seal support can enlarged the stable operation range. Qualitatively different nonlinear behaviours occur, depending on the specific pair of complex conjugated eigenvalues becoming unstable. Co-existing stable periodic solutions are separated by an unstable quasi-periodic solution induced by two incommensurable autonomous frequencies. The Fourier-Galerkin method is used to find periodic solutions and quasi-periodic repellors: a general Fourier series with a priori unknown frequencies approximates the solution. The series coefficients are determined by a Newton-Algorithm and a Galerkin projection.

[1] R. Gasch, R. Nordmann, H. Pfützner. Rotordynamik. Springer-Verlag.

[2] C. Bai, Q. Xu, J. Wang, (2011). Effects of flexible support stiffness on the nonlinear dynamic characteristics and stability of a turbopump rotor system. Nonlinear Dynamics, 2006, 64(3), 237-252.

[3] L. San Andres, A. Anderson. An All-Metal Compliant Seal Versus a Labyrinth Seal: A Comparison of Gas Leakage at High Temperatures. Journal of Engineering for Gas Turbines and Power, 2005, Vol. 137, No. 5, ASME (2015), 052504 (8 pages).

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[5] B. Marx, W. Vogt. Dynamical Systems: Theory and Numerics. Springer, 2010 (in German).

[6] A. Muszynska. Whirl and whip – rotor/bearing stability problems. Journal of Sound and Vibration, 1986, 110(3):443–462.

Stability Analysis of Numerically Approximated Quasiperiodic Motions

Robert Fiedler (*Mechanical Engineering - Engineering Dynamics, University of Kassel*), Hartmut Hetzler (*University of Kassel*) 17:50–18:10

This contribution deals with the stability analysis of flows on invariant manifolds based on the theory of LYAPUNOV-exponents. The description using an invariant manifold for quasiperiodic motions allows an analysis of a finite p-dimensional interval, which dimension is given through the parametrization, instead of an investigation through time integration of an one dimensional infinite interval. This assumption is admissible since a characteristic of a quasiperiodic motion on a invariant manifold is that a trajectory starting on the manifold fills it dense. An immediate consequence of the later is the mean-value theorem, which characterizes in the neighborhood of a manifold the ergodicity of semitrajectories. A requirement for the validity of the mean-value theorem is the presence of a parallel flow on the manifold. In general calculated manifolds, which are parametrized with physical phase angles, do not exhibit a parallel flow and an approach for a diffeomorphism is proposed transforming the physical flow into a parallel flow.
To demonstrate the use of this approach the LYAPUNOV-exponents of a periodic and quasiperiodic motion of a forced VAN-DER-POL equation are calculated by applying the diffeomorphism to the invariant manifolds. The verification of the proposed method is carried out by comparing the results to an alternative approach based on a time integration using a continuous GRAM-SCHMIDT orthonormalization.

Some Remarks on Parametric Excitation in Circulatory Systems

Artem Karev (*Institute of Numerical Methods in Mechanical Engineering, Technische Universität Darmstadt*), Lara De Broeck (*Technische Universität Darmstadt*), Peter Hagedorn (*Institute of Numerical Methods in Mechanical Engineering, Dynamics and Vibrations Group, Technische Universität Darmstadt*) 18:10–18:30

Dynamical systems with time-periodic coefficients, i.e. with parametric excitation, have been studied in different fields for over a hundred years. It is well known that the presence of parametric excitation acts mostly destabilizing, leading to the emergence of instability regions depending on the amplitude and frequency of excitation. However, most of the work is done on systems with synchronous parametric excitation, while there are only few papers dealing with out-of-phase time-periodicity. At the same time little to no research is done on systems containing nonconservative (gyroscopic and circulatory) terms in the context of parametric excitation. Still, both of the effects (asynchronous parametric excitation as well as gyroscopic and circulatory terms) can be observed in equations of motion of technical problems. The present paper emphasizes the importance of a generalized investigation of parametrically excited systems. An example containing both circulatory terms and out-of-phase time-periodic terms is treated numerically, but also analytically by means of the normal form theory. The derived stability boundaries in the parameter space of amplitude and frequency of parametric excitation show that the interaction of both features leads to the occurrence of unexpected resonance areas. The results extend the understanding of the influence of parametric excitation and encourage study of more general systems.

S06 | Material modelling in solid mechanics

Organiser Ralf Denzer (*Division of Solid Mechanics, Lund University*)
Andreas Menzel (*Institute of Mechanics, TU Dortmund University and Division of Solid Mechanics, Lund University*)

S06.01 | Material modelling in solid mechanics

Date 20.03.2018
Room 0220

An extended exponentiated Hencky energy for transverse isotropy

Markus von Hoegen (*Institut für Mechanik, University of Duisburg-Essen*), Jörg Schröder (*University of Duisburg-Essen*), Patrizio Neff (*Mathematics, University of Duisburg-Essen*) 08:30–08:50

From a theoretical point of view there is no reason to favor a specific finite strain tensor in constitutive modeling since any material law can be equivalently reformulated in terms of any other strain tensor. In this context already in 1928 Heinrich Hencky [1] introduced a strain-energy function based on the logarithm of the right stretch tensor $\log \mathbf{U}$ which is nowadays also called Hencky strain. Very recently it was discovered by [3] that the incorporated isotropic invariants can be uniquely motivated by purely geometric considerations based on the geodesic distance of the deformation gradient to the special orthogonal group $\mathrm{SO}(n)$. Building on those achievements the exponentiated Hencky energy was developed in [2] and subsequent contributions, showing remarkable properties on mathematical grounds. In this contribution we aim to formally extend this promising strain-energy in view of anisotropic problems, especially for transverse isotropy, making use of additional anisotropic logarithmic strain invariants, see also [4]. The potential of the formulation is studied for a number of numerical examples in order to discuss the logarithmic-strain driven material response.

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An anisotropic model for fiber-reinforced elastomers at finite strains

Vladimir Zatko (*Institut für Mechanik, Universität der Bundeswehr München*), Alexander Lion (*Universität der Bundeswehr München*), Michael Johlitz (*Institute of Mechanics, Universität der Bundeswehr München*) 08:50–09:10

Fiber-reinforced elastomers play an important role in a large number of industrial applications. Simulations accounting truly the heterogeneous nature of such polymers are very time-consuming and in many cases not feasible. Instead, the presented model uses the theory of continua and is such restricted to materials in which the fibers are assumed to be continuously distributed in the matrix material. The modeling approach is primary based on the existence of the Helmholtz free-energy function. In the present case, this is not only dependent on deformation but also on the set of preferred material directions (fiber orientations). The anisotropic hyper-elastic material behaviour has been further extended by the viscous properties of matrix material. This leads to the additive decomposition of the stress tensor into equilibrium and non-equilibrium parts. The behaviour of the model under simple loadings, as well as its numerical implementation is discussed in the article.

Constitutive modelling of hypererlastic rubber-like materials considering damage

Elisabeth Toups (*Institute of Applied Mechanics, RWTH Aachen*), Jaan-Willem Simon (*Institute of Applied Mechanics, RWTH Aachen*), Stefanie Reese (*Institute of Applied Mechanics, RWTH Aachen*) 09:10–09:30

Adhesives are used in numerous applications such as in the automotive industry, packaging industry, civil engineering, and many others. The use of multi-side bonded joints become increasingly common in glass-façade structures instead of bolted point fixings, inter alia, for aesthetic reasons.
For the simulation of glass-façade component behaviour, it is essential to investigate constitutive models which ensure a representation of rubber-like material behaviour. Several hyperelastic material models are available in the literature, but most of them are not suitable to represent large deformations, damage behaviour (i.e. Mullins-Effect), and multiaxial stress states all in one. Hence, the main goal of the present work is to develop a material model which considers the mentioned properties.
For this reason, different models are compared and adjusted accordingly. In the first step, the well-known Ogden model is used to represent the material behaviour undergoing large deformations. Then, in order to take damage into account, the micromorphic based formulation of a gradient-extended two-surface damage-plasticity model developed by Brepols et al. is considered. In this model damage and plasticity are treated independently from each other. This fact is very useful in order to describe the damage behaviour of hyperelastic materials without considering plasticity if needed. This model also enables the calculation of multi-axial stress states and thus offers a good starting point for further investigations. Thus, the above mentioned model will be developed and tested in its suitability by comparison to experimental test data.

Rari- and multi-constant theories of elasticity and related aspects of anisotropy in soft biological tissues

Alexander E. Ehret (*Empa, Swiss Federal Laboratories for Materials Science and Technology*), M. B. Rubin (*Faculty of Mechanical Engineering, Technion - Israel Institute of Technology*) 09:30–09:50

In the 19th century the founders of elasticity theory debated about the number of constants needed to characterise a general anisotropic linear elastic solid [1]. One line of thought followed the assumption that elastic behaviour is only due to coaxial forces between atoms, arising from their pair potentials, which led to the rari-constant theory, that is characterised by only 15 independent constants, while the multi-constant theory, that was strongly supported by Green's energetic approach to elasticity, is characterised by 21 [1, 2].

In modern terms, pair potentials are expressed through the squares of scalar products between strain and rank-one second order structural tensors of the form $\boldsymbol{M}_i \otimes \boldsymbol{M}_i$, where $\boldsymbol{M}_i$, $i = 1, 2, ...$, represent unit vectors that characterise the line of action. In this contribution, we show that infinitely many complete sets of 15 such tensors exist from which the multi-constant theory is obtained by including scalar products of 6 of these structural tensors with the squared strain tensor in addition to the 15 pair potentials that characterise the rari-constant theory.
Although these considerations are based on linear elasticity, they become relevant for models in finite elasticity which account for the anisotropy generated by the presence of distributed fibres providing reinforcement along their fibre axis. The present contribution therefore adds a new perspective on the discussion of differences between the structural [3] and structure tensor [4] approaches to model soft biological tissues with distributed collagen fibres.

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A new hyperelastic finite element model for graphene, carbon nanotubes and nanocones

Reza Ghaffari (*Aachen Institute for Advanced Study in Computational Engineering Science (AICES)*), Roger A. Sauer (*Aachen Institute for Advanced Study in Computational Engineering Science (AICES)*)

09:50–10:10

In this paper, the membrane and shell models of [1] and [2] are improved and a high performance model is obtained. The former works are based on the invariants of the logarithmic strain and the current work is based on the invariants of the right Cauchy-Green strain tensor. The speedup of the new model is 1.5 relative to the previous models. This material model is implemented in a rotation-free shell formulation based on curvilinear coordinates and isogeometric finite elements [3]. Exact quantum data is used to calibrate the model [1, 4]. The results of this model is very close to experimental and full ab-initio simulations [4, 5]. The first examples are bending and twisting of carbon nanotubes (CNTs) and carbon nanocones (CNCs). The second examples are contact of an atomic force microscope (AFM) which has a tip of CNT or CNC with a Lennard-Jones wall. The last examples are the modal analysis of graphene sheets under biaxial and uniaxial strains and CNTs under uniaxial strain. The results are compared with atomistic data from the literature [6, 7]. The contact between the Lennard-Jones wall and the AFM tips is modeled by the Lennard-Jones potential and the coarse grained contact model [8, 9]. The wall is modeled with a coarse grained contact model.

Keywords: Adhesive contact; carbon nanocones; carbon nanotubes; graphene; hyperelasticity; isogeometric finite elements.

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On construction of general solutions of equations of elastostatic problems for the elastic bodies with voids

Bakur Gulua (*I. Javakhishvili Tbilisi State University, Sokhumi State University*), Roman Janjgava (*I. Javakhishvili Tbilisi State University, I. Vekua Institute of Applied Mathematics*) 10:10–10:30

The linear theory of thermo-elastic materials with voids was for the first time considered in the work Ieșan. A two-dimensional system of equations of plane deformation is written in the complex form and its general solution is represented by means of two analytic functions of a complex variable and one solution of Helmholtz equation. The constructed general solution enables one to solve analytically a sufficiently wide class of plane boundary value problems of the elastic equilibrium with voids.

Acknowledgment. The designated project has been fulfilled by a financial support of Shota Rustaveli National Science Foundation (Grant SRNSF/FR /358/5-109/14).

S06.02 | Material modelling in solid mechanics

Date 20.03.2018
Room 2750

Thermodynamic dislocation theory: thermal softening and adiabatic shear banding

Khanh Chau Le (*Lehrstuhl für Mechanik - Materialtheorie, Ruhr-Universität Bochum*) 08:30–08:50

The statistical-thermodynamic dislocation theory developed in our earlier studies is used here in an analysis of the experimental observations of thermal softening and adiabatic shear banding in steel by Marchand and Duffy (1988). Employing a small set of physics-based parameters, which we expect to be approximately independent of strain rate and temperature, we are able to explain experimental stress-strain curves at six different temperatures and four different strain rates. We make a simple model of a weak notch-like disturbance that, when driven hard enough, triggers shear banding instabilities that are quantitatively comparable with those seen in the experiments.

Singularity-free dislocation continuum theory for anisotropic crystals

Markus Lazar (*Department of Physics, TU Darmstadt*), Giacomo Po (*University of California Los Angeles (UCLA), Los Angeles CA*) 08:50–09:10

A non-singular theory of three-dimensional dislocation loops in a particular version of Mindlin's anisotropic gradient elasticity with up to six length scale parameters is presented [1,2]. The theory is systematically developed as a generalization of the classical anisotropic theory in the framework of incompatible elasticity. The non-singular version of all key equations of anisotropic dislocation theory are derived as line integrals, including the Burgers displacement equation with isolated solid angle, the Peach-Koehler stress equation, the Mura-Willis equation for the elastic distortion, and the Peach-Koehler force. It is shown that all the elastic fields are non-singular, and that they converge to their classical counterparts a few characteristic lengths away from the dislocation core. In practice, the non-singular fields can be obtained from the classical ones by replacing the classical (singular) anisotropic Green tensor with the non-singular anisotropic Green tensor derived by [1]. The elastic solution is valid for arbitrary anisotropic media. In addition to the classical anisotropic elastic constants, the non-singular Green tensor depends on a second order symmetric tensor of length scale parameters modeling a weak non-locality, whose structure depends on the specific class of crystal symmetry. The anisotropic Helmholtz operator defined by such tensor admits a Green function which is used as the spreading function for the Burgers vector density. The anisotropic non-singular theory is shown to be in good agreement with molecular statics without fitting parameters, and unlike its singular counterpart, the sign of stress components does not show reversal as the core is approached. Compared to the isotropic solution, the difference in the energy density per unit length between edge and screw dislocations is more pronounced.

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The thermodynamic dislocation theory for the crystal undergoing anti-plane constrained shear

Yinguang Piao (*Lehrstuhl für Mechanik - Materialtheorie, Ruhr-Universitaet Bochum (RUB)*), Khanh Chau Le (*Lehrstuhl für Mechanik - Materialtheorie, Ruhr-Universität Bochum (RUB)*) 09:10–09:30

The present work proposes the thermodynamic dislocation theory for the crystal undergoing anti-plane constrained shear. The asymptotically exact energy of the crystal containing a moderately large dislocation density is found by the averaging procedure. This energy is extrapolated to the cases of extremely small or large dislocation densities. By incorporating the entropy of dislocations and the density of redundant dislocations, we develop the thermodynamic dislocation theory that extends the theory of Langer, Bouchbinder and Lookmann to non-uniform plastic deformations. The theory is applied to the problem of anti-plane constrained shear to calculate stress-strain curves and dislocation densities.

A new insight into the J-, M-, and L-integrals of dislocations

Eleni Agiasofitou (*Department of Physics, Technische Universität Darmstadt*), Markus Lazar (*Department of Physics, Technische Universität Darmstadt*) 09:30–09:50

In this work, the **J**-, M-, and **L**-integrals of dislocations are presented in the framework of Eshelbian dislocation mechanics; a unified framework of (three-dimensional) incompatible elasticity theory of dislocations and the so-called configurational or Eshelbian mechanics. A new insight is given into the physical interpretation of the M-, and **L**-integrals of dislocations, connecting them with established quantities in dislocation theory such as the interaction energy and the **J**-integral of dislocations, which is equivalent to the well-known Peach-Koehler force.
The explicit formulas of the **J**-, M-, and **L**-integrals for straight (screw and edge) dislocations in isotropic materials are derived [1]. The obtained results reveal the physical interpretation and significance of the M-, and **L**-integrals for straight dislocations. The M-integral between two straight dislocations (per unit length) is equal to the half of the interaction energy of the two dislocations (per unit length) depending on the distance and on the angle, plus twice the corresponding pre-logarithmic energy factor. The L_3-integral between two straight dislocations is the z-component of the configurational vector moment or the rotational moment about the z-axis caused by the interaction between the two dislocations.
Next, we derive the **J**-, M-, and **L**-integrals of a single (edge and screw) dislocation in isotropic elasticity as a limit of the **J**-, M-, and **L**-integrals between two straight dislocations. The M-integral of a single dislocation in anisotropic elasticity is also derived. The remarkable outcome is that the M-integral of a single dislocation represents the total energy (per unit length) of the dislocation which is given by the sum of the self-energy (per unit length) and the dislocation core energy (per unit length). The latter can be identified with the work produced by the Peach-Koehler force. It is shown that the dislocation core energy (per unit length) is twice the corresponding pre-logarithmic energy factor. This result is valid in isotropic as well as in anisotropic elasticity. The only difference lies on the pre-logarithmic energy factor which is more complex in anisotropic elasticity due to the anisotropic energy coefficient tensor which captures the anisotropy of the material [2].

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Stress-strain simulation of high temperature deformation in aluminum and steel under thermodynamic dislocation theory

Tuan Minh Tran (*Lehrstuhl fur Mechanik-Materialtheorie, Ruhr-Universität Bochum (RUB)*), Khanh Chau Le (*Institute for Mechanics-Material Theory, Ruhr-Universität Bochum (RUB)*), James S. Langer (*Physics, University of California, Santa Barbara, USA*) 09:50–10:10

The thermodynamic dislocation theory is used here in an analysis of high temperature deformation of aluminum and steel. For each of these materials, the experimental stress-strain curves for three different strain rates and three different temperatures are fitted using physics-based parameters which are expected theoretically to be independent of stain rate and temperature. Our theoretical curves include yielding transitions at zero strain in agreement with experiment. We find that thermal softening effects are important even at the lowest temperatures and smallest strain rates.

Continuum-mechanical aspects of modeling the dislocation motion including the effects of chemical impurities

Sandra Klinge (*Institute of Mechanics, TU Dortmund University*), Serhat Aygün (*Institute of Mechanics, TU Dortmund University*), Markus Bambach (*Chair of Constructions Design and Manufacturing, BTU Cottbus-Senftenberg*) 10:10–10:30

Dynamic recrystallization is a complex process which can be interpreted as the interplay between the motion and rearrangement of dislocations and of subgrain- and grain boundaries. External influences activating this process are mechanical load and temperature. The process is also dependent on the type of material and of the contents of the impurities in it. This presentation solely focuses on the simulation of the motion of dislocations and the change of their density during the process. For this purpose, a thermodynamically consistent mechanical model relying on the principle of maximum dissipation is proposed. Furthermore, the theory of small deformation is followed and three internal variables are introduced: the inelastic strains and the densities of both mechanically and thermally activated dislocations. In the next step, the free energy including two parts is considered: The first term goes back to the elastic deformations and the second one is due to the density of dislocations. The evolution of mechanically activated dislocations is approximated by the Kocks-Mecking model. Dissipation is expressed in terms of the velocity of the dislocations and of the dislocation mobility. The latter depends on the stacking fault energy which is suitable for the so-called "ab initio" simulations. The minimization process yields evolution laws in the form of a time-dependent nonlinear system of equations which is solved by using the Netwon method coupled with the backward-Euler. The numerical examples selected give insight into the influence of chemical contents on the dislocation motion.

S06.03 | Material modelling in solid mechanics

Date 20.03.2018
Room 0220

Parameter identification for thermo-mechanically coupled material models based on inhomogeneous field measurements

Lars Rose (*Institute of Mechanics, TU Dortmund University*), Andreas Menzel (*Institute of Mechanics, TU Dortmund University*) 16:30–16:50

Material models include material parameters, the identification of which is vitally important and the foundation of predictive simulations. Though data from homogeneous tests might be sufficient to fit the parameters of a simple model, the displacement and temperature field measured in experiments under inhomogeneous states of deformation are needed to identify the parameters of more advanced material models. For this reason a parameter identification based on inhomogeneous field measurements is presented. This includes the choice of an objective function which combines displacement and temperature values, the influence of weighting parameters within such a function, as well as the general algorithmic framework. Furthermore, the realisation of suitable experiments under inhomogeneous states of deformation is discussed, focusing on possible error sources and linking the formulation of the objective function to the minimisation of the impact of such errors.

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Modelling Thermo-Viscoplasticity of Case-Hardening Steels Over Wide Temperature Ranges

Philip Oppermann (*Division of Solid Mechanics, Lund University*), Ralf Denzer (*Division of Solid Mechanics, Lund University*), Andreas Menzel (*Institute of Mechanics, TU Dortmund University and Division of Solid Mechanics, Lund University*) 16:50–17:10

The aim of this work is the development of a thermodynamically consistent fully coupled thermo-viscoplastic material model for metals, especially for case hardening steels.
The model is based on a split of the free energy into a thermo-elastic, a purely plastic and a purely thermal part and covers nonlinear cold-work hardening and thermal softening.
Effects arising from phase transformations at austenitisation temperature are accounted for in the model as well as nonlinear temperature dependencies of the elastic moduli, the plastic hardening moduli, the thermal expansion, the heat capacity and the heat conductivity.
Moreover, strain rate dependency of the current yield stress is realized using a temperature dependent nonlinear Perzyna-type viscoplastic model. The model and its parameters are fitted against experimental data for case hardening steel 16MnCr5 (1.7131). Several numerical examples are discussed.

Single crystal plasticity - A mesoscale based approach for modeling the mechanics of additively manufactured Inconel 718

Andreas Kergaßner (*Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Julia Mergheim (*Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Paul Steinmann (*Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*) 17:10–17:30

Selective electron beam melting represents an additive manufacturing process. Complex parts are built in a layer-wise manner using metal powders. The powder is fused selectively by the energy of an electron beam guided by electromagnetic fields. The so called electromagnetic lens allows for a very fast deflection and thus very high beam velocities and different scan strategies. By using these scan strategies it is possible to tailor the resulting mesostructure in the material which may range from a columnar to an equiaxed grain structure.
For altered grain structures, different macroscopic mechanical properties are expected. Long grains oriented along the building direction cause highly anisotropic behavior. In contrast, a uniform grain structure results in isotropic mechanical behavior. Furthermore, different orientations of the unit cells, the effects of grain size and boundaries strongly influence the macroscopic mechanical properties.
In this contribution the mesoscopic material behavior is simulated by means of Finite Element simulations. A Voronoi tessellation based method is used to model the grain structure of columnar grained Inconel 718. The resulting grain structure of different scan strategies are taken into account. On the mesoscale, the thermo-mechanical behavior is modeled using a thermal gradient-crystal-plasticity model, allowing for relative misorientations on the grain boundaries. Computational homogenization and macroscopic experimental data are used to inversely identify elastic and plastic temperature-dependent mesoscopic mechanical parameters. With this approach at hand, the macroscopic mechanical properties, such as the anisotropic Youngs moduli and the yield surface, are obtained for varying grain structures.

Implementation of a Phase Mixture Model for Rate-Dependent Inelasticity

Johanna Eisenträger (*Institute of Mechanics, Otto-von-Guericke-Universität Magdeburg*), Konstantin Naumenko (*Institute of Mechanics, Otto-von-Guericke-Universität Magdeburg*), Holm Altenbach (*Institute of Mechanics, Otto-von-Guericke-Universität Magdeburg*) 17:30–17:50

Power plant components have to withstand complex thermo-mechanical loads, i.e. frequent start-ups and shut-downs in combination with long holding times at high temperatures induce creep-fatigue loads. Tempered martensitic steels with high chromium content feature high creep strength and corrosion resistance among other properties such that these alloys are often used for power plant components.
This contribution focuses on the simulation of the complex mechanical behavior of the alloy X20CrMoV12-1 based on a multi-axial phase mixture model. Within this model, we distinguish two phases: a hard and a soft phase. Both phases are connected via an iso-strain approach, and non-linear kinematic hardening as well as microstructural softening effects are taken into account by introducing a backstress and a softening variable as internal variables. The model is implemented into the commercial finite element code ABAQUS with a user material subroutine. For this purpose, the stress update algorithm and the consistent tangent operator are implemented based on the backward Euler method in combination with Newton-Raphson iteration. Next, a wide range of benchmarks for uni-axial as well as multi-axial stress states is taken into account in order to verify the numerical implementation. Furthermore, a thermo-mechanical fatigue test based on a typical sequence of start-ups and shut-downs of power plants is simulated.

On anisotropy evolution in finite strain plasticity

Tobias Kaiser (*Mechanical Engineering, Institute of Mechanics, TU Dortmund University*), Jia Lu (*Department of Mechanical and Industrial Engineering, University of Iowa*), Andreas Menzel (*Institute of Mechanics, TU Dortmund University*), Panayiotis Papadopoulos (*Department of Mechanical Engineering, University of California, Berkeley*) 17:50–18:10

In 2001, Lu and Papadopoulos derived a general theoretical framework to model the evolution of the elastic and plastic material symmetry groups of crystalline materials that are subjected to finite (plastic) deformation processes. Based on this foundation (see Comput. Methods in Appl. Mech. Eng. 190(48-51) 2001, 4889-4910 as well as Comput. Methods in Appl. Mech. Eng. 192(31-32) 2003, 3431-3470) a specific model is derived. We especially focus on the evolution equations for the structural tensors that are used to characterise the material symmetry group and prove the thermodynamic consistency of the model.
In a second step, the specific model is applied to simulate anisotropy evolution observed in experiments. To this end, the tension-test based experimental findings by Kim and Yin (J. Mech. Phys. Solids 45(5) (1997), 841-851) are taken into account. Their experiments suggest that the initially orthotropic yielding behaviour of cold rolled sheet metal is maintained throughout a finite plastic deformation process. However, the preferred material directions seem to rotate such that an alignment of the (plastic) material symmetry group with the principal loading directions is observable. By comparing the experimental findings with the finite element based simulation results, we show that the model is capable of reproducing the experimental observations, i.e. the change in the directional dependence of the yield limit which suggests a reorientation of the crystals.

Modeling the anisotropic in-plane and out-of-plane elastic-plastic response of paper

Yujun Li (*Department of Advanced Manufacturing Engineering, Northwestern Polytechnical University*), Ahmad Alajami (*RWTH Aachen University, Institute of Applied Mechanics*), Jaan-Willem Simon (*RWTH Aachen University, Institute of Applied Mechanics*) 18:10–18:30

Laminated paperboard is one of the most common packaging materials in industry due to its beneficial characteristics, such as low price, sustainability, and recyclability. This material exhibits a highly anisotropic mechanical behavior due to its manufacturing process; including anisotropic elasticity, initial yielding, strain hardening, and tensile failure.
Furthermore, there is a significant difference of behavior in the in-plane and the out-of-plane direction. While permanent deformations can be observed after unloading, indicating a typical elastic-plastic behavior in both directions, the thickness direction shows several specific characteristics, particularly during the compression. It appears to evolve exponentially because compression results in an apparent densification effect of the paper network, which is generally not found during in-plane deformation. Examples of other differences include the large deformation range and the internal friction effect, which are all more significant in the out-of-plane direction. In general, the experimentally observed mechanical behavior of paper includes: (i) elastic-plastic anisotropy, (ii) different yielding between tension and compression, (iii) pressure dependent yield behavior, (iv) densification effect in the out-of-plane compression, and (v) internal friction effect in the out-of-plane direction under combined shear and compression. According to the several studies in the literature, it is reasonable to study the in-plane and out-of-plane behavior in an uncoupled way. Therefore, an elastic-plastic model is developed, including an in-plane and an

out-of-plane part that do not interact with each other. This model is able to represent all the above-mentioned critical aspects of the mechanical response.

S06.04 | Material modelling in solid mechanics

Date 20.03.2018
Room 2750

Variational Principles for Thermo-Mechanics of Gradient-Extended Dissipative Solids

Stephan Teichtmeister (*Institute of Applied Mechanics, University of Stuttgart*), Aref Nateghi (*Institute of Applied Mechanics, University of Stuttgart*), Marc-André Keip (*Institute of Applied Mechanics, University of Stuttgart*) 16:30–16:50

We present an extension of the general variational framework of gradient-extended dissipative solids proposed in [1] towards the evolution of thermodynamic states at small as well as large strains. Starting point is the formulation of a canonical stored (gradient-type) energy and (gradient-type) dissipation potential function in terms of the entropy and the rate of entropy, respectively, determining a pure minimization principle for the coupled evolution problem. For practical applications, these constitutive functions are transformed into mixed potentials depending on the entropy as well as the temperature, and the rate of entropy as well as a dissipative driving force, respectively. These potentials yield fundamental mixed variational principles of thermo-mechanics. The associated incremental variational principles are solved via an intrinsic mechanical-thermal operator split algorithm. Alternative variational updates for the thermal evolution problem within a local plasticity theory are presented in [2, 3, 4]. We specify our proposed general framework for the thermo-mechanical coupling in gradient plasticity and gradient damage and give an outlook towards thermo-elasto-dynamics.

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Incorporation of deformation twinning in the framework of gradient crystal plastity

Edgar Husser (*Institute of Continuum Mechanics and Material Mechanics, Hamburg University of Technology*), Swantje Bargmann (*Chair of Solid Mechanics, Bergische Universität Wuppertal*) 16:50–17:10

Magnesium (Mg) alloys have attracted considerable attention in the early past due to its high potential for a variety of industrial applications in which weight reduction is of major priority.

Still, the technological potential of Mg-based alloys has not been fully utilized. For that reason, there is a great interest in understanding the mechanical behavior of the primary metal whose deformation behavior depends strongly on the crystal orientation. Tensile twinning represents an essential deformation mode in hcp materials such as Mg because it provides additional ability for deformation along the crystallographic c-axis and, hence, can be used to steer the ductility of Mg-based alloys.
On the basis of a well-established gradient crystal plasticity framework, deformation-induced twinning is consistently incorporated in terms of dissipative-like processes. A nucleation criterion is proposed which considers the natural competition between slip and twinning in a continuum sense. The morphological characteristics of twinning in terms of twin band formation and growth are modeled by a non-local approach. Microcompression of Mg single crystal favored oriented for activation of {1 0 -1 2}-tensile twins is exemplarily studied. Numerical results are quantitatively compared against experimental data.

Gradient-enhanced ductile damage - a finite deformation framework with application to DP800

Leon Sprave (*Institute of Mechanics, TU Dortmund University*), Andreas Menzel (*Institute of Mechanics, TU Dortmund University*) 17:10–17:30

Gradient-enhanced ductile damage is implemented in a finite element framework by means of an additional field variable, representing nonlocal damage, which is linked to the local damage variable. At material point level the isotropic damage formulation uses exponential damage functions to circumvent further constraints on the local damage variable. The ductility of the model is achieved by a coupling to finite strain plasticity. In a multisurface approach the onset of damage and plasticity is each governed by damage and yield criteria respectively. Linear and exponential isotropic hardening is implemented and the intricacies of the interaction between damage evolution and plastic hardening are discussed.
The simulation results are compared to experiments on tensile specimens made from DP800 sheets. With the help of a DIC-System the inhomogeneous displacement field is captured during the experiments and afterwards used in a parameter identification. The feasibility to identify the regularisation parameter controlling the width of the damage zone is analysed.

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3. T. Waffenschmidt, C. Polindara, A. Menzel and S. Blanco, A gradient-enhanced large-deformation continuum damage model for fibre-reinforced materials, Computer Methods in Applied Mechanics and Engineering, vol 268, p. 801-842 (2014)

Texture in polycrystalline nickel based superalloys

Lukas Munk (*Leibniz Universität Hannover, Institut für Kontinuumsmechanik*), Silvia Reschka (*Leibniz Universität Hannover, Institut für Werkstoffkunde*), Stefan Löhnert (*TU Dresden, Institut für Mechanik und Flächentragwerke*), Hans Jürgen Maier (*Leibniz Universität Hannover, Institut für Werkstoffkunde*), Peter Wriggers (*Leibniz Universität Hannover, Institut für Kontinuumsmechanik*) 17:30–17:50

For at least 60 years, Ni based superalloys have attracted scientific attention due to their good high temperature properties under load. In this study, focus is on the mechanical modelling of polycrystalline superalloys, which in contrast to single crystal alloys necessitates an appropriate description at the grain level. Tracking of grain orientation during inelastic deformation at high temperature has been accomplished by means of a new Electron Backscatter Diffraction (EBSD) method [1]. These data allow for the validation of a phenomenological and a physics-based local crystal plasticity model, which can be rapidly extended to account for additional constitutive equations. The second physics-based model employing the Dyson approach [2] incorporates temperature and parameters of the sub grain scale. The constitutive equations are presented and numeric results are compared to experimental data.

[1] S. Reschka, L. Munk, P. Wriggers, H. J. Maier, An EBSD Evaluation of the Microstructure of Crept Nimonic 101 for the Validation of a Polycrystal–Plasticity Model, Journal of Material Engineering and Performance (2017). https://doi.org/10.1007/s11665-017-3046-3

[2] B. F. Dyson, Microstructure based creep constitutive model for precipitation strengthened alloys: theory and application, Materials Science and Technology (2009). https://doi.org/10.1179/174328408X369348

Effect of grain orientations on the thermal grain boundary grooving in a three-dimensional setting

Asim ullah Khan (*Lehrstuhl für Mechanik - Materialtheorie, Ruhr-Universität Bochum (RUB)*), Klaus Hackl (*Lehrstuhl für Mechanik-Materialtheorie, Ruhr-Universität Bochum (RUB)*) 17:50–18:10

The object of this work is to study the effect of grain orientation on thermal grooving by surface diffusion. Hackl et al. have presented a finite element model for thermal grooving in three-dimensions [1]. This variational model involves surface energy, grain boundary energy, external and internal triple line energy and quadruple point energy. We use an orientation dependent surface energy. For {1 0 0} grain orientation in the normal direction, we have self-similar groove profiles under different degree of anisotropy of the surface energy. For {1 1 0} and {1 1 1} orientations, there is formation of facets for critical anisotropic cases. These formations are due to so-called missing orientations concerning the shape of an unconstrained crystal in equilibrium. The rate of grooving varies with change in surface free energy anisotropy. Flux along the triple line is also important in determining the groove root shape. Triple line energy and its mobility lead to deviate from a typical $t^{\frac{1}{4}}$ scaling law. Grain boundary energies are constant in all these simulations, satisfying Herring's relation. Comparisons are made for different values of mobilities for groove shape and its growth rate, using different grain orientations.

Cyclic plasticity modelling with a new type of nonlinear kinematic hardening

Volodymyr Okorokov (*Mechanical and Aerospace Engineering, University of Strathclyde*), Yevgen Gorash (*Mechanical and Aerospace Engineering, University of Strathclyde*), Donald MacKenzie (*Mechanical and Aerospace Engineering, University of Strathclyde*), Ralph Rijswick (*Weir Minerals*) 18:10–18:30

Material behavior of low carbon structural steels are investigated extensively in a wide range of industrial fields, especially in applications with dynamic loading conditions. Within these applications there are cases when the material yield strength is exceeded. Therefore, knowledge of the plastic response of low carbon steels is of high importance for an accurate prediction of the

structure behavior. Despite comprehensive research in cyclic plasticity, there are still deviations between mathematical modelling and experimental results, especially when specific loading conditions are considered. Recently developed models show good agreement with experiments for prediction of ratcheting rate and stabilized stress strain state of cyclic softening or hardening. However, for applications where prediction of an accurate stress strain state after a few cycles of loading is required, these models might not be as accurate as for prediction of the stabilized stress strain state. For low carbon steel, the simulation of cyclic plasticity is complicated by the fact that the initial monotonic stress-strain curve differs significantly from the cyclic stress strain curves. This study aims to develop a plasticity model which can simulates different plasticity phenomena with high accuracy. This is achieved through a new non-saturation type of nonlinear kinematic hardening without back stress decomposition and introducing a new type of internal variable to describe the transition effects between stress strain curves in cyclic loading. The new model is able to accurately describe the stress strain curve shape with a minimum number of material constants, which are determined in a straightforward manner.

S06.05 | Material modelling in solid mechanics

Date 21.03.2018
Room 2750

A variational framework for distance-minimizing data-driven computing method

Lu Trong Khiem Nguyen (*Civil and Environmental Engineering, Institute of Applied Mechanics (CE) - Chair of Material Theory, University of Stuttgart*), Matthias Rambausek (*Civil and Environmental Engineering, Institute of Applied Mechanics (CE) - Chair of Material Theory, University of Stuttgart*), Marc-André Keip (*Civil and Environmental Engineering, Institute of Applied Mechanics (CE) - Chair of Material Theory, University of Stuttgart*) 08:30–08:50

The distance-minimizing data-driven computing method initiated by Kirchoerfer and Ortiz [1] is revisited in the present work. Basically, a boundary value problem of continuum mechanics consists of three ingredients: The compatibility condition on the primary field, the conservation laws, and the material laws that relate the work conjugates such as the linearized strain and the Cauchy stress. The material laws are usually expressed in terms of a functional relationship that fits empirical observations based on experimental data. Thus, there are uncertainties in this approach of calibrating the constitutive laws. In the data-driven computation such functional relation is replaced with an abundant collection of material data. In this manner, we may control the errors in the material laws, conservations laws and compatibility conditions in contrast to the classical approach in which one may produce high numerical precision using FEM with material laws of far less accuracy. The data-driven problem can be expressed as an optimization problem: Find the point in the collection of material data points that minimizes the errors in the conservation laws, compatibility conditions and essential constraints [1, 2]. The present contribution proposes a variational framework for the distance-minimizing method using Lagrange multipliers for both the conservation laws and the compatibility condition in the continuous setting [3]. An interpretation of the resulting algorithm as a staggered scheme is also provided. As a consequence, the Galerkin-based methods with different possibilities of interpolation functions can be used. Several representative examples are illustrated in order to justify the proposed variational formulation.

[1] T. Kirchdoerfer, M. Ortiz, Data-driven computational mechanics, Computer Methods in Applied Mechanics and Engineering 304 (2016) 81–101.

[2] L. T. K. Nguyen, M.-A. Keip, A data-driven approach to nonlinear elasticity, Computers and Structures 194 (2018), 97–115.

[3] L. T. K. Nguyen, M. Rambausek, M.-A. Keip, A variational framework for distance-minimizing data-driven computing method, in preparation.

Thermo-mechanical modelling and finite element analysis of self-piercing riveting processes

Marvin Nahrmann (*University of Kassel*), Anton Matzenmiller (*University of Kassel*) 08:50–09:10

The self-piercing riveting is an innovative mechanical joining technique widely used in modern lightweight constructions. Within product development, many time-consuming and cost-intensive experimental tests are needed creating a feasible joining process. Therefore, the finite element analysis of self-piercing riveting processes is of high interest preventing faulty joint design. In this contribution, a thermo-mechanical simulation of the riveting process of two steel sheets is carried out taking into account the conversion of plastic work into heat. Thereby, a recently proposed user defined constitutive model is applied considering the highly temperature and rate dependent characteristics of metals. The user model is based on an enhanced concept of rheological elements and describes the temperature-dependent YOUNGS's modulus, initial yield stress, nonlinear isotropic and kinematic hardening, thermally activated recovery effects and strain rate sensitivity. All constitutive parameters are identified with test data of the microalloyed steel HX340LAD typically used for car body structures. The numerical results of the self-piercing riveting process are compared to the according test data for model validation by means of the final joint geometry as well as the setting force. Thereby, a twodimensional axisymmetric finite element model is applied reducing the numerical effort of the process simulation.

The strain rate intensity factor in plasticity and its application

Sergey Alexandrov (*Beihang University*) 09:10–09:30

This research is motivated by numerous experimental observations that demonstrate that a narrow layer with drastically modified microstructure is generated near frictional interfaces. This layer is usually called white layer in papers devoted to machining processes and fine grain layer in papers devoted to metal forming processes. Two of the main contributory mechanisms responsible for the generation of such layers are: (a) the mechanism of rapid heating and quenching and (b) the mechanism of intensive plastic deformation. The latter can be described by means of the strain rate intensity factor. This factor is the coefficient of the leading singular term in a series expansion of the equivalent strain rate near maximum friction surfaces. This expansion shows that the equivalent strain rate is infinite at the friction surface. Therefore, the strain rate intensity factor controls the magnitude of the equivalent strain rate in its vicinity. A necessary condition for the existence of the strain rate intensity factor is the friction boundary condition in the form of the maximum friction law. This boundary condition is often adopted at the tool - chip interface (at least, over a portion of this interface) in machining processes. This zone is usually called the sticking zone. The existence of such zones has been reported in deformation processes as well. However, it is worthy of note that the actual seizure (the velocity vector is continuous across the interface) may or may not occur in theoretical solutions. It depends on the constitutive equations chosen. The present paper deals with an approach for using the strain intensity factor in constitutive modeling for predicting the evolution of material properties in a narrow layer in the vicinity of frictional interfaces. The theory developed is supported by experiment on extrusion of a magnesium alloy.

S06.06 | Material modelling in solid mechanics

Date 21.03.2018
Room 2750

Investigation of size effects due to material interfaces

Tim Heitbreder (*Institute of Mechanics, TU Dortmund University*), Niels Saabye Ottosen (*Division of Solid Mechanics, Lund University*), Matti Ristinmaa (*Division of Solid Mechanics, Lund University*), Jörn Mosler (*Institute of Mechanics, TU Dortmund University*) 14:00–14:20

Interface models are well established and frequently applied in material science. However, the thermodynamical consistent combination of classical non-coherent cohesive zone models with surface elasticity is relatively new, cf. [1]. In this, talk a compact and direct derivation of the framework [1] is presented that relies on the variational structure of the underlying problem. Afterwards, the framework is embedded into the finite element method in order to investigate the mechanical influence of interfaces within RVEs. Due to the displacement and traction discontinuities at the interfaces, the homogenization concept has to be extended accordingly (see [2]). Based on the resulting numerical framework, different RVEs are studied. It is shown that the combination of the novel interface model [1] and models for bulk materials leads to a complex size effect covering the frequently observed "the smaller the stiffer" relation, but also the less often observed "the smaller the softer" relation. Furthermore, depending on the parameters defining the interface model, a complex non-monotonic size effect can also be obtained.
[1] N. S. Ottosen, M. Ristinmaa and J. Mosler, "Framework for non-coherent interface models at finite displacement jumps at finite strains", JMPS, 90, 124-141, (2016).
[2] A. Javili, P. Steinmann, J. Mosler, "Micro-to-macro transition accounting for general imperfect interfaces", CMAME, 317, 274-317, (2017).

Bulk material models in cohesive zone elements

Felix Toeller (*Leibniz Universität Hannover, Institut für Kontinuumsmechanik*), Stefan Löhnert (*Technische Universität Dresden, Institut für Mechanik und Flächentragwerke*), Peter Wriggers (*Leibniz Universität Hannover, Institut für Kontinuumsmechanik*) 14:20–14:40

Tailored Forming is a manufacturing process where two metallic materials are joined and formed subsequently. This processing order allows for new designs of hybrid material components. However, the joining zone is heavily loaded during forming. The thickness of the joining zone depends on manufacturing process parameters but is small in general. To evaluate the possibly occurring damage of the joining zone in a coarse scale simulation, a material model has to be developed that captures the complex microstructural behaviour effectively on a macroscopic length scale.
An initially flat element like a cohesive zone element (CZE) is beneficial for meshing and parameter studies due to the small thickness of the joining zone. The material behaviour in CZEs is characterized by traction separation laws (TSLs). TSLs are curves modelled using e.g. the maximum strength and the decohesion energy that depend on the stress triaxiality [2], i.e. TSLs phenomenologically describe specific decohesion situations. Using TSLs is not sufficient for this application as different not previously known stress triaxialities may arise and further damage causing deformation modes (shearing or size changes of the joining zone) may occur.
Continuum material models are able to take all deformation modes into account and their material parameters are independent of a pre-known stress triaxiality. In contrast to TSLs they use

relative variables (strain) instead of absolute ones (separation). Hence continuum material models are not directly combinable with initially flat elements like CZEs. An approach to overcome this limitation is presented along with specialities of its discretisation.

A strong discontinuity approach to crystal plasticity theory

Volker Fohrmeister (*Institute of Mechanics, TU Dortmund University*), Guillermo Díaz (*Institute of Mechanics, TU Dortmund University*), Jörn Mosler (*Institute of Mechanics, TU Dortmund University*) 14:40–15:00

In this talk, a novel, displacement-driven approach to crystal plasticity based on embedded strong discontinuities (ESDA) is presented, cf. [1] and [2]. In contrast to the classical strain-driven approach, which connects the Schmid stress to the slip strain at a certain slip system, the novel approach applies a traction-separation law to connect the Schmid stresses to the slip displacements. Surprisingly, both models show similar mathematical structures which allows to develop a unifying algorithmic formulation. The elaborated algorithmic formulation is fully implicit and the inequalities characterizing rate-independent crystal plasticity theory are solved efficiently by means of so-called Fischer-Burmeister NCP functions, cf. [3]. The resulting solution scheme is extremely robust – even for an arbitrary number of simultaneously active slip systems.

[1] J. Mosler, L. Stanković and R. Radulović, *Efficient modeling of localized material failure by means of a variationally consistent embedded strong discontinuity approach.* International Journal for Numerical Methods in Engineering, 88:10, 1008-1041, 2011.

[2] R. Radulovic, O. Bruhns and J. Mosler, *Effective 3D failure simulations by combining the advantages of embedded Strong Discontinuity Approaches and classical interface elements.* Engineering Fracture Mechanics, 78:12, 2470-2485, 2011.

[3] M. Schmidt-Baldassari. *Numerical concepts for rate-independent single crystal plasticity.* Computer Methods in Applied Mechanics and Engineering, 192:1261–1280, 2003.

Developing a model for the microscopic material behaviour of a tailored formed joining zone of an aluminium-steel hybrid solid component

Martina Baldrich (*Institut für Kontinuumsmechanik, Leibniz Universität Hannover*), Stefan Löhnert (*Institute of Mechanics and Shell Structures, TU Dresden*), Peter Wriggers (*Institute of Continuum Mechanics, Leibniz Universität Hannover*) 15:00–15:20

Tailored Forming is a technology in which two different metallic materials are joined before being formed together. This has the advantage of possible weight reduction of the engineering part and optimised material distribution with regard to the applied loads. One weakness of the technique however is the joining zone which due to the significant differences of the material properties of the joined materials may suffer from high stresses during the forming process that might lead to damage and failure. As a result, it is important to accurately predict the material behaviour of the joining zone during and after the tailored forming process. For this reason a micromechanically motivated material model needs to be developed.
Because of the strong dependence of the effective, macroscopic material behaviour on the thermomechanical and chemical influences on the microscopic level, the polycrystalline material is investigated on the microscopic length scale. Therefor, on the one hand the morphology of the joining zone (according to [1]) and on the other hand the material behaviour of the different components, ferrite, pearlite and aluminium as well as the intermetallic phases, are considered

in detail. Based on [2] the microscopic material behaviour of the components with thermoplastic material behaviour is described considering the atomic lattice and its orientation, the slip systems and dislocation densities as well as the critical stresses and deformation rates.

[1] S. Beese, S. Loehnert and P. Wriggers: Modeling of Fracture in Polycrystalline Materials. In Advances in Discretization Methods, pp. 79-102, 2016.

[2] S. Zeller, S. Löhnert and P. Wriggers, Modelling thermoplastic material behaviour of dual-phase steels on a microscopic length scale. Proc. Appl. Math. Mech., 15: 373–374, 2015

Finite Element Simulation and Analytical Estimation of Eigenstresses in Multi-Layer Thin-Film-Substrate Systems

Melanie Todt (*Institute of Lightweight Design and Structural Biomechanics, TU Wien*), Antonia Wagner (*Institute of Lightweight Design and Structural Biomechanics, TU Wien*), Michaela Nagler (*Institute of Lightweight Design and Structural Biomechanics, TU Wien*), Matthias Bartosik (*Institute of Materials Science and -Technology, TU Wien*), Helmut J. Böhm (*Institute of Lightweight Design and Structural Biomechanics, TU Wien*) 15:20–15:40

Multi-layer thin films are a special type of coating consisting of hundreds of layers with each layer being only a few nanometer in thickness. When simulating the mechanical behavior of such thin films, the high number of layers in combination with the small layer thickness usually leads to a high numerical effort. To overcome this issues a new finite element modeling strategy is developed which is based on the so called stacked shell approach. Within this approach the individual layers are discretized using shell elements leading to a high computational efficiency. The interfaces between the layers are represented using cohesive zone elements making it also possible to simulate delamination between the layers. A further increase in computational efficiency is achieved by using periodic or semi-periodic boundary conditions describing a plate-like periodic structure. The developed finite element model can handle various loading conditions, such as thermal or mechanical loading and can also be used to predict eigenstresses resulting from the manufacturing process. Furthermore, damage within the layers or the substrate as well as delamination can be accounted for. It should be noted that with this model the stress distribution within each layer can be resolved.
The capabilities of the developed finite element modeling strategy are exemplified by simulating the residual stresses in an infinitely large plate-like multi-layer thin-film-substrate system. The results are compared with an semi-analytic model that allows to estimate the eigenstresses resulting from the growth of the layers as well as stresses due to cooling down from manufacturing temperature.

The Particle Finite Element Method for the Modelling and Simulation of Solid Body Interactions

Markus Schewe (*Institut für Mechanik, Technische Universität Dortmund*), Andreas Menzel (*Technische Universität Dortmund*) 15:40–16:00

The simulation and, in particular, the underlying algorithmic treatment of effects such as fracture or abrasive wear are generally very complex in nature and thus time-consuming. The Particle Finite Element Method (PFEM) according to [1] constitutes a promising compromise between physical accuracy and computational efficiency. PFEM is based on two key aspects: (i) the continuous remeshing of particle clouds which represent the bodies under consideration and (ii) a shape detection algorithm, where the α-shape algorithm [2] is used in the present framework.

Conceptually speaking, this algorithm detects, for example, formerly neighboring points of the same particle cloud which then may exhibit a significantly larger distance from each other during loading. If this distance exceeds a certain threshold, the points may be regarded as separated and the connectivity between these points is deleted. Such applications of the PFEM may be incorporated in simulations of fracture and wear. In contrast, the shape detection algorithm may also be used in the complete opposite sense: When two points, which belong to two different particle clouds, approach each other, the α-shape algorithm can detect contact surfaces. In such contact regions, interface patches are generated which can directly be used to formulate the related contact constraints. In this contribution the focus is placed on the basics of the PFEM as well as details on the modelling and simulation of interacting solids along with illustrative numerical examples.

[1] Onate et al. Int. J. Comput. Methods, 1(2): 267-307, 2004. [2] Edelsbrunner, Mücke. ACM Trans. Graph., 13(1): 43-71, 1994.

S06.07 | Material modelling in solid mechanics

Date 21.03.2018
Room 2750

Identification of hyper- and viscoelastic properties of different flexible FDM printed specimens

Thomas Reppel (*Mechanical engineering, University of Siegen*), Kerstin Weinberg (*University of Siegen*) 16:30–16:50

Additive manufacturing, also known as 3D printing, has become a well-established method in many different fields of fabrication. It is a preferred method to produce small series or even individual parts of components. One common 3D-printing technology is fused deposition modeling (FDM), where the basic material, a coiled filament, is heated up and extruded at the desired position.
For applications demanding a highly elastic behavior, thermoplastic elastomers in particular thermoplastic polyurethanes (TPU) and thermoplastic copolyester elastomers (TPC) are frequently used materials in additive manufacturing.
The present work aims at the experimental identification of the hyper- and viscoelastic properties of two different highly flexible filaments, a TPU and a TPC. To this end several uniaxial tensile tests, as well as relaxation and creep experiments of printed specimens are performed. From the measured data we identify the parameters of different hyperelastic models. For the viscoelastic part we find the parameters of a prony series with N elements in a general Maxwell model. We also consider a model based on generalized fractional elements [1, 2, 3].

[1] R. L. Bagley and P. J. Torvik, On the Fractional Calculus Model of Viscoelastic Behavior, J. Rheol. **30**, 133–155 (1986).

[2] R. C. Koeller, Applications of Fractional Calculus to the Theory of Viscoelasticity. J. Appl. Mech. **51**, 299-307 (1984).

[3] F. Mainardi and G. Spada, Creep, relaxation and viscosity properties for basic fractional models in rheology. Eur. J. Phys. **193**, 133–160 (2011).

Identification of parameters on an interpolated function with measurement errors

Niklas Nostitz (*Deutsches Institut für Kautschuktechnologie e.V.*), Jörn Ihlemann (*Chemnitz University of Technology*), Nils Hendrik Kröger (*Deutsches Institut für Kautschuktechnologie e.V.*) 16:50–17:10

While the identification of material parameters via FEM is an important source for efficient simulations, leads the identification itself to new problems. The evaluation of a gradient for a n-parameter-modell with differential quotients requires n+1 function values. Each value is gained after different simulations, which itselves need computational effort of the FEM.
To reduce the effort and to speed up the identification, an alternative optimization is needed with a cheaper evaluation of the function values. An approximation, which is built with supporting points, of the functional landscape owns the disadvantage of not reproducible function values at the supporting points. Therefore, an interpolation algorithm is more suitable. Typical interpolation algorithms for landscape creation are Kriging, Radial base functions (RBF) or NURBS. Due to the fact, that NURBS for higher dimensional usage are complex, this work examines the advantages of Kriging and RBF.
To compare both types and the difference to a usual used Levenberg-Marquardt-algorithm, an optimizer was written. The optimizer uses the supporting points, which are gained after a design of experiments, build up the landscape and find the minimum on it. This point is used to compute a value of the original function, which is a new supporting point for the further optimization.
While there exist some problems of the stability at accumulation of supporting points, the interpolation variant has some advantages with uncertain data. Therefore, some test functions are chosen to give a short overview about the functionality of the algorithms.

Goal-oriented adaptivity for parameter identification in linear micromorphic elasticity

Xiaozhe Ju (*Chair of Engineering Mechanics, University of Paderborn*), Rolf Mahnken (*University of Paderborn*) 17:10–17:30

It is well-known that the classical Cauchy-Boltzmann continuum has limitations, e.g. on the simulation of strain localization phenomena or size effects. For a remedy, one may resort to the so-called generalized continuum theories, see e.g. [1]. Amongst others, we consider a class of higher order continua, namely the micromorphic continua, where the kinematics is enriched by means of a microstructure undergoing an affine micro deformation. As a drawback, the enriched kinematics leads to additional constitutive equations, increasing the number of material parameters, and therefore making the parameter identification procedure more involved. Here, the parameter identification is viewed as an inverse problem minimizing a least-square function. For simplicity, we consider a small strain theory. Moreover, we consider some stability indicators for several different situations. For an effective parameter identification, we adopt a two-step strategy, splitting the identification of macro and micro parameters, see [2]. The increasing number of the degrees of freedom and the material parameters clearly motivates an application of adaptive methods. For direct micromorphic problems, we refer to [3]. Here for the inverse micromorphic problems, we follow the general ansatz by [4] for goal-oriented error estimation and adaptivity, to control the discretization errors of the FEM.

[1] T. Dillard, S. Forest, P. Ienny, *European Journal of Mechanics A/Solids*, **25**, 526-549 (2006).

[2] W. Ehlers, B. Scholz, *Arch. Appl. Mech.*, **77(12)**, 911-931 (2007).

[3] X. Ju, R. Mahnken, *Int. J. Numer. Meth. Engng.*, **112**, 1017-1039 (2017).

[4] R. Becker, B. Vexler, *Numerische Mathematik*, **96(3)**, 435-459 (2004).

On the back calculation of material strength values from strength test results

Martin Schagerl (*Institute of Structural Lightweight Design, Johannes Kepler University Linz*), Markus Grillenberger (*Institute of Structural Lightweight Design, Johannes Kepler University Linz*) 17:30–17:50

The determination of material strength parameters from structural test measurements yields in general an inverse problem. The measured test values are e.g. finite loads and displacements applied on the specimen. The unknown material parameters are e.g. local stress values at particular strain states. Naturally, material models should only contain material parameters which can be identified by such back calculation. However, if material models want to be practically useful, the back calculation should be a simple procedure, which is derived from adapted analytical and numerical models, and where the material parameters are gained in a most direct way. In a complete approach the introduction of a new constitutive model is accompanied with the specification of an according test setup and a validated evaluation procedure, with which the engineer can determine the occurring material parameters. The current contribution discusses this approach on hand of two simple, but non-standard material strength values for metals: First, the flow curve under pure shear, which is determined by using a plane torsion test rig, and second, the compressive strength under high strain rates, which is determined by using a cam drive test rig. For both examples analytical considerations build the basis to develop an appropriate test rig and a validated numerical Finite Element model for evaluation.

Modelling and experimental testing of expanded granules as crash-absorber for double hull ships

Christian Woitzik (*Numerical Structural Analysis with Application in Ship Technology, Hamburg University of Technology*), Mohsin Ali Chaudry (*Institute of Continuum Mechanics, Leibniz Universität Hannover*), Peter Wriggers (*Institute of Continuum Mechanics, Leibniz Universität Hannover*), Alexander Düster (*Numerical Structural Analysis with Application in Ship Technology, Hamburg University of Technology*) 17:50–18:10

In modern shipbuilding double hulls are an established design to increase the stability and collision behaviour of ships. To gain further improvement of the collision safety innovative types of ship side hull structures can be used. Alternatively the filling of the void space between the hulls with energy absorbing and strength increasing material can be considered. This approach was suggested in [1] to be used with existing double hull structures to improve the penetration resistance in case of the collision with a bulbous bow using lightweight granular materials.
The present contribution deals with the experimental testing of lightweight granules like expanded cellular glass beads in a simplified collision test. To do so, two steel plates are used as outer and inner side hull structure. A rectangular steel box is welded in between these panels, which can be filled with granular material. As model for the bulbous bow a hemisphere is used and is driven into this structure. The glass beads considered have a diameter of about two millimeters and a multicellular structure as described in [2, 3]. During the experiment, force-displacement curves and strain values are monitored. Furthermore an optical measurement system is used to obtain additional information about the deformation of the structure.
The described experiment will be used to validate the finite element simulation of the penetration of the double hull with the bulbous bow. To model the granules the Mohr-Coulomb material model is taken advantage of. Based on the experimental data the suitability of the Mohr-Coulomb model will be discussed.

[1] M. Schöttelndreyer, I. Tautz, W. Fricke, E. Lehmann. Side Structure filled with multicellular glass hollow spheres in a quasi-static collision test. Collision and Grounding of Ships and Offshore Structures (Ed: J. Amdahl, S. Ehlers, B. Leira), 101-108. Taylor & Francis Group, London, 2013.

[2] C. Woitzik, A. Düster. Modelling the material parameter distribution of expanded granules. J. of Gran. Matter, 2017. doi: 10.1007/s40571-017-0169-0.

[3] M. A. Chaudry, C. Woitzik, A. Düster. P. Wriggers. Experimental and numerical characterization of expanded glass granules. J. of Comp. Part. Mech, 2017. doi: 10.1007/s40571-017-0169-0.

Computational modelling of particle filled structures with application in ship building

Mohsin Ali Chaudry (*Institute of Continuum Mechanics, Leibniz Universität Hannover*), Christian Woitzik (*Numerical Structural Analysis with Application in Ship Technology (M10), Hamburg University of Technology*), Alexander Düster (*Numerical Structural Analysis with Application in Ship Technology (M10), Hamburg University of Technology*), Peter Wriggers (*Institute of Continuum Mechanics, Leibniz Universität Hannover*) 18:10–18:30

With growth in traffic of ships, the risk of collision is increasing. Efforts are being made to improve the crashworthiness of ships and one promising design approach is to use granular materials in the cavity of double hull ships [1].
Numerical modelling of such a problem can be very challenging as it requires implementation of a robust contact model for the interaction of the ship with the colliding body and a finite strain based elasto-plastic material model for describing the large deformation of the structure. Furthermore, a particle-based method is also required to model granular materials. In this study, a mortar based method is used for the contact formulation which involves a segment-to-segment strategy with weak enforcement of contact constraints. Such a weak coupling leads to a rather robust formulation in case of large deformation and sliding. Regarding the material behaviour, a finite strain based elasto-plastic model is considered, where a multiplicative split of the deformation gradient is applied.
For numerical modelling of granular materials, the discrete element method (DEM) is used where the analysis of particles is carried out at the micro-mechanical level. In this study, expanded glass granular materials are considered, where the bulk and particle level properties of such materials were studied in detail in [2, 3]. The DEM-FEM coupling, as discussed in Wellmann and Wriggers [4], is employed to study the load transfer between granular particles and the confining structure. Finally, a homogenization technique for granular materials will be presented, where macroscopic quantities are derived from volume averaged properties of particles. Such a technique is helpful in the continuum based description of mechanical properties of granular materials.

[1] M. Schöttelndreyer, I. Tautz, W. Fricke, E. Lehmann. Side Structure filled with multicellular glass hollow spheres in a quasi-static collision test. Collision and Grounding of Ships and Offshore Structures (Ed: J. Amdahl, S. Ehlers, B. Leira), 101-108. Taylor & Francis Group, London, 2013.

[2] C. Woitzik, A. Düster. Modelling the material parameter distribution of expanded granules. J. of Gran. Matter, 2017. doi: 10.1007/s40571-017-0169-0

[3] M. A. Chaudry, et al., Experimental and numerical characterization of expanded glass granules. J. of Comp. Part. Mech, 2017. doi: 10.1007/s40571-017-0169-0.

[4] C. Wellmann, P. Wriggers. A 3D Coupled Finite-Discrete Element Method for Modeling the Interaction of Granular Materials and Solid Structures. *Particle-Based Methods, Fundamentals and Applications* pp. 72-75, 2009.

S06.08 | Material modelling in solid mechanics

Date 22.03.2018
Room 2750

An analytical approach to the accurate modeling of visco-elastic materials with stochastic microstructure

Philipp Junker (*Institute of Mechanics of Materials, Ruhr-Universität Bochum*), Jan Nagel (*TU Eindhoven*) 08:30–08:50

Stochastic fluctuations of material properties, i.e. the elastic constants, result in stochastic fluctuations of the material's response to mechanical loading, i.e. the stresses. In this talk, we present an semi-analytical approach to the time-efficient and mathematically accurate modeling of visco-elastic materials with stochastic microstructure. The material behavior is modeled using a viscous strain as an internal variable whose evolution is described by a differential equation. Since the stochastic material properties enter the evolution equation, a stochastic differential equation has to be treated which renders the problem rather uncomfortable. However, we present a precise investigation of the problem that yields a treatment similar to the deterministic case but resulting in the analytical estimation both of the expectation value and the variance (standard deviation) of the stresses. A numerical comparison to Monte Carlo simulations proves the reliability of our approach. Furthermore, first results of a finite element implementation will be presented.

A review on finite thermo-viscoelasticity models – based on hyperelasticity and MORPH

Nils Hendrik Kröger (*Simulation and Continuum Mechanics, Deutsches Institut für Kautschuktechnologie e.V.*), Abhiram Sarmukaddam (*Deutsches Institut für Kautschuktechnologie e.V.*), Jan Plagge (*Deutsches Institut für Kautschuktechnologie e.V.*) 08:50–09:10

Modern polymers (compounds) are developed to endure high stresses and strains on a long-time scale. In order to predict the material behaviour, the polymers has to be examined for their long-term relaxation behaviour. Besides hyperelastic effects, the investigated polymer types shows strong viscoelastic and, especially, strain rate and temperature dependencies for highly-filled compounds, e.g. with Carbon black in case of elastomers.

Tthe applicability of the modelling approach is evaluated for two materials – a polymer used in modern adhesive tapes as well for a technical elastomer compound (EPDM, Carbon black filled).

In order to characterize the polymers mechanically numerous stress-relaxations test with varying loading types, varying strain rates at varying temperature are conducted. Slightly simplified material models for finite thermo-viscoelasticity based on a combination of a hyperelastic basis model, resp. MORPH, a Prony-Series ansatz and a classic Williams-Landel-Ferry extension are identified for different polymers types. The simplification is carried out to overcome the ill-posed identification problem for total free relaxation times and corresponding weights. We present

different approaches for their functional dependencies.

The parameter identification of the models is conducted stepwise. At first the equilibrium stress states are extracted to estimate the hyperelastic response. Hereby, we review the required number of experiments to obtain a stable (unique) parameter combination for the first estimation of the equilibrium. Before the parameter are identified simultaneously for all experiments, in a second step the distribution of relaxations times needed to describe the time dependent effects are estimated as well.

The resulting material model for the adhesive tapes are validated with experiments considering the angle dependency from pull out test, over 45°-loading to simple shear loading and a "stick-on installation process".

Rubber viscoelasticity based on the analytical network-averaging concept

Sugeng Waluyo (*Department of Continuum Mechanics, RWTH Aachen*), Vu Ngoc Khiêm (*Department of Continuum Mechanics, RWTH Aachen*), Mikhail Itskov (*Department of Continuum Mechanics, RWTH Aachen*) 09:10–09:30

Real-life rubber components are frequently subjected to harmonic loads and exhibit complex viscoelastic response. In this contribution, we present a physically-motivated full network model for rate-dependent behavior of elastomers on the basis of the analytical network-averaging concept [1, 2]. Accordingly, we replace all polymer chains in the rubber network by a representative chain. Microscopic boundary conditions of the representative chain can be averaged from the macroscopic deformation via a directional distribution of polymer subnetworks. This orientational distribution function is driven by fluctuation of free chains through entanglements. By this means, the viscoelastic effects of rubber-like materials can be described. The purely analytical model includes very few physically motivated material constants and demonstrates good agreement with a wide range of rate-dependent experimental data of elastomers.

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[2] Khiêm, V. N., and Itskov, M. (2017), Analytical network averaging of the tube model: Mechanically-induced chemiluminescence in elastomers, *International Journal of Plasticity* (DOI:10.1016/j.ijplas.2017.11.001).

Elastic and viscoelastic modeling of pure and fiber reinforced thermoset- and thermoplast-based polymers based on dynamic mechanical analysis

Daniel Wicht (*KIT - Karlsruhe Institute of Technology*), Loredana Kehrer (*Chair for Continuum Mechanics, Institute of Engineering Mechanics, KIT - Karlsruhe Institute of Technology*), Jeffrey Wood (*Department of Mechanical and Materials Engineering, Western University*), Thomas Böhlke (*Chair for Continuum Mechanics, Institute of Engineering Mechanics, KIT - Karlsruhe Institute of Technology*) 09:30–09:50

A thermoplastic-based and a thermoset composite material and their respective polymer matrices are characterized and modeled based on dynamic mechanical analysis (DMA). The first composite is a short glass fiber reinforced polypropylene (PP) with a fiber content of 30wt.% [1]. Additionally, a composite system based on unsaturated polyester-polyurethane hybrid (UPPH)

resin reinforced with 41wt.% long discontinuous glass fibers is introduced [2]. Employing dynamic mechanical analysis, the time, temperature and load-dependent behavior of both materials is investigated. Based on the measured storage and loss moduli, the temperature-dependent degradation of stiffness and the glass transition temperature for all materials are observed. Moreover, PP and its composite system exhibit nonlinear viscoelastic behavior in the investigated range. These effects are also observed for the UPPH based materials, however they are far less pronounced. Based on the obtained matrix stiffnesses, the elastic behavior of the composites is predicted through a Hashin-Shtrikman mean-field homogenization [3] and compared to the experimental results. In addition, the viscoelastic behavior of the polymer matrices is modeled and characterized using a free volume based approach [4].

[1] V. Müller: Micromechanical modeling of short-fiber reinforced composites *Vol. 6. KIT Scientific Publishing*, (2016).

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[4] N. Tschoegl, W. Knauss, I. Emri: The effect of temperature and pressure on the mechanical properties of thermo-and/or piezorheologically simple polymeric materials in thermodynamic equilibrium - A critical review. *Mechanics of Time-Dependent Materials*, **6**, 53–99 (2002).

A Lagrangian Logarithmic Strain Space Formulation of Glass-Rubber Constitutive Model for Amorphous Polymers

Syed Hasan Raza (*Institute of Product and Process Innovation, Leuphana University of Lüneburg, Lüneburg, Germany*), Celal Soyarslan (*Chair of Solid Mechanics, School of Mechanical Engineering and Safety Engineering, University of Wuppertal, Germany*), Swantje Bargmann (*Chair of Solid Mechanics, School of Mechanical Engineering and Safety Engineering, University of Wuppertal, Germany*), Benjamin Klusemann (*Institute of Product and Process Innovation, Leuphana University of Lüneburg, Lüneburg, Germany*)

09:50–10:10

The available glass-rubber constitutive model presented by Buckley et al. [C. Buckley and D. Jones, "Glass-rubber constitutive model for amorphous polymers near the glass transition," Polymer, vol. 36, no. 17, pp. 3301-3312, 1995.] and extended by Adams et al. [A. Adams, C. Buckley, and D. Jones, "Biaxial hot drawing of poly (ethylene terephthalate): measurements and modelling of strain-stiffening," Polymer, vol. 41, no. 2, pp. 771-786, 2000.], exhibit a wide range of physical features such as yielding and strain hardening, observed during the deformation of amorphous polymers. However, these models are formulated using Eulerian (spatial) kinematic measures and their work conjugated stresses, resulting in the need to use objective stress rates where the associated numerical implementation becomes cumbersome. In this work, we reformulate the constitutive model by computing all constitutive response functions in terms of quantities associated with the Lagrangian (reference) state, allowing a transparent and naturally objective implementation. The accuracy assessment of the implementation is realized via quadratic convergence obtained during Newton-Raphson scheme. As an application problem, a combined tension-torsion test of a unit cube is selected.

Modelling and Finite Element Analysis of viscoelastic adhesive joints

Thomas Rehbein (*Department of Mechanical Engineering, Institute of Mechanics, University of Kassel*), Anton Matzenmiller (*University of Kassel*) 10:10–10:30

A finite viscoelasticity model for a polyurethane adhesive is investigated in regard to its capability to describe the rate dependent behaviour of bonded steel joints. Generally, polyurethane adhesives exhibit a nonlinear elastic response at finite strains, which is modelled commonly by the theory of hyperelasticity. The strain energy function is split into a volumetric and isochoric part additively describing the adhesive's nearly incompressibility separately. The Mooney-Rivlin model is applied for the isochoric material response and the volumetric behaviour is described by a model for compressibility taking the Jacobian of the deformation gradient into account. Since the material response of the adhesive is rate dependent, a generalised Maxwell model is proposed for the consideration of viscous effects. The viscoelastic relaxation spectrum is determined based on test data gained from dynamic mechanical analysis at small strains. To this end, the test frequencies are extended by applying the time temperature correspondence principle. The relaxation times and normalised moduli as well as hyperelastic parameters are identified by using the commercial optimisation program LS-OPT. Finally, three-dimensional finite element analyses of the butt joint specimen and thick adherend shear specimen at both different test velocities and varying adhesive layer thicknesses are conducted and the results are compared to the according tests. Furthermore, the damping capacity of the adhesive is evaluated under free vibration and harmonic excitation.

S06.09 | Material modelling in solid mechanics

Date 22.03.2018
Room 1180

Computational stability analysis of magnetorheological elastomers across scales

Marc-André Keip (*Institute of Applied Mechanics, University of Stuttgart*), Elten Polukhov (*Institute of Applied Mechanics, University of Stuttgart*) 08:30–08:50

The present contribution discusses the computational multiscale stability analysis of magnetorheological elastomers (MRE) across multiple length scales. In this connection, the effective properties of the MRE are determined by means of computational homogenization over representative volume elements [1, 2]. Based on that, localization-type macroscopic instabilities are detected by checking the strong ellipticity condition of the homogenized moduli [3]. At micro-level, bifurcation-type instabilities are treated by means of a finite-element based Bloch-Floquet wave analysis [4]. The latter allows us to find changed periodicities of microstructures as well as critical macroscopic loading points, cf. [5]. Some representative numerical examples will demonstrate various aspects of instabilities occurring in MREs.

[1] K. Danas, Effective response of classical, auxetic and chiral magnetoelastic materials by use of a new variational principle, *J. Mech. Phys. Solids* 105:25–53, 2017.

[2] M.-A. Keip and M. Rambausek, Computational and analytical investigations of shape effects in the experimental characterization of magnetorheological elastomers, *Int. J. Solids Struct.* 121:1–20, 2017.

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[4] K. Bertoldi and M. Gei, Instabilities in multilayered soft dielectrics, *J. Mech. Phys. Solids* 59:18–42, 2011.

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Investigations on different Fischer-Burmeister functions applied to the modelling of ferroelectrics

Robin Schulte (*Institute of Mechanics, TU Dortmund University*), Thorsten Bartel (*Institute of Mechanics, TU Dortmund University*), Andreas Menzel (*Institute of Mechanics, TU Dortmund University*), Björn Kiefer (*Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg*), Bob Svendsen (*Chair of Material Mechanics, RWTH Aachen University*) 08:50–09:10

Constitutive frameworks are often subjected to inequality constraints. These occur for example in the modelling of rate-independent evolution of internal state variables and result from physical restrictions. Different techniques – such as penalty methods and Augmented Lagrangian approaches – have been proposed in order to solve related energy minimization problems. Analytical forms of such inequality constraints are provided by the Karush-Kuhn-Tucker conditions (KKTC) which, however, turn out to be rather cumbersome with respect to their algorithmic treatment in general. A more sophisticated method is to reformulate the KKTC via Fischer-Burmeister Non-Complementarity-Problem Functions, which can directly be incorporated into the solution of (non-linear) systems of equations. However, such extended schemes are prone to numerical instabilities caused by the Fischer-Burmeister functions. In this contribution, several alternative Fischer-Burmeister formulations, e.g. a regularised approach, shall be discussed in the context of a micromechanical material model for ferroelectrics. These different formulations are compared to each other in terms of numerical stability and computational efficiency.

Finite element investigations on the cyclic behavior of shape memory alloys

Johanna Waimann (*Institute of Mechanics of Materials, Ruhr-Universität Bochum*), Philipp Junker (*Institute of Mechanics of Materials, Ruhr-Universität Bochum*), Klaus Hackl (*Institute of Mechanics of Materials, Ruhr-Universität Bochum*) 09:10–09:30

Shape memory alloys show the effect of functional fatigue under cyclic loading. This fatigue comes along with a decrease of the stress plateaus in the characteristic hysteresis curve which is also accompanied by an accumulated permanent strain. Cyclic experiments detected that a formation of dislocations trigger a stabilization of martensite and thus, are responsible for this kind of functional degradation. Our model takes into account the inelastic behavior by splitting the phase transformation from austenite to martensite into a reversible and an irreversible process. In addition to that, we will include an orientation distribution function to account –in a numerically very advantageous way– for the shape memory alloy's polycrystalline structure, see [1].

After presenting the material model [2], we will comment on the implementation into a finite element framework. Starting with the simulation of a cyclic loaded wire, we will compare the results with experimental data and also investigate the influence of a cycle-wise changing maximal applied displacement. Additionally, we will demonstrate the mesh-independency of our material model and comment on the good numerical performance regarding calculation times and stability. The presentation is closed by the geometrically more ambitious and application-oriented examples of a plate with a whole and a clamping ring.

[1] P. Junker. A novel approach to representative orientation distribution functions for modeling and simulation of polycrystalline shape memory alloys. Int. J. Numer. Meth. Eng. 98(11) (2014), 799–818.

[2] J. Waimann, P. Junker, K. Hackl. Modeling the Cyclic Behavior of Shape Memory Alloys. Shap. Mem. Superelasticity 3(2017), 124–138.

A normalization concept for smart material actuation by the example of hydrogels

Adrian Ehrenhofer (*TU Dresden*), Thomas Wallmersperger (*Institut für Festkörpermechanik, TU Dresden*) 09:30–09:50

In analogy to the normalization for the mechanical behavior of classic (passive) materials using *stress* σ and *strain* ε, the actuation behavior of smart (active) materials can be normalized as well [2]. In the present research, we show the normalization using the example of hydrogels that swell and deswell under different stimuli like temperature, chemical concentrations, pH or light intensity changes.
The HENCKY strain measure $\varepsilon^{\mathrm{H}}_{KL} = 1/2\ \ln(F_{mK}F_{mL})$ is used to describe the strain of material points due to activation. This can be e.g. the so-called first order volume phase transition due to the Lower Critical Solution Temperature (LCST) behavior of poly(N-isopropylacrylamide) (PNiPAAm) [4, 1]. The HENCKY strain measure is valid in the context of finite deformations, which is needed for most smart materials providing large deformations.
The activation stimulus $S^{\mathrm{activation}}$ has to be normalized consistently as well, in order to acquire a measure similar to the mechanical stress. Then, a sensitivity parameter $\mathcal{D}^{\alpha}$ which depicts a mechanical compliance to an outer stimulus α (e.g. temperature, pH), has to be derived. For isotropic swelling the scalar representation of the activation stimulus with subsequent swelling can be formulated in analogy to the stress-strain relation.
The normalized swelling behavior was numerically implemented using the resemblance of the phenomenon with thermal expansion. The Temperature Expansion Model [3] is then used to perform numerical simulations in a commercial finite element tool for the swelling of hydrogels without any further implementation of specialized subroutines.

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[2] Ehrenhofer, A.; Elstner, M.; Wallmersperger, T.: Normalization of Hydrogel Swelling Behavior for Sensoric and Actuatoric Applications. In: *Sensors and Actuators B: Chemical* 255 (2018), 1343 - 1353.

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[4] Gerlach, G.; Arndt, K.-F.: *Hydrogel Sensors and Actuators: Engineering and Technology.* Bd. 6. Springer Science & Business Media, 2009

An efficient model for the frictional contact of transverse isotropic functionally graded magneto-electro-elastic material

Haibo Zhang (*School of Mechanical Engineering, Beijing Institute of Technology*), Wenzhong Wang (*School of Mechanical Engineering, Beijing Institute of Technology*) 09:50–10:10

Composite material consisting of magneto-electro-elastic components have been increasingly used in engineering applications, particularly in smart material or intelligent structure systems. Functional graded magneto-electro-elastic (FGMEE) materials is the promising alternative to the conventional homogeneous material because they resist more the contact deformation and damage. This paper proposes the three dimensional semi-analytical solution of sliding frictional contact between a rigid insulating sphere and a transverse isotropic FGMEE film based on frequency response functions (FRFs). The multilayered approximation is used to model the FGM, and the FRFs for each MEE layer are derived by applying double Fourier transform to the general solution of governing equations. According to the loading on top surface and continuity conditions on interfaces, the unknown coefficients in FRFs are assembled as two matrix equations and solved through recursive and direct method respectively, which have no limits on the number or the thickness of layers. Based on the obtained FRFs, a highly efficient semi-analytical model (SAM) is developed to solve the frictional contact of FGMEE materials with any layer designs. The conjugate gradient method (CGM) is used to solve the pressure distribution and the fast Fourier transform (FFT) is used to speed up the field related calculation. The model is validated with literature and finite element method. Furthermore the pressure/stress distribution and electric/magnetic potential are studied in different FGM designs to investigate the influence of material layout.

S06.10 | Material modelling in solid mechanics

Date 22.03.2018
Room 2750

Constitutive modeling of the thermal induced crystallization in semicrystalline polymers

Christoph Mittermeier (*LRT 4 Institut für Mechanik, Universität der Bundeswehr München*), Michael Johlitz (*Universität der Bundeswehr München*), Alexander Lion (*Universität der Bundeswehr München*) 14:00–14:20

Depending on their tacticity respectively the collocation of their lateral, the macromolecules of a polymer can be arranged in a partial alignment. This effect is called polymer crystallization and occurs for example when a polymer melt solidifies due to cooling. With isotactic polymers or copolymers comprising isotactic parts a distinct dependence of the crystallisation behaviour on the cooling rate can be observed. These polymers are called semicrystalline, since even at very small cooling rates a considerable amorphous phase is present. Due to this, a glass transition occurs at temperature levels below the crystallisation temperature. The specific volume of the polymer also depends on the temperature history, because both phases exhibit different densities. These constitutive relations can be determined experimentally. In the talk some exemplary experimental results will be presented in order to motivate a thermodynamically consistent model which represents these relations in the time domain [1]. The model is based on an approach for the Gibbs Energy which is partitioned in order to represent the crystalline, the amorphous and the rigid amorphous phase. Therefore the energy approach takes also the mixture entropy of the

phases into account. The rigid amorphous phase represents the interface between the amorphous and the crystalline phase. It arises parallel to the crystalline phase [2]. Thus only two types of internal state variables are necessary to describe the degree of crystallinity and the configuration of the amorphous phase. By using the Coleman-Noll procedure, the energy approach results in constitutive and evolutionary equations which describe the relations with reference to the pressure- and temperature-history. The talk will close with a comparison between numerical and experimental results.
[1] Lion, A.: A thermodynamic approach to model the caloric properties of semicrystalline polymers, Coontinuum Mech. Thermodyn. 28, 799-819 (2016) [2] Wunderlich, B.: Reversible crystallisation and the rigid-amorphous phase in semicrystalline macromolecules. Prog. Polym. Sci. 28, 383–450 (2003)

Study of the microstructure evolution caused by the strain-induced crystallization in polymers

Serhat Aygün (*Institute of Mechanics, TU Dortmund University*), Sandra Klinge (*Institute of Mechanics, TU Dortmund University*) 14:20–14:40

The strain-induced crystallization (SIC) in polymers, such as in natural rubber, is a phenomenon manifesting itself as the natural reinforcement caused by the high deformation. Experimental data obtained from tensile tests show that the crystallization starts at a strain of 200-400%, whereas, at maximum possible stretches of up to 700%, the volume fraction of the crystallinity reaches its highest degree. The growth and reduction of the crystalline regions cause a hysteresis in the stress-stretch curve which indicates that the process has a dissipative character. In our work, the described material behavior is simulated by a micromechanical continuum model which involves the degree of network regularity as an internal variable. The focus is on the formulation of the dissipation potential simulating the reduction of the crystallinity degree during the unloading phase. The current approach furthermore simulates the dependence of the crystal orientation and form on the applied external load, which is achieved by assuming a specific coupling condition between the inelastic deformations and network regularity. Another aspect considered in the contribution is the study of the effective material behavior regarding the stress hysteresis by using the multiscale FEM. This, for example, enables the reconstruction of the possible material microstructure on the basis of the macroscopic experimental data. The latter is of crucial importance since crystalline regions appear at the nanoscale and thus are not yet accessible by any type of microscope. Presently, simulations are the only way to access this type of information.

Modeling and simulation of curing processes using time-adaptive, high-order time integration

Chris Leistner (*Division of Solid Mechanics, Institute of Applied Mechanics, Clausthal University of Technology*), Dilmurat Abliz (*Institute of Polymer Materials and Plastics Engineering, Clausthal University of Technology*), Gerhard Ziegmann (*Institute of Polymer Materials and Plastics Engineering, Clausthal University of Technology*), Stefan Hartmann (*Institute of Applied Mechanics, Clausthal University of Technology*) 14:40–15:00

Fiber composite materials offer many advantages in lightweight construction. They combine at least two components, fibers and matrix material. Epoxy resins are widely used as matrix material. During production process, these epoxy resins cure when exothermic chemical reaction proceed. Due to low thermal conductivity, commonly, an inhomogeneous temperature distribution occurs, which further influences the curing process. Especially for thick-walled structures,

warpage or cracks can be observed inside the final components. Even combustion might occur during curing. The cracks are a result of residual stresses introduced by the chemically shrinking material. This requires an accurate simulation of the process.
In this presentation, the curing properties of a pure epoxy system are investigated. From a set of DSC measurements, the development of the degree of cure is exploited. A special focus lies on the material parameter identification process, which turns out to be a challenging task due to non-uniqueness of the parameters. A particular focus lies on quality measures and identifiability of the parameters. As a result, curing functions commonly applied, can be simplified. In this view, a concept to identify the parameters is proposed. Due to the evolution of the parameters in the heat equation during the curing process - and, of course, in further constitutive equations as well - the dependence on the temperature and the curing state is provided as well. Finally, thermal simulations of boundary-value problems are provided showing the necessity of high-order, time-adaptive time-integration schemes to obtain reliable results. The results are validated by experimental results, where we draw on thermography.

Thermo-hygro-mechanical characterization and modeling of fast-curing polyurethane adhesives

Rebecca Jennrich (*Institute of Mechanics, Universität der Bundeswehr München*), Alexander Lion (*Institute of Mechanics, Universität der Bundeswehr München*), Michael Johlitz (*Institute of Mechanics, Universität der Bundeswehr München*), Sarah Ernst (*Institute of Joining and Welding, Technische Universität Braunschweig*), Elisabeth Stammen (*Institute of Joining and Welding, Technische Universität Braunschweig*) 15:00–15:20

In the context of lightweight construction and modern hybrid technologies, the importance of structural and soft adhesives in the automotive industry is increasing. Polyurethane adhesives are relatively soft, show nonlinear viscoelastic behavior at room temperature and can endure large deformations. Therefore, they are well suited for applications under dynamic loadings and can compensate gap changes generated by materials with different thermal expansion coefficients. Theoretically, the examined adhesive can be cured either thermally or through humidity, resulting in the same mechanical characteristics. In order to minimize the process time in industrial applications the curing temperature must be increased without negatively affecting the mechanical properties of the bond. To this end, the metallic join partner can be induction heated resulting in high heating rates of about 100 to 150 K/min on the adhesive's surface. In comparison with metals polyurethane conducts the heat with a much smaller rate which results in higher temperature gradients within the adhesive layer. The goal of this project is the modeling of a fast-curing polyurethane adhesive under consideration of the changes in the density and the thermomechanical material properties induced by curing, followed by the identification of material parameters to ultimately optimize the curing process.

A finite strain elasto-plastic material model incorporating kinematic and isotropic hardening for thermoplastic polymers

Sebastian Felder (*Institute of Applied Mechanics, RWTH Aachen*), Stefanie Reese (*Institute of Applied Mechanics, RWTH Aachen*), Jaan-Willem Simon (*Institute of Applied Mechanics, RWTH Aachen*) 15:20–15:40

For numerous technically relevant forming processes the springback effect, i.e. the undesired distortion of a part after unloading and removal from tooling, depicts a major problem. To counteract this effect, time-consuming and cost-intensive trial and error approaches are typically conducted to carefully determine the optimal set of process parameters (e.g. tool shape, part

positioning and forming velocity). Hence, a strong demand for computational models, which accurately predict the material and structural response of the part during forming, arises in order to eliminate trial and error approaches.
In this work, a thermodynamically consistent, finite strain elasto-plastic material model is developed. The dependence of the springback on the Bauschinger effect is well known, particularly for bend/unbend operations. Thus, isotropic and kinematic hardening are incorporated into the model to accurately predict the part distortions. The model is based on the formulation proposed by Vladimirov et al. [1] for metallic materials. It is founded on the multiplicative split of the deformation gradient in the context of hyperelasticity. In particular, the well-established Neo-Hookean form is used to formulate the elastic free energy contribution. Therefore, extending the model to simulate the material behaviour of thermoplastic polymers during forming is straight forward [2]. Further, utilizing the multiplicative split of the plastic deformation gradient, an additional strain like internal variable is introduced to describe the kinematic hardening. In addition, to preserve plastic incompressibility an exponential map algorithm is employed for the numerical integration of the internal variables, which has been proposed by Dettmer and Reese [3].

[1] I. Vladimirov, M. Pietryga and S. Reese, "On the modelling of non-linear kinematic hardening at finite strains with application to springback - comparison of time integration algorithms," International Journal of Numerical Methods in Engineering, Vol.: 75, pp. 1-28, 2008.

[2] T. Brepols, I. Vladimirov and S. Reese, "Numerical comparison of isotropic hypo- and hyperelastic-based plasticity models with application to industrial forming processes," International Journal of Plasticity, Vol.: 63, pp. 18-46, 2014.

[3] W. Dettmer and S. Reese, "On the theoretical and numerical modelling of Armstrong-Frederick kinematic hardening in the finite strain regime," Computer Methods in Applied Mechanics and Engineering, Vol.: 193, pp. 87-116, 2004.

Simulation of Anisotropic Diffusion due to Large Deformations in Polymer Blends

Jannik Voges (*Institute of Mechanics, Otto-von-Guericke-University Magdeburg*), Daniel Juhre (*Otto-von-Guericke-University Magdeburg*) 15:40–16:00

Blending polymers with different properties is a popular method to customize the behavior of a polymer material. For this, in some cases, the materials are mixed in molten form. At high temperatures, this usually yields a single phase, consisting of both the polymers. At lower temperatures, the blend often starts to decompose into two or more phases, which can yield a complex microstructure. One way to control this resulting structure, is to treat the cooling melt mechanically, whereby lamellar patterns are often observed. Performing computer simulations can help to understand the behavior of the mixture and thus help to be able to better control the microstructure of the polymer blends in the manufacturing process. This can improve the performance of the material.
Following a well-known approach, a phase-field determines the material distribution in a domain, representing the microstructure of the polymer blend. Here, the Cahn-Hilliard equation describes the evolution of the mentioned phase-field, starting with a random initial distribution. The domain is strongly deformed to force a rearrangement of the structure while the blend is decomposing, thus a large deformation framework is considered, cf. [1]. The decomposition process is investigated, using simulations for different deformations and by comparing them to a simulation free from deformations. Anisotropic diffusion occurs in the deformed domains, which yields regular patterns.

[1] W Hong and X. Wang, A phase-field model for systems with coupled large deformation and mass transport, J. Mech. Phys. Solids 61 (2013) 1281 - 1294.

S06.11 | Material modelling in solid mechanics

Date 23.03.2018
Room 1180

A consistent multi-scale derivation of a micro-plane model within the framework of RVE homogenisation

Johannes Storm (*Institut für Statik und Dynamik der Tragwerke, TU Dresden*), Michael Kaliske (*Institut für Statik und Dynamik der Tragwerke, TU Dresden*) 08:30–08:50

The micro-plane model is an elegant approach to describe complex anisotropic material behaviour by a set of uniaxial deformation states. The model is widely applied in the context of concrete materials and has various formulations for anisotropic damage, creep and plastic material behaviour. In the last three decades, several important extensions have been introduced in order to overcome some issues discovered.
The talk contributes to this class of material models by a consequent multi-scale derivation of a micro-plane-like model within the framework of RVE homogenisation. The new approach preserves the elegant and efficient model structure and yields a thermodynamic consistent scale transition. The model derivation allows to clearly state the conditions on the micro-structure and thereby to classify the micro-plane models and the known extensions with respect to their micro-structural motivations.
The present approach comes with additional freedom regarding the model geometry (number, size, shape and orientation of the planes) and the applicable material models at the micro-scale. Furthermore, micro-structural and numerical argumentations are separated (e.g. definition of the planes) and arbitrary model extensions can be avoided.
The talk presents the new approach and its properties considering classical micro-plane formulations.

Micromechanical modeling of filled elastomers based on the directional hydrodynamic strain amplification

Ehsan Darabi (*Department of Continuum Mechanics, RWTH Aachen University*), Mikhail Itskov (*Department of Continuum Mechanics, RWTH Aachen University*), Manfred Klüppel (*Deutsches Institut für Kautschuktechnologie e. V.*) 08:50–09:10

A constitutive model for filled elastomers is proposed based on the combination of the continuum damage [1] and the dynamic flocculation [2] framework. Damage takes place in both the network rubbery matrix and inside the filler aggregates. Accordingly, the probability density functions of the number of segments and the filler size distribution in all spatial directions evolve with deformation, which causes the stress softening, Mullins effect and induced anisotropy. Multiple breakage and reaggregation of filler clusters with different sizes in the spatial directions are the main sources of the directional hydrodynamic strain amplification. The model includes a few number of physically motivated material constants characterizing the average filler cluster dimension, filler-filler and filler-matrix interaction properties.

[1] S. Govindjee and J. Simo (1991). A micro-mechanically based continuum damage model for carbon black-filled rubbers incorporating Mullins' effect. Journal of the Mechanics and Physics of Solids, 39(1), 87-112.

[2] M. Klüppel (2003). The role of disorder in filler reinforcement of elastomers on various length scales. Advances in Polymer Science, 164, 1-86.

Numerical analysis of reinforced concrete structures with particular focus on bond behaviour

Timo Stein (*Institut für Statik, TU Braunschweig*), Marco Schauer (*Institut für Statik, TU Braunschweig*), Ursula Kowalsky (*Institut für Statik, TU Braunschweig*), Dieter Dinkler (*Institut für Statik, TU Braunschweig*) 09:10–09:30

Due to the broad field of application of reinforced concrete structures, a great importance is attached to the prediction of stress-strain behaviour affected by mechanical loads as well as environmental influences. Up to now, a model has been developed, by which numerical simulations of concrete structures can be performed, where the essential influences during lyfe-cycle are considered. Hereby, coupled THMC-processes are modelled for pure concrete in the framework of continuum mechanics of porous media. Model equations are discretized by the finite element method.
The existing model will be extended by the presented bond model, capturing bond behaviour between concrete and reinforcing ribbed steel bars. The work to be presented aims at systematic analysis of thermo-mechanical behaviour of reinforced concrete structures in the event of fire, as a potential specific influence during life-cycle. Against this background and due to the resulting requirements the approach of a geometrically consistent consideration of the reinforcement is chosen, neglecting the bar ribs in the geometric model. The bond mechanisms are considered by the additional bond model in between concrete and reinforcement. The bond model is discretized by interface elements and incorporates the mechanical interaction of the bar rips with adjacent concrete as well as the damage of the bond zone.
Results of numerical analysis of reinforced concrete structures are discussed with particular respect to the stress-strain behaviour in the bond zone.

Experimental study and discrete element simulation of auger dosing of different pharmaceutical powders

Bilal El Kassem (*RWTH Aachen University in Partnership with Bosch Packaging Technology*), Thomas Brinz (*Bosch Packaging Technology*), Yousef Heider (*Institute of General Mechanics, RWTH Aachen University*), Bernd Markert (*Institute of General Mechanics, RWTH Aachen University*) 09:30–09:50

In pharmaceutical solid dosage forms development, the mechanical properties of powders play a significant role in the flowability and help in understanding the flow behavior and optimizing the design of powder handling equipment. In particular, powder flow depends strongly on the interparticulate interactions between the particles, where with more interactions, i.e. internal friction between particles, the less is the powder flowability and, thus more power is required to accelerate the flow in the dosing machine. One of the main goals of this project is to implement high speed first-in-first-out powder dosing of small quantities and accomplishing high dosing accuracy. Shear cell analysis and empirical methods are used to characterize powder flow. Experimental studies and discrete element method (DEM) simulations on the auger dosing of different pharmaceutical powders are performed. Different parameters including powder properties, geometry design and operating process conditions are used and altered accordingly based

on design of experiments (DoE). Moreover, an approach to correlate between the experimental findings and the DEM simulations is introduced.

Constitutive modelling of sheet-layered lamination stack

M. Volkan Baloglu (*Department of Mechanical Engineering, FAU Erlangen-Nürnberg*), Kai Willner (*Department of Mechanical Engineering, FAU Erlangen-Nürnberg*) 09:50–10:10

The special microstructure of sheet-layered lamination stacks, which is dependent on the manufacturing process, is responsible for difficulties in predicting their deformation behavior. The individual sheets of these components, which are used in electric motors for the rotor and stator, are stacked together with the help of a bonding varnish or with clamps and welded joints, respectively. For the latter case, these sheets are in frictional contact to each other, which makes things even worse in terms of simulating these stacks and eventuates in a nonlinear deformation behavior.
In general, the individual sheet interactions have to be incorporated in any FE-simulation to achieve reasonable results. To avoid a full discretization of the sheet-layered lamination stack, this can be done by homogenization, cf. [1] and [2], to identify a transversely isotropic material model, where the stacking direction represents the preferred direction. For the case of two alternating isotropic layers (sheet and bonding varnish) or for some constitutive contact equations, it is possible to formulate analytically a strain energy function and the elasticity tensor, respectively. Otherwise, these quantities can be derived with the help of a linearization at an operating point.

[1] M. Volkan Baloglu and Kai Willner: *Material modelling of a sheet-layered lamination stack by homogenization.* In *PAMM*, Vol. 16. Wiley Online Library, pp. 509–510, 2016.

[2] M. Volkan Baloglu and Kai Willner: *Numerical homogenization and simulation of a lamination stack.* In 6^{th} *International Electric Drives Production Conference (EDPC)*. IEEE, pp. 67–72, 2016.

Modelling and simulation of HPFRC structural elements

Mieczyslaw Kuczma (*Poznan University of Technology*), Michal Demby (*Division of Concrete Structures, Poznan University of Technology*), Arkadiusz Denisiewicz (*Division of Structural Mechanics, University of Zielona Gora*) 10:10–10:30

Concrete is one of the most widely used construction material nowadays. The concept of high-performance fibre-reinforced concrete (HPFRC) is to enhance the functionality and sustainability of conventional (plain) concrete, especially by its greater ductility as well as higher compressive, tensile and flexural strengths. In the presentation, multiscale constitutive modelling of this heterogeneous multi-phase material will be considered and numerically solved by a two-scale computational homogenization approach, taking into account also the behaviour of HPFRC in its strain softening regime due to development of damage (micro-cracks) leading eventually to failure. Results of numerical simulations for HPFRC cubes and beams, obtained by our own FEM computer programs and by the Abaqus package will be presented. The developed constitutive model was validated by means of our own experimental tests on the HPFRC elements. The obtained experimental and theoretical results are in good agreement.

S06.12 | Material modelling in solid mechanics

Date 23.03.2018
Room 2750

Investigation of the network topology in amorphous silica during tensile load

Franz Bamer (*Institute of General Mechanics, RWTH Aachen University*), Firaz Ebrahem (*Institute of General Mechanics, RWTH Aachen University*), Bernd Markert (*Institute of General Mechanics, RWTH Aachen University*) 08:30–08:50

We investigate the behavior of silica glass using the molecular dynamics method by applying tensile strain until fracture occurs. The inter-atomic forces are calculated using two- and three-body potentials as proposed by Vashista et al. [1]. While the short-range order of the structure of amorphous SiO_2 is defined by the radial distribution function and the bond angle distribution, it is accepted in the literature that the medium-range order is defined by the distribution of the rings within the atomistic ensemble [2,3]. Dependent on the quenching rate, vitreous silica consists of N-fold rings composed of N corner-sharing tetrahedra. In this contribution, the statistics of the rings within the atomistic ensemble is evaluated during increasing tensile strain until fracture occurs. It is shown that the increasing strain and finally the fracture process have a big influence on the distribution of the N-fold rings.

[1] Vashishta, P., Kalia, R.K., Rino, J.P., Ebbsjö, I.: *Interaction potential for SiO_2: A molecular-dynamics study of correlations*, Vol. 41 of Physical Review B. American Physical Society, pp.12197-12209 (1990).

[2] Yuan, X., Cormack, A.N.: *Efficient algorithm for primitive ring statistics in topological networks*, Vol. 24 of Computational Material Science, pp.343-360 (2002).

[3] Pedone, A..: *Properties Calculations of Silica-Based Glasses by Atomistic Simulations Techniques: A Review*, Vol. 113 of Journal of Physical Chemistry C, pp.20773-20784 (2009).

Investigation of austenitic TRIP/TWIP steels by means of a phase field model

Simon Schmidt (*Institute of Applied Mechanics, University of Kaiserslautern*), Matthias W. Klein (*Institute of Materials Science and Engineering, University of Kaiserslautern*), Marek Smaga (*Institute of Materials Science and Engineering, University of Kaiserslautern*), Tilmann Beck (*Institute of Materials Science and Engineering, University of Kaiserslautern*), Ralf Müller (*Institute of Applied Mechanics, University of Kaiserslautern*) 08:50–09:10

Austenitic TRansformation Induced Plasticity/TWinning Induced Plasticity (TRIP/TWIP) steels offer an outstanding combination of formability and strength. Using Electron Backscatter Diffraction (EBSD) technique, the grain orientation and morphology of f.c.c. and b.c.c. phases can be clearly detected in initial state and at definite strains [1].

In order to qualify the driving mechanisms a phase field model is used. The martensitic transformation is modelled by means of a non-conserving Allen-Cahn type equation. The order parameter ϕ is introduced to distinguish between an austenitic parent phase and martensitic phases. In contrast to a sharp interface approach this allows to account for bulk and surface energies without the necessity of explicitly tracking the interface.

For the modelling, we follow [2] in order to focus on the twinning behaviour of the material. The field equations are solved using the finite element method with bi-linear shape functions on 4-node elements. Features of this model are demonstrated by illustrative numerical examples.

[1] M.W. Klein, M. Smaga, R. Skorupski, T. Beck [2017], "Phase transformation and deformation behavior of steels with different content of metastable austenite", Engineering Transactions, **65**, 69–75

[2] R. Schmitt, C. Kuhn, R. Müller [2017], "On a phase field approach for martensitic transformations in a crystal plastic material at a loaded surface", Continuum Mechanics and Thermodynamics, **29**(4), 957–968

The Influence of Cooling Nozzle Positions on the Transient Temperature Field during Cryogenic Turning of Metastable Austenitic Steel AISI 347

Steven Becker (*Institute of Applied Mechanics, University of Kaiserslautern*), Hendrik Hotz (*University of Kaiserslautern*), Benjamin Kirsch (*University of Kaiserslautern*), Jan C. Aurich (*University of Kaiserslautern*), Erik von Harbou (*University of Kaiserslautern*), Ralf Müller (*University of Kaiserslautern*)

09:10–09:30

Metastable austenitic steels offer the opportunity of a surface layer hardening integrated in the machining process. The hardening effect is achieved by a deformation induced austenite-martensite phase transformation, for which high mechanical loads and low temperatures are necessary, typically below room temperature. These conditions can be accomplished during cryogenic turning, allowing a phase transformation in the surface layer of the workpiece. To study the austenite-martensite transformation behavior, information about the temperatures in the contact zone between tool and workpiece during machining is necessary, which can be hardly measured. Thus, an inverse method is utilized to evaluate the inner workpiece temperature distribution during cryogenic turning of metastable austenitic steel AISI 347 via a FE model of the process. The necessary model parameters to describe the boundary conditions are determined by comparing the simulated transient temperature field of the inner workpiece to corresponding experimental data in a least squares sense. Temperature data from experiments is provided by thermocouples and an infrared thermography system. A heat flux from tool to workpiece as well as heat transfer coefficients for forced convection by air and by carbon dioxide as cryogenic coolant are identified for different cutting parameters. Additionally, predictive temperature field simulations for different settings of the cooling system are performed. Rigid body rotation in the model is considered applying convective time derivatives of the temperature field, resulting in an Eulerian representation of the process. Unphysical oscillations occurring in regions of high Péclet numbers are suppressed utilizing a streamline-upwind/Petrov-Galerkin scheme.

Effects of aging on the mechanical response of a die casting alloy

Maria Angeles Martinez Page (*Insitut of Applied Mechanics, Clausthal University of Technology*), Stefan Hartmann (*Clausthal University of Technology*)

09:30–09:50

Zamak alloys can be found in a wide variety of components of the automotive, building, electronic, and toys industry. They are preferred to other materials for die casting foundry for their several advantages. For example, they have a low melting point which allows an economic manufacturing process, they allow the production of components with tight tolerances and are characterized by good mechanical properties. Nonetheless, these alloys also exhibit a change in their mechanical behavior over time. This phenomenon is known as aging and it is associated to microstructural transformations such as diffusion and precipitation of alloying elements and phase transformations.

The influence of aging on the mechanical response of the alloy is first investigated with tension and torsion tests on specimens with different aging times and at different temperatures. Moreover, the aging process is also investigated with measurements of the thermal diffusivity of the alloy, which grows with the microstructural changes over the time. Based on these experimental results, we propose a phenomenological model in which aging is modeled making use of an internal variable. After that, the model is calibrated to the experiments within a parameter identification. Finally, the model is implemented into a finite element code and the behavior of the model is demonstrated with the help of simulations.

Deformation behaviour of small scale cp-titanium specimen with large grains

Robert Bischof (*University of Kaiserslautern*), Luisa Böhme (*Materials Testing, University of Kaiserslautern*), Charlotte Kuhn (*Computational Mechanics, University of Kaiserslautern*), Ralf Müller (*Institute of Applied Mechanics, University of Kaiserslautern*), Eberhard Kerscher (*Materials Testing, University of Kaiserslautern*) 09:50–10:10

Manufacturing processes on small scales are necessary to satisfy the need of increasing production accuracy. The Finite-Element-Method (FEM) is an important tool to predict the workpiece behaviour in the development of such manufacturing processes. In micro machining processes the machining tool is about the same scale as the grains of the crystalline workpiece. Thus the crystal structure has to be considered in the FEM material model.
The influence of the microstructure of commercially pure (cp-) titanium is modeled by a crystal plastic material model. It considers the reversible elastic behaviour through a compressible Neo-Hookean material law. The anisotropic plastic deformation is considered by specifying the slip systems of the hexagonal-closed-packed crystal structure. To circumvent the difficulties associated with possible non-uniqueness of the set of active slip systems, a viscoplastic material is used. The viscoplastic parameters are chosen such that the viscoplastic material behaviour approximates the elasto-plastic limit. Due to the volume preserving plastic deformation, locking effects can arise, which is dealt with by a modified F-bar deformation gradient.
The results of the FEM-Simulations are compared with the experimental data for further development and validation of the material model. To investigate the material behaviour of cp-titanium small scale tensile tests are performed. The dimension of the sample are small enough that the crystal structure has an influence on the material behaviour, but large enough that the material can be considered as polycrystal. Electron backscatter diffraction (EBSD) investigations of the sample provides the specific grain orientations of microstructure to perform realistic simulations.

Boundary value problems in the theory of thermoelasticity for materials with a triple porosity structure

Merab Svanadze (*Institute for Fundamental and Interdisciplinary Mathematics Research, Ilia State University*) 10:10–10:30

This talk concerns with the linear theory of thermoelasticity for materials with a triple (macro, meso and micro) porosity structure. The system of the governing equations based on the equations of motion, the constitutive equations, the concept of the mechanics of materials with voids and Fourier's law of heat conduction. The system of equations of motion is expressed in terms of the displacement vector field, the changes of volume fractions from the reference configuration corresponding to the three pore systems and the temperature.
In this talk the 3D basic boundary value problems (BVPs) of steady vibrations of the theory of thermoelasticity for materials with a triple porosity structure are investigated. The representations of general solutions for the system of equations of steady vibrations and Green's formulae

in the considered theory are obtained. The Sommerfeld-Kupradze type radiation conditions are established and the uniqueness theorems for solutions of the BVPs of steady vibrations are proved. The basic properties of surface and volume potentials are established. On the basis of the potential method and the theory of singular integral equations the existence theorems for solutions of the BVPs of steady vibrations are proved.

S07 | Coupled problems

Organiser Alexander Düster (*Numerical Structural Analysis with Application in Ship Technology, TU Hamburg (TUHH)*)
Ralf Jänicke (*Department of Industrial and Materials Science, Chalmers University of Technology*)

S07.01 | Coupled problems

Date 20.03.2018
Room N1190

Quasi-Newton – A Universal Approach for Coupled Problems and Optimization

Miriam Mehl (*Institute for Parallel and Distributed Systems, University of Stuttgart*), Benjamin Uekermann (*Computer Science, Technische Universität München*), Klaudius Scheufele (*University of Stuttgart*), George Biros (*University of Texas at Austin*), Andreas Mang (*University of Texas at Austin*) 08:30–09:10

Quasi-Newton methods are used in many fields to solve non-linear equations without explicitly known derivatives. This is the case, e.g., in coupled multi-physics applications such as fluid-structure interactions where we combine several independent solvers in a partitioned approach to a coupled simulation environment. To do so, we have to solve a (in general non-linear) interface equation that contains operator contributions from all involved single-physics solvers. If we assume that these solvers are black-box, quasi-Newton methods are the best known method to accelerate pure interface fixed point iterations. In PDE-constrained optimization, i.e., inverse solvers that are based on gradient descent, we have to find the root of the (reduced) gradient of the objective function. Though the Hessian can usually be calculated and used in an inner Krylov method, these calculations are typically costly as they involve the solution of forward and adjoint problems. Thus, quasi-Newton methods are an efficient alternative. In both cases, coupled problems and optimization, an additional advantage of quasi-Newton over Newton methods is the fact that we can directly approximate the inverse Jacobian or Hessian such that no inner linear solver is required. We present a comparison of known quasi-Newton methods for multi-physics such as interface quasi-Newton with methods usually used in optimization, in particular the BFGS method that is, e.g., used in PETCs's TAO package. Results for two applications – fluid-structure interaction and inverse tumor simulation – demonstrate their potential in terms of robustness, generality, and efficiency.

A numerical approach for fluid-structure interaction in biological applications

Marco D. de Tullio (*Department of Mechanics, Mathematics and Management (DMMM), Politecnico di Bari*) 09:10–09:30

Numerical simulation of biological applications can be particularly challenging, especially in cases involving very thin bodies interacting with the fluid, undergoing large deformations. The numerical method should be able to describe the fluid and the complex deforming geometries in an efficient way, while preserving accuracy. In this work, a versatile numerical method is presented to predict the interaction of thin structures immersed in an incompressible fluid, with the aim of simulating different biological engineering applications. The fluid-structure-interaction problem is handled by a partitioned approach. A direct-forcing immersed boundary method is adopted, based on a moving-least-squares approach to reconstruct the solution in the vicinity

of the immersed surface. A simple and efficient interaction-potential approach is considered for describing the dynamics of deformable structures, so as to easily model and simulate different biological systems, without affecting the computational time and simplicity of the overall method. The fluid and structure solvers are coupled in a strong way, by means of an iterative predictor-corrector approach, in order to avoid instabilities related to large accelerations of the bodies. The effectiveness of the method is validated by means of several test cases involving thin elastic structures, with a very good agreement with available data in literature. Finally, the blood dynamics through heart valves in realistic configurations is selected as a case study. The tool presented is shown to reproduce accurately the flow and structure dynamics, giving results in good agreement with experimental data obtained for similar configurations.

Monolithic fluid-structure interaction formulations for membranes and their application to liquid contact

Roger A. Sauer (*RWTH Aachen University*) 09:30–09:50

A computational framework is presented for fluid-structure interaction (FSI) between fluids and membranes, considering both solid and liquid membranes [1]. The membrane discretization is based on curvilinear surface finite elements that can describe large deformations and rotations [2], and also provide a straightforward description for contact. The fluid is described by the incompressible Navier-Stokes equations, and its discretization is based on stabilized Petrov-Galerkin FE. In the special case of Stokes flow, also boundary element methods can be used within the proposed framework. The coupling between fluid and structure uses a conforming sharp interface discretization, and the resulting non-linear FE equations are solved monolithically within the Newton-Raphson scheme. An arbitrary Lagrangian-Eulerian formulation is used for the fluid in order to account for the mesh motion around the structure. The formulation is very general and admits diverse applications that include contact at free fluid surfaces. This is demonstrated by various analytical and numerical examples. They include rolling droplet, flowing melts and flapping flags.

[1] R.A. Sauer and T. Luginsland (2017), "A monolithic fluid-structure interaction formulation for solid and liquid membranes including free-surface contact", https://arxiv.org/abs/1710.02128

[2] R.A. Sauer, T.X. Duong and C.J. Corbett (2014), "A computational formulation for constrained solid and liquid membranes considering isogeometric finite elements", Comp. Methods Appl. Mech. Engrg., 271:48-68

Coupled simulations involving light-weight structures within turbulent flows: a complementary experimental and numerical application

Guillaume De Nayer (*Department of fluid mechanics, Helmut Schmidt University*), Jens Nikolas Wood (*Department of fluid mechanics, Helmut Schmidt University*), Michael Breuer (*Department of fluid mechanics, Helmut Schmidt University*), Andreas Apostolatos (*Chair of Structural Analysis, Technical University of Munich*), Roland Wüchner (*Chair of Structural Analysis, Technical University of Munich*) 09:50–10:10

In order to accurately simulate coupled problems involving practically relevant light-weight structures exposed to turbulent flows, an ongoing cooperation between the Helmut-Schmidt University Hamburg and the University of Technology Munich was established. It led to an enhanced computational methodology based on the following ingredients: For the fluid side a modern eddy-resolving simulation methodology based on the large-eddy simulation technique [1] is applied. To

ensure appropriate inflow conditions mimicking a turbulent boundary layer a digital filter based inflow generator is used, which was recently extended by a source term formulation [5] allowing to inject the inflow turbulence in well-resolved regions. Finally, advanced grid deformation techniques based on hybrid methods were developed [4]. For the structure side a specialized FEM and IGA solver for membranous structures is applied. A coupling software for the exchange of the fluid loads and structure displacements exchanges completes the methodology, which was validated based on 2D benchmarks [2]. Presently, a more realistical case towards civil engineering applications is considered: A wall-mounted air-inflated membranous hemisphere in a turbulent boundary layer. In a first step, complementary experimental and numerical investigations were conducted based on a rigid dome to evaluate the flow complexity [3]. In the second step, the rigid structure is replaced by a deformable membrane. The challenging case is simulated applying the described framework. FSI phenomena are studied in detail and compared with measurements carried out in parallel [6].

[1] Breuer, M., De Nayer, G., Münsch, M., Gallinger, T., Wüchner, R.: Fluid-structure interaction using a partitioned coupled predictor-corrector scheme for the application of large-eddy simulation. *J. of Fluids and Structures*, **29**, 107-130, (2012).

[2] De Nayer, G, Kalmbach, A., Breuer, M., Sicklinger, S., Wüchner, R.: Flow past a cylinder with a flexible splitter plate: A complementary experimental-numerical investigation and a new FSI test case (FSI-PfS-1a). *Computers and Fluids*, **99**, 18-43, (2014).

[3] Wood, J. N., De Nayer, G., Schmidt, S., Breuer, M.: Experimental investigation and large-eddy simulation of the turbulent flow past a smooth and rigid hemisphere. *Flow, Turbulence and Combustion*, **97**, 79-119, (2016).

[4] Sen, S., De Nayer, G., Breuer, M.: A fast and robust hybrid method for block-structured mesh deformation with emphasis on FSI-LES applications. *Int. Journal for Numerical Methods in Engineering*, **111**, 273-300, (2017).

[5] De Nayer, G., Schmidt, S., Wood, J. N., Breuer, M.: Enhanced injection method for synthetically generated turbulence within the flow domain of eddy-resolving simulations. *Computers & Mathematics with Applications*, in press, (2018).

[6] Wood, J. N., Breuer, M., De Nayer, G.: Experimental Studies on the Instantaneous Fluid-Structure Interaction of an Air-Inflated Flexible Membrane in Turbulent Flow. *J. of Fluids and Structures*, under review, (2018).

Coupled simulations involving light-weight structures within turbulent flows: FSI strategy and non-matching interface treatment for isogeometric B-Rep analysis

Roland Wüchner (*Chair of Structural Analysis, Technical University of Munich*), Andreas Apostolatos (*Chair of Structural Analysis, Technical University of Munich*), Guillaume De Nayer (*Professur für Strömungsmechanik, Helmut-Schmidt Universität (HSU) Hamburg*), Michael Breuer (*Professur für Strömungsmechanik, Helmut-Schmidt Universität (HSU) Hamburg*), Kai-Uwe Bletzinger (*Chair of Structural Analysis, Technical University of Munich*)

10:10–10:30

The safe design of light-weight shell and membrane structures within wind flows is typically characterized by the treatment of complex free-form shapes, the appearance of large deformations, and the occurrence of potentially critical flow-induced vibration effects. The characteristic of natural wind is very complicated and it is a highly turbulent flow with huge Reynolds number. In

order to capture properly the relevant flow-induced effects and the transient interaction between structure and wind flow, one needs to couple LES with geometrical nonlinear structural dynamics simulation. The resolution of the complex flow patterns requires (especially around curved shapes) very fine fluid meshes which are typically not needed in the structural field. Moreover, the fluid requires a highly accurate surface description, also in case of large deformations. The latter corresponds well with one of the core ideas of Isogeometric Analysis (IGA). Typically, real-world geometries are composed of multiple NURBS patches with non-matching parametrizations at their seam lines and these complex geometries are built by heavily using trimming operations. The structural analysis on such design models is enabled by the isogeometric B-Rep analysis (IBRA) which is therefore the basis of the presented structural analysis. To enable the coupling to a dedicated and approved LES solver, a non-matching grid treatment between IBRA for thin-walled structures and "classical" fluid discretizations (like FVM and low-order FEM) is elaborated and investigated. A special focus is set on the discussion of peculiarities originating from the multi-patch coupling and the trimming.

S07.02 | Coupled problems

Date 20.03.2018
Room 0606

Multiscale and Multiphase Problems in Elastic Porous Media

Tim Ricken (*Institute of Mechanics, Structural Analysis and Dynamics, Stuttgart University*), Lena Lambers (*Institute of Mechanics, Structural Analysis and Dynamics, Stuttgart University*), Florian Bartel (*Chair of Mechanics, Structural Analysis, and Dynamics, TU Dortmund University*), Lukas Moj (*Institute of Mechanics, Structural Analysis and Dynamics, Stuttgart University*) 08:30–09:10

In this talk we will give an overview about recent developments for the description of multiscale and multiphase problems in elastic porous media based on the theory of porous Media (TPM). Multiphase materials we will consider consist of two, three or more immiscible phases. Partly, the phases carry concentrations of miscible chemical or electrical active components. We will address different kinds of nonlinear phenomena as phase transformation (solidification or growth), biodegradation, detoxification or remediation. Depending on the investigate phenomena, different kinds of multiscale techniques will be presented as the FE2 approach, the PDE-ODE coupling or a two-scale phase field model. After presenting the general framework, examples of numerical simulations will be given including steel solidification, liver detoxification and microstructure depending flow in porous media.

Modeling and Computational Homogenization of Pressure Diffusion in Fluid-Saturated Fractured Rock

Sophie Tunger (*University of Kassel*), Ralf Jänicke (*Industrial and Materials Science, Chalmers University of Technology*), Detlef Kuhl (*University of Kassel*) 09:10–09:30

Fluid-saturated fractured rock is well-known to exhibit a pronounced attenuation of seismic waves. Attenuation is caused by a local redistribution of fluid in networks of intersecting fractures associated with fluid pressure diffusion. Pressure diffusion is a dissipative process and, thus, part of the wave energy is attenuated. Hereby, the morphology of the fracture network strongly influences the particular characteristics of seismic attenuation. Therefore, a deeper understanding of how attenuation signatures depend on the morphology of underlying fracture networks is of utmost importance for the exploration of unconventional hydro-carbon or geothermal reservoirs.

In this contribution, we numerically investigate pressure diffusion in fracture networks which are embedded in a poroelastic rock matrix. We employ a sharp interface formulation to model the fractures as mechanically and hydraulically open conduits. We incorporate pressure diffusion along the fractures and in the poroelastic matrix as well as the exchange of fluid mass ("leak-off") between the fracture network and the rock matrix. All numerical investigations are carried out on the basis of Statistical Volume Elements (SVE). We compute the overall stress response of the medium in terms of computational homogenization.

Computational homogenization and numerical model reduction of pressure diffusion in fractured porous media

Ralf Jänicke (*Industrial and Materials Science, Chalmers University of Technology*), Beatriz Quintal (*Institute of Earth Sciences, University of Lausanne*), Fredrik Larsson (*Industrial and Materials Science, Chalmers University of Technology*), Kenneth Runesson (*Industrial and Materials Science, Chalmers University of Technology*) 09:30–09:50

This contribution deals with the computational homogenization and numerical model reduction of deformation driven pressure diffusion in fractured porous rock. Exposed to a seismic stimulation, the heterogeneity of the material leads to local fluid pressure gradients which are equilibrated via pressure diffusion. However, a macroscopic observer is not able to measure the pressure diffusion process directly. In fact, the observer senses the intrinsic attenuation of an apparently monophasic viscoelastic solid. The aim of this paper is to establish a reliable yet numerically efficient method to identify the properties of the apparently viscoelastic substitute model for pressure diffusion in fractured rock. To this end, we model the fractures as fluid-filled interfaces embedded in a higher-dimensional poroelastic matrix and develop a computational homogenization technique to link the hybrid-dimensional fracture model to the macroscopic viscoelastic model. Inspired by the Nonuniform Transformation Field Analysis, we incorporate numerical model reduction and approximate the space-time dependent fluid pressure field by a linear-combination of a finite number of pressure modes that span a reduced basis. The pressure modes result from a Proper Orthogonal Decomposition of a series of training computations. This decomposition of the fluid pressure field allows us to derive a set of evolution equations of the Maxwell-Zener type for the viscoelastic substitute model. Altogether, this numerical model reduction method only requires a small amount of "offline" computations that do not burden the "online" simulation of macroscopic boundary value problems. This enables us to run full FE^2 computations with reasonable numerical efforts. The proposed method is validated for several scenarios.

Investigations of hydro-mechanical phenomena in fluid-filled fractures using a hybrid dimensional formulation

Patrick Schmidt (*Continuum Mechanics, Institute of Applied Mechanics, University of Stuttgart*), Holger Steeb (*Continuum Mechanics, Institute of Applied Mechanics, University of Stuttgart*) 09:50–10:10

Numerical studies of flow processes in fractured porous media contribute information about underground matter and heat transport properties as well as fluid underground storage capacity characteristics. In the literature diffusion-based models describe subsurface flow precisely. Nevertheless, diffusion-based models lack to reproduce phenomena related to hydro-mechanical effects such as inverse waterlevel fluctuations (Noordbergum effect). Potentially direct numerical (fluid-fracture interaction) methods or coarse grained approaches (Biot's theory) can model such

phenomena. However, when it comes to fractures with high aspect ratios (length vs. aperture, i.e.$l/\delta > 1000$) technical issues arise due to explicit discretization of the fluid domain. The hybrid dimensional approach assumes Poiseuille flow to avoid explicit numerical discretization and reduces the problems dimension by one. The stiffness of the coupled system varies with the bulk modulus of the fluid within the fracture and the elastic moduli of the surrounding matrix. For moderate fluid bulk moduli an iterative coupled system using non-conformal meshes is proposed. In case of large bulk moduli/low compressibilities the governing equations are strongly coupled on the fracture boundary in an implicit fashion. This work proposes and compares two consistent schemes for coupling the hybrid dimensional formulation with the surrounding bulk material. Besides the validation of both methods an outlook on more complex geometries is presented.

Analysis of instabilities in a quasi-static hydraulic fracturing model

Alina Juan-Lien Ramirez (*Institut für Mechanik und Flächentragwerke, Technische Universität Dresden*), Insa Neuweiler (*Institut für Strömungsmechanik und Umweltphysik im Bauwesen, Leibniz Universität Hannover*), Stefan Löhnert (*Institut für Mechanik und Flächentragwerke, Technische Universität Dresden*) 10:10–10:30

The numerical simulation of hydraulic fracturing poses many challenges when it comes to incorporating relevant processes and choosing adequate assumptions under which these should be modelled.
If the model is assumed to behave quasi-statically, an inconsistency between the static behavior of the solid and the dynamic behavior of the fluid is introduced. This has been observed to lead to instabilities in the simulation if the saturated rock matrix (solid deformation and fluid flow through pores) and the fluid flow within the fracture are modelled separately, but coupled through the interface.
We analyze the origin of these instabilities in a two-dimensional poroelastic model with a single embedded fracture and present a stability criterion. The solid component is assumed to be linear elastic and the propagation of the fracture follows the energy release rate criteria. The fluid flow within the pores is described by Darcy's law. A one-dimensional model is used to simulate the fluid flow inside the fracture following the cubic law. The models are fully coupled via Lagrange Multipliers and are solved iteratively in a staggered manner.
Both models are discretized with the Extended Finite Element Method, which has been proven to be effective for the simulation of discontinuities.

S07.03 | Coupled problems

Date 20.03.2018
Room N1190

Advanced isogeometric fluid-structure interaction applications

Alessandro Reali (*Institute of Advanced Study, Technical University of Munich, Department of Civil Engineering and Architecture, University of Pavia*) 16:30–16:50

Isogeometric Analysis (IGA) is a recent simulation framework, originally proposed by Hughes et al. in 2005 [1], to bridge the gap between Computational Mechanics and Computer Aided Design (CAD). The basic IGA paradigm consists of adopting the same basis functions used for geometry representations in CAD systems - such as, e.g., Non-Uniform Rational B-Splines (NURBS) - for the approximation of field variables, in an isoparametric fashion. This leads to a cost-saving simplification of the typically expensive mesh generation and refinement processes required by standard finite element analysis. In addition, thanks to the high-regularity properties of its basis

functions, IGA has shown a better accuracy per-degree-of-freedom and an enhanced robustness with respect to standard finite elements in a number of applications ranging from solids and structures to fluids and fluid-structure interaction (FSI), opening also the door to geometrically flexible discretizations of higher-order partial differential equations in primal form, as well as to highly efficient (strong-form) collocation methods. Within this context, this work aims at presenting two recent interesting applications, where the unique features of IGA have been exploited to obtain powerful simulation frameworks for some specific FSI problems. The first application is related to an IGA approach for FSI which exploits a boundary integral formulation of Stokes equations to model the surrounding flow and a nonlinear Kirchhoff-Love shell theory to model the elastic behavior of the structure [2]. The proposed method seems to be particularly attractive for the simulation of falling objects, since only the boundary representation (B-Rep) of the thin structure middle surface is indeed constituting the mesh for the entire studied problem. The goal of the second considered application is to show the high flexibility and potential of IGA immersed methods to study complex problems as those typically found in Biomechanics (see, e.g., [3]). Within this context, FSI simulations of patient-specific aortic valve designs are successfully carried out (and also compared with medical images) [4].

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Free-surface flows interacting with structures represented via isogeometric shell analysis

Thomas Spenke (*Chair for Computational Analysis of Technical Systems (CATS), RWTH Aachen University*), Norbert Hosters (*Chair for Computational Analysis of Technical Systems (CATS), RWTH Aachen University*), Marek Behr (*Chair for Computational Analysis of Technical Systems (CATS), RWTH Aachen University*), Stefanie Elgeti (*Chair for Computational Analysis of Technical Systems (CATS), RWTH Aachen University*) 16:50–17:10

For many engineering applications the analysis of fluid-structure interaction is complicated by the occurrence of free-surface flows, e.g., in case of sloshing tanks or ship structures. In such cases a geometrically exact representation of the interface is essential not only for the interaction itself, but also for the movement of the free-surface along the deforming structure.
In the presented work a partitioned algorithm is pursued, successively calling the in-house single-field solvers XNS and FEAFA. While XNS is based on the Deforming Spatial Domain/Stabilized Space-Time (DSD/SST) [1] procedure, FEAFA solves the elastodynamic problem using isogeometric shell analysis [2]. The fluid mesh is adapted to free-surface movements via an interface-

tracking approach [3].
The required slip conditions for both the fluid and the mesh have been adjusted to deforming walls with arbitrary shapes. Beyond that, further improvements of interface Quasi-Newton methods allow for a stable and efficient solution of the fluid-structure interaction problem.

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[2] W. Dornisch and S. Klinkel, "Treatment of Reissner–Mindlin Shells with Kinks without the Need for Drilling Rotation Stabilization in an Isogeometric Framework", Computer Methods in Applied Mechanics and Engineering, 276:35-66, 2014.

[3] S. Elgeti and H. Sauerland, "Deforming Fluid Domains within the Finite Element Method: Five Mesh-Based Tracking Methods in Comparison", Archives of Computational Methods in Engineering, 23(2):323-361, 2016.

Model order reduction for monolithic fluid-structure interaction

Davide Baroli (*Institute of Computational Engineering,FTCS, University of Luxembourg*), Andreas Zilian (*University of Luxembourg*) 17:10–17:30

In this talk we deal with Reduced Order Methods (ROM) applied to a monolithic fluid-structure problem (incompressible and small-deformation structure) regarding harvest energy application. The high-fidelity and reduced order method are based on the one-field fluid-structure formulation where the velocity field is defined over the whole domain. Thus, the pressure and stress are the additional unknown for fluid and structure respectively. A proper orthogonal decomposition enhanced by a reduced assemble is proposed to perform the model order reduction of the parameterized system of PDEs. The method is validated on academic test for the piezoelectric scenarios.

An efficient splitting scheme for fluid-solid interaction

Henk Seubers (*Computational Mechanics and Numerical Mathematics, University of Groningen*), Arthur Veldman (*Computational Mechanics and Numerical Mathematics, University of Groningen*) 17:30–17:50

In hydrodynamical applications, considerable masses of water are moving around vessels and solid structures. When these large masses are coupled to the solid motion, strong interactions between fluid and solid occur. Traditional coupling approaches based on separate fluid and solid models may show numerical instabilities when the effective fluid mass exceeds the solid mass. This could be overcome by one combined numerical model for the fluid and solid, which is not always desirable given the way in which models are developed.
However, we may apply a splitting to the coupled problem, where the inertial forces are treated separately from the remaining dynamics within the fluid and solid. Since the inertial part dominates the coupling, it is treated implicitly whereas the other parts are treated explicitly. This provides a stable method, similar to a fractional step method. The inertial part of the fluid-solid problem can then be solved efficiently within the fluid model as a modified boundary condition for the pressure. Using this strategy, the solver structure remains intact.

Simulation of thermoforming processes with directed air-flow

Simon Wagner (*Lehrstuhl für Strömungsmechanik, FAU*), Fabian Kayatz (*Fraunhofer IVV Dresden*), Manuel Münsch (*Lehrstuhl für Strömungsmechanik, FAU*), Antonio Delgado (*Lehrstuhl für Strömungsmechanik, FAU*) 17:50–18:10

For simply shaped thin-walled plastic mass products, thermoforming is a standard manufacturing method. A plastic sheet is heated and clamped air-tight between a pressure-box above and a mold with the end product's shape below the plastic sheet. Injection of pressurized air into the pressure-box deforms the plastic into the mold. In general the end products exhibit inhomogeneous wall thickness distributions, causing excess raw material consumption in order to achieve the desired properties like for example diffusion resistance[1]. This problem can be alleviated by using plug-assisted pre-stretching of the material[2] or an optimized temperature distribution in the raw material, which leads to a favourable deformation behaviour due to local differences in material strength. While pre-stretching requires more complicated thermoforming machines and locally different pre-heating is rather difficult, a further possibility to influence the plastic sheet temperature during the process is by directing jets of pressurized air onto the areas of the plastic sheet that require local cooling. In cooperation with the Fraunhofer IVV in Dresden, the Institute of Fluid Mechanics of Friedrich-Alexander-Universität Erlangen-Nürnberg is setting up a coupled TFSI model of the thermoforming process with directed air flow, so that numerical parameter studies allow the process to be optimized towards more homogeneous wall thickness distributions. Experimental parameter studies are used for validation and back-up of the process model. The model setup and preliminary results from the (experimental) parameter studies will be shown.

preCICE Coupling Library for Multi-Physics Simulation

Amin Totounferoush (*IPVS, University of Stuttgart*), Miriam Mehl (*Computer Science, University of Stuttgart*) 18:10–18:30

We present the coupling library preCICE providing full functionality to couple different black-box solvers to a partitioned multi-physics simulation environment. Generally there are two approaches for solving multi-physics problems: monolithic approaches and partitioned approaches. While monolithic solutions seem to be less problematic regarding stability issues, the possibility of using existing solvers makes partitioned approaches very attractive. In order to use previously developed solvers in multi-physics simulations, a coupling tool is necessary to connect different solvers to each other. The coupling library preCICE provides communication, data mapping and equation couplings for surface coupled multi-physics applications in a modular way. Up to now preCICE has been used to couple various open-source solvers Open-FOAM, SU2, foam-extend and Calculix and commercial solvers Fluent, FEAP and COMSOL. The applications studied by preCICE include, but not limited to, fluid-structure interaction, fluid-structure-acoustics interaction and heat transfer problems. To obtain accurate results, high grid resolution is required and accordingly multi-physics simulations are run on massively parallel computers and this would result in a large number of communications. A scalable coupling tool must be able to efficiently handle such a large number of communications. This presentation is aimed to introduce different features of preCICE with focus on new communication schemes. Substituting central communication with point-to-point communication and using better communication initialization approaches enhance the preCICE library's scalability.

S07.04 | Coupled problems

Date 20.03.2018
Room 0606

Variational inequalities for saddle point functionals in continuum mechanics and their relevance for satisfying error estimates

Andreas Krischok (*Stanford University*), Christian Linder (*Stanford University*) 16:30–16:50

We present a variational approach towards identifying conditions for stability and uniqueness of Galerkin methods based on saddle point problems in continuum mechanics and continuum thermodynamics. The framework aims to generalize the inf-sup theory in the context of general problems in an arbitrary number of fields for both linear and nonlinear settings. In utilizing a linearized second derivative test for admissible variations, the proposed framework is purely based on uniqueness properties of a mixed Lagrangian around the solution, thus combining requirements that descend from variational calculus with error estimates for finite-dimensional Galerkin methods. In particular, due to its universal form and its straightforward connection to generalized numerical tests, the proposed framework is trusted to provide a helpful tool for the development of mixed methods that arise in many novel engineering problems due to the coupling of multiple physical phenomena.

Examining errors and correction techniques for SPH

Jan-Philipp Fürstenau (*Institut für Kontinuumsmechanik, G. W. Leibniz Universität Hannover*), Christian Weißenfels (*G. W. Leibniz Universität Hannover*), Peter Wriggers (*G. W. Leibniz Universität Hannover*) 16:50–17:10

The Smoothed Particle Hydrodynamics (SPH) method is a Lagrangian meshfree method for the simulation of large motions and deformations. After being developed in the late seventies for astrophysical applications a large community evolved working on many engineering problems like fluid or machining simulations.
Despite its popularity, it is well known that the SPH method in its original form is not even C0-consistent [1]. This inconsistency results from the SPH-ansatz function, the so-called kernel, only depending on the chosen smoothing length, ignoring the current particle distribution. For the examination of the resulting error, the heat conduction equation has been chosen. Heat conduction test cases have the advantage, that their particle distribution remains constant during the whole simulation. In SPH there are two common possibilities to calculate the Laplacian. One is to use the second derivative of the kernel and the other is to replace the second derivative by the first derivative in a finite difference manner [2].
Beside these two general approaches, common and simple correction techniques are tested in one- and two-dimensional test cases. The following questions are adressed: which approach comes closest to the analytical solutions? Which correction technique is insensitive according to irregular particle spacings and free surfaces?

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[2] Fatehi, R., Fayazbakhsh, M., & Manzari, M. T. (2008, April). On discretization of second-order derivatives in smoothed particle hydrodynamics. World Acad Sci Eng Technol (Vol. 30, pp. 243-246).

Numerical modeling of solid particles motion in suspensions using Smoothed Particle Hydrodynamics

Nadine Kijanski (*Institut für Mechanik (Bauwesen), Universität Stuttgart*), Holger Steeb (*Institut für Mechanik (Bauwesen), Universität Stuttgart*) 17:10–17:30

Suspensions and their applications can be found in many fields of mechanical, civil and environmental engineering. The rheological behavior of suspensions strongly depends on their concentration. To consider the flow behavior as well as fluid-solid interactions in dilute suspensions, we present 3D Direct Numerical Simulations (DNS) of a single-phase fluid with discrete solid particles. We therefore present an implementation using the general-purpose particle simulation toolkit HOOMD-blue [1, 3] extended for the usage of Smoothed Particle Hydrodynamics (SPH) [2, 5]. Since both the fluid and the solid part can be discretized by particles, SPH as a Lagrangian particle method presents a good choice to model this particular non-linear problem. To describe solid contact and interaction forces, a simplified Hertz-Mindlin contact model [4] was implemented and applied on all solid particles representing the solid phase in the suspension. Thus, in case of contact, an additional particle force is added to the prescribed forces in the local momentum conservation equation. To review the results of the approach, we discuss an example with multiple spherical solid grains in a single-phase fluid in different configurations as for example gravity or parallel flow. Resulting local particle properties as velocity and shear stresses are considered and compared to known analytical solutions. We focus on particle scale effects as for example the evolution of shear flow dependent on the number of suspended particles.

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[5] R. Sivanesapillai, H. Steeb, and A. Hartmaier. Transition of effective hydraulic properties from low to high reynolds number flow in porous media. *Geophys Res Letters*, 41:4920–4928, 2014. doi:10.1002/2014GL060232.

Smoothed Particle Hydrodynamics model of poroelasticity-fluid coupling

Maria Osorno (*Institut für Mechanik, Universität Stuttgart*), Holger Steeb (*Institut für Mechanik, Universität Stuttgart*) 17:30–17:50

Analysis of hydraulic fracturing is highly relevant in the exploration and production of geothermal energy. The simulation of fluid-filled fractures in porous media requires to model the coupling between a fracture saturated with a compressible fluid and a surrounding (fluid-saturated)

poroelastic rock. A numerical investigation of hydraulic fracturing in poroelastic media includes the treatment of evolving fractures and possible large deformations. The use of classical mesh-based methods in these cases implies computationally expensive geometrical meshing and remeshing pre-processing. Furthermore, employing mesh-based methods may entail other error sources, such as mesh distortions and fracture mesh-alignment. To overcome these difficulties, we use the meshless method Smoothed Particle Hydrodynamics (SPH).
The poroelastic model assumes rigid solid grains (bulk modulus of the grains $K^{\mathfrak{s}} \to \infty$) and negligible effective pore fluid density. In contrast to other poroelastic-SPH methods, the porous domain in our approach is discretized with a single set of particles that carry mixture properties. Further, the fluid-filled fracture is modeled with the Navier-Stokes equations, and solved with a quasi-incompressible single-phase flow SPH scheme. In the presented approach we concentrate on crystalline rock (leak-off could be neglected), therefore we only analyse pressure diffusion in the fracture and the hydro-mechanical coupling with the surrounding porous rock matrix.
We apply our model to low-ratio fractures, and present study cases for smooth fractures and fractures with asperities. Future work includes computation optimization for simulation of higher ratio fractures.

Coupling Peridynamic Continuum Mechanics with analytical solutions

Moritz Becker (*Chair of Structural Mechanics, TUM BGU*), Gerhard Müller (*TUM Department of Civil, Geo and Environmental Engineering, Chair of Structural Mechanics, Technische Universität München*) 17:50–18:10

Peridynamics is a nonlocal formulation of continuum mechanics which uses integral equations for the balance of momentum and an internal length scale called the peridynamic horizon. Therefore, the theory is able to deal with discontinuous displacement fields and shows dispersive behavior. However, the computational costs of peridynamic algorithms are higher than e.g. Finite Element methods. Thus, it is desirable to limit the peridynamic discretization to regions where discontinuities are likely. Investigated is a 1-D bar which is separated in two regions. One region is discretized with Peridynamics. Coupled to this region is a 1-D classical continuum, for which analytical solutions exist. In the scope of this talk, the coupling of both regions is presented. Subsequently investigated is the influence of the length of the peridynamic horizon in the coupling region and the dispersive effect of the peridynamic waves on the solution. The results are compared to a Finite Element analysis.

Metal Particle Melting Analysis for Additive Manufacturing Using the Stabilized Optimal Transportation Meshfree Method

Henning Wessels (*Institute of Continuum Mechanics, Leibniz Universität Hannover*), Tobias Bode (*Institute of Continuum Mechanics, Leibniz Universität Hannover*), Christian Weißenfels (*Institute of Continuum Mechanics, Leibniz Universität Hannover*), Peter Wriggers (*Institute of Continuum Mechanics, Leibniz Universität Hannover*) 18:10–18:30

Selective Laser Melting (SLM) is an Additive Manufacturing (AM) process where a powder bed is locally melted. Layer by layer, complex three dimensional geometries including overhangs can be produced. Non-melted powder thereby acts as a support structure. The process is held under an inert gas atmosphere to prevent oxidation. The principal machine parameters in SLM processes are the laser power, the scan rate and the laser spot radius. The powder bed is characterized by the material, the packing density and the particle size distribution. These factors define the structure of SLM finished parts. Up to date, the material and process development of SLM mainly relies on experimental studies that are time intensive and costly. Simulation tools offer

the potential to gain a deeper understanding of the process - structure - property interaction. This can help to find optimal process parameters and to individualize AM manufactured parts. A continuum framework for the finite deformation phase change problem is presented. For its numerical solution the stabilized Optimal Transportation Meshfree Method [1] is employed. The advantage of meshfree over conventional mesh based techniques is that the treatment of particle fusion is intrinsic to the formulation. This is important to resolve the complex moving boundaries between liquid melt flow and solid metal. The melting and consolidation of two powder particles is analyzed as a primary stage towards a SLM process simulation. Different heat source model approaches, namely a volumetric heat source and a ray tracing scheme, are compared and evaluated regarding their influence on modeling the fusion process of metal particles.

[1] Weißenfels, C. and Wriggers, P.: Stabilization Algorithm for the Optimal Transportation Meshfree Approximation Scheme. *Computer Methods in Applied Mechanics and Engineering 2018*. 329:421-443

S07.05 | Coupled problems

Date 21.03.2018
Room N1190

Exact model reduction for nonlinear thermo-mechanical systems

Shobhit Jain (*D-MAVT, ETH Zürich*) 08:30–08:50

We propose a method to reduce a general nonlinear thermo-mechanical system to a lower-dimensional model using slow manifolds. In doing so, we exploit the dichotomy of time scales, featured between the slow thermal dynamics and fast structural dynamics of the potentially high-dimensional thermo-mechanical system. This mathematically rigorous procedure results in a global reduced-order model, whereby the structural dynamics is enslaved to the thermal dynamics. We show that within the thermal buckling limits, such a manifold is globally attracting, i.e., the full system trajectories are attracted to the reduced-order model trajectories at rates faster than the typical rates within the manifold.

A hierarchical computational model for moving thermal loads and phase changes with applications to selective laser melting

Stefan Kollmannsberger (*Chair for Computation in Engineering, TU München*), Ali Özcan (*Chair for Computation in Engineering, TU München*), Massimo Carraturo (*Computational Mechanics and Advanced Materials Group, University of Pavia*), Davide D'Angella (*Chair for Computation in Engineering, TU München*), Nils Zander (*Chair for Computation in Engineering, TU München*), Ferdinando Auricchio (*University of Pavia*), Alessandro Reali (*Civil Engineering and Architecture, University of Pavia*), Ernst Rank (*Chair for Computation in Engineering, TU München*) 08:50–09:10

SLM as an additive manufacturing process bears numerous computational challenges. It is a thermomechanically coupled process in which material coefficients depend non-linearly on the state of the material and the temperature. Moreover, the energy input is highly localized which leads to strong temperature gradients and rapid changes of state in the material. Although the underlying physics of these processes have been investigated in the context of welding, the large span of the involved spatial and the temporal scales call for highly efficient computational

techniques. It is well known that hp-finite elements yield very accurate results for problems with strong gradients or even singular solutions. hp-finite elements are, therefore, an ideal candidate for the simulation of SLM processes. In this contribution, we present a computational framework, which was specifically designed to resolve moving singularities or sharp fronts [1]. Its core employs the multilevel-hp method for the resolution of strong gradients in the solution field [2]. This is complemented by a spatially hierarchic management of material coefficients in the spirit of the finite cell method [3]. We will discuss the computation of the SLM process and evaluate the accuracy as well as efficiency of the presented computational approach by means of comparison to benchmark solutions.

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[3] A. Düster, J. Parvizian, Z. Yang and E. Rank, The finite cell method for three-dimensional problems of solid mechanics, Comp. Meth. Appl. Mech. Eng., 3768–3782, 2008.

S07.06 | Coupled problems

Date 21.03.2018
Room N1190

Numerical and Experimental Investigations of Hydroelasiticity Effects on Wave Induced Loads

Ould el Moctar (*Mechanical Engineering, Universität Duisburg-Essen*) 14:00–14:20

Water entry experiments and computations were performed to identify the effects of hydro-elastic elasticity on impact-induced loads acting of flat bottom structures and to analyze the two-phase flow during water entry. Two bodies were tested. One body was fitted with stiffened, rigid bottom plating; the other body, with thin elastic plating. Bottom pressures and forces acting on the flat bottom plating as well as impact-induced elastic bottom strains were measured and computed High-speed videos of water entry sequences were analyzed to investigate rigid as well as hydroelastic water entry phenomena. Further on, the fluid-structure interaction was computed based on Navier Stokes equations solver (two-way) coupled with a structure solver. Computation and experiments were compared.

Numerical Analysis of the Response of Thin Flexible Membranes to Free Surface Water Flow

Mahtab Makaremi Masouleh (*Mechanical Engineering, TU-Chemnitz*), Günter Wozniak (*Fluid Mechanics, TU Chemnitz*) 14:20–14:40

This work is part of a major research project concerning the design of a light temporary installable textile flood control structure. The motivation for this work is the great need of applying light structures for the protection of coastal areas from detrimental effects of rapid water runoff. In the previous work, the behavior of down scale membrane was examined under hydrostatic pressure by the Abaqus explicit solver, which is part of the finite element based commercially available SIMULIA software. In the current contribution, the procedure to achieve a stable and convergent solution for strongly coupled media including fluids and structures is explained. A partitioned

strategy is imposed to make both structures and fluids be discretized and solved with appropriate formulations and solvers. In this regard, finite element method is again selected to analyze the structural domain. Moreover, computational fluid dynamics algorithms are introduced for solutions in flow domains by means of a commercial package of Star CCM+. Likewise, SIMULIA co-simulation engine and an implicit coupling algorithm, which are available communication tools in commercial package of the Star CCM+, enable powerful transmission of data between two applied codes. This approach is discussed for two different cases and compared with available experimental records. In one case, the down scale membrane interacts with open channel flow, where the water wave is produced by movement of a rigid baffle. The second case illustrates, how the full scale flexible flood barrier behaves, when a massive flotsam is accelerated towards it.

Applied Mechanics on Docking Sequences

Charlott Weltzien (*Institut of Ship Design and Ship Safety, Hamburg University of Technology (TU Hamburg-Harburg)*) 14:40–15:00

Nowadays many shipyards have their own floating docks for both new buildings and repairs. In view of all the challenging projects these days, many yards have to produce designs which are close to or even beyond the structural limits of their docking facilities. This paper presents a first principle based method to calculate the key numeric values to extend the scope of application of floating docks and platforms.
The method calculates the hydrostatic stable equilibrium of the interacting bodies for selected floating situations. The subsequent structural calculations results in the block force distribution by applying the deformations method. In the process the load redistribution of the non-linear wood layers is calculated and the righting levers of the keel blocks are displayed. Moreover the deflection lines of ship and dock are presented. In the case of high deflections of the platform the deflection line is considered in the hydrostatic calculations. The modified buoyancy distribution is then included in the structural calculations.
The described method provides a useful tool to minimize local and global stresses and deformations of the interacting bodies during the docking procedure by fast optimization of the block system arrangement and the ballasting sequences. Different applications to docking sequences have been calculated and are presented in the paper. For validation, measurements on a full-scale docking process have been done.

Numerical Simulation of Wind Turbine Considering the Soil-Structure-Interaction

Marco Schauer (*Instistut für Statik, TU-Braunschweig*) 15:00–15:20

Whenever vibrations are emitted to soil, they induce waves traveling through the ground. This work is focused on the the Soil-Structure-Interaction effects on the dynamic behavior of operating wind turbines. Two different mechanical problems have to be addressed and to be solved simultaneously. The structure of the wind turbine and its foundation as well as parts of the soil are modeled by the Finite Element Method. The surrounding infinite half-space is discretized by the Scaled Boundary Finite Element Method. Both domains are discretized separately in order to reduce the effort of the preprocessing. This leads to non-matching meshes in general. To overcome this issue state projection methods are utilized to exchange state variables at the common interface, while solving the couped FEM/SBFEM approach.

Partitioned simulation of multi-field problems - efficient and robust coupling of fluids and structures

Lars Radtke (*Numerische Strukturanalyse mit Anwendung in der Schiffstechnik, Institut für Konstruktion und Festigkeit von Schiffen, Technische Universität Hamburg*), Tobias Lampe (*Institut für Fluiddynamik und Schiffstheorie, Technische Universität Hamburg*), Marcel König (*Numerische Strukturanalyse mit Anwendung in der Schiffstechnik, Institut für Konstruktion und Festigkeit von Schiffen, Technische Universität Hamburg*), Moustafa Abdel-Maksoud (*Institut für Fluiddynamik und Schiffstheorie, Technische Universität Hamburg*), Alexander Düster (*Numerische Strukturanalyse mit Anwendung in der Schiffstechnik, Institut für Konstruktion und Festigkeit von Schiffen, Technische Universität Hamburg*)

15:20–15:40

Fluid-structure interaction (FSI) constitutes a prominent example for a coupled two-field problem [1]. FSI problems range from biomechanics, where, for example, the blood flow in arteries is of interest to marine applications including the simulation of ship propellers or floating wind turbines. In order to describe the mechanical behaviour of these systems in an efficient way, three-dimensional models cannot be used in the entire problem domain. Instead, computationally less expensive approaches are taken for regions, where a high accuracy is not needed. To this end, some parts of a wind turbine plant, for example, may be considered as rigid bodies (e.g. the platform), while others are modeled as elastic continua (e.g. the rotor blades). Regarding blood flow through arteries, the local flow strongly depends on the up- and downstream vessel network as well as the surrounding tissue, which have to be described using reduced order models that interact with the fully resolved FSI problem. Regardless of the application, the resulting multi-field problems demand for a suitable solution approach. We favor partitioned approaches over monolithic ones as existing field solvers can be reused and coupled in a flexible way using the coupling software comana [2]. In our presentation, we will give an overview of possible applications and focus on the special techniques needed to realize the coupled simulations. This includes interpolation methods needed to couple structural elements (beams and shells) commonly used in maritime applications as well as convergence acceleration methods that circumvent stability problems encountered, for example, in blood flow simulations due to the high added mass effect [3].

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[2] M. König et al. A flexible C++ framework for the partitioned solution of strongly coupled multifield problems. Computers and Mathematics with Application, 72:1764-1789, 2016.

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Partitioned simulation of the fluid-structure interaction of flexible marine propellers in unsteady flow conditions

Tobias Lampe (*Fluid Dynamics and Ship Theory, Technical University of Hamburg-Harburg*), Lars Radtke (*Institute for Ship Structural Design and Analysis, Technical University of Hamburg-Harburg*), Alexander Düster (*Institute for Ship Structural Design and Analysis, Technical University of Hamburg-Harburg*), Moustafa Abdel-Maksoud (*Institute for Fluid Dynamics and Ship Theory, Technical University of Hamburg-Harburg*) 15:40–16:00

Regarding new propeller materials and designs, vibrations and large deformations are becoming increasingly relevant. Therefore, simulation methods need to be developed which take into account the interaction of fluid and structure while retaining a computational effort suitable for the design stage. In the approach to be presented, the fluid mechanical subproblem is solved by means of the software *pan*MARE, which is based on the potential theory. The structural-mechanical subproblem is engaged using different structural solvers as well as modelling approaches. Information exchange between the subproblems is managed by the software *comana*. In addition to a study regarding flexible propeller geometries in unsteady flow conditions, a suitable implicit coupling algorithm, validation of the method and an investigation of different structural modelling approaches are presented in the paper.

S07.07 | Coupled problems

Date 21.03.2018
Room N1190

Thermodynamically consistent modelling and simulation of multicomponent gas transport in elastic porous media within the Theory of Porous Media (TPM)

Andrea Thom (*Institute of Mechanics and Structural Analysis in Aerospace Engineering, Universität Stuttgart*), Tim Ricken (*Universität Stuttgart*) 16:30–16:50

Multicomponent gas transport in elastic porous media includes diffusion in the presence of advection. The interaction between these transport mechanisms can be significant since e.g. the diffusion of light to heavy gas is faster which causes a pressure difference which in turn causes advection into the opposite direction. One basic modelling approach is the linear addition of advection, calculated by Darcy's law using the pressure gradient, and diffusion, modelled by Fick's law using the gradient of the molar concentration of each gas component. Both laws have to be adjusted for the porous media context.
A theoretical and numerical framework is presented based on a biphasic continuum mechanical approach using the well-known Theory of Porous Media (TPM) extended by the mixture theory for the description of a multicomponent gas mixture. The presentation gives an overview of the underlying coupled differential physical equations considering the basic principles of thermochemistry, starting with the evaluation of the entropy inequality in order to receive restrictions for the thermodynamically consistent framework of the constitutive relations. The balance equations of momentum, mass and energy as well as the constraints for phase interaction and mass exchange of the reacting materials and the explicit formulation for the molar flux of the gas components build the governing equations of the model. Weak formulations are numerically implemented into and solved for the primary variables with the Finite-Element-Code FEAP. An academic example is presented using a reacting four-component-gas mixture diffusing through soil.

Investigation the effect of Nano-silica on the depth of water penetration in concrete used in seawater: Case study of Caspian Sea

Omolbanin Arasteh Khoshbin (*Civil Engineering, Institute of Mechanics Statics Dynamics, TU Dortmund University*), Seyed Morteza Seyedpour (*Institute of Mechanics Statics Dynamics, TU Dortmund University*), Tim Ricken (*Institute of Statics and Dynamics of Aerospace Structures, University of Stuttgart*) 16:50–17:10

One of the requirements of concrete structures is functional continuity for which it is considered to be resistance in a certain period. Water during cementing process causes hydration to cause concrete hardness, whereas after hardening of concrete in most cases damages its structure and properties. Dams, waveguides, docks and oil platforms in the seawater are subject to gradual erosion, which is very slow but measurable. Seawater due to the properties of sulphate, acid and alkali is a major threat to concrete durability. Reducing the water absorption into the concrete body is the main step in coping with the erosion and change of particular characteristics, which makes it with high density, low porosity and more durable. One way is adding fine-grained additives as filler in the concrete mixture and fill all the cavities and porosities of the concrete body. Nano derivatives are the additives that have been considered by researchers over recent years. In this research, we study the effect of Nano-silica with 1% and 5% replacement ratios instead of cement on compressive strength and water penetration depth for concrete in environments of the Caspian Sea. Furthermore, we have simulated the water penetration depth and compare the numerical results with experiments.

Keywords:Nano silica, water penetration, Caspian Sea

A fully coupled thermo-hygro-mechanical model for the description of phase transitions in plant tissues

Lukas Eurich (*Institute of Applied Mechanics, University of Stuttgart*), Arndt Wagner (*Institute of Applied Mechanics, University of Stuttgart*), Wolfgang Ehlers (*Institute of Applied Mechanics, University of Stuttgart*) 17:10–17:30

Plants have developed several strategies to cope with freezing events without being damaged. Understanding the strategies is of high interest, as they could potentially be used for the development of bio-inspired construction materials with optimised properties in terms of frost resistance. Since the involved thermo-hygro-mechanical processes in plants upon freezing are strongly coupled, a modelling approach based on the Theory of Porous Media is applied. The phase transition of water is characterised by a jump in physical quantities at a singular surface. The corresponding mass transfer of (liquid) water to (solid) ice is formulated using the energy jump at this interface. This formulation enables a derivation of the velocity of the frost front in the intercellular space. Furthermore, the pore water freezing has two main impacts on the pore space and the notion of porosity: (1) the material descriptions need to account for the so-called compaction point, as the bulk material may undergo a transition from a porous to a solid material and (2) the reduction of the pore space also needs to be considered in the intrinsic permeability of the Darcy-type approach for the fluid flow in the intercellular space. By including also structural properties via spatially varying anisotropic permeability conditions, the description of the so-called water management in plant tissues is reasonably characterised. Moreover, the dehydration of the tissue cells, which is assumed to be crucial for the frost resistance of plants, is included by a Darcy-type approach for the cell-wall perfusion. Selected numerical examples illustrate these effects.

Modeling and simulation of the groundwater level with respect to weirs and river water levels

Jonas Boungard (*Institute of Mechanics and Dynamics, University of Kassel*), Christian Seidel (*Institut für Statik, TU Braunschweig*), Lars Ostermann (*Institut für Statik, TU Braunschweig*) 17:30–17:50

The groundwater level in a certain area has a high impact on both the infrastructure as well as the ecology. As the groundwater level decreases the upwelling decreases too and buildings may be damaged by subsidence. A decreasing groundwater level also leads to problems with the water supply for the flora and fauna. Therefore the estimation of the groundwater flow is of high interest.
The groundwater level in an area is governed by the water level in the rivers in that certain area. As weirs change the water level of the river they also influence the groundwater level. We discuss the impact of a certain weir - the "Allerwehr Hademstorf" - on the groundwater level for the perspective weir replacement. Therefore we derive a numerical model and simulate the groundwater flow close to this weir. Due to the permeable soil in that area we choose to model the groundwater as a phreatic aquifer which leads to a system of nonlinear partial differential equation. The system of governing equations is solved by means of the finite element method. We discuss the results for different water levels at the weir and different domains of interest.

An investigation on residual stresses in gas tungsten arc welding

Baharin Rahim Ali Ali (*Institute of General Mechanics (IAM), RWTH Aachen University*), An Danh Nguyen (*Institute of General Mechanics (IAM), RWTH Aachen University*), Bernd Markert (*Institute of General Mechanics (IAM), RWTH Aachen University*) 17:50–18:10

It is known that the gas tungsten arc welding (GTAW) generates high and localised heat gradients in the welded components, leading to the formation of weld bead and residual stresses that affect their fatigue life. In this work a finite element model of GTAW is presented to estimate the residual stresses for lifetime prediction. Coupling the heat and fluid flow (HFF) approach using the enthalpy-porosity model and the finite element multiphase modelling allows us to simulate the rapid melting and solidification. Moreover, Marangoni effect due to a thermally caused surface tension gradient and the electromagnetic force distribution are also studied. The performance of the proposed finite element model is demonstrated via a simulation of GTAW process with appropriate boundary conditions on temperature and velocity fields. The simulated results are validated with the existing ones in the literature.

S07.08 | Coupled problems

Date 22.03.2018
Room N1190

Numerical Design for Primary Shaping Manufacturing Processes

Stefanie Elgeti (*CATS, RWTH Aachen University*), Sebastian Eusterholz (*RWTH Aachen University*), Markus Frings (*RWTH Aachen University*), Daniel Hilger (*RWTH Aachen University*), Florian Zwicke (*RWTH Aachen University*) 08:30–08:50

Using a mold or die, primary shaping manufacturing processes form material from an initially unshaped state (usually melt) into a desired shape. All of these processes have in common that the exact design of the mold cannot be determined directly and intuitively from the product shape. This is due to the non-linear behavior of the material regarding the flow and solidification processes. Consequently, shape optimization as a means of numerical design can be a useful tool in mold development. The core of our optimization tool is the in-house flow solver XNS, which is based on the finite element method with GLS stabilization. It is able to exploit the common communication interfaces for distributed-memory systems. XNS has been coupled with an optimization framework. Furthermore, a geometry kernel has been developed, which internally describes the geometry of the mold in a CAD-based fashion. The optimization tool has been applied to three melt-based manufacturing processes: plastics profile extrusion, injection molding and high-pressure die casting. Topics discussed will be our approach to shape optimization as well as methods for simulating the flow through, in and behind the mold/die. Recent examples in 2D and 3D will compare different design objectives, material models, and geometry descriptions, giving insight into the influence of these factors on the optimization result.

Behaviour of Anionic and Cationic Hydrogels

Karsten Keller (*ISD, Universität Stuttgart*), Thomas Wallmersperger (*Institut für Festkörpermechanik, Technische Universität Dresden*), Tim Ricken (*ISD, Universität Stuttgart*) 08:50–09:10

Ionic polyelectrolytic gels in aqueous solution – hydrogels – also known as smart materials, react to different kinds of environmental changes, e.g. chemical, electrical, mechanical and thermal stimulation. As a reaction, they show enormous swelling capabilities due to the delivery or uptake of ions and solvent. These properties make them attractive for chemo-electro-mechanical energy converters and for the application as actuators or sensors.
Polyelectrolyte gels consist of a crosslinked polymer network. This network consists of a liquid phase with mobile ions and either bound anionic or cationic charged groups. Ampholytic gels consist of both kinds of bound charges.
The hydrogel is more or less sensitive in its reaction depending on the type of the stimulus. The reaction under chemical stimulation is far beyond the reaction under electrical stimulation. The applied multi-field formulation is capable of giving local concentrations, electric potential distributions and displacements. The swelling of the gel results from changes of fixed charges in the gel as well as from the variation of mobile ion concentrations. The change of the fixed charges is due to dissociation reactions and locally different strains. In this research the reaction of a modelled hydrogel sample under multifield stimulation is investigated. The swelling ratio is assumed to be in the regime of small volume changes and corresponding displacements.
Acknowledgements: This research has been financially supported by the Deutsche Forschungsgemeinschaft (DFG) in the framework of the Priority Programme 1259 (SPP) Intelligente Hydrogele under the grant number Wa 2323/2.

A multi-phase continuum model to model the swelling behavior of SAP-enhanced mortars

Malte Sauerwein (*Continuum Mechanics, Institute of Applied Mechanics, University of Stuttgart*), Holger Steeb (*Continuum Mechanics, Institute of Applied Mechanics, University of Stuttgart*) 09:10–09:30

In this contribution, a novel two-component grouting mortar with adjustable rheological properties is presented. One promising application can be found in the field of mechanized tunneling, where the cavity between the tunnel lining and the surrounding soil needs to be grouted with an adequate mortar. Initially, a low shear viscosity is required in order to pump the complex fluid through pipes to its final position. Once the gap is filled completely, a rapid evolution of shear stiffness is necessary in order to ensure a safe bedding of the tunnel structure. Since a high water content is needed to meet the first requirement, a consolidation process of the grouting mortar is used to get rid of the excess pore water. However, the permeability of the surrounding soil restricts the efficiency and duration of the consolidation process. To overcome this limitation, the innovative concept of adding super absorbent polymers (SAPs) as an additive to the mixture in order to accelerate the gelation process is investigated. SAPs have the ability to absorb large amounts of the aqueous pore liquid depending on the specific polymer characteristics and the chemical composition of the pore liquid. The three-phase material is modeled within a continuum mixture theory based on the Theory of Porous Media (TPM). The solid phase represents the porous skeleton, while the pore space is simultaneously filled with a pore liquid and the SAPs. The mechanical properties of the mixture and the inter-phase mass exchange are linked by the evolution of the internal state variables.

[1] M. Alexandersson, H. Askfelt and M. Ristinmaa. Triphasic Model of Heat and Moisture Transport with Internal Mass Exchange in Paperboard. *Transport Porous Med*, **112**:381-408, 2016.

[2] M. Ristinmaa, N.S. Ottosen and B. Johannesson. Mixture theory for a thermoelasto-plastic porous solid considering fluid flow and internal mass exchange. *Int J Eng Sci*, **49**:1185-1203, 2011.

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Digital Material Laboratory: advantages of controlling the complete workflow of X-ray computed tomography

David Uribe (*Institute für Mechanik - Lehrstuhl für Kontinuumsmechanik, Universität Stuttgart*), Holger Steeb (*Institut für Mechanik - Lehrstuhl für Kontinuumsmechanik, Universität Stuttgart*) 09:30–09:50

The transport, chemical, electrical and mechanical properties of geophysical and engineering materials is highly influenced by its microstructure. The study of a material's microstructure can result in the possibility to enhance its technical application, e.g.investigating porous rock samples

could improve the amount and safety of C02 sequestration in related reservoirs or studying man-made metallic foam could reduce the weight of the material by a parallel increase in stiffness. The use of micro X-ray computed tomography (XRCT) to obtain the material's microstructure has increasingly gained attention, since advances in X-ray sources, computing power in consumer computers, and electronics in digital detectors have increased the quality and decreased the costs of a single tomographic acquisition.
The workflow of XRCT to study materials is straightforward. It can be separated into three steps: sample preparation, tomographic acquisition and tomogram analysis. In the present work, the advantages of an integrated workflow are shown. This includes the design and setup of the XRCT system, and the flexibility we gain from developing an in-house operation software tool. The software and algorithms used to postprocess the tomographic data and analyse are presented and also the use of open source solutions is motivated. Furthermore, the experimental hardware for fluid flow phenomena developed in our laboratory is presented with a case study. A brief comparison of the hardware used for in-situ and ex-situ experiments shows the challenges that XRCT introduces to do this kind of studies. Finally, we compare the results of fluid flow simulations using Smoothed Particle Hydrodynamics based on XRCT data sets.

Coupling Brain-Tumor Biophysical Models With Medical Image Registration

Klaudius Scheufele (*Institute for Parallel and Distributed Systems, SGS,, University of Stuttgart*), Andreas Mang (*Department of Mathematics, University of Houston*), Amir Gholami (*EECS, Berkeley, University of California, Berkeley*), George Biros (*ICES, University of Texas at Austin*), Miriam Mehl (*IPVS, University of Stuttgart*) 09:50–10:10

We present the SIBIA (Scalable Integrated Biophysics-based Image Analysis) framework for joint image registration and biophysical inversion and we apply it to analyse MR images of glioblastomas (primary brain tumors). In particular, we consider the following problem. Given the segmentation of a normal brain MRI and the segmentation of a cancer patient MRI, we wish to determine tumor growth parameters and a registration map so that if we 'grow a tumor' (using our tumor model) in the normal segmented image and then register it to the patient segmented image, then the registration mismatch is as small as possible. We call this '*the coupled problem*' because it two-way couples the biophysical inversion and registration problems. In the image registration step we solve a large-deformation diffeomorphic registration problem parameterized by an Eulerian velocity field. In the biophysical inversion step we estimate parameters in a reaction-diffusion tumor growth model that is formulated as a partial differential equation (PDE). In SIBIA we couple these two steps in an iterative manner. We will present the different Picard iterative schemes to solve the PDE-constrained optimization formulation of the coupled problem. In addition, we perform several tests to experimentally assess the performance of our method on synthetic and clinical datasets. We demonstrate the convergence of the SIBIA optimization solver in different usage scenarios. We demonstrate that using SIBIA, we can accurately solve the coupled problem in three dimensions (256^3 resolution) in a few minutes using 11 dual-x86 nodes. Also, we demonstrate that, with our coupled approach, we can successfully register normal MRI to tumor-bearing MRI while obtaining Dice coefficients that match those achieved when registering of normal-to-normal MRI.

S07.09 | Coupled problems

Date 22.03.2018
Room 0606

Kinetic Modeling and Simulation of Reactive Transport Phenomena in resolved Porous Media

Hussein AliHussein (*Institute for Computational Modeling in Civil Engineering, TU Braunschweig*), Martin Geier (*Institute for Computational Modeling in Civil Engineering, TU Braunschweig*), Manfred Krafczyk (*Civil Engineering, TU Braunschweig*), Konstantin Kutscher (*Institute for Computational Modeling in Civil Engineering, TU Braunschweig*) 08:30–08:50

A coupled Lattice Boltzmann model (LBM) is proposed to simulate advection-diffusion-reaction of multiple species in geometrically resolved porous media based on the Cumulant LBM [1]. The approach is intended to capture solid matrix evolution due to chemical precipitation / dissolution reactions. In this presentation we focus on numerical and algorithmic aspects of coupling flow, advection-diffusion and reaction in a complex three-dimensional pore space and address issues related to different time-scales of the underlying processes.

[1] M. Geier, M. Schönherr, A Pasquali, M. Krafczyk, "The cumulant lattice Boltzmann equation in three dimensions: Theory and validation", Computers & Mathematics with Applications, Vol. 70, pp. 507-547, (2015).

Optimizing the quasi-simultaneous coupling method for viscous-inviscid boundary-layer interaction

Arthur Veldman (*Mathematics and Computer Science, University of Groningen*) 08:50–09:10

The viscous-inviscid interaction (VII) philosophy for coupling an aerodynamic boundary layer to an external inviscid flow is discussed. Traditionally the shear-layer equations are solved with pressure prescribed by the inviscid flow, but then the solution breaks down in a singularity related to flow separation. This singularity is named after Sydney Goldstein, who analyzed its possible cause in 1948. Yet, it took thirty years before the actual cause was identified: a two-way interaction with reversing hierarchy.
After that insight, coupling methods were designed that could cope with this singularity. In the quasi-simultaneous coupling approach (developed four decades ago), the singularity is overcome by making use of a so-called interaction law. The latter describes, in a simple approximate way, how the external flow reacts to changes in the shear layer. In modern domain-decomposition terms, it could be called an approximate Dirichlet-to-Neumann (Steklov-Poincare) operator. In this abstraction, the quasi-simultaneous coupling method can be readily generalized to other multi-physics problems, like fluid-structure interaction, fluid-solid body interaction and multi-body robotics.
In the paper, a mathematical analysis is presented of the essential properties of such quasi- simultaneous interaction laws, based on classical Perron-Frobenius theory for non-negative matrices. Herewith, the interaction law can be optimized in terms of efficiency and robustness. As a demonstration, simulations of separated flow past an airfoil beyond maximum lift are presented.

An algorithm to couple the 2D shallow water equations with the 3D Reynolds averaged equations

Hao Zeng (*TU München,Chair of Hydromechanics*), Michael Manhart (*TU München, Chair of Hydromechanics*), Florian Mintgen (*TU München, Chair of Hydromechanics*) 09:10–09:30

Shallow Water Equations (SWE), a 2D approach, is widely used in current urban flood simulation assessment tools, e.g. Bradford and Sanders [1]. This 2D approach reproduces well the surface run-off phenomenon in large river basins. However, for flood assessment in complex environments, such as urban areas, it is not accurate enough. Thus a 3D Reynolds-averaged Navier-Stokes Equations (RANS) solver with free surface should be used for representing the interaction between flow and building structures. Due to computational cost, it is hardly possible to use RANS for the whole domain. A coupling of the shallow water solver with a full solution of the RANS is needed in the cases when the flow interacts with buildings, bridge piers, or bridge abutments for instance.
A coupling between SWE and RANS has been done in Kilanehei [2], but only steady state problems can be covered. This work focuses on a full coupling between the SWE and the RANS with free surface which has been implemented in the Finite Volume Open Source code OpenFOAM, giving robust and accurate results for a wide variety of flows. Test cases will be presented as well as the limitations of this method and future research possibilities.
The coupling has been achieved by exchanging flow variables depending on the respective conditions. A Dirichlet-Neumann coupling, based on an exchange of values and fluxes at the 2D-3D interface, is employed in two regions. The two solvers have been implemented in one single executable, which can be fully parallelized.

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[2] Kilanehei F. et. al. (2011). Coupling of 2DH-3D hydrodynamic numerical models for simulating flow around river hydraulic structures. World Applied Sciences Journal, 15(1), 63-77

Multiple Reference Frames Formulation for Blood Damage Modeling in Medical Devices

Stefan Haßler (*Chair for Computational Analysis of Technical Systems, RWTH Aachen University*), Lutz Pauli (*Chair for Computational Analysis of Technical Systems, RWTH Aachen University*), Marek Behr (*Chair for Computational Analysis of Technical Systems, RWTH Aachen University*) 09:30–09:50

Heart failure is the main cause of death in developed countries; heart transplants often being the only permanent medical treatment. Since the number of donor hearts is not sufficient for all patients in need of one, artificial blood pumps, such as Ventricular Assist Devices (VADs), are often the only alternative.
With Computational Fluid Dynamics (CFD) it is possible to predict both the hydraulic performance and the biocompatibility of VADs in development. Hemolysis, the release of hemoglobin from red blood cells (RBCs) to the blood plasma, is a major cause of blood damage. While an empirical power law model to estimate the produced hemolysis is commonly used, we think that it is crucial to account for the complex RBC behavior in blood flow. Our morphology model is able to predict the relaxation, elongation and rotation of RBCs [1]. The results from the

morphology simulation are used in a power law model with modified parameters to estimate the produced hemolysis [2, 3]. There is a one-way coupling between the blood flow and the hemolysis equations, i.e., the RBCs shape or the plasma free hemoglobin do not influence the blood flow. VADs often contain rotating parts that have to be dealt with during the simulation. An arbitrary Lagrangian-Eulerian formulation can produce very accurate results, but is computationally expensive. A multiple reference frames (MRF) formulation can give a good approximation of the steady-state behavior at low computational cost [4]. We will present the derivation of the hemolysis equations in a rotating reference frame and will show the application of the MRF hemolysis simulations to VADs.

[1] D. Arora, M. Behr, and M. Pasquali. A tensor-based measure for estimating blood damage. *Artificial Organs*, 28:1002–1015, 2004. Errata in *Artificial Organs*, 36(5):500, 2012.

[2] L. Pauli and M.Behr. On the significance of exposure time in computational blood damage estimation. In *High-Performance Scientific Computing*, volume LNCS 10164 of *Lecture Notes in Computer Science*, pages 24–36. Springer, 2017.

[3] L. Pauli, J. Nam, M. Pasquali, M. Behr. Transient Stress-Based and Strain-Based Hemolysis Estimation in a Simplified Blood Pump. *International Journal for Numerical Methods in Biomedical Engineering* 29:1148–1160, 2013.

[4] L. Pauli, J. W. Both, M. Behr. Stabilized finite element method for flows with multiple reference frames. *International Journal for Numerical Methods in Fluids*. 78(11):657–669, 2015.

Towards pressure-robust mixed methods for the incompressible Navier-Stokes equations

Alexander Linke (*Numerical Mathematics & Scientific Computing, WIAS*)
 09:50–10:10

For more than fourty years it was thought that the efficient construction of pressure-robust mixed methods for the incompressible Navier–Stokes equations, whose velocity error is pressure-independent, was practically impossible. Indeed, classical inf-sup stable mixed methods like the Taylor–Hood element relax the divergence constraint and are thus not pressure-robust. Therefore, classical inf-sup stable *lowest order methods* like the Bernardi–Raugel element are not accurate and are never used in computational practice, since even relatively easy continuous pressures may dramatically spoil their discrete velocities.
However, a novel, quite universal construction approach shows that it is indeed rather easy to construct inf-sup stable, pressure-robust mixed methods. The approach repairs a certain L^2 orthogonality between gradient fields and discretely divergence-free test functions. It is rather universal in the sense that it works for families of arbitrary-order mixed finite element methods, arbitrary-order discontinuous Galerkin methods, and finite volume methods. Novel benchmarks for the incompressible Navier–Stokes equations show that the approach promises significant speedups in computational practice, whenever the continuous pressure is complicated. The main benefit of pressure-robust methods seems to be a potential reduction of the approximation order of the applied algorithms without losing accuracy in many benchmarks problems.

A CFD-DEM approach to model the orientation and distribution of non-spherical fibers in fresh concrete

Florian Gerland (*Universität Kassel*), Olaf Wünsch (*Universität Kassel*)
 10:10–10:30

Modern high performance concretes are reinforced by fibers to cast complex parts without reinforcing bar. The orientation and distribution of fibers influence the properties of the final solid and the flow properties of fresh concrete. Therefore it is important to predict the casting process adequately. A promising method for this is CFD-DEM. The suspending phase is described as a continuum and can be solved using suitable methods such as Finite Volume Method. The suspended particles are modeled as rigid bodies and simulated using the Discrete Element Method.
Commonly the particles used in DEM are spherical. More complex particle geometries can be modeled by bonded spheres and the drag forces can be approximated from drag relations of single spheres by various methods such as in [1].
This work is based on the CFDEM® engine which uses OpenFOAM® for the suspending phase and LIGGGHTS® for the particles. The modeling of fluid-particle interaction forces and the momentum coupling between the phases is of outstanding relevance for the applicability of this method. Therefore the influence of various drag models and further discretization parameters and interpolation schemes, e.g. CFD mesh resolution and time step of CFD and DEM as well as the coupling interval between the two subsolvers on the solution accuracy, will be investigated in this contribution.

[1] R. Sun, H. Xiao, H. Sun, Realistic Representation of Grain Shapes in CFD-DEM Simulations of Sediment Transport: A Bonded-Sphere Approach, Adv. Water Resour. (2017).

S07.10 | Coupled problems

Date 22.03.2018
Room N1190

Multi-field modeling of thermomechanical coupled fracture problems

Jonathan Schulte (*University of Siegen*), Melanie Krüger (*University of Siegen*), Maik Dittmann (*University of Siegen*), Christian Hesch (*University of Siegen*) 14:00–14:20

In this contribution we focus on a novel variationally consistent formulation for thermomechanical coupled fracture problems. To be specific, we aim on a phase-field approach to fracture such that the resulting system consists of three fields, the deformation map, the absolute temperature field as well as the crack phase-field.

In the sense of Griffith energy criterion for brittle fracture, a crack initiates or continues upon the attainment of a critical crack energy density. This critical energy exhibits strong temperature dependence, which is approximated by a linear interpolation within our framework.

The material behaviour is governed by a modified Helmholtz free energy function in terms of the elastic part of the deformation gradient and the temperature. Postulating that fracture requires a local state of tension, we apply an anisotropic decomposition of the principle stretches of the deformation gradient and reduce the tensile contributions by a suitable degradation function, see [1] for more details. Accordingly, we are able to derive local constitutive relations for the first Piola-Kirchhoff stress tensor, the entropy density and the phase-field driving force in variationally consistent manner, see [2].

A further constitutive relation is the Duhamel's law of heat conduction. In case of fracture, the conduction degenerates locally such that we achieve a pure convection problem and the heat transfer depends on the crack opening width. Here, we formulate the conductivity tensor in

terms of the phase-field parameter.

Eventually, various numerical examples will show the accuracy and capability of the proposed multi-field approach to fracture.

[1] C. Hesch and K. Weinberg: Thermodynamically consistent algorithms for a finite deformation phase-field approach to fracture, *Int. J. Num. Meth. Engng*, 99:906-924, 2014.

[2] M. Dittmann, C.Hesch. M. Krüger, F. Schmidt and S. Schuß, Modeling and simulation of thermomechanical fracture and contact problems, *in preparation.*

Multi-field formulation of large deformation ductile fracture

Maik Dittmann (*University of Siegen, Chair of Computational Mechanics*), Christian Hesch (*University of Siegen, Chair of Computational Mechanics*), Jonathan Schulte (*University of Siegen, Chair of Computational Mechanics*), Fadi Aldakheel (*Leibnitz University Hannover, Institute of Continuum Mechanics*)

14:20–14:40

In the present contribution we focus on a novel computational framework for the simulation of ductile fracture in elastoplastic solids. In particular, a fully non-linear formulation of gradient plasticity is applied together with a higher order phase-field approach to fracture to account for large elastic and plastic deformations along with three dimensional crack propagation.

The proposed formulation is based on a multiplicative decomposition of the deformation gradient into elastic and plastic contributions and a subsequent multiplicative decomposition of the elastic part into a fracture sensitive and a fracture insensitive contribution, see [1]. Postulating that fracture requires a local state of tensile/shear deformation, the latter decomposition is used to formulate the isochoric and tensile contributions to the elastic strain energy, whereas the compressive contribution remains unaffected by the crack phase-field and vice versa.

The modification of the Griffith brittle fracture theory to ductile fracture is most crucial and has to be adjusted carefully. Within our framework, this adaptation is considered as dependency of the critical fracture energy density by the equivalent plastic strain.

Concerning the elastic/plastic decomposition, we assume an isochoric plastic flow which requires special attention for the update procedure of the plastic deformation. To be specific, we apply an exponential time integration scheme such that we preserve the deviatoric state of the plastic deformation and obtain a correct evaluation of the phase-field driving force, see [2,3] for more details.

Eventually, a number of numerical examples will demonstrate the accuracy and capability of the proposed multi-field approach to ductile fracture.

[1] C. Hesch and K. Weinberg: Thermodynamically consistent algorithms for a finite deformation phase-field approach to fracture, *Int. J. Num. Meth. Engng*, 99:906-924, 2014.

[2] M. Dittmann, F. Aldakheel, J. Schulte and C. Hesch: On the Phase-Field Formulation of Ductile Fracture in Multi-Field Environments, in preparation, 2017.

[3] M.J. Borden, T.J.R. Hughes, C.M. Landis, A. Anvari and I.J. Lee: A phase-field formulation for fracture in ductile materials: Finite deformation balance law derivation, plastic degradation, and stress triaxiality effects, *Comput. Methods Appl. Mech. Engrg.*, 312:130-166, 2016.

Variational Homogenization for Phase-Field Modeling of Micro-Magneto-Mechanics at Finite Deformations

Daniel Vallicotti (*Institute of Applied Mechanics, University of Stuttgart*), Ashish Sridhar (*Institute of Applied Mechanics, University of Stuttgart*), Marc-André Keip (*Institute of Applied Mechanics, University of Stuttgart*) 14:40–15:00

Smart or functional materials have received significant attention in recent times due to their application as advanced sensors and actuators. Magnetorheological elastomers (MREs) are a special class of these materials, where micron-sized ferromagnetic particles are embedded in an elastomeric matrix material. The large deformations capable by these materials coupled with their high operating frequency, make them very attractive for engineering applications.

The behavior of MREs is a complex phenomenon that spans over multiple length-scales. The ferromagnetic inclusions show magnetic domain wall motions on the micro-scale, which drives the magneto-mechanical deformations seen on the macroscopic level. To capture this behavior we propose a *large-deformation variationally consistent micro-magnetic framework* embedded into a scale-bridging scenario by using *computational homogenization techniques* in order to define the macroscopic overall response. Starting point is a *rate-type saddle-point variational principle* yielding the famous *Landau-Lifshitz-Gilbert* equation for the temporal evolution of the magnetization order parameter. The physical unity constraint of the magnetization vector is realized by a staggered solution scheme on the micro-structure with additional normalization routine. A macroscopic driving routine enables the magneto-mechanical loading of the periodic micro-structure based on a generalized Hill-Mandel homogeneity condition.

The presentation focuses on the algorithmic implementation of the two-scale solution scheme and displays its capabilities by numerical examples. Interactions of the neighboring magnetic particles based on evolving magnetic domains and their influence on the overall macroscopic material response are demonstrated.

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2. K. Danas, S.V. Kankanala, N. Triantafyllidis, Experiments and Modeling of Iron-particle-filled Magnetorheological Elastomers, *Journal of the Mechanics and Physics of Solids*, **60**, 120-138, 2012.

3. A. Javili, G. Chatzigeorgiou, P. Steinmann, Computational Homogenization in Magneto-Mechanics, *International Journal of Solids and Structures*, **50**, 4197-4216, 2013.

4. A. Sridhar, M.-A. Keip, C. Miehe, Homogenization in Micro-Magneto-Mechanics, *Computational Mechanics*, **58**, 151-169, 2016.

5. C. Miehe, D. Vallicotti, S. Teichtmeister, Homogenization and multiscale stability analysis in finite magneto-electro-elasticity. Application to soft matter EE, ME, and MME composites, *Computer Methods in Applied Mechanics and Engineering*, **300**, 294-346, 2016.

6. M.-A. Keip, M. Rambausek, Computational and Analytical Investigations of Shape Effects in the Experimental Characterization of Magnetorheological Elastomers, *International Journal of Solids and Structures*, **121**, 1-20, 2017.

An Anisotropic Phase-field Approach to Fracture in Coupled Electro-Mechanics

Ashish Sridhar (*Civil Engineering, Institute of Applied Mechanics, University of Stuttgart*), Stephan Teichtmeister (*Institute of Applied Mechanics, University of Stuttgart*), Marc-André Keip (*Institute of Applied Mechanics, University of Stuttgart*) 15:00–15:20

The advancements in technology dictate the demand for materials that are more adaptable and efficient whilst being more reliable. Smart or functional materials have received significant attention in recent times due to this. Coupled electro-mechanical materials such as piezoelectric ceramics and electroactive polymers are used as actuators, sensors, motors as well as noise and vibration control devices. This entails the need for structural stability analyses of such devices which requires the modeling of failure under coupled electro-mechanical actions.
From a purely mechanical perspective numerical simulations of failure due to fracture based on sharp crack discontinuities may suffer in situations with complex crack topologies. This can be overcome by a diffusive crack modeling based on the introduction of a crack phase field. Such a phase-field model has to be extended to account for the behavior of electro-mechanically coupled materials, in particular, the coupled electro-mechanical anisotropy in these materials has to be taken into account.
We propose a variational three-field formulation that couples the displacement with the electric potential and the fracture phase field. The proposed framework allows for the definition of mechanical and electrical parts of the fracture driving force, which follows in a natural format from the proposed kinematic assumption, that decomposes the strain and the electric field into energy producing and fracture parts, respectively. The choice of the driving forces and proposed degradation functions are explained from a fundamental viewpoint. Appropriate numerical examples that showcase the capability of the proposed model to capture the coupled and anisotropic electro-mechanical fracture phenomenon are presented.

Recent Publications

1. C. Miehe, F. Welschinger, M. Hofacker [2010], *A phase field model of electromechanical fracture*, Journal of Mechanics and Physics of Solids, **58**, 151–169.

2. Xu et. al. [2010], *Fracture simulation of ferroelectrics based on the phase field continuum and damage variable*, International Journal of Fracture, **166**, 163-172.

3. A. Abdollahi, I. Arias. [2011], *Phase field simulation of anisotropic crack propagation in ferroelectric single crystals: effect of microstructure on fracture process*, Modelling and Simulation in Materials Science and Engineering , **19**, 074010.

4. A. Abdollahi, I. Arias. [2012], *Phase field modeling of crack propagation in piezoelectric and ferroelectric materials with different electromechanical crack conditions*, Journal of Mechanics and Physics of Solids, **60**, 2100-2126.

5. Z.A. Wilson, M.J. Borden, C.M. Landis [2013], *A phase-field model for fracture in piezoelectric ceramicss*, International Journal of Fracture, **183**, 135-153.

6. S. Teichtmeister, D. Kienle, F. Aldakheel, M.-A. Keip [2017], *Phase field modeling of fracture in anisotropic brittle materials*, International Journal of Non-Linear Mechanics **97**, 1–21.

Phase-field predictive model for the setting of fresh self-compacting concrete

Haiqin Huang (*Faculty of Science, Technology and Communication, University of Luxembourg*), Andreas Zilian (*Faculty of Science, Technology and Communication, University of Luxembourg*) 15:20–15:40

The initial setting of fresh concrete is mainly caused by the dissolution of cement grains and the precipitation of calcium-silicate-hydrates during cement hydration. From a more global perspective it describes the transition from dense liquid phase to porous solid phase. Fresh mixture of self-compacting concrete (SCC) can be considered as a phase-changing multi-component material. It can be described as a continuum at the macro scale, driven by a set of coupled transport-reaction-diffusion processes at the level of the microstructure. This contribution focuses on a predictive model for the setting of fresh SCC where the liquid-solid phase transition is captured by a phase-field variable using the Ginzburg-Landau type free energy function. Hydration-related chemical reactions together with heat and mass transfer are volume-coupled with the mechanical behaviour and determined by the environmental conditions. Implementation of the predictive model is demonstrated using the FEniCS framework, together with numerical examples supporting model validation.

Simulation of upper and lower bainitic transformation with a coupled phase field/diffusion/deformation framework

Martin Düsing (*Lehrstuhl für Technische Mechanik, Fakultät für Maschinenbau, Paderborn University*), Rolf Mahnken (*Lehrstuhl für Technische Mechanik, Fakultät für Maschinenbau, Paderborn University*) 15:40–16:00

The bainitic transformation is one of the most complex transformations in steel. The transformation from austenite to bainitic ferrite is assumed to be displacive [1] in contrast to the perlitic growth which is highly dependent on the carbon movement and therefore is ranked as a diffusive transformation. However, regarding the whole microstructure named bainite, consisting of bainitic ferrite, carbides and (residual) austenite, the movement of the carbon is of major importance. In lower bainite the carbon within the ferrite separates [1] and precipitates as carbides. In upper bainite the carbon diffuses across the interface into the austenite. In this work the phase-field method is utilized to simulate the phase transformations from austenite to bainitic ferrite and the precipitation of carbides. An elaborate diffusion model considers the separation of carbon within the supersaturated bainitic ferrite and the diffusion across the interface. It is based on a Cahn-Hilliard diffusion equation coupled with deformations and the phase field equations. The simulation is based on a thermodynamic framework of generalized stresses as introduced by Gurtin [2] for a two phase Ginzburg-Landau system and a Cahn-Hilliard equation. We extend this framework to multiphase-field models coupled to a viscous Cahn-Hilliard equation and deformations [3]. The numerical examples show the qualitative mechanism of the bainitic transformation as discussed above.

[1] Bhadeshia, H. K. D. H. Bainite in steels, Cambridge, Second Edition (2001).

[2] Gurtin, M. E., Physica D: Nonlinear Phenomena (1996) 92:178–192.

[3] Düsing, M. and Mahnken, R., Int J Solids Struct (2017) doi:10.1016/j.ijsolstr.2017.11.018

S07.11 | Coupled problems

Date 22.03.2018
Room 0606

Towards structural optimization of lithium battery anodes

Kerstin Weinberg (*Maschinenbau, Universität Siegen*), Marek Werner (*Maschinenbau, Universität Siegen*) 14:00–14:20

In lithium batteries, multicomponent compositions like $LiCoO_2$ or $LiFePO_4$ are used as cathode material and single substances like silicon or graphite are developed as anode material. In the latest battery developments anodes of silicon are introduced. However, the high volumetric changes of silicon during intercalation — sometimes a factor of four has been reported — lead to pulverization and capacity fade of the anode.
To account for the intercalation induced volumetric swelling and phase segregation, the mechanical, thermal, chemical, electrical and diffusion field equations have to be coupled which leads to a complex description based on fourth order partial differential equations. Additionally, the structure of the anode needs to provide minimal compliance but maximal conductivity. In our contribution we provide a concept to combine these competing objectives with a the multi-physics model of battery charging.

Microscale analysis of interactions in magnetorheological elastomers

Philipp Metsch (*TU Dresden, Institute of Solid Mechanics*), Karl A. Kalina (*TU Dresden, Institute of Solid Mechanics*), Jörg Brummund (*TU Dresden, Institute of Solid Mechanics*), Günter K. Auernhammer (*Leibniz Institute for Polymer Research Dresden*), Markus Kästner (*TU Dresden, Institute of Solid Mechanics*) 14:20–14:40

Magnetorheological elastomers (MREs) represent a class of active composite materials which typically consist of micron-sized magnetizable particles that are embedded in a cross-linked elastomer matrix. Due to mutual interactions of the particles, MREs are able to alter their effective material behavior reversibly if subjected to an external magnetic field. This strong coupling between magnetic and mechanical fields facilitates a variety of applications in the fields of actuators and sensors, valves or tunable vibration absorbers. Within this contribution, a modeling approach for MREs is presented: starting from the properties of the magnetizable particles and the elastomer matrix, a microscale continuum formulation of the coupled magneto-mechanical problem is applied [1].
While macroscopic properties of MREs have been determined via a computational homogenization approach in former applications of our modeling strategy [2, 3], the current contribution focusses on an analysis of the influence of microstructural geometric as well as constitutive properties on the behavior of MREs with only few particles. In a first study, the discrepancy between widely used two-dimensional approaches and a full three-dimensional solution of the underlying field problem is examined qualitatively and quantitatively for the behavior of simple MRE samples - the identification of characteristic deformation mechanisms facilitates the understanding of interactions in complex, realistic specimens. Afterwards, the simulations are compared to experiments [4]: the versatility of our approach allows for a very good agreement of the results for different MRE samples, independent of the particle positions and distances.

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[2] Metsch, P., Kalina, K. A., Spieler, C., Kästner, M., A numerical study on magnetostrictive phenomena in magnetorheological elastomers, Computational Materials Science, 124, pages 364-374 (2016)

[3] Kalina, K. A., Metsch, P., Kästner, M., Microscale modeling and simulation of magnetorheological elastomers at finite strains: A study on the influence of mechanical preloads, International Journal of Solids and Structures, 124–103, pages 286-296 (2016)

[4] Puljiz, M., Huang, S., Auernhammer, G. K., Menzel, A. M., Forces on rigid inclusions in elastic media and resulting matrix-mediated 1interactions, Physical Review Letters, 117, page 238003 (2017)

Modeling and Simulation of Hysteresis Effects in Magnetorheological Elastomers

Karl A. Kalina (*Institute of Solid Mechanics, TU Dresden, Institute of Solid Mechanics*), Jörg Brummund (*TU Dresden, Institute of Solid Mechanics*), Philipp Metsch (*TU Dresden, Institute of Solid Mechanics*), Markus Kästner (*TU Dresden, Institute of Solid Mechanics*) 14:40–15:00

Magnetorheological elastomers (MREs) are a class of composites which can alter their macroscopic properties if a magnetic field is applied. These materials consist of a polymer matrix with embedded micron-sized magnetizable particles. If the MREs are filled with magnetically hard particles as NdFeB, they reveal strong hysteresis effects. Recently published experiments [1, 2] indicate a significant dependence of the hystereses on the stiffness of the matrix. In this contribution we investigate the microstructural causes of this effect by the use of a computational modeling approach.
The analyzed MREs are described by a microscopic model [2], i. e. the heterogeneous microstructure consisting of magnetizable inclusions embedded into a polymer matrix is taken into account explicitly. The constitutive models for the particles and the matrix are formulated separately. To describe the magnetic behavior of the NdFeB-particles a hysteresis model based on [3] is used. The governing equations of the coupled magnetomechanical problem are solved by a nonlinear finite element formulation [4, 2]. Therein, the evolution equation of the hysteresis model is solved by means of an implicit integration scheme. In order to connect the macroscopic and the microscopic magnetic and mechanical quantities, a suitable homogenization scheme is applied.
The simulations presented in this contribution indicate a rotation of the particles within the soft polymer material. Due to this effect, the effective hystereses of the MRE are significantly smaller than the hystereses of pure NdFeB. The presented computational results are qualitatively in good agreement with the results in [1].

[1] J. M. Linke, D. Yu. Borin, S. Odenbach, RSC Adv., 6, 2016.

[2] K. A. Kalina, J.Brummund, P. Metsch, M. Kästner, D. Yu. Borin, J. M. Linke, S. Odenbach, Smart Mater. Struct., 26, 2017.

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A numerical study of the influence of inclusion geometries in heterogeneous dielectric elastomers

Markus Klassen (*Chair of Structural Analysis and Dynamics, RWTH Aachen*), Sven Klinkel (*RWTH Aachen*), Ralf Müller (*TU Kaiserslautern*) 15:00–15:20

The investigation and study of dielectric elastomers has emerged as an important research field in the last years with regard to the development of so called dielectric elastomer actuators (DEAs). The main advantage of this technology lies in the possibility of the design of soft actuators which are capable of large deformations. The main drawback is given by the high electric fields, which are necessary to drive such actuators. This drawback emerges from the reduced relative permittivity of dielectric elastomers, which leads to a low electromechanical coupling. In order to improve this handicap, a heterogeneous material structure, consisting of an elastomer matrix with bariumtitanate inclusions, is suggested. This contribution is concerned with the numerical analysis of the heterogeneous material including the electromechanical coupling for the dielectric elastomer. A mixed finite element formulation is employed to account for the nearly incompressibility of the dielectric elastomer. The importance of a mixed element formulation is shown by some numerical examples. The numerical results show that the proposed material inclusions are capable to improve the stretch ratios of the elastomers. Different geometries of the inclusion are investigated with respect to the actuator deformation range.

Comparison of experimental data and FEM simulation for a multiferroic nanocomposite

Veronica Lemke (*Institut of Mechanics, Universität Duisburg-Essen*), Matthias Labusch (*Universität Duisburg-Essen*), Jörg Schröder (*Universität Duisburg-Essen*), Samira Webers (*Universität Duisburg-Essen*), Heiko Wende (*Universität Duisburg-Essen*) 15:20–15:40

The combination of ferromagnetic and ferroelectric materials, i.e. producing multiferroic composites, increases the opportunities for technical sensors and data storage devices, see [1]. Together the magneto-electric (ME) materials have the property to affect each other e.g. an applied electric field modifies the magnetization of the magnetic phase. In nature also single-phase materials exist with magneto-electric properties. Though, the interoperation of the magnetization and the polarization is exclusively activated at very low temperature. Therefore, they are not favorable for most of the known technical applications. Considering this, the ME composites can be seen as a good option since their synergy of the magneto-electric properties is active at room temperature [2] and can be differentiated in two different effects, the direct and the converse ME effect. The first one describes a magnetically induced polarization, where an applied magnetic field provokes a deformation in the piezomagnetic material. The piezoelectric phase is then forced to perform a deformation which causes a polarization in this material. The reversed reactions are the second observed effect where an electrically caused magnetization is noticable. We will focus on (1-3) nanocomposite grounded on the experiments made in [3] and [4]. In the experiments, cobalt ferrite nanopillars, embedded in a barium titanate matrix, are determined. Then, for the numerical FEM-simulations the material coefficients from [5] and [6] are taken. The change of the strain-induced in-plane polarizations of the ferroelectric matrix around one cobalt ferrite nanopillar is calculated. These computed results are compared to the ones of the experimental measurement outcomes. Additionally, we investigate the magneto-electric coupling coefficient.

[1] N. A. Spalding and M. Fiebig, The renaissance of magnetoelectric multiferroics. *Materials Science*, **309**, 391–392, 2005.

[2] J. van Suchtelen, Product properties: a new application of composite materials. *Philips Research Reports*, **27**, 28–37, 1972.

[3] C. Schmitz-Antoniak, D. Schmitz, P. Borisov, F. de Groot, S. Stienen, A. Warland, B. Krumme, R. Feyerherm, E. Dudzik, W. Kleemann and H. Wende, Electric in-plane polarization in multiferroic $CoFe_2O_4/BaTiO_3$ nanocomposite tuned by magnetic fields. *nature communications*, **4**, 1–8, 2013.

[4] C. Schmitz-Antoniak, D. Schmitz, P. Borisov, F. de Groot, S. Stienen, A. Warland, B. Krumme, R. Feyerherm, E. Dudzik, W. Kleemann and H. Wende, Electric in-plane polarization in multiferroic $CoFe_2O_4/BaTiO_3$ nanocomposite tuned by magnetic fields: Supplementary information. 2013.

[5] M. Labusch, M. Etier, D. C. Lupascu, J. Schröder and M. A. Keip, Product properties of a two-phase magneto-electric composite: Synthesis and numerical modeling. *Computational Mechanics*, **54**, 71–83, 2014.

[6] J. Schröder, M. Labusch, and M. A. Keip, Algorithmic two-scale transition for magneto-electro-mechanically coupled problems FE^2-scheme: Localization and homogenization. *Computer methods in applied mechanics and engineering*, **302**, 253–280, 2016.

Analytical investigation of non-local deformation-mediated magneto-electric coupling

Matthias Rambausek (*Institute of Applied Mechanics, University of Stuttgart*), 15:40–16:00
Marc-André Keip (*Institute of Applied Mechanics (CE), University of Stuttgart*)

During the past decade the search for magneto-electric materials concentrated on multi-ferroics and hard-matter composites[1]. However, rather recently strain-mediated magneto-electric coupling in soft composites was brought up as an alternative [2]. Such composites, might be realized with hard ferroic inclusions embedded in a very soft matrix material. The importance of non-local effects contributing to the total coupled *magneto*-mechanical response of such composites has been discussed in [3].
Motivated be these findings we investigate deformation-mediated magneto-electric coupling in an abstract setting: We assume the existence of a soft body with magnetic and electric properties regardless of their origin. Hence, we consider simple but reasonable relations for the magnetical, electrical and mechanical material behavior. Based on that we demonstrate that even in such a reduced setting considerable magneto-electric coupling can be achieved. The observed effect originates from the combination of non-local magneto- and electro-mechanical coupling phenomena in a finite-strain setting [4]. Thus, one may either regard this effect as an additional source of coupling in device design or as a mechanism for the creation of new magneto-electrically coupling composites.
In order to assess the strength of this coupling effect, we provide extensive parameter studies based on analytical estimates. Besides that we present more detailed results in terms of numerical simulations for selected model parameters.

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S07.12 | Coupled problems

Date 22.03.2018
Room N1190

Uncoupled Thermoelasticity Boundary Element Formulation with Variable Time Step Size

Martin Schanz (*Graz University of Technology/Institut of Applied Mechanics*), Michael Leitner (*Graz University of Technology/Institut of Applied Mechanics*) 17:30–17:50

In this talk, we propose a Boundary Element formulation for thermoelasticity. The application for such a method can be found in the simulation of tools in hot forming processes, where the temperature distribution is essential for designers to obtain the requested strength in the formed metal. But also the elastic deformation of the tool influences the shape of the formed metal. These tools are an optimal application of Boundary Element Method because the governing equations are linear and only the physical data at the surface are of interest. A simplification can be used, the Uncoupled Quasistatic Thermoelasticity is applicable. Therein the effects of the deformation onto the temperature distribution is neglected and consequently, the heat conduction equation can be solved separately.
In the proposed formulation convolution integrals occur. Several approaches exist to discretize this time-domain integral equation. Utilizing the Laplace domain fundamental solutions the Convolution Quadrature Method can be applied to establish a time stepping procedure. The system develops a steady state over time and for such a behavior an adaption of the time resolution is justified. Therefore, we implement the Generalized Convolution Quadrature Method to our system to allow non-uniform time discretization. Numerical results are presented and compared to analytic solutions.

A thermo-mechanical model of ultrasonic metal welding process with the focus on the mating interface

Shimaalsadat Mostafavi (*Mechanical Engineering, RWTH Aachen University, Institute of General Mechanics*), Yousef Heider (*Mechanical Engineering, RWTH Aachen University, Institute of General Mechanics*), Bernd Markert (*Mechanical Engineering, RWTH Aachen University, Institute of General Mechanics*) 17:50–18:10

In this study, a thermo-mechanical model of the interface of two mating metal parts in the process of ultrasonic welding is presented. Ultrasonic metal welding, as a joining technique, is a combined process of applying pressure and ultrasonic frictional vibrations on the surfaces of the mating parts. Ultrasonic metal welding is counted as a solid state consolidation of the involved parts, in which the growing interface temperature is far below the melting point of the material [1]. Energy consumption in this process is relative low compared to the common welding processes, such as arc welding and no weld deposit is needed. This contribution is devoted to study the interactive effect of the process parameters, namely, the applied pressure and the amplitude of the ultrasonic vibrations on the interface stress as well as the interface temperature rise. Finally, the results of the proposed thermo-mechanical model are compared with the results from experiments [2].

[1] Siddiq, A., Sayed, T. El, 2012. A thermomechanical crystal plasticity constitutive model for ultrasonic consolidation. Comput. Mater. Sci. 51, 241–251. doi:10.1016/j.commatsci.2011.07.023

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Thermomechanically coupled simulation of cracks in aero engine components using the XFEM in 3D

Artsem Boris Kunin (*Institute of Continuum Mechanics, Leibniz Universität Hannover*), Stefan Löhnert (*Institute of Mechanics and Shell Structures, Technical University Dresden, Germany*), Peter Wriggers (*Institute of Continuum Mechanics, Leibniz Universität Hannover*) 18:10–18:30

In the Collaborative Research Center(CRC) 871 "Regeneration of complex capital goods" new repair procedures are investigated and further developed. Among other things the compressor and turbine blades are taken as a subject of research. In addition to the real repair procedures numerical simulations are carried out in order to estimate the quality of the repair. Another goal of the project is to investigate worn blades during the usage in order to predict component behavior and operational life span. In turbine blades of aero-engines typical defects are cracks in the range of several centimeters down to 40-70 microns. In addition to the high centrifugal forces, the temperature near the surface can reach up to 1000°C. To accurately simulate 3D crack propagation in an inelastically and thermo-mechanically behaving material leads to an extensive numerical effort. Therefore, the extended finite element method (XFEM) is widely used for simulations of fracture mechanics problems considering cracks directly at the element level. Discontinuities in the displacement and temperature field are allowed and simultaneously the crack opening displacement and crack tip stress field are reproduced accurately with the XFEM. Since crack closing and non-physical penetration of the crack surfaces may occur at element level under certain load conditions, it becomes necessary to enforce the non-penetration condition (for crack surfaces) like in multi body systems with contact. Additionally, pressure depended heat transfer across crack surfaces should be taken into account for thermo-mechanically coupled problems which are investigated in this work.

S07.13 | Coupled problems

Date 23.03.2018
Room N1090

Modelling delamination in ferromagnetic-ferroelectric composites via an extended cohesive zone model

Alexander Schlosser (*Institute of Mechanics, Universität Kassel*), Andreas Ricoeur (*Group of Engineering Mechanics/Continuum Mechanics, Universität Kassel*) 08:30–08:50

Exhibiting interactions between magnetical and electrical fields at room temperature makes magnetoelectric (ME) composites interesting for various applications in technical devices. The ferroelectric matrix as well as the magnetostrictive inclusions of particle composites and the layers of laminates are mostly ceramics or other brittle materials, thus being prone to cracking. Due to this brittleness, the consideration of damage is crucial in numerical analyses of ferroelectric and ferromagnetic devices. Especially the delamination behavior of boundary layers in ME composites is of a great interest due to its large influence on coupling factors. In order to

investigate delamination processes in ME composites, cohesive elements are being developed and applied in combination with nonlinear ME finite elements [1], [2]. The mechanical behavior of the cohesive zone is prescribed by a bilinear traction-separation-law. Magnetical and electrical fields are based on an approach of the potential gradient between the two constituents, taking into account the electrostatic stresses at the interface. Electrical and magnetical properties change during damaging processes, being controlled by damage variables which in turn are determined by the separation between the boundaries. Some numerical results are presented, giving insight into interface and matrix crack growth under combinded loading conditions

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Leakage current and polarization domains in ferroelectric nanogenerators for energy harvesting

Franziska J. Wöhler (*Institute for Structural Analysis, Karlsruhe Institute of Technology (KIT)*), Ingo Münch (*Institute for Structural Analysis, Karlsruhe Institute of Technology (KIT)*), Werner Wagner (*Institute for Structural Analysis, Karlsruhe Institute of Technology (KIT)*) 08:50–09:10

Energy harvesting based on the transformation of mechanical into electrical energy is under investigation. Mechanical deformations from ambient parasitic vibrations serve as energy source for our nanogenerator concept with the ferroelectric material barium titanate. The energy harvesting process is enabled by the designed polarization domain topology. Due to the deformation in the ferroelectric film, the polarization domains reorder and result in an electron flow between the surface electrodes, which is required for energy harvesting.
Defects and other imperfections are the physical background turning the ferroelectric film into a semiconductor. We account for leakage current mechanisms in our finite element phase field model phenomenologically. Linear and quadratic functions present the Ohm's law and the space-charge-limited- current (SCLC), respectively. Both effects are implemented for the bulk ferroelectric film. Additionally, Schottky emission is simulated for the interface between electrodes and ferroelectric film. The Schottky emission has an exponential dependency on the electric field.
The distance between the electrodes as well as the ferroelectric film thickness have an immense influence on the leakage current density regarding the electric potential. Further investigations focus on the influence of leakage current on the polarization domain topology.

Influence of domain switching and phase transition on temperature changes in ferroelectric materials

Marius Wingen (*Institute of Mechanics, University of Kassel*), Andreas Ricoeur (*Institute of Mechanics, University of Kassel*) 09:10–09:30

Due to their special electromechanical properties, nowadays ferroelectric materials are widely used in many technical applications, mostly as actuators or sensors. Advantages compared to other smart devices are their extremely fast reaction times in a range of $\mu s - ms$ and large

actuation forces. In the past, temperature changes inside the material were rather disturbing during the investigation and usage of these materials and were mostly neglected in numerical models, although they may have a non-negligible impact on issues like phase transitions, domain wall motion or reliability and lifetime. One example is the dynamic operation of piezoelectric actuators, resulting in self-heating. In case of insufficient heat dissipation, phase transformations may arise in addition to structural problems due to thermal stresses. In materials with low Curie temperature, such as barium titanate, even depolarization may occur. Experiments have shown, that transient electromechanical fields in ferroelectric materials lead to two types of temperature changes [1, 2]. There is a reversible temperature change, which can heat up or cool down the material and a much stronger irreversible heating caused by domain switching.
In this work, the theoretical background and a Finite Element (FE) approach based on a micromechanically and physically motivated nonlinear constitutive model are presented. The model considers the mutual nonlinear coupling of thermal and electromechanical fields. Numerical calculations show the effects of temperature on the electromechanical field quantities and vice versa. They also reveal switching processes in ferroelectrics and associated heating or cooling, taking into account phase transitions and their dependence on temperature changes.

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[2] Molin, C., Sanlialp, M., Shvartsman, V. V., Lupascu, D. C., Neumeister, P., Schönecker, A. and Gebhardt, S. *Effect of dopants on the electrocaloric effect of 0.92 $Pb(Mg_{1/3}Nb_{2/3})O_3$-0.08 $PbTiO_3$ ceramics*. Journal of the European Ceramic Society, Volume 35, Issue 7, p. 2065-2071 (2015).

A finite-element framework for the modelling and simulation of phase transforming magnetic solids using energy relaxation concepts

Thorsten Bartel (*Mechanical Engineering, Institute of Mechanics, TU Dortmund University*), Björn Kiefer (*Mechanical Engineering, Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg*), Karsten Buckmann (*Mechanical Engineering, Institute of Mechanics, TU Dortmund University*), Andreas Menzel (*Mechanical Engineering, Institute of Mechanics, TU Dortmund University and Division of Solid Mechanics, Lund University*)

09:30–09:50

The macroscopic behavior of ferroic functional materials such as magnetic shape memory alloys is highly affected by microscopic mechanisms such as the formation and further evolution of microstructures. Thus, the modelling of these effects is important for establishing micromechanically well-motivated constitutive frameworks with high physical plausibility. In the present approach, the switching between different crystallographic variants of martensite as well as the propagation of magnetic domains is treated by the evolution of phase volume fractions on the basis of energy relaxation methods. In addition to these mechanisms, possible deviations of the local magnetization vectors with respect to the easy axes also need to be taken into account in order to simulate the material behavior accurately. For homogeneous problems (e.g. elliptic bodies), the influence of the demagnetization field can be captured by demagnetization tensors and the effective quantities such as stresses and the magnetic induction can be calculated in a post-processing step. However for inhomogeneous problems, the demagnetization field has to be treated as an independent field variable. An intermediate conclusion of the present research project states that a conventional Finite-Element-based implementation, where internal state variables are locally determined at the integration points in a condensed manner, is hardly, if at

all, realizable. Thus, the variables describing the microstructure are also treated as global field variables and the related Biot-type evolution equations are solved at the macroscopic level. In this contribution, the theoretical approach as well as the Finite Element implementation will be elaborated along with a comparison between different parametrizations.

Modeling of Electromechanically Induced Phase Transitions in Lead Zirconate Zitanate (PZT) Based on the Condensed Method

Philip Uckermann (*Institute of Mechanics Chair of Engeneering Mechanics, Universität Kassel*), Stephan Lange (*Universität Kassel*), Andreas Ricoeur (*Universität Kassel*)

09:50–10:10

Ferroelectric materials are used for a variety of technical applications, for example fuel injections and thermal sensors. Despite containing lead, PZT remains one of the most common actor materials because of its favorable electromechanical properties, particularly at the morphotropic phase boundary (MPB). PZT at the MPB consists of both tetragonal and rhombohedral unit cells. One of the most accepted theories for those properties is the existence of fourteen instead of six (tetragonal) or eight (rhombohedral) domain variants.
The condensed method was developed to calculate e.g. hysteresis loops or residual stresses for polycrystalline materials without spatial discretization, resulting in low computational effort and large numerical stability [1]. It is suitable for efficient implementation of various constitutive behaviors, accounting for interactions of grains or different constituents of a material compound. Hitherto it has been applied to tetragonal ferroelectrics, ferromagnetics and multiferroic compounds [2] as well as to life time predictions in ferroelectrics [3].
In this research the approach is expanded towards transitions of tetragonal and rhombohedral phases. Therefore, an additional evolution law is implemented. It contains energy barriers which can be reached by electrical and mechanical loads. Some alternatives for modeling these barriers and the related consequences on material responses will be presented. Finally, the influences of the existence of two different types of unit cells and of possible phase transitions on properties of PZT at the MPB will be critically discussed.

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S08 | Multiscales and homogenization

Organiser Daniel Balzani (*Ruhr-Universität Bochum*)
Thomas Böhlke (*Institute of Engineering Mechanics, Chair for Continuum Mechanics, Karlsruhe Institute of Technology (KIT)*)

S08.01 | Multiscales and homogenization

Date 21.03.2018
Room 0220

A Hashin-Shtrikman Type Finite Element Method for the Model-Order Reduction of Nonlinear Homogenization Problems

Stephan Wulfinghoff (*Institut für Angewandte Mechanik, RWTH Aachen*), Fabiola Cavaliere (*Institut für Angewandte Mechanik, RWTH Aachen*), Stefanie Reese (*Institut für Angewandte Mechanik, RWTH Aachen*) 08:30–08:50

This talk presents a computational nonlinear homogenization approach, the starting point of which is a model order reduction method based on data-clustering. To this end, the micromechanical data from numerical experiments (snapshots) is analyzed in order to identify characteristic microstructural deformation patterns. These describe how the macroscopic strain typically localizes within the microstructure. The outcome of the procedure is a subdivision of the microstructure into a set of clusters of material points. Within each cluster the strain is then approximated as being constant.
The mechanical problem is formulated in terms of a three-field Hashin-Shtrikman type variational formulation which is based on the introduction of a linear-elastic reference medium. After discretization, most of the global unknowns can be eliminated via static condensation leaving the piecewise constant cluster strains as the primary unknowns.
The resulting homogenization scheme includes, as special cases, the finite element method as well as Hashin-Shtrikman and Talbot-Willis type homogenization approaches with phase-wise constant trial fields (as well as related bounds). The limit case 'finite element method' allows to transfer knowledge from finite element technology and thus provides new strategies for the choice of the stiffness of the reference material. The method is applied to several nonlinear microstructures with different inclusion volume fractions and varying degree of anisotropy. The results are shown to be in good agreement with full-field FE-simulations. Furthermore, the method is used to compute a refined upper bound of the Talbot-Willis type (compared to phase-wise constant trial fields), which converges to the finite element solution with increasingly refined discretization.

An efficient reduced computational method for nonlinear homogenization problems: the Hashin-Shtrikman type Finite Element method (HSFE)

Fabiola Cavaliere (*Institut für Angewandte Mechanik, RWTH Aachen*), Stephan Wulfinghoff (*Institut für Angewandte Mechanik, RWTH Aachen*), Stefanie Reese (*Institut für Angewandte Mechanik, RWTH Aachen*) 08:50–09:10

An efficient reduced computational method for nonlinear homogenization problems: the Hashin-Shtrikman type Finite Element method (HSFE) A numerically efficient homogenization approach for nonlinear microstructures, which combines the small computational effort of the Hashin-Shtrikman type approach with the accuracy of full-field finite element solutions (HSFE), has

been recently proposed by the authors [1]. The key point of the method is a model order reduction scheme based on data-clustering, which is performed by means of FE-simulations of microstructures (snapshots) driven by characteristic macroscopic deformations. The analysis of these snapshots provides a description of the strain localization within the microstructure. The method exploits this feature to perform the model order reduction by subdividing the RVE into a set of clusters of material points where the strain is approximated as being homogeneous. The mechanical problem is formulated in terms of a three-field Hashin-Shtrikman type variational formulation [2]. After discretization, most of the global unknowns can be eliminated via static condensation leaving the piecewise constant cluster strains as the primary unknowns. As a consequence, the presented microscopic model has significantly less degrees of freedom in comparison to the classic FE2-method. In addition the number of stress computations within the microstructure is highly reduced. The computation of the analytical tangent operator realises the coupling between the microscopic and macroscopic scale, allowing to compute two-scale simulations of complex macrostructures. The presented approach is tested in the context of small strains. Different numerical examples are carried out, where a nonlinear RVE is attached to each integration point of a macrostructure. A comparison to the FE-simulations shows that the macro-response is well captured by the HSFE method.

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Consistent FFT-based homogenization in nonlinear electroelasticity

Felix Selim Göküzüm (*Institute of Applied Mechanics (CE, Chair 1), University of Stuttgart*), Lu Trong Khiem Nguyen (*Institute of Applied Mechanics (CE, Chair1), University of Stuttgart*), Marc-André Keip (*Institute of Applied Mechanics (CE, Chair1), University of Stuttgart*)

09:10–09:30

Motivated by the recent progress in research and development of electroactive polymers (EAP) [1], the goal of the present contribution is to formulate a *fast-Fourier-transform-based multiscale framework for the simulation of electroelastic composites*. In the context of numerical homogenization, the FFT-based method suggested by Moulinec & Suquet [2] has increased in popularity due to its high computational speed and the straight-forward processing of micrograph images. The algorithm is based on the solution of the Lippmann-Schwinger equation on a periodic representative volume element (RVE) of a composite, where the Lippmann-Schwinger equation is formulated in terms of the deformation gradient and its dual variable, namely the first Piola-Kirchhoff stress tensor, using an appropriate *linear reference medium*. It is usually solved by means of a fixed-point iteration or conjugate gradient method [3]. Recently, the method has been successfully incorporated into multiscale frameworks [4,5].
Our present work focuses on the rigorous extension of the Lippmann-Schwinger equation to coupled problems with a special focus on the influence of the coupled linear reference medium on the convergence behaviour. Additionally, a consistent macroscopic coupled tangent operator is derived by means of the Lippmann-Schwinger equation [6,7]. Finally, aspects of using a *reduced macroscopic tangent operator* for coupled problems are discussed.

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.5627 (2018).

[7] F. Göküzüm, L. T. K. Nguyen, M.-A. Keip: Consistent FFT-based multiscale homogenization of electromechanically coupled materials, *in preparation*, (2018).

S08.02 | Multiscales and homogenization

Date 21.03.2018
Room 0220

Nonlinear dynamic mechanical metamaterials

Dennis Kochmann (*Department of Mechanical and Process Engineering, ETH Zürich*) 14:00–14:40

Mechanical metamaterials are periodic or more complex structures whose small-scale architecture gives rise to controllable macroscopic (meta)material properties with applications ranging from acoustic wave guiding and cloaking to controllable stiffness and strength. Here, we discuss a new paradigm: the exploitation of small-scale instabilities and nonlinearities to produce interesting nonlinear dynamic effective behavior at the macroscopic scale. Instability entails a nonconvex energy landscape and the associated formation of microstructure (such behavior occurs frequently in materials undergoing, e.g., phase transformations or ferroelectric and -magnetic switching). Under applied external fields domain boundaries move and give rise to nonlinear hysteresis. We will demonstrate how such effective behavior can be reproduced by periodic structures with intrinsic instabilities, both qualitatively and quantitatively. To this end, we discuss selected examples of nonlinear mechanical metamaterials and emphasis the micro-to-macro transition of their dynamic phenomena (both analytically by taking continuum limits and numerically by studying realistic systems). Finally, experimental realizations are shown to validate the model and give evidence of this class of nonlinear dynamic mechanical metamaterials.

Numerically robust two-scale full-field finite strain crystal plasticity simulations of polycrystalline materials

Julian Kochmann (*Institute of Applied Mechanics, RWTH Aachen University*), Tim Brepols (*Institute of Applied Mechanics, RWTH Aachen University*), Stephan Wulfinghoff (*Institute of Applied Mechanics, RWTH Aachen University*), Bob Svendsen (*Chair of Material Mechanics, RWTH Aachen University*), Stefanie Reese (*Institute of Applied Mechanics, RWTH Aachen University*) 14:40–15:00

The work is concerned with the development of two-scale numerical scheme for the prediction of the local and effective mechanical behavior of polycrystalline materials with elasto-viscoplastic constitutive behavior at finite strains. Assuming scale separation, the microstructural deformations are dictated by the kinematics of the macroscopic continuum body. The macroscopic constitutive behavior is in turn determined by the mean response of the point-wise attached microstructure which is represented by a statistically similar periodic unit cell. The algorithmic formulation and numerical solution of the two locally-coupled boundary value problems is based on the FE-FFT method (e.g. Spahn et al. 2014, Kochmann et al. 2016, 2017). In particular, this work deals with the development of a numerically robust and an efficient numerical scheme for two-scale full-field finite strain crystal plasticity simulations of polycrystalline aggregates. The results of two- and three-dimensional problem settings indicate that the proposed method is characterized by numerically robust computations for relatively large time increments and high rate sensitivity parameters, an accurate representation of micromechanical fields and moderate overall computation times.

A thermomechanically coupled FE2-framework - application to thermoviscoplasticity

Rolf Berthelsen (*Institute of Mechanics, TU Dortmund University*), Andreas Menzel (*Institute of Mechanics, TU Dortmund University*) 15:00–15:20

In many technological applications, it is essential to understand the coupling between thermal and mechanical loading during the whole process. In order to reduce the costs during the development of new processes or during the optimisation of existing processes, numerical simulations play a major role. While many of todays engineering processes involve materials which consist of different constituents - with their own physical properties - the prediction of the effective material behaviour of such composite materials is a key aspect of numerical process analysis. Amongst other methods, the so called FE^2-method is one option to transfer the behaviour from the lower scale, at which the heterogeneities are explicitly resolved, to the effective material response at the upper scale. In this contribution, a nonlinear thermomechanically coupled two-scale finite element framework is elaborated and applied to the simulation of thermoviscoplasticity. The performance of the framework is presented by means of representative examples.

An adaptive FE^2 method for the thermomechanical behaviour of a SMA-Fiber matrix composite

Maximilian Praster (*Lehrstuhl für Baustatik und Baudynamik, RWTH Aachen University*), Sven Klinkel (*Lehrstuhl für Baustatik und Baudynamik, RWTH Aachen University*) 15:20–15:40

This contribution deals with the multiscale analysis of a reinforced matrix with shape-memory-alloys (SMA). An FE^2 approach is employed to capture the nonlinear behavior of the microstructure. SMA has a complex behavior with a high-temperature dependency in the loading

and unloading case. The microstructure of the macroscopic problem consists of a linear-elastic matrix and a random fiber distribution. The stress response of the composite depends nonlinear on the deformation, the fiber orientation and the temperature in the integration point. This necessitates an accompanying homogenization during the loading of the macro structure. One disadvantage of the FE^2 method is the high computational effort by solving a boundary value problem (BVP) in every integration point and every iteration step. This motivates an adaptive scheme, where the accompanying homogenization is performed only if necessary. Here, an indicator for the accompanying FE^2 analysis is presented. Due to the temperature dependency, on the macroscale, a coupled thermo-mechanical problem is solved on the microscale. In the first homogenization step, the BVP of the RVE is performed with Neumann Boundary conditions. This leads to an underestimation of the stiffness and accordingly to an overestimation of the strains. The SMA will stay linear elastic until the phase transition condition is reached, which is defined by a critical strain and temperature level. From the phase transition condition, the temperature dependent indicator is defined as a limit strain for the linear behavior of the SMA-fibers. An accompanying homogenization is only necessary when the limit strain is exceeded, aftet that the accompanying homogenization is performed.

A multi-phase/-scale numerical model for temperature driven solidification processes

Lukas Moj (*ISD: Institute of Mechanics, Structural Analysis and Dynamics, University of Stuttgart*), Tim Ricken (*ISD: Institute of Mechanics, Structural Analysis, and Dynamics, University of Stuttgart*), Rüdiger Deike (*Chair of Metallurgy for Iron and Steel Production, University of Duisburg-Essen*) 15:40–16:00

Numerical simulations of hot working processes, like casting and forming have gained significant importance for steel making industries in order to improve manufacturing. Hence, a continuum-mechanical, bi-phasic, two-scale model has been developed for thermally driven phase transition during solidification processes. The solid and liquid physical states, representing the solid and molten metallic material are formulated in the framework of the theory of porous media (TPM) [1], including thermal coupling [2], finite plasticity superimposed by a secondary power creep law as well as visco-elasticity associated by Darcy's permeability for the solid and the liquid phase. The phase transition is formulated by a two-scale approach considering the phase-field model on the micro-scale [3]. However, a double-well potential consisting of two local minima at completely solid and liquid physical states is utilized. The inter-scale, energetic consistent micro-macro linking scheme is formulated, where the homogeneity condition must be fulfilled.The finite element method and the finite difference method are employed to solve the macroscopic and the microscopic boundary value problem. The numerical performance as well as its validation is shown by two numerical examples. The first example denotes a solidification experiment, where a cube-shaped specimen is cooled down by the atmosphere. Moreover, the temperature and the shrinkage have been recorded during the experiment. The second experiment is a controlled cooling process of a cylindrical specimen in a Bridgman oven.

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S08.03 | Multiscales and homogenization

Date 21.03.2018
Room 0220

Microstructure modelling using the scaled boundary finite element method

Carolin Birk (*Universität Duisburg-Essen*), Xinran Tian (*Hohai University*) 16:30–17:10

Innovative and classical composite materials such as ceramic matrix composites and concrete are characterized by a heterogeneous microstructure. Their macroscopic behaviour is determined by the physical and mechanical properties of their constituents as well as by their morphology. Moreover, microstructures often exhibit random geometrical features. For engineering applications, effective properties of homogenized micro-heterogeneous materials are required. Stochastic approaches to uncertainty quantification of effective properties require highly efficient numerical procedures.
In this paper a scaled boundary finite element approach to calculate effective material properties of random microstructures is proposed. Here, circular and elliptical inclusions with varying number of inclusions, aspect ratio, location and orientation are randomly distributed in a homogeneous matrix. For each random topology, a structured quadtree or octree mesh is generated using image-based modelling techniques. Such meshes are beneficial when highly irregular geometries prevail and allow for a rapid transition in mesh size when geometrical features of very different scale are present.
Despite its versatility, the use of the finite element method on structured meshes has been largely precluded by the existence of hanging nodes. In this paper, linear elastic structural analysis on structured meshes is facilitated by the scaled boundary finite element method (SBFEM). Only the boundaries of a domain are discretized with line or surface elements, thus avoiding the hanging nodes issue. Generalized polygon and polyhedral elements are constructed which can be used in a finite element framework, thus allowing for the extension to nonlinearity. In combination with automatic mesh generation techniques the SBFEM provides a potentially highly efficient alternative approach to uncertainty quantification of effective properties. This will be illustrated using several examples.

Effective description of anisotropic wave dispersion in mechanical metamaterials via the relaxed micromorphic model

Angela Madeo (*INSA Lyon*), Marco Valerio d'Agostino (*INSA Lyon*), Gabriele Barbagallo (*INSA Lyon*), Ionel-Dumitrel Ghiba (*Alexandru Ioan Cuza University of Iasi*), Patrizio Neff (*Mathematik / Nonlinear Analysis, Universität Duisburg-Essen*), Bernhard Eidel (*Heisenberg-Group, Department of Mechanical Engineering, University Siegen*) 17:10–17:30

The relaxed micromorphic model for anisotropic elasticity is used to describe the dynamical behavior of a band-gap metamaterial with tetragonal symmetry. Unlike other continuum models (Cauchy, Cosserat, second gradient, Mindlin-Eringen micromorphic), the relaxed model is endowed to capture the main microscopic and macroscopic characteristics of the targeted metamaterial, namely, stiffness, anisotropy, dispersion and band-gaps. The simple structure of our material model, which simultaneously lives on a micro-, a meso- and a macroscopic scale, requires only the identification of a limited number of frequency-independent truly constitutive parameters, valid for both static and wave-propagation analyses in the plane. The static macro- and microparameters are identified by numerical homogenization in static tests on the unit-cell level. The

3 macro-parameters are obtained by imposing periodic boundary conditions thus mimicking the structure at large. The 3 micro-parameters can be uniquely identified for a unit-cell, which (i) represents the unit-cell with maximal stiffness and (ii) preserves its tetragonal symmetry. Both conditions (i) and (ii) are built on the inherent rationale of the relaxed micromorphic model. The missing mesoscopic elastic parameters directly follow from a recently developed harmonic-mean type micro-macro homogenization rule, which establishes the general relation between the elasticities in the micromorphic model on its three scales. The remaining inertia parameters for dynamical analyses are calibrated on the dispersion curves of the same metamaterial as obtained by Bloch-Floquet analysis for two wave directions. We demonstrate via polar plots that the obtained material parameters describe very well the response of the structural material for all wave directions in the plane, thus covering the complete panorama of anisotropy of the targeted metamaterial.

Numerical Homogenization for Linear Elasticity in Translation Invariant Spaces

Ronny Bergmann (*Fachbereich Mathematik, TU Kaiserslautern*), 17:30–17:50
Dennis Merkert (*Fachbereich Mathematik, TU Kaiserslautern*)

In homogenization the quasi-static equation of linear elasticity with periodic boundary conditions is used to characterize the macroscopic elastic properties of composite materials, with material data often sampled on voxel grids.
This partial differential equation allows for a different formulation where the strain is given as a fixed-point of the Lippmann-Schwinger equation. For data on a regular grid, i.e. an equispaced tensor product grid, the Lippmann-Schwinger equation can be discretized by a Galerkin projection onto spaces of truncated Fourier series on the torus. Based on this approach, Moulinec and Suquet formulated a matrix-free algorithm that makes heavy use of the fast Fourier transform to decompose the occurring linear operators. The computational effort is dominated by the fast Fourier transform resulting in very fast computations applicable to large numbers of degrees of freedom.
This talk introduces a generalization of this discretization approach to anisotropic spaces of translates, i.e. spaces generated by translating a single function on an anisotropic lattice on the torus. Such ansatz functions include periodized Box splines (and thus simplified finite elements) and anisotropic de la Vallée Poussin means. The truncated Fourier series approach emerges as a special case.
By choosing the anisotropic lattice when generating the translation invariant space, the sampling grid can be adapted to dominant directions occurring in the composite material. De la Vallée Poussin means then further provide a way to smoothen these directions independent from each other which can further reduce disturbances from jumps at interface boundaries, as will be demonstrated on numerical examples.

Computational homogenization of nematic liquid crystal elastomers based on Landau-de-Gennes theory

Omkar Nadgir (*Institute of Applied mechanics, University of Stuttgart*), 17:50–18:10
Matthias Rambausek (*Institute of Applied Mechanics, University of Stuttgart*),
Marc-André Keip (*Institute of Applied Mechanics, University of Stuttgart*)

Nematic liquid crystal elastomers (LCEs) represent an important class of materials with a complex microstructure [1, 2, 3]. In this talk, we present techniques of computational homogenization of LCEs based on Landau-de Gennes theory. A symmetric and traceless tensor $\mathbf{Q}$ is employed as an internal variable in order to capture the nematic behavior [4]. An Allen-Cahn type phase-field equation is used to describe the evolution of $\mathbf{Q}$, whereas the coupling with a small-strain

elastic energy provides the elasto-nematic character to the model. Computational homogenization techniques are adopted [5, 6] in order to account for the scale-bridging scenerios between micro- and macro-scale of LCEs. Numerical simulations of initial- and boundary-value-problems are presented in order to investigate the underlying material characteristics.

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S08.04 | Multiscales and homogenization

Date 22.03.2018
Room 0220

A nonlinear FE-HMM formulation along with a novel algorithmic structure for finite deformation elasticity

Bernhard Eidel (*Heisenberg-Group, Department of Mechanical Engineering, University Siegen*), Andreas Fischer (*Heisenberg-Group, Department of Mechanical Engineering, University Siegen*)

08:30–08:50

This contribution presents a general, nonlinear formulation of the Finite Element Heterogeneous Multiscale Method (FE-HMM) for the homogenization of microheterogeneous solids. It is based on the precursor work [1] dealing with the setting of linear elasticity in a geometrical linear frame and the general framework of FE-HMM established in [2-4]. The second thrust is the proposal of a novel algorithmic structure which enables for the broad range of hyperelastic constitutive laws a considerable speed-up in comparison to the standard algorithmic structure. The novel idea is equally applicable for FE^2 and related homogenization methods. A set of numerical examples underpins the improved efficiency.

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Micromorphic, micropolar and microstrain continua: a comparative study based on homogenisation of particle simulations

Sami Bidier (*Institute of Applied Mechanics, Institute of Applied Mechanics, University of Stuttgart*), Wolfgang Ehlers (*Institute of Applied Mechanics, Institute of Applied Mechanics, University of Stuttgart*) 08:50–09:10

Extended continuum-mechanical theories, such as the micromorphic, the micropolar or the microstrain continuum, are suitable formulations when additional characteristic microstructural deformation modes should be included into macroscopic modelling techniques. This is especially the case when the microscopic view of the considered material reveals a granular or particulate structure. Then, by means of a particle-centre-based homogenisation technique, it is possible to link the microstructural information that can be gained, for example, from discrete-element simulations, to the extended deformation and stress states of the above mentioned extended continua. In this context the present contribution focuses on two main aspects: at first, different granular microstructures, in particular bonded, unbonded or rotation-free particle systems, are investigated using a discrete-element formulation with the emphasis on the evolution of strain localisation phenomena. Secondly, the obtained results of these initial-boundary-value problems are homogenised towards micropolar, microstrain and micromorphic stresses and strain measures. Depending on the microstructural characteristics, the activation of the different deformations and stresses of the extended continua are compared and evaluated.

Cosserat parameters of foams by homogenization

Geralf Hütter (*Institute of Mechanics and Fluid Dynamics, Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg*) 09:10–09:30

Classical Cauchy-Boltzmann continuum theory comes to its limits when the dimensions of a specimen (and thus the distances over which gradients occur) become comparable to the length scales of the microstructure. For instance it has been shown that the bending and torsion stiffnesses of foams are strongly underestimated by classical theory if only few cells are present over the cross section of the specimen, Fig. 1. However, in order to simulate such behavior numeric-

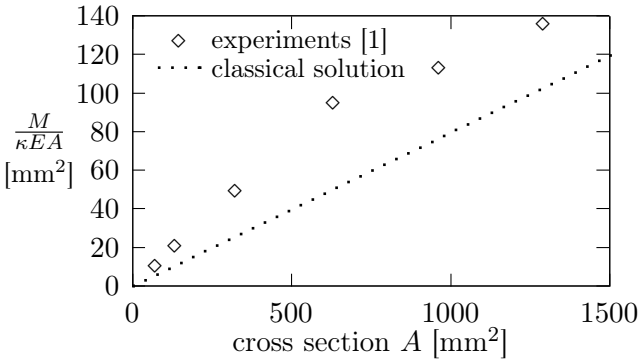

Figure 1: Normalized bending stiffness of a foam in dependence of specimen cross section

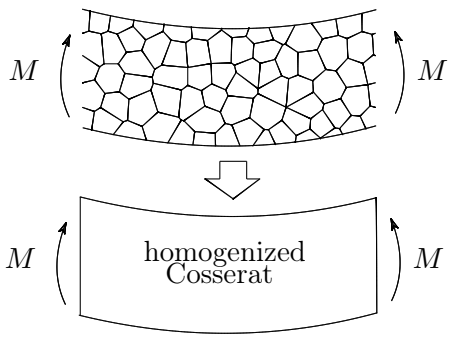

Figure 2: Micromorphic homogenisation for a porous medium

ally, the microstructure can hardly be resolved discretely, especially not in 3D simulations. That is why generalized continuum theories like the Cosserat theory were employed to model such

size-effects at the macroscale. Mostly, the necessary constitutive laws are formulated heuristically and the corresponding large number of parameters must then be identified from experiments.

Recently, the author developed a homogenization framework which allows to derive the micromorphic constitutive law from the microstructure of a material [2]. The Cosserat theory, also known as micropolar theory, is a special case of the micromorphic theory. In the present contribution, this framework is applied to compute the Cosserat constitutive parameters of a foam material. The *predicted* size-effect is compared to corresponding experimental results from literature.

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Towards a unified Lagrangian multi-scale model for interacting particles

Jens Bender (*Transport Processes, Fraunhofer ITWM*), Axel Klar (*Technische Universität Kaiserslautern*), Jörg Kuhnert (*Fraunhofer ITWM*)

09:30–09:50

The simulation of interacting particle systems by individual tracking in a Lagrangian framework can become virtually impossible in feasible time frames and for large problem sizes. This is why there are many approaches to describe the resulting behavior by continuous equations which are usually much more efficiently solved using an Eulerian grid on a larger scale. Motivated by the development of a Lagrangian generalized finite difference solver using moving point clouds, we work towards a method that can blend between the different scales in a unified framework. To this end, we derive a macroscopic model which still contains microscopic information in the form of an integral term. Different approximations of this term based on the point cloud configuration then allow for a scaling between the representation of microscopic particles and the solution of a purely macroscopic model by the point cloud. We will evaluate the model performance based on the classical spring-damper forces known from discrete element methods and compare to previous results on a multi-scale meshfree method for interacting particle systems.

On the Identification of Contact Parameters of the Discrete Element Method for Complex Particle Ensembles

Golnaz Hoormazdi (*Theory of Materials, Ruhr-Universität Bochum (RUB)*), Klaus Hackl (*Materialtheorie, Ruhr-Universität Bochum (RUB)*)

09:50–10:10

The Discrete Element Method (DEM) is a particle-based approach, which is applied in a wide range of engineering fields. One problem of the DEM is the identification of the required input parameters. In this study, we develop an analytical prediction based on an energy minimization approach relating the macroscopic elastic parameters to the microscopic contact parameters. In order to validate these relations, a series of confined and unconfined compression tests are performed by PFC3D. A more complex version of materials containing a mixture of different types of particle ensembles are used to study the effect of bonding and grain shape on the elastic properties of the materials. These results are compared to the previous study of materials with all spherical grains for both solid (bonded) and granular (unbonded) materials.

Homogenization of Kirchoff-Love plate equation

Krešimir Burazin (*Department of Mathematics, University of Osijek*), Marko Vrdoljak (*Department of Mathematics, Faculty of Science, University of Zagreb*), Jelena Jankov (*Department of Mathematics, University of Osijek*) 10:10–10:30

We are interested in general homogenization theory for fourth-order elliptic equation describing the Kirchhoff-Love model for pure bending of a thin solid symmetric plate under a transverse load. Such theory is well-developed for second-order elliptic problems, where a key role plays H-convergence, which was introduced by Spagnolo through the concept of G-convergence (1968), and further generalised by Tartar (1975) and Murat and Tartar (1978) as H-convergence. While some results for general elliptic equations were established by Zhikov, Kozlov, Oleinik and Ngoan (1979), we push forward currently known results by proving a number of properties of H-convergence for stationary plate equation, including metrizability of H-topology and corrector result.
We give special emphasis to calculating the first correction in the small-amplitude homogenization limit of a sequence of periodic tensors describing material properties of the plate. We also discuss smooth dependence of H-limit on a parameter and calculate H-limit of a periodic sequence of tensors.

S08.05 | Multiscales and homogenization

Date 22.03.2018
Room 0220

Mean field homogenization schemes for short fiber reinforced thermoplastics based on real microstructural information

Patrick Arthur Hessman (*Robert Bosch GmbH, Karlsruhe Institute of Technology (KIT)*), Kurt Hornberger (*Robert Bosch GmbH*), Fabian Welschinger (*Robert Bosch GmbH*) 14:00–14:20

Mean field homogenization models have been an ongoing subject of academic research and have seen widespread industrial application due to the introduction of efficient schemes that allow the description of complex composite materials, e.g. short fiber reinforced thermoplastics.
This work focuses on the application of different mean field models to an injection-molded short glass fiber reinforced polyamide 6.6 thermoplastic polymer with a fiber mass fraction of 30%. The material's process-induced microstructure is characterized by means of x-ray micro-computed tomography, yielding morphological data including the fiber orientation and fiber length distributions. Based on this information, models such as the Mori-Tanaka [1], Interaction Direct Derivative [2] and Two-Step [3] homogenization schemes are employed to describe the composite's micromechanical state.
The models are compared with regard to their predictions for the effective elastic moduli as well as the stress localization, the latter playing a crucial role in the onset and development of inelastic material behavior. Finally, the influence of the microstructural morphology is discussed and limits to the models' applicability are highlighted.

[1] Benveniste, Y.: A new approach to the application of Mori-Tanaka's theory in composite materials. Mechanics of Materials **6**, 147–151 (1987).

[2] Zheng, Q.-S., and Du, D.-X.: An explicit and universally applicable estimate for the effective properties of multiphase composites which accounts for inclusion distribution. Journal of the Mechanics and Physics of Solids **49**, 2765–2788 (2001).

[3] Pierard, O., Friebel, C., and Doghri, I.: Mean-field homogenization of multi-phase thermoelastic composites: a general framework and its validation. Composites Science and Technology **64**, 1587–1603 (2004).

Efficient Simulation of Short Fibre Reinforced Composites

Rolf Springer (*Mathematics, TU Chemnitz*) 14:20–14:40

Lightweight structures became more and more important over the last years. One special class of such structures are short fibre reinforced polymers (SFRPs), produced by injection moulding. To avoid expensive experiments for testing the mechanical behaviour of these composites proper material models are needed. Thereby, the stochastic nature of the fibre orientation is the main problem.
In this talk the simulation of such materials in a linear thermoelastic setting is considered. So, the stress-strain relation

$$\sigma = \mathfrak{C} : (\varepsilon - (\theta - \theta_0)\mathbf{T}),$$

is used. Here, $\mathfrak{C}$ is the fourth order stiffness tensor, $\mathbf{T}$ is the second order thermal expansion tensor, $(\theta - \theta_0)$ is the temperature difference, and ε is the second order linearised strain tensor. Furthermore, the temperature θ is described by the stationary heat equation

$$-\nabla(\cdot\kappa \cdot \nabla\theta) = \Theta,$$

with the second order heat conduction tensor κ.
The occurring material quantities of SFRPs can be obtained in a quite easy and straightforward manner with the "Tucker Averaging Procedure". However, this approach does not consider the stochastic nature of the underlying partial differential equations. In this talk a way is presented how this common approach can be extended for a better incorporation of the stochastic nature of the orientation of the short fibres.

Numerical material testing based on statistically similar representative volume elements for discontinuous fiber composites

Takashi Sasagawa (*Toyota Central R &D Labs., Inc., Japan*), Masato Tanaka (*Toyota Central R &D Labs., Inc., Japan*), Ryuji Omote (*Toyota Central R &D Labs., Inc., Japan*), Daniel Balzani (*Institute of Mechanics and Shell Structures, Technical University Dresden, Germany*) 14:40–15:00

Discontinuous fiber composites (DFCs) are one of the most important advanced materials for lightweight vehicle design. To ensure the safety and reliability of the automobiles, it is essential to accurately predict mechanical properties of materials used in the vehicles, which are typically obtained by a series of material tests. Numerical material testing (NMT) [1] based on computational homogenization methods [2] is a more efficient alternative to estimate the nonlinear material properties of the composites. The NMT can compute macroscopic stress-strain relationships by solving microscopic boundary value problems (BVP) using representative volume elements (RVEs). However, the NMT usually requires high computational cost especially for DFCs due to the high aspect ratio of fibers. To overcome this difficulty, a method for the construction of statistically similar RVEs (SSRVEs) for fiber-reinforced composites is proposed. The SSRVE can be interpreted as simplified RVE reflecting real microstructures in terms of statistical

measures which characterizes the microstructure morphology, see details in Balzani et al. [3][4]. In this contribution, the power spectral density is used as the statistical measure to construct the SSRVE of the fiber reinforced composites. The resulting mechanical properties of the SSRVE are in good agreement with the target RVE and the computational cost can be significantly reduced compared to the target RVE.

D. Balzani's present affiliation is Chair of Continuum Mechanics, Ruhr-University-Bochum, Department of Civil- and Environmental Engineering, Germany.

[1] K. Terada, J. Kato, N. Hirayama, T. Inugai, K. Yamamoto, A method of two-scale analysis with micro-macro decoupling scheme: application to hyperelastic composite materials, Computational Mechanics, 52 (2013) 1199-1219.

[2] C. Miehe, J. Schotte, J. Schröder, Computational micro–macro transitions and overall moduli in the analysis of polycrystals at large strains, Computational Materials Science, 16 (1999) 372-382.

[3] D. Balzani, D. Brands, J. Schröder, C. Carstensen, Sensitivity analysis of statistical measures for the reconstruction of microstructures based on the minimization of generalized least-square functionals, Technische Mechanik, 30 (2010) 297-315.

[4] D. Balzani, L. Scheunemann, D. Brands, J. Schröder, Construction of two- and three-dimensional statistically similar RVEs for coupled micro-macro simulations, Computational Mechanics, 54 (2014) 1269-1284.

Seeding and growing RVEs of electrospun fibre networks

Sebastian Domaschke (*Empa - Swiss Federal Laboratories for Materials Science and Technology*), Alexander E. Ehret (*Empa - Swiss Federal Laboratories for Materials Science and Technology*)

15:00–15:20

Electrospinning proved to be a versatile method, to produce nano-fibrous networks with a wide range of mechanical and structural properties. Despite the broad application of electrospun materials [1], the mechanical understanding of the relation between the micro structure on the fibre scale and the macroscopic response is still limited. To shed light on this relation, 3D representative volume elements (RVEs) created by a virtual spinning process, in which fibres discretized by finite beam elements are deposited and form a network. This procedure allows considering fibre orientation, shape, interaction properties and fibre material behaviour over a wide range. From the networks RVEs characteristic quantities such as cross-link density or fibre segment orientation can be extracted. Moreover, these RVEs serve as reference configuration for subsequent simulations, where the network undergoes prescribed macroscopic deformations, and from which the homogenized network response is computed.
In the present contribution we focus on steps of generating a statistically representative fibre shape, and of seeding the fibres such that a final random network structure within the RVE is obtained. The first aspect is addressed by treating fibres as worm-like chains [2], allowing for the generation of representative random fibre shapes in-silico by extracting a single parameter from electron microscopy images. For the second step, analytical approaches and Monte Carlo simulations are employed to characterise randomness by isotropy and homogeneity criteria. A major influence of the size and shape of the seeding domain on both these criteria is revealed and quantified for both straight fibres and those described by worm-like chains. Methods to address these limitations are presented and discussed.

[1] Fang, J., et al., *Applications of electrospun nanofibers.* Chinese Science Bulletin, 2008.**53**(15):p.2265-2286.

[2] Rivetti, C., M. Guthold, and C. Bustamante, *Scanning force microscopy of DNA deposited onto mica: Equilibration versus kinetic trapping studied by statistical polymer chain analysis.* Journal of Molecular Biology, 1996.**265**(5):p.919-932.

Damage evolution in fiber reinforced polymer-metal joints - modeling and simulation

Franz Hirsch (*TU Dresden, Institute of Solid Mechanics*), Markus Kästner (*TU Dresden, Institute of Solid Mechanics*) 15:20–15:40

The application of fiber reinforced polymers (FRP) in lightweight structures requires innovative joint concepts since e.g. the large-scale production of critical components in automotive engineering necessitates the combination of FRP with classical lightweight metals. As established technologies like bolt joints induce unintentional damage to the material during the manufacturing process, interlocking joining concepts are promising alternatives [1].
In this contribution, the interface behavior of an aluminum component connected to an FRP is considered on the microscale [2]. The microsection of the interface zone between both materials exhibits different inhomogeneities, e.g. the rough metal-polymer interface and embedded carbon fibers. The structure can be divided into a homogeneous metal zone, an FRP zone and a transition zone with pure polymer material which fills the rough metal surface.
Based on the definition of a representative volume element, a microscale model is developed to investigate the interaction of the weak aluminum-polymer interface and the strength of the bulk material with their influence on the overall interface properties. Characteristic geometric interface parameters are used to generate generic surface structures with a defined roughness. The application of a numerical homogenization approach allows to derive effective traction-separation relations from the micromechanical simulations [3]. Arising adhesive damage is described by a cohesive zone model, while the large deformation behavior of the polymer is described by an elastic-plastic damage model.
The results of the numerical study show a strength enhancement with increasing roughness, caused by a shift from pure adhesive failure of the local interface to cohesive failure of the bulk material.

[1] R. Kießling, J. Ihlemann, M. Pohl, M. Stommel, C. Dammann, R. Mahnken, M. Bobbert, G. Meschut, F. Hirsch, M. Kästner, On the Design, Characterization and Simulation of Hybrid Metal-Composite Interfaces, *APPL COMPOS MATER* **23** (2016), 1–19.

[2] F. Hirsch, M. Kästner, Microscale simulation of adhesive and cohesive failure in rough interfaces, *ENG FRACT MECH* **178** (2017), 416–432.

[3] M.V.C. Alfaro, A.S.J. Suiker, C.V. Verhoosel, R. de Borst, Numerical homogenization of cracking processes in thin fibre-epoxy layers, *EUR J MECH A-SOLID* **29** (2010), 119–131.

Coupling of an explicit and implicit finite element model to simulate the draping behavior of a plain-woven fabric

Benjamin Kaiser (*Technische Hochschule Mittelhessen - University of Applied Sciences*), Thomas Pyttel (*Technische Hochschule Mittelhessen - University of Applied Sciences*), Fabian Duddeck (*Computational Mechanics, Technical University Munich*) 15:40–16:00

To simulate the draping behavior of a plain-woven fabric a complex interaction of kinematic between tows and continuous deformation of tows must be considered. Common methods just take continuous deformation into account on a macro scale. These methods for example model the fabric with an orthotropic material behavior.
The presented work overcomes this limitation by coupling a macroscopic explicit finite shell element with a mesoscopic implicit model of a 3D unit cell. This unit cell models the real fabric with 1D structure elements like beams, bars and torsion elements. The torsion element is also able to model contact between fibers. The created model has been set up with periodic boundary conditions and solved with a 3D implicit static nonlinear solver.
The macroscopic shell element is implemented in the nonlinear, dynamic PAM-Crash environment. All standard options like penalty contact and rigid bodies can be used to model the draping process. Due to coupling of macroscopic explicit simulation and the mesoscopic implicit simulation disadvantages for example of an explicit method, whit small element lengths which leads to small time steps, can be eliminated by the implicit method.

S08.06 | Multiscales and homogenization

Date 22.03.2018
Room 0220

Derivation of higher-order terms in FFT-based homogenization for periodic media in linear elasticity

Felix Dietrich (*FB Mathematik, AG Differential-Algebraische Systeme, Technische Universität Kaiserslautern*) 17:30–17:50

For industrial applications, it is crucial to have fast and efficient solvers at hand. In the context of continuum mechanics and linear elasticity, it is possible to reduce the computational cost by solving several homogenized problems on representative volume elements (RVE) on the microscale, before then solving the macroscopic one on a coarser grid, as it is done in recent FE-FFT multiscale methods [1].
One of these homogenization based algorithms, called *Basic Scheme*, was introduced in 1994 by Moulinec and Suquet [2]. It attracted the attention of many researchers, who in the following years developed faster or more specified versions of this scheme's idea to compute certain operations in the frequency domain as opposed to the time domain. Based on the work of Boutin from 1996 [3], Tran, Monchiet, and Bonnet extended the Basic Scheme such that macroscopic higher-order derivatives could be taken into account as well [4].
In this talk, the generalized homogenization problems

$$\nabla \cdot \Big(C(x) : \epsilon(x) + p(x) \Big) + g(x) = 0$$

will be derived as a hierarchy of linear equations that allows the inclusion of higher macroscopic derivatives in the computations in the RVE. Here, ϵ denotes the mean-free microscopic strain, C is a stiffness distribution, and p and g are order-dependent polarization and body force terms. We will mainly focus on the numerical differences between zeroth (standard) and first order problems.

[1] J. Spahn, H. Andrä, M. Kabel, R. Müller.
A multiscale approach for modelling progressive damage of composite materials using fast Fourier transforms. *Computer Methods in Applied Mechanics and Engineering 268 (2014): 871–883*

[2] H. Moulinec, P. Suquet.
A fast numerical method for computing the linear and nonlinear properties of composites. *Comptes Rendus de l'Académie des Sciences Paris II 318 (1994): 1417–1423*

[3] T. Tran, V. Monchiet, G. Bonnet.
A micromechanics-based approach for the derivation of constitutive elastic coefficients of strain-gradient media. *International Journal of Solids and Structures 49 (2012): 783–792*

[4] C. Boutin.
Microstructural effects in elastic composites. *International Journal of Solids and Structures 33 (1996): 1023–1051*

A two-scale homogenisation approach for fluid saturated porous media based on TPM and FE^2-Method

Florian Bartel (*Chair of Mechanics, Statics, Dynamics, TU Dortmund University*), Tim Ricken (*Stuttgart University*), Jörg Schröder (*Duisburg-Essen University*), Joachim Bluhm (*Duisburg-Essen University*) 17:50–18:10

Thinking about the description of porous materials, e.g. metal foam, human tissue, plants or soils, we always have to take into account a global design composed of various substructures with different characteristics on a lower level. Examples of such substructures are pores which can be saturated with fluids or gases, fibers with different orientations or cells which can be influenced by chemical reactions. For the theoretical description of the behavior, enhanced continuum mechanical models give promising approaches. Up to now, due to the high complexity, it has not been possible to simulate these systems with only one design model. Hence, it is necessary to think about techniques which simplify the model but still consider the essential characteristics.

It is clear, future applications will consider the discrete microstructure of materials. For example the topology can be received by CT-scanning and therefrom Representative Volume Elements (RVEs) can be designed. Therefore, we are preparing the Theory of Porous Media (TPM), see [1] and [2], for the usage in combination with the FE$^2-$Method, cf. [3] and [4].

This contribution will present a two-scale homogenization approach for fluid saturated porous media with a reduced two-phase material model, which covers the behavior of large poro-elastic deformation. The main aspects of theoretical derivation for the weak form, the lower level boundary conditions under consideration of the Hill-Mandel homogeneity condition and the averaged macroscopic tangent moduli will be pointed out and a numerical example will be shown.

Still, solving a coupled problem in FE^2 environment is extremely time consuming. Therefore, a parallel solution strategy is absolutely essential. Remarks on the investigation of High Performance Computation in this context will be given.

Finally, creating a suitable geometric model and finite element mesh for the macroscopic as well as for the microscopic structure of a real problem will be mandatory for the validation. Hence, we present the mentioned procedure of transferring CT images (.raw data) to a FE-model on an example of a concrete specimen.

[1] R. de Boer and W. Ehlers, *Theorie der Mehrkomponentenkontinua mit Anwendung auf bodenmechanische Problem,* Technical report, Teil I, Forschungsberichte aus dem Fachbereich Bauwesen, Heft **40**, Universität-GH-Essen, 1986.

[2] W. Ehlers, *Poröse Medien – ein kontinuumsmechanisches Modell auf der Basis der Mischungstheorie,* Technical Report **47**, Universität-GH Essen, 1989.

[3] C. Miehe, *Computational micro-to-macro transitions for discretised micro-structures of heterogeneous materials at finite strains based on the minimization of averaged incremental energy,* Computer Methods in Applied Mechanics and Engineering, 2002.

[4] J. Schröder, *A numerical two-scale homogenization scheme: the FE^2-method,* in J. Schröder, K. Hackl (editors), CISM course **550**, Plasticity and Beyond, Springer, 1-64, 2014.

S08.07 | Multiscales and homogenization

Date 23.03.2018
Room 0220

Reduced order modeling of the viscoelastic properties of asphalt concrete

Dennis Wingender (*Institute for Computational Engineering, Ruhr-University Bochum*), Felix Fritzen (*EMMA - Efficient Methods for Mechanical Analysis, Institute of Applied Mechanics (CE), University of Stuttgart*), Ralf Jänicke (*Department of Industrial and Materials Science, Chalmers University of Technology*) 08:30–08:50

Asphalt concrete is a highly heterogeneous mixture appearing as biphasic or triphasic material consisting of mineral aggregates, an bituminous binding agent and, in case of triphasic material, it contains voids additionally. The material data of the linear-elastic mineral aggregates are known from literature, while the material parameters of the bituminous suspension are extracted from Dynamic Shear Rheometer (DSR) tests. To obtain the mixture's overall material behaviour, we apply computational homogenization and model order reduction via the Non-uniform Transformation Field Analysis (NTFA). Therefore, we computationally generate multiple Statistical Volume Elements (SVE), that represent the asphalt concrete structure, based on real-data from X-Ray Computed Tomography or based on data obtained from DIN norms. We generate these structures by applying the Lubachevsky-Stillinger algorithm to find a dense sphere packing. Afterwards, we use the Voronoi tessellation to generate particles and shrink those statistically to their final forms similar to the mineral aggregates. For the verification of the structural generation and homogenization method, we execute the indirect tensile tests in laboratory experiments. Additionally, this test is simulated with the generated macroscopic material model based on homogenized asphalt concrete SVEs with the same geometrical properties as the physical specimens, to compare the results.

First Steps Towards the Direct Micro-Macro Simulation of Reinforced Concrete Under Impact Loading

Erik Tamsen (*Institute of Mechanics and Shell Structures, Technische Universität Dresden*), Wolfgang Weber (*Helmut-Schmidt-Universität - Universität der Bundeswehr Hamburg*), Daniel Balzani (*Ruhr-Universität Bochum*) 08:50–09:10

Reinforced concrete exhibits a strong heterogeneity at the microscale, which gives rise to sophisticated wave propagations at the microscale and thus, a complex macroscopic material behavior under dynamic loading. Especially in strain-hardening cement-based composites, where the favorable energy absorbing behavior under impact loading results from breaking of the concrete matrix and fiber pullout, microscopic dynamical effects may be significant. To establish a valid

model for the effective macroscopic material properties, the finite element method can be used. Then, a suitable RVE can be considered and based on its discretization a microscopic boundary value problem including dynamics can be solved to compute the homogenized mechanical fields at the macroscale. A micro-macro formulation based on kinematic admissibility and the principle of multiscale virtual power [1, 2] is presented, which allows for an energetically consistent scale-bridging. Implementation aspects will be discussed and an initial computational framework for the numerical simulation of reinforced concrete under impact loading is presented and applied to simple numerical examples.

[1] E.A. de Souza Neto, P.J. Blanco, P.J. Sánchez, R.A. Feijóo. An RVE-based multiscale theory of solids with micro-scale inertia and body force affects, Mechanics of Materials, 80:136-144, 2015.

[2] C. Liu and C. Reina. Variational coars-graining procedure for dynamic homogenization. Journal of the Mechanics and Physics of Solids, 104:187-206, 2017.

Multiscale modelling of alkali transport and ASR in concrete structures

Tagir Iskhakov (*Lehrstuhl für Statik und Dynamik, Ruhr-Universität Bochum*), Jithender J. Timothy (*Ruhr-Universität Bochum*), Günther Meschke (*Ruhr-Universität Bochum*) 09:10–09:30

The overall deterioration of concrete pavements is influenced, in addition to traffic induced loads by, continuously varying climatic conditions and its effect on the development of the Alkali-Silica Reaction (ASR). ASR is a microscopic process in concrete characterized by the formation of a hydrophilic alkali-silica gel due to the reaction of the alkali in the pore-fluid with silica in the aggregates. In the presence of moisture, the gel swells and induces an internal pressure that leads to microcracking, expansion and overall deterioration of the material. When subject to external alkali supply, the material is susceptible to higher levels of degradation. Ion and fluid transport in deteriorating concrete (characterized by a distributed network of microcracks) is quantified in terms of a homogenized effective diffusivity and permeability [1]. The effective transport properties are then incorporated into a finite element model to describe the penetration of alkali ions at the structural scale. The overall deterioration of concrete pavements due to ASR is then modelled by a synthesis of two sub-models: 1) the alkali concentration is coupled to a meso-scale finite element reaction diffusion model describing the formation and evolution of the alkali-silica gel in and around the reactive aggregates; 2) the gel induced microcracking in the material is estimated using a semi-analytical multiscale micromechanics model [2]. The model capabilities are evaluated using select numerical examples and comparison with experimental observations.

[1] Timothy, J. J. & Meschke, G. (2016) Cascade lattice micromechanics model for the effective permeability of materials with microcracks. Journal of Nanomechanics and Micromechanics (ASCE), 6, 04016009

[2] Iskhakov, T., Timothy, J. J., & Meschke, G. (2017) Multiscale model of ASR-induced damage in concrete. Proceedings of the 7th GACM Colloquium on Computational Mechanics, Stuttgart. DOI: 10.18419/opus-9334

Improving constitutive equations in multiscale modelling by means of the sufficiency criterion using the example of nano wire contraction

Patrick Kurzeja (*Institute of Mechanics, TU Dortmund University*), Christian Sievers (*Institute of Mechanics, TU Dortmund University*), Jörn Mosler (*Institute of Mechanics, TU Dortmund University*) 09:30–09:50

Statistical and mechanical models share the same challenge of determining closing equations, e.g., estimators in statistics and constitutive equations in multiscale systems. In statistics, there is a powerful tool that allows to improve a given estimator: the sufficiency criterion and its use in the Rao-Blackwell-Kolmogorov theorem. The improved estimator is never worse and only requires a sufficient set of parameters. [1,2]
This concept is however not well-known in mechanical modelling. Yet, it can be adapted to purely mechanical, multiscale problems. For instance, the constitutive equation takes the role of the estimator, the macroscopic parameters replace the random variables and an error norm supersedes the expected deviation. [3]
We will demonstrate how this concept can be adapted to non-statistical, multiscale problems using the example of contraction in relaxed nano wires. We start with a crude and simple equation for the unknown contraction strain excluding relevant geometric information. Then a set of sufficient parameters will be identified. This set is used to derive an improved equation that resembles the real solution in shape and quantity. Molecular simulations will finally highlight the multiscale interpretation of the scheme as implemented in the multiscale framework.

[1] D. Blackwell (1947): Conditional expectation and unbiased sequential estimation, Ann. Math. Stat., 18, 105 - 110.

[2] C.R. Rao (2001): Linear statistical inference and its applications. London, UK: Wiley-Interscience.

[3] P. Kurzeja (2016): The criterion of subscale sufficiency and its application to the relationship between static capillary pressure, saturation and interfacial areas. Proc. R. Soc. A, 472, 20150869.

Norm-Resolvent Convergence in Perforated Domains

Frank Rösler (*Applied Mathematics, Albert-Ludwigs-Universität Freiburg*), Patrick Dondl (*Albert-Ludwigs-Universität Freiburg*), Kirill Cherednichenko (*University of Bath*) 09:50–10:10

For several different boundary conditions (Dirichlet, Neumann, Robin), we prove norm-resolvent convergence for the operator $-\Delta$ in the perforated domain $\Omega \setminus \bigcup_{i \in 2\epsilon\mathbb{Z}^d} B_{a_\epsilon}(i)$, $a_\epsilon \ll \epsilon$, to the limit operator $-\Delta + \mu_\iota$ on $L^2(\Omega)$, where $\mu_\iota \in \mathbb{C}$ is a constant depending on the choice of boundary conditions.
This is an improvement of previous results [Cioranescu-Murat (1982)], [Kaizu (1985)], which show *strong* resolvent convergence. In particular, our result implies Hausdorff convergence of the spectrum of the resolvent for the perforated domain problem.

Kardar-Parisi-Zhang (KPZ) universality of the dynamic correlations in Fermi-Pasta-Ulam-type anharmonic chains

Christian Mendl (*Mathematics, TU Dresden*) 10:10–10:30

We study the time correlations for the conserved fields of Fermi-Pasta-Ulam-type anharmonic chains, and argue that their dynamic correlations can be predicted on the basis of nonlinear fluctuating hydrodynamics, a nonlinear system of conservation laws with noise. For a single mode it is equivalent to the spatial derivative of the one-dimensional Kardar-Parisi-Zhang (KPZ) equation. We find good agreement between the stochastic description on a mesoscopic scale and microscopic molecular dynamics simulations.

Christian B. Mendl, Herbert Spohn. Phys. Rev. Lett. 111, 230601 (2013) (arXiv:1305.1209)

Suman G. Das, Abhishek Dhar, Keiji Saito, Christian B. Mendl, Herbert Spohn. Phys. Rev. E 90, 012124 (2014) (arXiv:1404.7081)

Christian B. Mendl, Herbert Spohn. J. Stat. Mech. (2015) P08028 (arXiv:1505.04218)

S09 | Laminar flows and transition

Organiser Michael Manhart (*Civil, Enviromental and Geo Engineering, TUM Professorship for Hydromechanics*)
Ulrich Rist (*Universität Stuttgart*)

S09.01 | Laminar flows and transition

Date 22.03.2018
Room 2605

Internal Compressible Flow Simulations on Simplex Space-Time Meshes

Max von Danwitz (*Chair for Computational Analysis of Technical Systems, RWTH Aachen University*), Violeta Karyofylli (*Chair for Computational Analysis of Technical Systems, RWTH Aachen University*), Norbert Hosters (*Chair for Computational Analysis of Technical Systems, RWTH Aachen University*), Marek Behr (*Chair for Computational Analysis of Technical Systems, RWTH Aachen University*)

08:30–08:50

The efficiency of many technical applications heavily depends on proper sealing of employed valves and seals. An example of performance-critical seals are piston rings of an internal combustion engine. To improve the sealing effect, detailed knowledge of the leakage flow behaviour is necessary. In this contribution, we propose a numerical methodology to study leakage flow configurations.

Spatially-resolved simulations of leakage flow have to cope with particularly challenging problem geometries. In case of piston rings, the leakage gaps are of μm size while the piston ring pack measures approximately 1 cm in axial direction. Moreover, the topology of the fluid domain may change with time, e.g., a closing valve divides the domain into two separated ones. In contrast to space-time finite element meshes with a structured temporal discretisation, simplex space-time meshes [1] can account for topology changes.

Additionally, the unstructured temporal discretisation can be locally adjusted to the flow conditions. This in very beneficial considering the wide range of Reynolds and Mach numbers expected in leakage flow configurations. Large pressure gradients across sealings force the fluid to extremely high velocities in narrow gaps, so that compressibility has to be considered in the fluid model. To obtain a stable finite element solution to the compressible Navier-Stokes equations, we use an SUPG stabilisation.

[1] V. Karyofylli, M. Frings, S. Elgeti, and M. Behr. Simplex space-time meshes in two-phase flow simulations, to appear in *International Journal for Numerical Methods in Fluids* http://dx.doi.org/10.1002/fld.4414, 2017.

Implicit time discretization schemes for least-squares finite element formulations to model incompressible flows

Solveigh Averweg (*Universität Duisburg-Essen*), Alexander Schwarz (*Universität Duisburg-Essen*), Carina Nisters (*Universität Duisburg-Essen*), Jörg Schröder (*Universität Duisburg-Essen*)

08:50–09:10

In the present contribution different implicit time integration schemes to model incompressible flow problems are investigated. The accuracy and efficiency of lower as well as higher order integration schemes for the solution of the unsteady Navier-Stokes equations are studied. Amongst the tested methods are the fully implicit Newmark, Houbolt and Crank-Nicholson schemes and the singly diagonally implicit Runge-Kutta methods with four and six stages.
A least-squares finite element method (LSFEM) is applied to discretize the flow problem. The first-order system for the proposed formulation is given in terms of stresses and velocities as introduced in [2]. Raviart-Thomas and standard Lagrange interpolations of various orders are used to approximate the stresses and velocities, respectively.
For the comparison of all time discretization schemes, the unsteady two-dimensional laminar flow around a cylinder at the Reynolds number $Re = 100$ is chosen. The physical quantities lift and drag coefficient are evaluated for all investigated time integration methods. For a statement on the accuracy, all obtained results are benchmarked against reference solutions by [1].

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[2] A. Schwarz, J. Schröder, S. Serdas, S. Turek, A. Ouazzi, and M. Nickaeen. Performance aspects of a mixed s-v LSFEM for the incompressible Navier-Stokes equations with improved mass conservation. Proc. Appl. Math. Mech., 13:97-98, 2013

Investigation of a least-squares finite element formulation for sea ice modeling.

Jörg Schröder (*Institut für Mechanik, Universität Duisburg-Essen*), 09:10–09:30 Carina Nisters (*Institut für Mechanik, Universität Duisburg-Essen*), Tim Ricken (*Institut für Statik und Dynamik der Luft- und Raumfahrtkonstruktionen, Universität Stuttgart*)

In this contribution a mixed least-squares finite element method for the modeling of sea ice motion including a viscous-plastic (VP) sea ice rheology is investigated. The simulation of sea ice motion goes back to the findings in [4], who introduced a numerical model for the simulation of sea ice circulation and thickness evolution over a seasonal cycle. Hibler developed a basin-scale model treating the sea ice as a VP material enriched by an additional approach. The ice-thickness distribution on the basis of an evolution equation is explicitly described. Both models are still in use today and involved in climate models. Recent research in this field is devoted to finite element formulations based on the Galerkin variational approach. Here, special focus lies on the stabilization of the numerically complex scheme. It is therefore desirable to establish a least-squares formulation to overcome possible numerical drawbacks. The least-squares variational approach is well established in finite element formulations in the branch of fluid mechanics, see [2], [3] and [6], for instance. A great advantage of the method is its applicability to first-order systems, such that it results in stable and robust formulations also for not self-adjoint operators like in the Navier-Stokes equations, for instance.
The presented least-squares finite element formulation bases on the instationary sea ice equation consisting of the balance of momentum and a constitutive law describing the VP flow. A box test case, which is taken from [5] and [3] is investigated for the least-squares formulation and the results are compared to present results from literature.

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[2] Z. Cai, B. Lee, and P. Wang. Least-squares methods for incompressible Newtonian fluid flow: Linear stationary problems. SIAM Journal of Numerical Analysis, 42(2):843–859, 2004.

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[6] B.-N. Jiang. The least-squares finite element method, Scientific Computation. Springer-Verlag, Berlin, 1998.

A fluid-structure interaction approach with inherently fulfilled coupling conditions

Alexander Schwarz (*Universität Duisburg-Essen*), Solveigh Averweg (*University Duisburg-Essen*), Carina Nisters (*University Duisburg-Essen*), Jörg Schröder (*University Duisburg-Essen*) 09:30–09:50

In the present contribution a fluid-structure interaction (FSI) approach based on a mixed least-squares finite element method (LSFEM) is introduced. The LSFEM is an established variational approach in constructing finite element formulations, see e.g. [1] and [2]. The method provides some theoretical benefits compared to the well-known (mixed) Galerkin method, since it is not restricted to the LBB-condition. The construction of the finite elements leads to positive definite and symmetric system matrices, also for differential equations with non self-adjoint operators and is applied successfully especially in fluid mechanics, see e.g. [1], [5], [6]. Besides, the LSFEM offers a wide range of approaches based on different solution variables, since they can be included directly in the formulations. Therefore, the proposed FSI method is based on the formulation of mixed finite elements in terms of stresses and velocities for both the fluid and the solid regime. The conforming discretization of the stresses and velocities in the spaces $H(\mathrm{div})$ and H^1, respectively, leads to the inherent fulfillment of the coupling conditions of a FSI method. The idea of the LSFEM based FSI scheme is the solution of the full problem consisting of both domains in one triangulation at the same time. The general idea on this was firstly annotated in [3]. A numerical example considering an incompressible, linear elastic material behavior at small deformations (compare to [4]) and the incompressible Navier-Stokes equations demonstrates the applicability of the LSFEM-FSI approach.

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[2] Z. Cai, B. Lee, and P. Wang. *Least-squares methods for incompressible Newtonian fluid flow: Linear stationary problems*, SIAM J. Numer. Anal., 42(2):843-859, 2004.

[3] O. Kayser-Herold and H.G. Matthies. *A unified least-squares formulation for fluid-structure interaction problems.* Comput. Struct., 85:998-1011, 2007.

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S09.02 | Laminar flows and transition

Date 22.03.2018
Room 2605

Boundary Layer Transition on Rough Walls

Lars von Deyn (*Institute of Fluid Mechanics, Karlsruhe Institute of Technology - KIT*), Pourya Forooghi (*Institute of Fluid Mechanics, Karlsruhe Institute of Technology - KIT*), Bettina Frohnapfel (*Institute of Fluid Mechanics, Karlsruhe Institute of Technology - KIT*), Ardeshir Hanifi (*KTH Mechanics, Royal Institute of Technology (KTH)*), Dan Henningson (*KTH Mechanics, Royal Institute of Technology (KTH)*), Philipp Schlatter (*KTH Mechanics, Royal Institute of Technology (KTH)*) 14:00–14:20

It is well known that surface roughness affects the laminar-turbulent transition. In the present work, we study the influence of surface roughness on transition induced by free stream turbulence (FST) by means of direct numerical simulations (DNS). We consider the flow in a flat-plate boundary layer which is subjected to FST. A random surface roughness designed to represent relevant roughness properties on turbine blades, where transition is mainly caused by FST, is introduced via an immersed boundary technique. It is shown that surface roughness has a significant impact on the transition location, the details of which depend on roughness height and roughness density in agreement with experimental findings on turbine blades. Analysis of the generated DNS data reveals that the presence of surface roughness leads to more strongly amplified streaks in the boundary layer compared to the case of a flow over a smooth plate which is disturbed by FST only. The mechanism of the streak breakdown appears to be similar in both cases, however, the stronger streaks in case of the rough wall break down earlier. In addition, a case with no FST is also considered. In this case the generated streaks occur in fixed locations and show no time dependence in the earlier parts of their development. In this case the breakdown to turbulence is also due to the appearance of a secondary instability on the streaks, in a similar way as for bypass transition induced by FST.

Symmetry induced new non-modal stability analysis and algebraic growth rate of rotating wire flow in an infinite domain

Judith Kahle (*Fachgebiet Strömungsdynamik, TU Darmstadt*), Martin Oberlack (*Fachgebiet Strömungsmechanik, TU Darmstadt*) 14:20–14:40

Since Taylors experiment in 1923 [1], the Taylor Couette (TC) flow represents a paradigmatic system to study the stability of rotating shear flow. Nowadays it is common to study the stability by employing the normal-mode approach. Stability analysis has shown that the two dimensional TC flow is always longtime stable, although the non-normality of the eigenfunctions leads to a transient growth instability, which often appears to admit an algebraic growth rate [2]. It has been shown by the present group [3, 4, 5] that this ansatz has its basis in symmetries and,

moreover, that many classical shear flows admit new non-modal symmetry induced eigenfunctions. For the TC azimuthal base velocity $u_\varphi = Ar + Br^{-1}$ we obtain the new eigenfunction

$$\Psi(r, \varphi, t) = \widetilde{\psi}\left(\frac{r}{\sqrt{t}}\right) e^{im(-At+\varphi)} t^s, \tag{1}$$

where s represents the complex exponent of the algebraic growth rate. As the variable $x = \frac{r}{\sqrt{t}}$ of the eigenfunction is depending on the variables in time and space, the initial geometry of the Taylor Couette flow has been transformed into a rotating wire flow in an infinite domain, which is some kind of TC model system for the wide-gap TC flow. Together with the appropriate boundary conditions at $x \to 0$ and $x \to \infty$ the underlying eigenvalue problem was completely solved, yielding the restriction $\Re(s) < \frac{1}{2}$ for arbitrary $m \neq 0$. The stability analysis yields new instable modes for the plane TC model, i.e. $\Re(s) > 0$. Considering the vorticity of the disturbed flow, spiral movement can be observed. Hereby, the parameter m determines the number of spiral arms, the imaginary part of the eigenvalue defines the direction and degree of turns.

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Three-dimensional linear stability analysis of thermocapillary cavity flow

Pierre-Emmanuel des Boscs (*TU Wien, Vienna University of Technology*), Hendrik Kuhlmann (*TU Wien, Vienna University of Technology*)
 14:40–15:00

A liquid-filled cuboidal cavity with an indeformable top free surface and a solid bottom wall, both adiabatic, is heated differentially from the two facing side walls. In spanwise direction either periodic or adiabatic no-slip conditions are imposed. Thermocapillary stresses at the free surface and buoyancy forces, treated in Boussinesq approximation, drive a steady basic flow in the liquid. Two- and three-dimensional instabilities of the basic flow are computed numerically for Pr = 4.4 (acetone) using selective frequency damping for the basic flow and time marching of the linearized Navier–Stokes equations combined with an Arnoldi method.

Direct numerical simulations of unsteady porous media flow through hexagonal sphere-pack

Yoshiyuki Sakai (*Technical University of Munich*), Michael Manhart (*Technical University of Munich*)
 15:00–15:20

Unsteady flow through porous media can be seen in a wide range of engineering applications and environ- mental processes, such as heat and mass transport in a heat exchanger, interaction between an atmospheric boundary layer and a forest canopy, and so on. Despite such high technical and scientific relevance, however, our fundamental understanding on the unsteady porous media flow is still limited. On one hand, conducting precise measurements within such complex geometry is still a challenge even with the state-of-art experimen- tal techniques, whereas the high computational cost necessary to numerically resolve the complex topology within the porous media is equally a challenge, hence the slow progress. Recent progress in the development of the immersed boundary techniques, however, has enabled us to advance the frontier of the physical parameter for the numerical simulations, and consequently our understanding on the flow phenomena signif- icantly. In the current contribution, we perform a series of direct numerical simulations of the unsteady flow through hexagonal sphere-pack at different Reynolds numbers, ranging from linear, nonlinear, and turbulent flow regimes. We employ our inhouse flow solver MGLET which utilises a variant of the aforementioned immersed boundary techniques. In the analysis, our main focus is placed upon the onset of the turbulent flow regime and the corresponding flow behaviour. Moreover, we draw a comparison among those three flow regimes with respect to the temporal development of the integrated quantities such as bulk velocity, turbulent kinetic energy, and dissipation rate, and the associated time-scales will be discussed.

Couette flow with geometrically induced unsteady effects

Markus Scholle (*Mechatronics and Robotics, Hochschule Heilbronn*), Florian Marner (*Hochschule Heilbronn*), Philip H Gaskell (*Engineering and Computing Science, Durham university*) 15:20–15:40

Film flow over surfaces containing topography is a key feature of a number of coating technologies. To date, detailed theoretical investigations of the same, underpinned by the long-wave approximation, have been used to study the nature of the associated free-surface disturbance formed; the internal flow structure being more-or-less of secondary importance. In the work reported here, a recently developed approach is used to explore the internal flow, embodying both inertial and unsteady effects, for a related model problem in which the free-surface is replaced by a moving upper boundary with its own topographical profile. Perspectives toward generalised cases such as 3D flows over topography, two-layer flows and non-Newtonian liquids are provided. The introduction of an auxiliary potential field [1,2], enables the construction of a first integral of the two-dimensional Navier-Stokes equations which can be used in beneficial ways for the analysis of thin film flows, in particular, to explore material transfer between trapped eddies and the associated bulk flow, and vice versa, known as 'turnstile lobe' effect [3]. The existence of isolated or periodically occurring topographical features can give rise to the formation of closed eddy structures, leading to particle trapping and stagnant flow in separated flow regions, an undesired effect in many coating processes which might be controlled via lobe dynamics. An intriguing finding is that this effect occurs even in the absence of inertia.

[1] F. Marner, P.H. Gaskell, and M. Scholle *Phys. Mesomech.* **17(4)**, 341–348 (2014).

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[3] F. Marner, P.H. Gaskell, and M. Scholle *J. Math. Phys.* **58**(4), 043102 (2017).

Variational Multiscale or Eddy Viscosity: How to Deal with Blood Flow in Transitional Regimes?

Lutz Pauli (*Chair for Computational Analysis of Technical Systems, RWTH Aachen University*), Marek Behr (*RWTH Aachen University*) 15:40–16:00

Blood pumps like ventricular assist devices (VADs) operate in flow regimes, where a transition to turbulence occurs. Usually, RANS-based turbulence models are applied for the flow analysis. They can be efficiently solved and are known to predict global flow features like the pressure head with very good accuracy. However, local flow features are not represented in sufficient detail. Therefore, we focus on state-of-the-art LES modeling to capture more complex flow patterns. In particular, we consider a residual-based variational multiscale turbulence model and a wall-bounded eddy viscosity model, the σ-model. Both models are implemented in a stabilized finite element code with equal-order interpolation for velocity and pressure, and special treatment of the stabilization parameter [1].
The turbulence models are tested in a benchmark nozzle by the U.S. Food and Drug Administration (FDA) and compared to the available experimental data. In addition, we will introduce how the turbulence models are used for the analysis of full blood pumps.

[1] L. Pauli, and M. Behr. On Stabilized Space-Time FEM for Anisotropic Meshes: Incompressible Navier-Stokes Equations and Applications to Blood Flow in Medical Devices. *International Journal for Numerical Methods in Fluids*, 85(3):189–209, 2017.

S09.03 | Laminar flows and transition

Date 22.03.2018
Room 2605

Using magnetic fluids to model convection of planetary or stellar interiors in laboratory scale

Peter Szabo (*School of Engineering and Physics, Heriot-Watt University*), Wolf-Gerrit Früh (*School of Engineering and Physical Sciences, Heriot-Watt University*) 17:30–17:50

Experimental investigations of large-scale convection on stellar or planetary interiors are of great interest in geophysics. However, experiments are difficult to reproduce in laboratory scale, such as creating a central force field under terrestrial conditions. In 2005, Früh [1] developed a novel approach to simulate convection in a central force field for laboratory investigations by using magnetic fluids that are sensitive to temperature and external magnetic fields. This approach suggested a useful experimental tool to investigate convection in planetary interiors at the laboratory scale. However, Früh's computational simulation only provided a 2D section through a non-rotating spherical shell.

Here, we present a parametric numerical study that extends Früh's investigation by adding rotation around the central (vertical) axis of an equatorial plane of the spherical shell. The shell is heated at the inner wall and cooled at the outer wall. A permanent magnet was placed in the center of system to provide an external magnetic field which generates the central force field of the system.

The parametric computational study investigated a combination of sixteen different angular velocities and eight temperature differences to study the growth and saturation of baroclinic waves. The heat transfer was characterised by the Nusselt number and plotted versus a magnetic Rayleigh number which is the equivalent to the conventional Rayleigh number. To characterise the observed baroclinic wave solutions, a further non-dimensional parameter had to be developed that quantified the ratio of magnetic forces to rotational forces and is the equivalent to the thermal Rossby number. A regime diagram was developed that represented all observed flow regimes.

[1] W.-G. Früh. Using magnetic fluids to simulate convection in central force field in the laboratory. *Nonlinear Processes in Geophysics*, 12:877-889, 2005.

3-D Numerical Simulation and Analysis of The Flow Pattern in the Shot Sleeve of the Cold Chamber HPDC Process

Roudouane Laouar (*mechanical engineering, University Larbi Tebessi Tebessa*) 17:50–18:10

Incompressible viscous flow with moving free surfaces has drawn broad attention because of its important applications in environmental engineering, die casting, polymer processing and many other areas of interest. Many methods have been developed for their numerical resolution in various fields of the physics or the engineering. This work presents a 3-D numerical study of the flow of molten metal in the shot sleeve of horizontal high-pressure die casting machine during the injection process. The study includes the filling process of the shot sleeve and the plunger advancement. The analysis of the flow pattern caused by the filling and the plunger motion can be of help in reducing porosity in manufactured parts caused by air entrapment. A particular attention has been paid for the flow and temperature field below the filling hole. This one did not receive much regard in the die casting research. The importance of the understanding of this process can show us how to minimize the heat transfer, layer created on the sleeve (solidification layer), and sleeve protection from erosion and plunger problem. The used numerical model, which considers the problem as three-dimensional, is based on the conservation equations of mass, momentum and energy, and describes the free surface using the volume-of-fluid method. The motion of plunger is simulated by using a layering dynamic mesh method. The numerical results are obtained by using a CFD code that is based in the finite volume method. A linear plunger velocity profile is used to predict an optimum plunger movement without air entrapment. The influence of filling inlet velocity in the hydraulic jump and wave formation is to be discussed.

Simulation of a hollow profile extrusion process for a semicrystalline polymer

Stefan Descher (*Chair of Fluid Mechanics, University of Kassel*), Olaf Wünsch (*Chair of Fluid Mechanics, University of Kassel*) 18:10–18:30

Hollow profiles are of great interest in polymer processing industry. The most popular and simplest application is pipe extrusion. But there are more complex applications as well. Window profiles for example consist out of many thin elements connected to each other. Sometimes also the geometry is simple but the behavior of the polymer is complex. This is the case for the project this contribution originates from. The material used there, is a wood-plastic-composite, but in the stage presented here only its matrix polymer, polyethylene is considered.
The object of this work is to model an experimental setup operated with the unfilled polymer. It is a die connected to a cooling device in which the polymer solidifies. The shape of the profile formed is square. Simulations are carried out to get an insight of the solidification process.
A solver for non-isothermal crystallization as described in [1] is used, but in a substantially more developed state. It includes a modified function considering the suppression of crystallization

as published in [2]. The flow behavior is considered to be nonlinear viscoelastic described by the exponential form of the Phan-Thien Tanner Model. OpenFOAM was used to perform the calculations.

[1] S. Descher, O. Wünsch. Modelling and simulation of solidification processes in polymer melt flows. PAMM 14, 595-596. 12/2014

[2] J. E. K., Schawe. Cooling rate dependence of the crystallinity at nonisothermal crystallization of polymers: A phenomenological model. J. Appl. Polym. Sci. 133. 10/2015.

S10 | Turbulence and reactive flows

Organiser Nikolaus A. Adams (*Technical University of Munich, Chair of Aerodynamics and Fluid Mechanics*)
Wolfgang Schröder (*Aerodynamisches Institut, RWTH Aachen University*)

S10.01 | Turbulence and reactive flows

Date 20.03.2018
Room 0601

Space and scale fluxes of Reynolds shear stresses in turbulent channel flows

Alessandro Chiarini (*Politecnico di Milano*), Bettina Frohnapfel (*Karlsruhe Institute of Technology - KIT*), Maurizio Quadrio (*Politecnico di Milano*), Andrea Cimarelli (*Università Politecnica delle Marche*), Yosuke Hasegawa (*University of Tokyo*), Davide Gatti (*Karlsruhe Institute of Technology - KIT*) 08:30–08:50

The turbulent energy transport phenomena can be described through the generalized Kolmogorov equation (GKE) [Cimarelli, De Angelis, Jimenez & Casciola, *J. Fluid Mech.* (2016)], a budget equation for the second order structure function $\langle \delta u^2 \rangle$, where $\delta u^2 = \delta u_i \delta u_i$ and δu_i is the increment of the i-th velocity component at position $\mathbf{X_c}$ and separation $\mathbf{r}$, i.e. $\delta u_i = u_i\left(\mathbf{X_c} + \mathbf{r}/2\right) - u_i\left(\mathbf{X_c} - \mathbf{r}/2\right)$. $\langle \delta u^2 \rangle$ can be interpreted as the amount of kinetic energy at a *scale* (smaller than) $\mathbf{r}$ and in a channel flow is a function of space through the wall-normal position Y_c and of scale through the separation vector $\mathbf{r}$. In the present work we extend the GKE to fully account for anisotropic flows by deriving budget equations for the generic structure function $\langle \delta u_i \delta u_j \rangle$, which describes the production, dissipation and transport of each Reynolds stress component in the four-dimensional Y_c and $\mathbf{r}$ spaces.
In its most compact notation each one of the generic structure function budget equations reduces to:

$$\frac{\partial \Phi_c\left(Y_c, r_i\right)}{\partial Y_c} + \frac{\partial \Phi_{r_i}\left(Y_c, r_i\right)}{\partial r_i} = \xi\left(Y_c, r_i\right) + \Pi\left(Y_c, r_i\right),$$

in which Φ_c and Φ_{r_i} are the Reynolds stress fluxes in space and among scales, while ξ is the scale energy source, budget between production and dissipation of scale energya, and Π is the pressure-strain term, which redistrbute energy among the various compoents of the Reynolds stress tensor. The equation above, stemming from the Navier-Stokes equation, describes the path in space and among scales between the production and dissipation of Reynolds stresses.
In the present work we compute for the first time such budget equations for turbulent channels and exploit them to describe structural properties of turbulent channel flows, which can not be highlighted by single-point statistics.

Integral energy budgets in turbulent channels with and without drag reduction

Davide Gatti (*Institute of Fluid Mechanics, Karlsruhe Institute of Technology*), Bettina Frohnapfel (*Institute of Fluid Mechanics, Karlsruhe Institute of Technology - KIT*), Andrea Cimarelli (*Università Politecnica delle Marche*), Yosuke Hasegawa (*Institute of Industrial Science, University of Tokyo*), Maurizio Quadrio (*Department of Aerospace Science and Technologies, Politecnico di Milano*) 08:50–09:10

In canonical turbulent flows, skin-friction drag is directly linked to a wall-normal integral of the Reynolds shear stress via the FIK identity, an exact analytical expression introduced by Fukagata, K., Iwamoto, K. & Kasagi, N., Phys. Fluids, vol. 14, 2002, pp. L73–L76. In the present contribution, we derive new exact relationships between the Reynolds shear stress (i.e. turbulent skin-friction drag) and the dissipation rates of turbulent and mean kinetic energy, along with all terms in the kinetic energy budgets of turbulent channels.
A new decomposition of the kinetic energy dissipations is adopted, stemming from an extended Reynolds decomposition, in which the mean velocity is additionally split into a laminar component and a deviation from it. A compact representation of the energy fluxes is introduced to understand their relative importance at different values of the Reynolds number. The particular properties of the laminar and deviation component allow deriving exact relationships that link all the energy fluxes with two wall-normal integrals of the Reynolds shear stresses.
The relevance of the present results for improving present understanding of turbulent skin-friction drag reduction obtained via active means is discussed. Under the Constant Power Input (CPI) framework, in which the total power fed to the system is given and constant, the newly-derived relationships show that drag reduction and turbulent dissipation are linked via the two integrals of the Reynolds shear stresses and a power-based Reynolds number only.

Towards a hybrid turbulent mixing model based on hierarchical parcel-swapping and one-dimensional turbulence

Pedro Pupo Sá da Costa (*BTU Cottbus-Senftenberg, BTU Cottbus - Senftenberg*), Heiko Schmidt (*Lehrstuhl Numerische Strömungs- und Gasdynamik, BTU Cottbus - Senftenberg*) 09:10–09:30

One-dimensional turbulence (ODT) based models are able to generate good results for canonical flow problems compared to Direct Numerical Simulations. ODT has been successfully implemented as a sub-grid scale model for LES problems (ODTLES) delivering promising results. However, due to the computational cost of the ODT model in this scope, there is a need for an even faster model for real world parameter regimes. The Hierarchical Parcel Swapping (HiPS) algorithm used in combination with the ODT model to simulate a channel flow recently provided results with an acceptable quality in a fraction of the time of an ODT simulation. HiPS uses a binary tree to define the fluid domain, and stochastic eddy events are sampled in this tree. A local instantaneous and complete mixing of the cells is performed when an eddy event happens at the Kolmogorov scale. The biggest limitation of this model is that the viscosity of the solution is implicitly defined by the number of cells in a mesh. A more complex mixing model is introduced in order to introduce the viscosity of the flow as an explicit variable of the problem, providing a more versatile implementation of HiPS-ODT. This version of HiPS-ODT will serve to provide a computationally cheaper alternative for the ODT model, e.g. to be used in areas of less activity in 3D ODTLES flow simulations.

One-Dimensional Turbulence investigation of incompressible and low Mach number variable density pipe-flow

Juan Medina (*Lehrstuhl Numerische Strömungs- und Gasdynamik, BTU Cottbus - Senftenberg*), Heiko Schmidt (*Lehrstuhl Numerische Strömungs- und Gasdynamik, BTU Cottbus - Senftenberg*) 09:30–09:50

Cylindrical pipe-flow is evaluated by means of the One-Dimensional Turbulence (ODT) model applying both an incompressible and a low Mach number variable density framework. Several Direct Numerical Simulations (DNS) studies have already shown similarities and differences between compressible and incompressible formulations (with noted focus on channel and pipe-flow configurations, as in [1]). ODT formulations incorporating variable density effects, conversely, have

been mostly restricted so far to the combustion field in planar cartesian configurations (e.g. [2, 3]).
In this study, we decompose the velocity field into density-related (non-divergence-free) and density-unrelated (divergence-free) contributions, analogous to the method applied in [2]. Both contributions are subject to the separate effects of diffusion and turbulent transport, as it is normally the case in the incompressible ODT formulation. The turbulent transport is implemented by means of stochastic eddy events. Eddy events are influenced by the available kinetic energy given by the divergence-free (rotationally charged) velocity contribution. An eddy may arise from the different regions of shear caused by varying velocity gradients in the 1-D domain, but also as a consequence of the temperature-varying dynamic viscosity.
Results comparing the incompressible and low Mach number variable density frameworks are presented and compared to the results from Xu et al [J. Comput. Phys. 203 (2005) 22-48] [4], who summarised DNS results and additionally performed Large Eddy Simulations (LES) in pipe-flow configurations. ODT model parameters were assumed to remain constant for both formulations and were taken from the incompressible pipe-flow evaluation already performed in [5].

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[4] X. Xu, J. S. Lee, R. H. Pletcher, A compressible finite volume formulation for large eddy simulation of turbulent pipe flows at low Mach number in Cartesian coordinates, J. Comput. Phys. 203 (2005) 22-48.

[5] D. Lignell, V. Lansinger, J. Medina, A. R. Kerstein, H. Schmidt, M. Fistler, M. Oevermann, One-dimensional turbulence modeling for cylindrical and spherical flows: model formulation and application, submitted to Theor. Comput. Fluid Dyn. (2017).

Investigating incompressible temporally developing turbulent boundary layers using One-Dimensional Turbulence

Rakhi (*Mechanical Engineering, BTU Cottbus-Senftenberg*), Heiko Schmidt (*Mechanical Engineering, BTU Cottbus-Senftenberg*)
 09:50–10:10

We investigate incompressible temporally developing turbulent boundary layers using the One-Dimensional Turbulence (ODT) model. ODT is spatially fully resolved along the 1-D domain, only turbulent advection is represented by stochastic mapping events. Due to the reduction in dimensions, the model is suitable for high Reynolds number computations. We use ODT for the first time to study temporally developing boundary layers. We apply no-slip and impermeable boundary conditions at the top boundary with velocity u=0 and at the bottom boundary with velocity u=ub. Constant velocity at the bottom wall triggers the transition to turbulence by bringing the fluid at rest into motion. The skin friction coefficient and velocity statistics for different Reynolds number are compared with DNS results [3]. The study demonstrates that ODT has the capability to systematically investigate developing boundary layers.

Keywords: turbulent boundary layers, One-Dimensional Turbulence, turbulent flows

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Investigating the Reynolds number dependency of the scalar transfer to a wall using a stochastic turbulence model

Marten Klein (*Numerische Strömungs- und Gasdynamik, BTU Cottbus - Senftenberg*), Heiko Schmidt (*Numerische Strömungs- und Gasdynamik, BTU Cottbus - Senftenberg*) 10:10–10:30

The turbulent transport of scalar quantities, like temperature or chemical species, is of importance for various applications. A model for such problems is given by a passive scalar, which is governed by two non-dimensional numbers: the Reynolds number Re and the Schmidt number Sc. Re is related to the range of scales (integral to Kolmogorov) on which the scalar is mixed by turbulent advection (eddies). Sc is related to the molecular diffusion of the scalar, where $Sc \gg 1$ means low diffusivity and emergence of very small (Batchelor) scales. The high values of Re and Sc encountered in applications can only be simulated with the aid of modeling. Unfortunately, gradient-diffusion models do not represent satisfactorily the effects of crucial scale interactions. Therefore, we make use of a different modeling strategy using the One-Dimensional Turbulence (ODT). ODT resolves all scales of the flow along a notional line of sight. Along this line, turbulent advection is modeled by discrete mapping (eddy) events, which are selected stochastically with highest probability where velocity shear is strongest. In this study we use ODT as stand-alone tool to simulate turbulent channel flows with prescribed scalar concentrations at the walls.
In the talk we will show velocity and scalar statistics by comparing ODT results to reference data. We will address the scaling of the scalar transfer coefficient and the Sherwood number with the focus on Re-dependency at moderate Sc. Preliminary results show very good agreement with theory based on extrapolated DNS results.

S10.02 | Turbulence and reactive flows

Date 20.03.2018
Room 0601

Dynamics of flexible fibers in turbulent channel flow

Diego Dotto (*University of Udine*), Cristian Marchioli (*Department of Engineering and Architecture, University of Udine*) 16:30–16:50

In this paper, we investigate the dynamics of flexible fibers in turbulent channel flow. Fibers are longer than the Kolmogorov length scale of the carrier flow, and their velocity relative to the surrounding fluid is non negligible. Our aim is to examine the effect of local shear and turbulence anisotropy on the translational and rotational behaviour of the fibers, considering different elongation (parameterized by the aspect ratio) and inertia (parameterized by the Stokes number). To these aims, we use a Eulerian-Lagrangian approach based on direct numerical simulation of turbulence in the dilute regime. Fibers are modelled as chains of sub-Kolmogorov rods (referred to as segments hereinafter) connected through ball-and-socket joints that enable bending and twisting under the action of the local fluid velocity gradients [1]. Velocity, orientation and concentration statistics, extracted from simulations at shear Reynolds number $Re_\tau = 300$ (based on the channel half height) are presented to give insights into the complex fiber-turbulence interactions that arise when non-sphericity and deformability add to inertial bias. These statistical observables are examined at varying aspect ratio (namely $\lambda_s = b_s/a = 2$ and 5, with b_s the length of each segment s composing the fiber and a its cross-sectional diameter) and varying fiber inertia (considering values of the segment Stokes number, $St_s = 1$, 5, 30). To highlight the effect of flexibility, statistics are compared with those obtained for fibers that translate and rotate as rigid bodies relative to the surrounding fluid. Flexible fibers exhibit a stronger tendency to accumulate in the near-wall region, where they appear to be trapped by the same inertia-driven mechanisms that govern preferential concentration of spherical particles in bounded flows [2]. In such region, however, the mean shear is strong enough to reduce bending and stretch the fibers. Preferential segregation into low-speed streaks and preferential orientation in the mean flow direction is also observed.

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Viscosity-modulated breakup and coalescence of large drops in bounded turbulence

Alessio Roccon (*TU Wien, Vienna University of Technology*), Marco De Paoli (*TU Wien, Vienna University of Technology*), Francesco Zonta (*TU Wien, Vienna University of Technology*), Alfredo Soldati (*TU Wien, Vienna University of Technology*) 16:50–17:10

In this work, we examine the influence of viscosity on breakup and coalescence of a swarm of large drops in a wall-bounded turbulent flow. We consider several values of surface tension and a wide range of drops to fluid viscosity ratios $\lambda = \eta_d/\eta_c$ (with η_d the viscosity of drops and η_c the viscosity of the carrier fluid), from $\lambda = 0.01$ to $\lambda = 100$, while we maintain the same density for drops and carrier fluids. Drops can coalesce and break following a complex dynamics that is

primarily controlled by the interplay between turbulence fluctuations (measured by Re_τ), surface tension (measured by We) and λ. We use Direct Numerical Simulations (DNS) of turbulence coupled with a Phase Field Method (PFM) to describe the drops dynamics. We consider three different values of We (which is the inverse of the surface tension): $We = 0.75$, $We = 1.5$ and $We = 3$. For each value of We, we assume five values of λ: $\lambda = 0.01$, $\lambda = 0.10$, $\lambda = 1.00$, $\lambda = 10.0$ and $\lambda = 100$. We observe a consistent action of increasing λ, which, especially for the larger Weber numbers decreases significantly the breakup rate of the drops. Qualitatively, an increase of drop viscosity decreases the breakup rate, very much like an increase of surface tension does. The mechanism by which drop viscosity acts is a modulation of turbulence fluctuations inside the drop, which reduces the work surface tension has to do to preserve drop integrity. We believe that this may give important indications in many industrial applications to control drop coalescence and fragmentation via the ratio of drop-to-fluid viscosity.

Verification and validation of a low-Mach OpenFOAM solver for reacting multiphase flows

Louis Dreßler (*Fachgebiet Energie- und Kraftwerkstechnik, Technische Universität Darmstadt*), Florian Ries (*Fachgebiet Energie- und Kraftwerkstechnik, Technische Universität Darmstadt*), Johannes Janicka (*Fachgebiet Energie- und Kraftwerkstechnik, Technische Universität Darmstadt*), Amsini Sadiki (*Fachgebiet Energie- und Kraftwerkstechnik, Technische Universität Darmstadt*) 17:10–17:30

Despite the upcoming popularity and acceptance of Computational Fluid Dynamics in industry, less consideration is given to verification of the numerical tools applied. Indeed, often greater attention is paid to validation of specific models, neglecting the underlying numerics. However, the necessity of dealing with complex flow environment including turbulent flows, combustion or multiphase imposes the constant consideration of both, verification and validation. Recently, a low-Mach OpenFOAM solver has been developed to deal with turbulent single phase flows in which strong density variations, as typically observed in reacting flows and supercritical two phase flows, take place. This is extended to be coupled with Lagrangian particle tracking as given in OpenFOAM [1]. This contribution adresses the issue of code verification with respect to the transport equations of thermofluid dynamics of the implemented low-Mach solver. The approach used is the Method of Manufactured Solutions [2]. The analysis is done by means of order-of-accuracy analysis. Additionally, a validation of the implemented solver coupled with a Lagrangian particle tracking will be presented. The validation will be carried out in terms of comparison with a non-evaporating as well as an evaporating, non-reacting case of the Sydney dilute spray burner [3].

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A mass conserving approach for large-scale advection in large eddy simulations that use the linear eddy model as a sub-grid mixing and combustion model

Salman Arshad (*Mechanics and Maritime Sciences, Chalmers University of Technology*), Alan Kerstein (*Consultant*), Michael Oevermann (*Mechanics and Maritime Sciences, Chalmers University of Technology*) 17:30–17:50

The present study aims to test a new mass conserving approach for large-scale advection (splicing) in Large Eddy Simulations (LES) that use the Linear Eddy Model (LEM) as a sub-grid mixing and combustion model called LES-LEM. Previous splicing approaches were not consistent with mass conservation on non-uniform unstructured meshes, which is demonstrated by doing combustion simulations. An important property of the new splicing approach is to keep the LEM length in each LES cell equal to its initial length. In addition, the sub-grid contributions to splicing are made solenoidal in order to be consistent with mass conservation.

Flame Propagation in Arbitrarily Shaped Vessels

Clemens Gößnitzer (*Institute of Fluid Mechanics and Heat Transfer, TU Wien, Vienna University of Technology*), Herbert Steinrück (*Institute of Fluid Mechanics and Heat Transfer, TU Wien, Vienna University of Technology*) 17:50–18:10

We will present a new method for capturing the flame front for premixed, laminar combustion inside a closed vessel using a flame sheet model, and the Markstein correction.
Darrieus and Landau showed that the flame front is unstable for all wavelengths for a constant laminar burning velocity. Markstein introduced a curvature-dependent laminar burning velocity which stabilizes the flame front for high frequencies.
We are interested in explosions which have an expansion ratio much bigger than unity inside a closed vessel. Thus, the pressure rises considerably. Furthermore, we assume inviscid flow, neglect heat conduction, and expand the solution with respect to a low Mach number.
Thus, to leading-order, the pressure depends only on time. The front is modeled as a gas-dynamic discontinuity along which heat is instantaneously released due to reaction enthalpy. We decompose the velocity field in an irrotational and solenoidal part. The vector potential is determined by a Poisson equation. The boundary condition at the flame front and the vessel wall are satisfied by the potential flow part computed by a panel method. The flame front is represented by a set of moving points forming a polygon. Special care has to be taken to simulate the unstable front. We expect that this method is faster and more efficient predicting the pressure and position of the flame than a level-set based simulation method used by other authors. To validate our approach, we compare our results to the pole solution of the unstable front at constant pressure of Rastigejev and Matalon.

S10.03 | Turbulence and reactive flows

Date 21.03.2018
Room 0601

Conservation laws, DNS and statistical invariants of helically invariant turbulence

Dominik Dierkes (*Strömungsdynamik, TU Darmstadt*), Martin Oberlack (*Strömungsdynamik, TU Darmstadt*) 14:00–14:20

In turbulence theory it is well known that for three-dimensional turbulence, dissipation is a statistical invariant for small scales, whereas for two-dimensional turbulence, enstrophy is an invariant for large scales. The aim of this work is to determine invariants for flows which lie between two and three dimensions. Therefore, we focus on helical flows, which may be considered $2\frac{1}{2}$-dimensional. Helical flows admit a three-dimensional velocity field, and, moreover, vortex stretching in the helical vorticity transport equations is active, if the velocity u^η along the helix is non-zero. Nevertheless, similar to 2D flows, helical flows live on a 2D manifold, i.e. all variables depend on only two spatial coordinates: the cylindrical radius r and the helical variable given

by $\xi = az + b\varphi$, $a \cdot b \neq 0$. In order to determine the underlying invariants of helical turbulence we consider conserved quantities of helically invariant flows by using the recently discovered new conservation laws of the helically invariant Navier-Stokes equations [1].
Even for the case where $u^\eta \neq 0$, several vorticity conservation laws still persist including three for non-zero viscosity. At this point of the analysis we suppose that for this case at least one of these vorticity conservation laws correspond to a statistical invariant for small scales, such as the dissipation for 3D flows. To determine the various statistical invariants, and to verify the above hypotheses, presently we numerically solve the helically symmetric Navier-Stokes equations using a high-order discontinuous Galerkin code [2].

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Statistical One-Point Turbulence Modelling Using Symmetries

Dario Klingenberg (*Chair of Fluid Dynamics, TU Darmstadt*), Martin Oberlack (*Chair of Fluid Dynamics, TU Darmstadt*), Dominik Plümacher (*Chair of Fluid Dynamics, TU Darmstadt*)

14:20–14:40

The present work introduces a fundamentally new approach to turbulence modeling motivated by insights provided by the theory of Lie symmetry groups.
The nine Lie point symmetries of the Navier-Stokes system are connected to the axiomatic properties of classical mechanics, which, since around the 1990s, are intuitively fulfilled by turbulent models. An analysis of the Reynolds-averaged Navier-Stokes equations has however yielded an infinite additional amount of symmetries[1]. A subset of these, referred to in the following as statistical symmetries, has been linked in previous works to some special statistical properties of turbulent flows, i.e. intermittent and non-gaussian behaviour [2]. No currently available turbulence model generally preserves these additional symmetries. It is the aim of this work to develop a new turbulence model that complies with the statistical symmetries, which is motivated by the assumption that the predictive quality of a turbulence model is closely connected with the symmetries it preserves from the exact system.
As is shown, the statistical symmetries introduce significant restrictions on the form of possible model equations, resulting in the failure of all classical modeling approaches. It is demonstrated that this problem can be overcome if modifications are made to the convective term in the model transport equations. This will be accomplished through the introduction of an artificial velocity field as a new model variable. The implementation of a statistically invariant turbulence model is beyond the scope of this work, but a preliminary analysis of some simple flow configurations already produces very promising results.

Acknowledgements

The funding of Mr. Klingenberg's work by the Graduate School of Computational Engineering is gratefully acknowledged.

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Study of Decaying Two-Dimensional Turbulence with the Help of the Karman–Howarth Equation

Igor Vigdorovich (*Institute of Mechanics, Lomonosov Moscow State University*) 14:40–15:00

The decaying two-dimensional isotropic turbulence is investigated on the basis of the Karman-Howarth equation, which includes two unknown functions: two-point correlations of the velocity field of the second and third order. A method for closing this equation is proposed, based on the fact that the flow according to Batchelor is determined by the two parameters: the mean turbulence energy at the initial instant of time and the fluid viscosity. At initial instants of time, the energy dissipation is not small, as a result of which a rapid change in the mean turbulence energy to a certain value occurs, which subsequently remains almost unchanged. Next, a self-similar flow regime develops. There are two regions of self-similarity. In the first one, the flow occurs at small scales of the order of the scale of enstrophy dissipation, in the second one it occurs on large scales that are much larger then the dissipation scale. It turns out that the solution to the second self-similar problem is not unique and is determined within an arbitrary constant that is related to the value of Loitsyansky's integral. This constant must be determined from the solution for the initial instants of time.

Experimental and Numerical investigation of a Nozzle at different operating conditions for a Clean in Place System

Anand Sivaram Sivaramakrishnan (*Lehrstuhls für Strömungsmechanik (LSTM), Technischen Fakultät der Friedrich-Alexander-Universität Erlangen-Nürnberg*), Harish Abubaker (*Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Manuel Münsch (*Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Roman Murcek (*Fraunhofer-Institut für Verfahrenstechnik und Verpackung IVV*), Andre Boye (*Fraunhofer-Institut für Verfahrenstechnik und Verpackung IVV*), Antonio Delgado (*Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*) 15:00–15:20

Selection and optimization of a Clean In Place (CIP) system is a complex process. The CIP nozzles used in the system plays a huge role in the efficiency of the entire system. Therefore, numerical investigations are widely employed by many industrial processes, especially in the hygiene critical industries, such as Food, Beverage and Pharmaceutical industries. An enormous quantities of cleaning agent and water are consumed on a daily basis during their cleaning processes. Hence finding reliable and efficient design and operating condition of the cleaning nozzle based on understanding the internal and external flow properties and their optimization is a priority for these companies.
This paper presents the comparison between experimental measurement and the numerical prediction of the flow features and spray characteristics of a currently available CIP nozzle which are widely used for the industrial cleaning in place application. The flow features are measured experimentally using the optical measurement technique, Phase Doppler Anemomerty (PDA) system which is then compared numerically. Computations of the CIP nozzle system were conducted using a finite volume based commercial computational fluid dynamics (CFD) solver, StarCCM+ V12.04. The Eulerian based unsteady multiphase simulation (Volume of Fluid method) is carried out and is presented here. The achievement of good agreement between the numerical predictions and the experimental results has presented the opportunity to study the flow behaviour in unsteady state conditions. Based on these studies further optimization will be carried out with the help of some evolutionary algorithms or artificial neural networks.

Application and adaption of Dynamic Mode Decomposition to experimental and numerical data of turbomachinery flow

Christian-Henrik Walter (*Institut für Technische Mechanik, Technische Universität Clausthal*), Marinho Krieg (*Institut für Technische Mechanik, TU Clausthal*) 15:20–15:40

Unsteady turbomachinery flows are challenging in terms of resolving turbulent characteristics and instability mechanisms like rotating stall, rotor-stator interaction and von Karmán vortex streets. Furthermore, in part load conditions these flow phenomena can induce vibrations leading to resonance problems and high cycle fatigue. Flowfield measurements of a centrifugal fan were taken by high-speed particle image velocimetry (PIV). CFD results, calculated as unsteady Reynolds averaged Navier Stokes (URANS) and based on Menter's shear-stress transport (SST) model, are the source of numerical data. In former examinations discrepancies between experiment and simulation in time-averaged velocity profil data of part load conditions have been stated. The source of theses discrepancies is still unknown. Hence, a new approach is needed for further examination of measured and calculated flowfields. The Dynamic Mode Decomosition is executed in order to compare experimental and numerical datasets. Information about coherent structures and the dynamical behaviour are contained in the eigenvalues and their associated eigenvectors offered by DMD. While the eigenvectors are describing the coherent structures, the associated eigenvalues describe the dynamical behaviour of the structure. The approached eigenvectors are denoted as DMD-Modes. The results acquired by DMD of experimental and numerical data are compared to investigate congruent behaviour and therefore if it is possible to obtain reliable information about dynamical behaviour of a system even with URANS simulations. Comparisons between singular values, dynamic modes and eigenvalues are presented and discussed.

S10.04 | Turbulence and reactive flows

Date 21.03.2018
Room 0601

Large-eddy simulation of the flow in a scour geometry

Wolfgang Schanderl (*Civil Enviromental and Geo Engineering, TUM Professorship for Hydromechanics*), Michael Manhart (*Civil, Enviromental and Geo Engineering, TUM Professorship for Hydromechanics*) 16:30–16:50

A large fraction of stability problems of bridge piers is related to scour if the bridge pier is located in a sandy river bed. The flow which has to bypass the pier accelerates and thus causes an enhanced wall shear stress on the river bed, which in turn can trigger the erosion of the bed material. As the flow structure is complex and bears rich dynamics, it is hard to model in a numerical simulation and its estimation - especially the estimation of the near-wall flow - requires a high spatial resolution.
We have conducted highly-resolved large-eddy simulation of the flow around a circular cylinder placed in a scour hole at a moderate Reynolds number to investigate the flow structure inside this hole. In the region of interest, the Cartesian grid was fine enough to resolve the wall and to ensure that the influence of the turbulence model was small. The focus of this contribution is on the computational grid and the corresponding grid study. Furthermore, we discuss the requirements for this grid to capture the near-wall flow originating from the complex flow structure.

Near Wall Turbulence Structure of Flow Over Periodic Hills

Daniel Quosdorf (*Chair of Hydromechanics, Technical University of Munich*), Michael Manhart (*Chair of Hydromechanics, Technical University of Munich*) 16:50–17:10

The flow over periodically arranged hills in a closed rectangular flow channel features a strong speed-up at the windward slope, which leads to the formation of a near wall maximum of the tangential velocity component at the crest. Flow detachment and the formation of an oscillating separation zone can be studied [1, 2, 3].
Numerical methods e.g. LES cannot predict the velocity distribution and the size of the recirculation zone in a satisfactory manner, which we suspect is due to an inappropriate determination of the turbulence structures at the windward side of the hill. The error made, propagates downstream and leads to deviant results.
To clarify on the near wall turbulence quantities, PIV-measurements with high spatial resolution have been carried out at two different measuring positions (middle part of the slope and the crest region) for two Reynolds numbers $Re = 10600$ and $Re = 37000$.
From the asymptotic theory [4] it is suggested to divide the boundary layer into an inner and an outer region. Regarding the results of the PIV-measurements inner and outer layer can be clearly distinguished based on the distribution of the Reynolds shear stress. Their thickness can be quantified and put into context with the Reynolds number. The wall shear stress could be determined as well.
The distribution of the Reynolds shear stress follows the one of a classic channel flow for the close wall region. With increasing wall distance the distribution becomes approximately linear which shows a strong influence of the outer flow that splashes onto the hill.

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Heat transfer in a heat exchanger channel with dimples and passive inserts

Shanshan Wei (*Karlsruhe Institute of Technology - KIT*), Pourya Forooghi (*Karlsruhe Institute of Technology (KIT)*), Bettina Frohnapfel (*Karlsruhe Institute of Technology (KIT)*) 17:10–17:30

Study of convective heat transfer plays a key role in a wide range of applications in the industry, including improving the efficiency of heat exchangers. In this article, two possible heat transfer enhancement techniques, namely use of dimples and passive inserts (bumps), in a channel are numerically studied and compared. The working conditions correspond to those at the liquid side of a typical heat exchanger used in the automative air-conditioning systems. Quasi-Direct Numerical Simulations (Q-DNS) is conducted using OpenFOAM(C) to examine the detailed heat

transfer and flow field inside the heat exchanger channels. The computational mesh is generated by SnappyHexMesh application. For minimizing the computational costs, periodic boundary conditions are used in the streamwise and spanwise directions. The results are used to compare the heat transfer enhancement and pressure drop obtained from the two techniques and the underlying mechanisms. Keywords: heat transfer enhancement; heat exchanger; dimples

Proper orthogonal decomposition of a cylinder wall junction flow

Ulrich Jenssen (*Bau Geo Umwelt, Professur für Hydromechanik*), Julia Hüttmann (*Bau Geo Umwelt, Professur für Hydromechanik*), Michael Manhart (*Professur für Hydromechanik*) 17:30–17:50

The flow in front of a cylinder wall junction is dominated by a horseshoe vortex wrapping around the cylinder. This vortex is a result of a downflow in front of the cylinder and the stretching of the flow around the cylinder. The horseshoe vortex is an important agent for the performance and losses in junction flows. It has also been brought in connection to local scour development around bridge piers. It has first been demonstrated by Devenport and Simpson (Journal of Fluid Mechanics, 210, 1990) and later confirmed by many other authors that the horseshoe vortex undergoes a complex dynamics which leads to bimodal velocity and wall shear stress distributions. However there is still a controversy on the individual flow modes contributing to this dynamics.
We investigate the dynamics of this horseshoe vortex in front of a cylinder wall junction by Proper Orthogonal Decomposition (POD). 2D velocity fields were measured by Particle Image Velocimetry (PIV) in the symmetry plane in front of the cylinder. Horizontal oscillations of the horseshoe vortex core lead to strongly amplified turbulent kinetic energy levels around the vortex core. The POD decomposes the data set into orthogonal, thus independent, basis functions (modes) and provides information about the most energetic flow structures. Two main results can be provided by this study: (i) identification of the most relevant modes contributing to the TKE, and (ii) motion of the HV system due to the most energetic flow modes.

Numerical approaches for the simulation of a real multiphase flow in a fermentation tank

Daniel Klembt (*Mechanical Engineering, University of Applied Sciences Stralsund*), Heiko Meironke (*Mechanical Engineering, University of Applied Sciences Stralsund*) 17:50–18:10

In the context of investigations of multiphase flows, the beer production is currently being investigated, especially fermentation, maturation and storage in cooperation with the local brewery.
The university has its own 350 litre fermentation tank with comprehensive acoustic flow and temperature measurement technology for the systematical investigation, of the influence of the fermentation activity, distribution of yeast and occurring convection phenomena.
In addition to many other problems, in a real fermenting fluid only acoustic or magnetic resonance tomography measurement technology can be used. Due to the high turbidity of the fluid, optical measuring techniques are not suitable. Another, but a non-experimental method is to simulate the process numerically. Numerical approaches for the natural convection and bubble rise have already been presented in earlier publications.[1, 2]
This paper is about combining the two numerical approaches with the two Fluid Eulerian-Eulerian time-averaged model.[3]. This model enables that two sets of governing equations, continuity and momentum equations are solved for either phase and their interactions are modelled using interface transfer terms for interfacial heat, mass and momentum exchanges. Finally, its planned to simulate the different phases interactions between the yeast, carbon dioxide bubbles and the beer wort.

In this investigation, the flow is assumed to be adiabatic and only the momentum exchange has to be considered. For the liquid a turbulence shear stress (SST) model according to Menter will be applied, because the SST model switches between the standard k-ϵ- (for the flow away from walls) and the k-ω-turbulence model (for the vicinity of walls) using a blending function, excluding the user influence modelling the near wall conditions.[4]
Modelling the influence of the gas bubbles on the liquid turbulence the SatoŽs eddy viscosity model for bubble-induced turbulence will be applied.[5]
The goal of the Eulerian-Eulerian model is to simulate as realistic a simulation of the flow processes in the fermentation tank as possible, taking into account the natural convection and the actual bubble behaviour.
For the validation of the numerical simulation different experimental results from a real fermentation tank are used, e.g. measured velocity fields with the Ultrasonic Doppler Velocimetry (UDV).

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S11 | Interfacial flows

Organiser Dieter Bothe (*Mathematical Modeling and Analysis, TU Darmstadt*)
Michael Schlüter (*Hamburg University of Technology*)

S11.01 | Interfacial flows

Date 20.03.2018
Room N1090

Modelling and simulation of foams with convective and diffusive momentum transport

Antonio Delgado (*Lehrstuhl für Strömungsmechanik, FAU Erlangen-Nürnberg*), Katharina Gladbach (*Lehrstuhl für Strömungsmechanik, FAU Erlangen-Nürnberg*), Cornelia Rauh (*TU Berlin*), Nan Chen (*Lehrstuhl für Strömungsmechanik, Friedrich-Alexander-Universität Erlangen-Nürnberg*) 08:30–08:50

Foams are of essential importance in nature and in a wide range of technical fields that deal with matter of biological origin. There are several methods to incorporate bubbles within the biomatter structures: mixing, steam generation, gas injection, vacuum expansion, fermentation etc. However, due to the structural complexity and the corresponding macroscopic appearance of rheological effects there exists only few methods for modelling, simulating and predicting foams. Here, the suitability of the model suggested by Piesche et al (2008) for describing food foams is studied. The foam growth is induced by a pressure drop and diffusion of volatile components. The related fluid mechanical transport processes are divided into two consecutive models that concern spherical foam and polyhedral foam, respectively. The foam growth is calculated by solving problem-specific conservation equations for mass, momentum and thermal energy. Numerical simulations are carried out for different two-phase systems that are of intermediate or low viscosity and that differ only in the viscosity at a temperature of 20°C. As the typical Reynolds number takes on values in the order of magnitude of unity, no terms in the momentum transport equation can be neglected. The numerical method used for solving the model equations has been analyzed with respect to stability, consistency and convergence. The simulations show that the less viscous the liquid is, the faster the hydrodynamic and thermodynamic equilibrium is reached. Consequently the characteristic times for balancing pressure differences between the bubbles and their environment and concentration differences in the liquid decrease.

A novel method for the measurement of flotation recovery by means of 4D particle tracking velocimetry

Anna-Elisabeth Sommer (*Transport processes at interfaces, Helmholtz-Zentrum Dresden-Rossendorf*), Mitra Nikpay (*Helmholtz-Zentrum Dresden-Rossendorf*), Sascha Heitkam (*Technische Universität Dresden*), Kerstin Eckert (*Helmholtz-Zentrum Dresden-Rossendorf, Technische Universität Dresden*) 08:50–09:10

Froth flotation is a fundamental technique to separate minerals. Hydrophobized target particles attach to the fluidic interface of gas bubbles rising in a suspension. The success of the process depends on the surface chemistry for the hydrophobization of particles as well as the hydrodynamics for an encounter between bubble and particle. To quantify this performance in terms of recovery, the number of target particles at various times in a reference volume is measured. Previous researchers developed analytical models to predict the recovery. Thus, a direct way to

measure recovery at defined hydrodynamic conditions would be helpful to verify these models and to advance our understanding of particular microprocesses.
This work focuses on the analysis of flotation recovery through a simultaneous time-resolved measurement of particle and bubble trajectories. We introduced a new method that determined the probability of collision and attachment through a 3D particle tracking method with a high temporal (1000 fps) and spatial (0.03 mm/pixels) resolution. A tomographic particle image velocimetry device with three high-speed cameras recorded the three-phase flow in a rectangular bubble column (bubble chain, 2 mm). Fluorescent polystyrene particles (5000 particle/ml) were employed so that particles appeared bright and bubbles dark on the captured images. An attachment occurred if the trajectory of a particle coincided with that of a bubble. The recovery was calculated based on the number of particles attached to a bubble compared to the total particle density.
With this method, we investigated various particle diameter (30-100 μm) and compared the results with existing models of the bubble-particle attachment microprocess.

Behavior of a single bubble and its wake in swarm like background turbulence

Katharina Haase (*Institut für Strömungsmechanik und Aerodynamik, Universität der Bundeswehr München*), Christian Kähler (*Institut für Strömungsmechanik und Aerodynamik, Universität der Bundeswehr München*) 09:10–09:30

Multiphase flows are used in various applications not only in industry but also in science or energy production. In real technical applications mainly small bubbles, 1-10 mm, are used with up to 10% volume fraction. An important variable to control the behavior are the size and amount of the gaseous phase. In order to fully understand the individual mechanics, it is necessary to investigate the interaction between bubbles, as well as with the induced wake turbulence. Special value has to be placed on characteristic variables (bubble size, gas volume fraction and liquid agitation) and their influence on the mass transport in the surrounding fluid. By using optical methods only swarms with low volume fractions 1-2% can be investigated. Therefor a swarm turbulence is generated artificially in order to study a single or small amount of bubbles in a swarm like background turbulent environment. The presented method to imitate the hydrodynamic behavior of a bubble swarm uses plastic particles organized in a flexible grid. It was shown [2] [3] that those grids create turbulence that is comparable to real bubble swarm hydrodynamics taken from literature [1] [4]. To visualize the mass transport from a single bubble in the surrounding fluid a chemical tracer [6], that is designed to darken when in contact with oxigen. Thus with a tomographic camera setup the 3D motion, shape and deformation of the bubble as well as the mass transport can be reconstructed. To complete the analysis a simultaneous PIV system recorded the flow field around the bubble. This will give further insight in how the turbulence influences the transport.

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Active control of foams by physically based destruction mechanisms

Christopher McHardy (*Fachgebiet Lebensmittelbiotechnologie und -prozesstechnik, TU Berlin*), Julian Thünnesen (*Lehrstuhl für Strömungsmechanik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Tobias Horneber (*Fachgebiet Lebensmittelbiotechnologie und -prozesstechnik, TU Berlin*), Jordanka Kostova (*Fachgebiet Lebensmittelbiotechnologie und -prozesstechnik, TU Berlin*), Mohamed Hussein (*Lehrstuhl für Strömungsmechanik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Antonio Delgado (*Lehrstuhl für Strömungsmechanik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Cornelia Rauh (*Fachgebiet Lebensmittelbiotechnologie und -prozesstechnik, TU Berlin*) 09:30–09:50

Foams may be undesired in technical processes and need, thus, to be actively controlled. In Life Science Engineering it is often not possible to apply chemical measures due to the required purity of the processed products. To overcome this challenge, it is necessary to apply physically based foam destruction mechanisms. These physical measures include thermal, fluid mechanical and acoustic mechanisms. The presented contribution deals with these mechanisms from an experimental as well as numerical point of view. The results show that it is possible to classify the foamability of different fluids by a correlation of dimensionless numbers containing purely physico-chemical properties (i.e. density, surface tension, viscosity). The foam stability is a consequence of the net balance of the foam generation and the foam decay. The respective time scales may be influenced by the process conditions, the fluid properties, and the selected physically based destruction mechanism. In the case of resonance excitation of foam bubbles by acoustic waves of defined frequencies, selective foam destruction can be achieved. The bubbles in the foam start to oscillate and absorb energy depending on the bubble size, fluid properties, and ultrasound frequency. The resulting bubble breakdown leads to a shortening of the time scales of the foam decay. The active control of foams may be designed and optimized based on numerical simulations of the coupled effects of fluid flow and acoustic wave agitation of the foam and by experimental investigation by high speed imaging, particle tracking velocimetry, and particle image velocimetry.

Mixing characteristics of turbulent flow in a T-mixer

Tobias Schikarski (*Lehrstuhl für Strömungsmechanik, FAU*), Wolfgang Peukert (*Lehrstuhl für Feststoff- und Grenzflächenverfahrenstechnik*), Marc Avila (*Zentrum für angewandte Raumfahrttechnolgie und Mikrogravitation*), Holger Trzenschiok (*Lehrstuhl für Feststoff- und Grenzflächenverfahrenstechnik*) 09:50–10:10

A T-mixer is one of most simple test beds to study chemical reactions or precipitation processes, which both usually demand fast and well mixing. The latter method is driven in a Reynolds numbers regime (here $Re \approx 2200$), where beyond a substantial increase of energy input only

results in a marginal improvement of the process outcome, e.g., the mean size of the precipitated nanoparticles approaches an almost constant value. At such conditions, the flow (assuming a mixture with equal fluid properties) is found to be turbulent in the mixing channel, which involves the advantage of narrowly distributed nanoparticles with a small mean size. It is, thus, surprising that the flow and its induced mixing characteristics at these conditions have been only rarely studied with experiments leave alone direct numerical simulations.
In this talk, I will focus on the inherent mixing processes to be present in the formally unknown chaotic regime considering Reynolds numbers $650 < Re < 4000$. For this purpose, we apply different inflow condition being either laminar or turbulent or both. We do obtain that the decay of the generated turbulence by the colliding streams to the final duct flow state is primarily affected by the inflow condition resulting in different turbulent intensity and dissipation histories. This observation allows us to explain satisfyingly the various mixing regimes obtained in experiments for the Reynolds number regime considered.

Neutron imaging of froth structure and particle motion

Sascha Heitkam (*Institute for Process Engineering, TU Dresden*), Martin Rudolph (*Helmholtz-Institute Freiberg for Resource Technology*), Sven Eckert (*Magnetohydrodynamics, Helmholtz-Zentrum Dresden-Rossendorf*), Tobias Lappan (*Magnetohydrodynamics, Helmholtz-Zentrum Dresden-Rossendorf*), Kerstin Eckert (*Institute for Process Engineering, TU Dresden*)

10:10–10:30

Froth flotation, exploiting differences in surface properties of mineral particles, is the most important process in ore beneficiation in mineral processing. In the froth zone, the bubble-particle aggregates, crossing the pulp-froth interface, move upwards towards the concentrate launder. Ressource efficiency calls for an increase of recovery and grade of the flotation concentrate. This is ultimately coupled to the need of a refined understanding of the froth dynamics, including drainage, the bursting and coalescence of bubbles and the respective impact on particle motion. This also requires the availibility of reliable experimental data. However, local measurements and detection of particles in flotation froths are challenging due to their opaqueness. This article reports on the simultaneous measurement of foam structure and attached particles employing neutron imaging. An aqueous foam sample is placed in the NEUTRA beamline at PSI, enabling a spatial resolution of less than 200 μm to be achieved at a frame rate of more than 1 Hz. A forced drainage setup allows the liquid content of the foam to be controlled. The averaged attenuation of the neutrons is demonstrated to yield the liquid fraction of the foam. Hydrophobized gadolinium particles with a diameter of 200 μm are added to the foam. Using two surfactants, different levels of hydrophobicity are achieved. Depending on the drainage flow and the hydrophobicity, the particles are washed out of the foam at different rates. An avalanche-like motion of particle clusters is observed. Neutron radiography is demonstrated to yield unique insights into the unsteady froth flotation process.

S11.02 | Interfacial flows

Date 20.03.2018
Room N1090

Instabilities of a liquid metal/oil interface caused by magnetic stirring

Christian Resagk (*Mechanical Engineering, Ilmenau University of Technology*), Andreas Wiederhold (*Mechanical Engineering, Ilmenau University of Technology*), Christian Cierpka (*Mechanical Engineering, Ilmenau University of Technology*) 16:30–16:50

We report about an experiment where the behavior of a liquid metal/oil interface is studied. This two-fluid experiment is a simplified model of a liquid metal battery (LMB) which is a promising energy storage device. LMBs generally consist of two liquid metal layers, which are the electrodes, and a separating electrolyte layer between them. Hydrodynamic stable interfaces are of highest importance for the operation of a LMB, because interface deflections could disrupt the electrolyte layer and cause a short circuit. The experiment contains a room temperature-liquid metal (Galinstan) as the lower phase and a silicone oil as the upper phase. Different geometries of the cell (cubic, cylindrical) and aspect ratios of the fluids were investigated. The flow inside the cell is driven by Lorentz forces, which corresponds to magneto-hydrodynamic instabilities like metal pad instability. For this a rotating disc equipped with permanent magnets is arranged below the cell. A Laser triangulation sensor and a Laser light sheet are used to scan and to measure the shape of the interface. The absolute deflection of the interface is the range of millimeter, which could impair the operation of a LMB negatively.

Experimental analysis of bubble entrapment during droplet impact on solid substrates

Sabrina Grünendahl (*TU Dortmund*), Lutz Gödeke (*Biochemical and Chemical Engineering, TU Dortmund*), Peter Ehrhard (*TU Dortmund*) 16:50–17:10

Droplet impact is fundamental for a wide variety of industrial processes, most notably for spray cooling and spray coating. The quality of the final coating is highly dependent on the layering of different paints. The dry-film thickness is in the range of $80 - 150\mu m$ and, thus, sensitive to small disturbances due to leveling and bubble entrapment caused by insufficient flash-off times or substrate-pinning.
The contribution is based upon the experimental investigation of droplet impact on solid substrates by use of high-speed imaging. Droplets ($d_p \cong 2mm$) are generated by a continuous flow through a thin capillary ($d_{cap} = 0.15mm$) and dripping on solid substrates. This process is filmed from an axis perpendicular to droplet trajectory, i.e. side-view, and for transparent substrates from below along the trajectory axis. The obtained pictures allow for diameter and velocity measurements shortly before impact and capture the spreading dynamics after impact. Dimensional analysis leads to a set of dimensionless groups that are used to create a map-of-occurrence for substrate-pinned bubbles. These numbers are varied by using mixtures of water and glycerol, thus changing material properties and by changing the capillary-to-substrate distance, thus changing impact velocity.
We are able to measure the fast process of substrate-pinned-bubble entrapment during droplet impact for a range of dimensionless groups. We show that the size of the bubbles is dependent on Weber- and Reynolds-numbers. The typical spray painting process has an overlap in these ranges of dimensionless groups.

Droplet deformation, oscillation and detachment on a vibrating plate by a controlled airflow

Beawer Barwari (*Chair of Fluid mechanics, Bergische Universität Wuppertal*), Sebastian Burgmann (*Chair of Fluid mechanics, Bergische Universität Wuppertal*), Uwe Janoske (*Chair of Fluid mechanics, Bergische Universität Wuppertal*) 17:10–17:30

Droplet movement can be initiated by external flow, vibration and other influencing factors. Droplet dynamics, when subjected to either vibration or shear flow has been extensively studied. The novelty of this work is hence an effort to study droplet movement when subjected to both vibration and shear flow.
Hydrodynamic instabilities of different droplets present in a rectangular channel on a substrate subjected to vibrations is studied experimentally. Both the effect of harmonic vibration induced by an shaker and shearing mechanism induced by airflow are discussed here. Experiments are carried out for a wide spectrum of water and glycerol mixture ratios. A new empirical correlation for the initiation of droplet motion is presented. A better insight of viscosity influence on droplet behavior is obtained by performing an FFT analysis.
Experiments indicate, that the critical velocity, at which the droplet motion starts, is a function of material properties, droplet sizes, and oscillation parameters. Increasing the droplet volume and vibration amplitude results in a decrease of the critical velocity, while the droplet deformation increases. On the contrary, increasing the glycerol content results in an increase in both the critical velocity and droplet deformation. The droplet movement is categorized into three motion patterns based on experimental observations: (i) the droplet retains its elliptical shape, while at rear side the droplet taking the shape of a tail; (ii) small droplets detach from the long tail at rear of the droplet; (iii) the droplet deforms over its entire length and assumes the shape of a film.

A new approach to non-linear droplet oscillations via the unified method for boundary value problems

Dominik Plümacher (*Maschinenbau, Fachgebiet Strömungsdynamik, Technische Universität Darmstadt*), Martin Oberlack (*Strömungsdynamik, Technische Universität Darmstadt*), Yongqi Wang (*Strömungsdynamik, Technische Universität Darmstadt*), Martin Smuda (*Strömungsdynamik, Technische Universität Darmstadt*) 17:30–17:50

Considering the surface oscillations of a liquid droplet in vacuum, the Unified Transform Method [1] is used analogous to [2] to derive a new system of two non-linear equations in two unknowns $q, \mathcal{R}$, the velocity potential on the surface and the surface's distance to the drop's centre, respectively. These equations constitute a new geometrically non-linear model describing the oscillation of almost arbitrary drop shapes. Accounting for the effects of surface tension and small viscosity via a stress balance on the surface and assuming a potential flow, the three-dimensional problem is transformed onto the unit sphere. This transforms the original problem from a time-dependent domain to a time-independent one. Furthermore the number of independents is reduced from $(3+1)$ to $(2+1)$ (two spatial, one temporal).
Subsequentially, by using asymptotic expansion up to terms second order and, additionally, by orthogonal expansion into spherical harmonics (modes), a system ordinary differential equations (ODEs) is derived. This approach is similar to and therefore extends previous results in [3] to three dimensions and generalise them by incorporating weak viscous effects.

1. Ablowitz M. J. , Fokas A. S. , Musslimani Z. H. On a new non-local formulation of water waves//J. Fluid Mech. 2006. Vol. 562. PP. 313–343

2. [Fokas2008] Fokas A. S. A unified approach to boundary value problems//CBMS-NSF Regional Conf. Series in Applied Math. 2008, Vol. 78

3. Tsamopoulos J. A., Brown, R. A. Nonlinear oscillations of inviscid drops and bubbles//J. Fluid Mech. 1983. Vol. 127. PP. 519–537

Numerical Investigation of Coalescing Filtration Process

Jayotpaul Chaudhuri (*Strömungsmechanik, TU Dortmund*), Peter Ehrhard (*Strömungsmechanik, TU Dortmund*) 17:50–18:10

Coalescing filtration is a mechanical process which is employed to remove dispersed aerosol particles from a gas stream. This kind of filtration is a depth-filtration process and is widely used in process industries to remove particulate matter from exhaust gases or in compressed-air applications to filter oil particles introduced during the compression process. Fibrous filters are often used due to low cost, high capture efficiency and low pressure drop. The droplets are first captured on the fibres, then coalesce, and eventually drain out. The performance of a filter medium is judged based on its capture efficiency and pressure-drop characteristics. Estimating these parameters without setting up experimental investigations of each filter medium would be beneficial for choosing optimal filters.
In the present study, numerical simulations are used to predict the behaviour of a fully-wetting fibrous filter using a Euler-Euler scheme in ANSYS CFX. Different theoretical models to predict single fibre capture efficiencies are compared and a novel extrapolation scheme to predict the net capture of oil particles is presented. Pressure-drop studies are carried out to find the pressure drop of a viscous fluid flowing through an array of fibres. A steady-state multiphase simulation with the influence of gravity is set up, and the physical relevance of the results is examined.

Numerical simulation of initial stages of liquid water drop explosion

Thomas Paula (*Technische Universität München*), Stefan Adami (*Technische Universität München*), Nikolaus A. Adams (*Technische Universität München*) 18:10–18:30

The initial stages of shock-driven explosion of liquid water microdrops is studied numerically with a high-resolution discretization of the axisymmetric Euler equations. A level-set based conservative interface-interaction method is extended to allow phase transition. For this purpose, a Riemann solver is employed that incorporates evaporation across the Knudsen layer. Furthermore, the rapid formation of vapor cavities is achieved through a surrogate model. The numerical method is applied to a configuration that has been investigated in recent experiments of high-speed drop breakup due to energy deposition by a high-energy X-ray free-electron laser (XFEL). The presented results show, that the numerical model predicts the initial stages of the violent liquid drop explosion dynamics accurately. Our results reveal that deformation of the cylindrical vapor cavity within the droplet is not induced by a negative-pressure wave as implied from the experimental data. Instead, the particular wave is a shock and the observed deformation is caused by interaction with a negative-pressure region preceding it. The simulation starts to deviate from experimental results when the drop deformation is dominated by cavitation effects that cannot be reproduced by the current approach which does not yet include nucleation and recondensation models.

S11.03 | Interfacial flows

Date 21.03.2018
Room N1090

Numerical simulation of bubble-collapse-driven penetration of biomaterial-surrogate liquid-liquid interfaces

Stefan Adami (*Technical University of Munich, Chair of Aerodynamics and Fluid Mechanics*), Shucheng Pan (*Technical University of Munich, Chair of Aerodynamics and Fluid Mechanics*), Xiangyu Hu (*Technical University of Munich, Chair of Aerodynamics and Fluid Mechanics*), Nikolaus A. Adams (*Technical University of Munich, Chair of Aerodynamics and Fluid Mechanics*) 08:30–08:50

Since the discovery of tissue damage incurred by cavitation bubble collapses during intraocular surgery or shock-wave lithotripsy, the potential of harnessing the strongly localized release of thermal and mechanical energy through a collapse-induced shock wave has moved into the focus of biomedical technology. Experimental access of such configurations is extremely challenging, and thus intense research on experimentally accessible surrogate configurations and accompanying numerical simulations has developed over the past decade. Such an experimental surrogate configuration we consider in this paper (Kodama & Tomita 2000) and discuss the late stages of bubble collapse and interaction with the tissue surrogate by highly-resolved axisymmetric numerical simulations. We use a recently developed multimaterial regional level-set approach to represent the sharp multi-material interfaces while employing high-resolution low-dissipation WENO schemes, adaptive multi-resolution with a conservative interface-interaction model. As we consider the evolution throughout the late stages of development we have to treat potential nonresolved interface structures in a consistent fashion. We investigate in detail bubble deformation and which configurations lead to which level of gelatin penetration. The detailed results help to assess the utilization of in-vivo generated cavitation bubbles or stabilized gas containers to generate collapse-induced tailored shock waves and re-entrant jets which cause nanoperforations of cell membranes. The results show that process parameters, in particular shock overpressure, control not only penetration depth but also the size of the interface perforation, indicating means to steer processes in biomedical applications.

Vapor bubble growth in a rectangular microchannel

Alexander Stroh (*ISTM, Karlsruhe Institute of Technology - KIT*), Sahba Sadir (*IMVT, ISTM, Karlsruhe Institute of Technology - KIT*), Roland Dittmeyer (*IMVT, Karlsruhe Institute of Technology - KIT*), Bettina Frohnapfel (*Karlsruhe Institute of Technology - KIT*) 08:50–09:10

Flow boiling heat transfer in microchannels plays an important role in micro process engineering and cooling of high-performance electronic devices. A precise knowledge about the microevaporation process can help to optimize the microstructure geometry for various application scenarios. In order to gain better understanding of the physical mechanism behind boiling in a microchannel, the growth and motion of a single bubble in laminar flow is investigated. We carry out a two-phase VOF simulation in OpenFOAM. The surface tension model of Brackbill (1992) is used, while thermally driven phase change is realized using the equilibrium interface model by Rattner & Garimella (2015). The contact line dynamics of the phase fraction is modelled with a dynamic contact angle model based on the correlation by Kistler (1993). The numerical domain represents a channel with superheated bottom wall with dimensions of 1200µm x 200µm x 100µm

and a resolution of 2.5µm on an equidistant grid. A laminar velocity profile is prescribed at the inlet with no-slip boundary conditions at the walls. An initial vapor bubble with a radius of 20µm is placed in the middle of the channel. Using this numerical setup we investigate the effects of the prescribed flow velocity, temperature distribution and contact angle on the growth and motion of the vapor bubble. The simulation results are compared to corresponding experimental data.

Diffusion under micro-gravity: Mass transfer from rising bubble in a stagnant fluid column

Md Ashfaqul Bari (*Lehrstuhl für Stromungsmechanik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Cemil Akbulut (*Lehrstuhl für Stromungsmechanik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Manuel Münsch (*Lehrstuhl für Stromungsmechanik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Antonio Delgado (*Lehrstuhl für Stromungsmechanik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*)

09:10–09:30

Bubble column reactors are intensively used in chemical, biological and petrochemical productions and are also useful for long space mission eg. biological treatment of waste water in international Space Station(ISS)[1]. Convective and diffusive mass transfer occurs sequentially with other phenomena in a multiphase system with system inherent convective and diffusive time scale and within which the diffusive transport is the slowest transport mechanism impacting the run-time of the system. Investigation of the diffusion process with the exclusion of buoyancy convection will enable to better understand the overall process and optimize the underlying transfer rate. In the absence of buoyancy convection the sole effect of local flow modulation on the overall diffusion process will be investigated. For this purpose experimental and numerical investigation of the diffusion process due to force modulation of the local flow field in a multiphase system under compensated gravity in a single bubble column reactor has been planned and are being performed within the framework of project PhaDi.
At this stage numerical simulation of Oxygen bubble rising in stagnant Silicon Oil column is being carried out to investigate bubble motion, shape and path instability as well as influence of Sharp Surface Force (SSF)[2] approach to mitigate spurious current magnitude and will be presented along with the Continuous Species Transport(CST)[3] implementation of OpenFOAM for mass transfer from rising bubble to surrounding liquid.

[1] Louis M. Kindt, Michael E. Mullins, David W. Hand, Andrew A. Kline, D. Layne Carter and John D. Garr *Catalytic Oxidation Model Development of the Volatile Reactor Assembly Unit of the International Space Station Water Processor*

[2] Raeini, Ali Q., Blunt, Martin J. and Bijeljic, Branko *Modelling two-phase flow in porous media at the pore scale using the volume-of-fluid method*

[3] Deising, Daniel, Marschall, Holger and Bothe, Dieter *A unified single-field model framework for Volume-Of-Fluid simulations of interfacial species transfer applied to bubbly flows*

S11.04 | Interfacial flows

Date 21.03.2018
Room N1090

Droplet and satellite droplet shedding in dewetting polymer films

Dirk Peschka (*Weierstrass Institute for Applied Analysis and Stochastics*), Andreas Münch (*Mathematics, University of Oxford*), Barbara Wagner (*Weierstraß-Institut für Angewandte Analysis und Stochastik*) 14:00–14:20

Thin liquid polymer films on hydrophobic substrates are susceptible to rupture and formation of holes, which in turn initiate a complex dewetting process leaving behind characteristic patterns of droplets. It is now possible to trace back the specific type of droplet patterns to the nature of the polymer-substrate interfacial condition. In the talk, we present results based on large-scale simulations that enable to follow the evolution of the dewetting process deep into the nonlinear regime of the thin-film model equation. This allows to capture the complex dynamics including shedding of droplets, showing excellent comparisons to experimental results. Furthermore, the thin-film models predict the shedding of satellite droplets during the destabilisation of a liquid ridge, as it occurs during the late phases of the dewetting process. While this behavior is well-known in the context of elongating fluid filaments and jets, we show that for liquid ridges this signature can be dramatically altered by the interfacial condition between polymer and substrate.

Shear driven drop break-up on smooth rigid substrates

Patrick M. Seiler (*Strömungslehre und Aerodynamik, TU Darmstadt*), Ilia V. Roisman (*Strömungslehre und Aerodynamik, TU Darmstadt*), Cameron Tropea (*Strömungslehre und Aerodynamik, TU Darmstadt*) 14:20–14:40

Shear driven drop motion on rigid substrate is a phenomenon which occurs in various industrial and natural processes, for example in prefilming airblast atomization, printing, ice accretion or vehicle soiling. At some critical velocity of air flow velocity the drop breaks up. Drop breakup and atomization are determined by drop volume, distribution of the aerodynamic pressure, substrate wettability and liquid material properties, like density, surface tension and viscosity.
In this experimental study drop motion and breakup on the wall of a well-controlled, fully developed turbulent Hagen-Poiseuille flow are observed using a high-speed video system. A regime map for different modes of drop deformation and breakup for various Weber and Ohnesorge numbers is obtained for different values of the average static contact angle and for the contact angle hysteresis. An analytic model is developed to capture the observed dependencies and comparisons are drawn with experimental results.

Acknowledgements This work is financially supported by Adam Opel AG as part of a cooperation with TU Darmstadt. The authors express appreciation to F. Werner and P. Klaus of Adam Opel AG, who provided feedback and valuable input for the experiments.

Kinematics of contact line motion

Mathis Fricke (*Mathematische Modellierung und Analysis, TU Darmstadt*), Matthias Köhne (*Applied Analysis, HHU Düsseldorf*), Dieter Bothe (*Mathematical Modeling and Analysis, TU Darmstadt*) 14:40–15:00

We address the moving contact line problem for two-phase incompressible flows by a novel kinematical (or geometrical) approach. The key idea is to derive an evolution equation for the contact angle if the transporting velocity field is given. It turns out, that the resulting equation has a simple structure and expresses the time derivative of the contact angle in terms of the gradient of the velocity field at the solid wall. The imposed boundary conditions provide additional information about the gradient of velocity, which can be used in the kinematical evolution equation. In this paper we consider the Navier slip boundary condition, which is frequently used for the modeling of moving contact lines. Finally we use the interfacial transmission condition for the viscous stress to derive an explicit form of the contact angle evolution for a large class of models, which only involves the contact line velocity and the slip length from the Navier condition. From this equation we can read off the qualitative behaviour of the contact angle evolution for these models, which turns out to be unphysical. In particular, if the contact angle is directly related to the contact line velocity, the contact angle is a monotonically increasing or decreasing function. We discuss consequences from this observation and possible generalizations of the model.

Acknowledgements: We kindly acknowledge the financial support by the German Research Foundation (DFG) within the Collaborative Research Centre 1194 "Interaction of Transport and Wetting Processes", Project B01.

Using sliding droplets to investigate numerical schemes for moving contact line simulations with a phase field model

Henning Bonart (*Dynamik und Betrieb technischer Anlagen, Technische Universität Berlin*), Christian Kahle (*Technische Universität München*), Jens-Uwe Repke (*Technische Universität Berlin*) 15:00–15:20

The wetting of liquids on solid surfaces occurs in many industrial processes like coating, painting and separation apparatuses involving trickle films. At the intersection of the gas-liquid interface with the solid surface a moving contact line is formed. Applying the common no-slip boundary condition at the solid surface, a non-physical divergent stress at the contact line occurs. One possibility to circumvent this difficulty in the context of continuum mechanics is the coupling of the incompressible Navier-Stokes equations with the Cahn-Hilliard (CH) equation. The CH equation models the interface between the fluids with a diffuse interface of positive thickness and describes the distribution of the different fluids by a smooth indicator function. Especially, the CH equation allows the contact line to move naturally on the solid surface due to a diffusive flux across the interface, which is driven by the gradient of a chemical potential.
To incorporate dynamic contact angles and allow for contact angle hysteresis, we apply the CHNS model by [1] augmented with complex boundary conditions by [2] for the accurate description of moving contact lines. As the resulting model forms a very tightly coupled and nonlinear system of equations a careful consideration of the discretization and solution strategy is needed for efficient and accurate simulations. In this talk, we compare simulation results of sliding droplets on inclined surfaces to investigate the accuracy and efficiency of several linearization and decoupling strategies as well as free energy density formulations.

[1] Abels et al. 2012. Math. Models Methods Appl. Sci. 22 (3): 1150013.

[2] Qian et al. 2006. J. Fluid Mech. 564 (2): 333.

Wetting With ALE Interface Tracking

Dirk Gründing (*Mathematics, TU Darmstadt*), Dieter Bothe (*Mathematics, TU Darmstadt*), Holger Marschall (*Mathematics, TU Darmstadt*) 15:20–15:40

We solve the governing equations of this multiphase flow problem using an ALE interface tracking method. This approach has excellent volume conservation properties while providing a surface mesh that allows to compute high quality surface curvature and to solve surfactant transport equations.
While a no slip condition on a wall boundary is a widely accepted approach to model fluid wall interaction, the interaction between two fluids and the wall at the so called contact line does lead to a paradox involving diverging pressure and dissipation towards the contact line. Here, the surface mesh does not only allow to use standard contact angle models in combination with Navier slip boundary conditions but also provides a suitable setting for more complex models that require the solution of additional surface equations and promise to resolve the contact line paradox.
Validating the static geometry of a liquid drop on a surface for varying Eötvös numbers, yields excellent agreement with analytic reference solutions and results from literature. With this approach, the evolution of the rise height of a liquid in a capillary gap can be reproduced adequately, if for a given mesh, the initial rise height and rise velocity is used for the analytic reference solution.

We kindly acknowledge the financial support by the German Research Foundation (DFG) within the Collaborative Research Centre 1194 "Interaction between Transport and Wetting Processes", Project B02"

Investigation of the behaviour of a Newtonian liquid regarding the picture framing coating error

Oliver Sommer (*Fakultät Maschinenbau, Technische Universität Chemnitz*), Sven Hehemann (*Fakultät Maschinenbau, Technische Universität Chemnitz*), Günter Wozniak (*Fakultät Maschinenbau, Technische Universität Chemnitz*) 15:40–16:00

Surfaces of solid objects are subject to manifold external influences in manufacturing and process engineering but also surface modifications are applied to achieve characteristic surface functionalities, e.g. coatings for protection and change of surface properties, respectively. For these purposes, continuous and homogeneous layers of the coatings are desired. Many coatings remain liquid on a solid substrate for a while after their application, independently of the method of application. This may lead to different effects regarding the coating surface, which reach from small disturbances up to serious errors in the final steady state, e.g. dewetting and crater formation. Of importance is equally the specific Fat-Edge/Edge-Thinning effect, also known as frame effect or edge bulge phenomenon, depending on the industrial sector of application. In this study, we examined the specific behaviour of thin liquid layers at curved solid edges experimentally and numerically. In experimental coating investigations, we used adapted laser-induced fluorescence technique (LIF) to measure the layer thickness distribution and the numerical film simulations were carried out with the so-called Volume-of-Fluid multiphase flow model (VOF) to compute the underlying capillary flow. The main motivation is to find optimal combinations of influencing quantities to reduce the picture framing effect in order to achieve a homogenously layer thickness distribution of the liquid coating on the surface of the substrate, especially at the edges. For this purpose, we varied the viscosity of the liquid, the edge radii of curvature of the substrate and it is orientation regarding the gravitational direction etc. and the coating process.

S11.05 | Interfacial flows

Date 22.03.2018
Room N1090

Incompressible fluid problems on embedded surfaces: Modeling and variational formulations

Arnold Reusken (*Mathematics, RWTH Aachen University*) 08:30–08:50

In the past decade, in numerical analysis there was extensive research devoted to the development of numerical methods for *scalar* surface PDEs. An important application of these methods is in the numerical simulation of interfacial flows with surfactants. Only very few results for *surface flow equations*, such as the surface (Navier-)Stokes equations are known. In recent work we derived some basic properties of surface Navier-Stokes equations, which will be presented in this contribution.
The governing (Navier-Stokes) equations of motion for a viscous incompressible *material surface* are derived from the balance laws of continuum mechanics. We use elementary tangential calculus to derive the governing equations in terms of exterior differential operators in Cartesian coordinates in an ambient Euclidian space. We consider a splitting of the surface Navier-Stokes system into coupled equations for the tangential and normal motions of the material surface. We then restrict ourselves to the case of a geometrically stationary manifold of codimension one embedded in $\mathbb{R}^n$. For this case, we present new well-posedness results for the simplified surface fluid model consisting of the surface Stokes equations. Finally, we propose and analyze several alternative variational formulations for these surface Stokes problem, including constrained and penalized formulations, which are convenient for Galerkin discretization methods, such as the finite element method. Results of finite element numerical simulations for a surface Stokes problem are presented.

PIV Measurements and Numerical Simulations in a 2D-Extruder

Stefan Hirschfeld (*Chair of Fluid Mechanics, University of Kassel*), Olaf Wünsch (*Chair of Fluid Mechanics, University of Kassel*) 08:50–09:10

Extruders are widely used in polymer processing to fulfil many different tasks like for instance conveying, melting, mixing and devolatilization. All of these compounding tasks are usually performed in different processing zones arranged in series within the extruder. The devolatilization of volatile organic compounds (VOCs) from highly viscous polymer melts is a complex separation process [1] that requires a partially filled section with a free surface. Both the complete process modeling itself and the numerical simulation of two-phase flows with extremely high viscosity differences are currently not state of the art [2, 3].
To develop this field, this contribution provides a detailed study of the fluid flow in a partially and fully filled extruder. An experimental setup with a 2D model has been established that allows single-screw and twin-screw measurements with a highly viscous model fluid (silicone oil) under ambient temperature. These results are compared with numerical investigations to validate the models used. On the experimental part, a Particle Image Velocimetry (PIV) system was applied to measure the 2D velocity field in a cross section. Fluorescent PMMA-Rhodamine B-Particles are used in combination with an optical filter that blocks the disturbing scattered laser light on the free surfaces. For the numerical calculations, a Finite Volume Method (FVM) implementation of a Volume of Fluid (VOF) based free-surface approach is applied [4], solving only the liquid phase flow with appropriate boundary conditions on the free surface [3]. The numerical results show a good agreement with the experimental measurements.

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A phase-field model for immiscible fluids in porous media

Marco De Paoli (*Institute of Fluid Mechanics and Heat Transfer, TU Wien, Vienna University of Technology*), Alessio Roccon (*Polytechnic Department of Engineering and Architecture, Università degli Studi di Udine*), Francesco Zonta (*Institute of Fluid Mechanics and Heat Transfer, TU Wien, Vienna University of Technology*), Alfredo Soldati (*Institute of Fluid Mechanics and Heat Transfer, TU Wien, Vienna University of Technology*) 09:10–09:30

Global energy consumption has doubled over the last 40 years and shows no sign of drop. A major proportion of the energy produced comes from combustion of fossil fuels, with corresponding emissions of carbon dioxide (CO2) in the atmosphere, responsible for the greenhouse effect. Injection of liquefied CO2 in underground reservoirs has been identified as a possible remedy to this global problem. However, carbon dioxide pumped in geological formations is not fully soluble in the surrounding fluid (brine), and complex phenomena may occur along the interface existing between these two phases. An accurate description of the interfacial dynamics is therefore required to improve the physical modeling of the transfer mechanisms between the fluids. Inspired by this geophysical problem, we propose a thermodynamically-consistent method for the description of two immiscible phases in a three-dimensional and satured porous medium. We used the Cahn-Hilliard model for the concentration field, whereas the velocity is computed with the Darcy law, where the effects of buoyancy and Korteweg stresses are also included. We performed direct numerical simulations to investigate the effect of surface tension on the finger dynamics. These results will lead to a deeper understanding of the dynamics occurring along the interface of two immiscible or partially miscible fluids.

A Quasi-Incompressible Navier-Stokes Cahn-Hilliard Model with Large Density Contrast and Volumetric Source Terms

Simon Praetorius (*Institute of Scientific Computing, Technische Universität Dresden*), Axel Voigt (*Institute of Scientific Computing, Technische Universität Dresden*), Steven Wise (*Department of Mathematics, University of Tennessee, Knoxville*) 09:30–09:50

Diffuse-interface models are a popular framework to study the flow of immissible fluid phases. In the recent years thermodynamically consistent models have been derived for variable density and viscosity, utilizing different modeling assumptions. The quasi-incompressible Navier-Stokes Cahn-Hilliard model by Lowengrub and Truskinovsky [3] introduces an order-parameter for mass concentration and a mass-averaged velocity field, resulting in a non-solenoidal velocity near the interface of the phases. On the other hand, Abels et al. [1] have formulated their model with a volume-averaged velocity, leading to divergence-free velocity fields.
We want to show a numerical comparison of two models similar to the models above but based on a volume fraction approach that differ in the definition of the global velocity field only, i.e., mass

averaged or volume averaged velocity. Therefore, we study benchmark systems with and without topological transitions, as postulated being of relevance for the quasi-incompressible approaches. The models are derived in the setting of a multi-component system, including source terms that may account for mass exchange via reaction or a phase transformation, and resulting in an energy-stable dynamical system. We want to show the corresponding energy stable and mass conservative discrete schemes for the full system, similar to the binary case, as given recently by Guo et al. [2].

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Higher-order surface FEM for incompressible Navier-Stokes flows on manifolds

Thomas-Peter Fries (*Civil Engineering, Graz University of Technology*) 09:50–10:10

For the modeling of transport processes on interfaces, e.g., in foams, biomembranes and bubble surfaces, Stokes and Navier-Stokes flows on two-dimensional manifolds have to be considered. Models for fixed or moving curved surfaces in three dimensions are available [1, 2]. Herein, the focus is on the approximation of stationary and instationary (Navier-)Stokes flows based on the surface finite element method as outlined in [3,4]. Individual orders for the geometry, velocities, pressure and Lagrange multiplier to enforce tangential velocities are chosen. Stabilization is employed for flows at high Reynolds numbers. Applications are presented which extend classical benchmark testcases from flat domains to general manifolds. Highly accurate solutions are presented and higher-order convergence rates confirmed.

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[4] T.P. Fries, D. Schöllhammer: Higher-order meshing of implicit geometries—part II: Approximations on manifolds, Comp. Methods in Appl. Mech. Engrg., 326, 270-297, 2017.

Simulation of particle collision rates in a bubbly liquid metal flow

Ronja May (*Institute of Fluid Mechanics, TU Dresden, George-Bähr-Str. 3c, 01062 Dresden, Germany*), Jochen Fröhlich (*Institute of Fluid Mechanics, TU Dresden, George-Bähr-Str. 3c, 01062 Dresden, Germany*) 10:10–10:30

Collision rates of particles in bubbly liquid metal flows are of major interest in different applications, such as flotation processes in steel making for the removal of small inclusion particles

from the liquid metal. For example, colliding inclusions can form larger aggregates that might get more easily entrained by the injected gas bubbles in flotation processes. Also the increased buoyancy of larger particles can be beneficial for the inclusion removal.
In the presented flow simulations spherical Argon gas bubbles rise in stagnant liquid metal with initially homogeneously distributed spherical alumina oxide particles of small inertia. Due to the vortex structures and increased shear rate in the developing bubble wakes, regions of higher and lower particle density can form. Depending on their relative position to the bubble particles are subjected to different forces and tend to collide in regions of increased strain rate.
The contribution presents Direct Numerical Simulations with bubbles being geometrically resolved and the inclusions represented as point particles. In the community, the boundary conditions at particle surfaces are discussed controversially. To elucidate their potential influence, two extreme cases are simulated, one with full no-slip condition, the other one with full slip condition. The contribution provides an analysis of the locations and the rate of particle collisions in the bubbly liquid metal flow and their potential impact on aggregation.

S11.06 | Interfacial flows

Date 22.03.2018
Room N1090

Finite Element Approximation of Coupled Bulk-Surface Navier-Stokes Equations and Applications to Fluidic Two-Phase Biomembranes

Harald Garcke (*Mathematik, Universität Regensburg*) 14:00–14:20

We consider two-phase Navier–Stokes flow taking viscous effects within the surface into account. In such a fluid the rheological behaviour at the interface includes surface viscosity effects, in addition to the classical surface tension effects. We introduce and analyze parametric finite element approximations, and show, in particular, stability results for semi-discrete versions of the methods, by demonstrating that a free energy inequality also holds on the discrete level. We perform several numerical simulations for various scenarios in two and three dimensions, which illustrate the effects of the surface viscosity.
As an application of our finite element approach we study the evolution of biomembranes. Biomembranes can be considered as a surface fluid and the governing equations for the evolution include the surface (Navier–)Stokes equations and forces steming from the Helfrich curvature energy, modelling the elasticity of the membrane, and from a Cahn–Hilliard type energy, modelling line energy effects.

Numerical methods for multi-region interfacial problems

Shucheng Pan (*Department of Mechanical Engineering, Technical University of Munich, Chair of Aerodynamics and Fluid Mechanics*), Xiangyu Hu (*Department of Mechanical Engineering, Technical University of Munich, Chair of Aerodynamics and Fluid Mechanics*), Nikolaus A. Adams (*Technical University of Munich, Chair of Aerodynamics and Fluid Mechanics*) 14:20–14:40

We present recently developed numerical methods for several multi-regions problems. Our method, based on regional level-set function, can capture the time evolution of multiple junctions via new mapping and remapping operators. This method automatically handles topology changes and does not generates any artifacts (voids and overlaps). High-order accuracy has been achieved. It has been applied to dry-foam dynamics and mean-curvature flows. We also develop a high-order redistancing method and a multi-region interface reconstruction method for those

probelms. For compressible multi-material flows, we couple this interface-capturing method with conservative finite volume method. The exchange flux across different materials are calculated by a reduced interface-interaction model and the HLLC Riemann solver to archive high computational efficiency. The multi-resolution method and local time-stepping scheme are incorporated into our multi-material method to speed up the high-resolution simulations. And during these high-resolution simulations a new multi-material scale separation model is proposed to consistently remove non-resolved interface scales and thus improves the robustness of our methods. Numerical test cases includes the multi-material shock tube problem, inertial confinement fusion implosion, triple-point shock interaction and shock interaction with multiple bubbles. At last we also consider that the domain-decompostion problem resembles the foam dynamics. Thus we propose a variational model for the domain-decompostion problem and solve it by our interface-capturing method. The minized load balancing error and communication volumes are smaller than traditional graph-based methods.

Application of the Stochastic Field Method to Multi-fluid flow

Martin Raquet (*KIT - Karlsruhe Institute of Technology*), Andreas Class (*Karlsruhe Institute of Technology - KIT*), Wilfried Edelbauer (*AVL LIST GmbH.*) 14:40–15:00

The Stochastic Field Method was originally derived in the field of combustion and firstly applied to a cavitation problem by our group [1]. Randomly distributed variables exist in both combustion and cavitating problems. Calculating strong nonlinear processes using mean values as input lead to unphysical results. The consideration of the variable's probability density function (PDF) becomes mandatory. The Stochastic Field Method approximates this PDF by samples similar to methods of Lagrangian particles where imaginary particles are introduced to the flow. In contrast to Lagrangian particles methods these samples are represented by Eulerian fields described by stochastic partial differential equations. This pure Eulerian interpretation makes the method attractive for CFD-codes: A coupling of a Eulerian and a Lagrangian perspective becomes obsolete which results in efficient computation times - especially in the presence of a vast number of bubbles. In contrast to other Eulerian methods the calculation of an arbitrary PDF is possible at low computational cost. The representation of samples as fields allows the visualization of PDFs within every computational cell. The first implementation into a commercial CFD-Code is presented. In addition industrial examples, i.e. cavitation in an automotive injection nozzle, are shown.

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Step formation in thin-film diblock-copolymers via a phase-field model with free surfaces

Quentin Parsons (*Computer Science, University of Oxford*), Andreas Münch (*Mathematical Institute, University of Oxford*), David Kay (*Computer Science, University of Oxford*) 15:00–15:20

Phase separation in diblock-copolymers is an important process in nanotechnology that yields highly regular structures on very fine length scales.
In this talk, we discuss the evolution of two-phase, thin-film diblock-copolymers using a three-phase Ohta–Kawasaki (non-local Cahn–Hilliard) phase-field model, with an obstacle homogeneous energy potential. The free surface is represented as an interface with a third, homopolymer phase for the void.

We develop energy estimates for stationary solutions, based on an appropriate sharp interface limit. These suggest that films with steps have lower free energy than their flat counterparts. We present supporting results of numerical solutions of energy-decaying, time-dependent dynamics of the copolymer-void model, based on a Moreau–Yosida regularisation of the obstacle potential. These provide insight into the evolution of stepped films, and their associated domain patterns.

Asymptotic analysis of a degenerate phase-field model involving bulk and surface diffusion

Andreas Münch (*Mathematical Institute, University of Oxford*), Alpha Lee (*Department of Physics, University of Cambridge*), Marion Dziwnik (*Technical University Berlin*), Endre Süli (*Mathematical Institute, University of Oxford*) 15:20–15:40

We study the evolution of solid surfaces and pattern formation by surface diffusion. Phase field models with degenerate mobilities are frequently used to model such phenomena, and are validated by investigating their sharp interface limits. We demonstrate by a careful asymptotic analysis involving the matching of exponential terms that a certain combination of degenerate mobility and a double well potential leads to a combination of both surface and non-linear bulk diffusion to leading order. We also discuss implications for the case with an anisotropic free energy.

Surface Navier-Stokes flows and related problems

Axel Voigt (*Mathematics, TU Dresden*), Ingo Nitschke (*TU Dresden*), Sebastian Reuther (*TU Dresden*) 15:40–16:00

We consider a surface Navier-Stokes equation on an evolving surfaces, derive the model, discuss numerical approaches and analyse the coupling between the topology of the considered surface, local geometric properties and the dynamics of the flow field. We further extend the model towards surface liquid crystals and show preliminary results.

S11.07 | Interfacial flows

Date 22.03.2018
Room N1090

Convective mass transfer from a square cavity

Tianshi Sun (*Hydromechanics, TUM BGU Chair of Hydromechanics*), Michael Manhart (*Hydromechanics, TUM BGU Chair of Hydromechanics*) 17:30–17:50

Non-aqueous phase liquids (NAPLs), such as gasoline, octanol, may enter the subsurface, for example, from a leaking underground pipe or tank. Due to their low solubility in water, it may take several decades for them to disperse by natural dissolution. Residual NAPLs will be trapped in soil and constitute a long-term threat to drinking water supplies. For this reason, a variety of techniques have been developed for remediating the NAPLs contaminated land.

A numerical investigation of the purging of NAPL from a 2D cavity model is undertaken. The 2D cavity is filled with a NAPL which is immiscible with water underneath a channel. A Direct Numerical Simulation (DNS) is performed using our in-house codes MGLET [1]. It is implemented with a finite volume (FV) solver on a Cartesian grid with the staggered variable arrangement for the computations. A conservative level set method [2][3] is used to track the interface between overflow and the NAPL in the cavity. Due to NAPLs low solubility, only

convective mass transfer will be taken into account. Different kinds of flow conditions, such as Richardson number, Weber number, density ratio and time scale, are simulated numerically, and the results show that these flow conditions not only have a significant impact on the mass transfer rate, but also on the behavior of the interface.

[1] M. Manhart. A zonal grid algorithm for DNS of turbulent boundary layer. Comput. Fluid, 33(3) (2004), 572–581.

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Numerical investigations of the hydrodynamics in aerated tanks

Ann Kathrin Höffmann (*Biochemical and Chemical Engineering, TU Dortmund*), Peter Ehrhard (*TU Dortmund*)

17:50–18:10

Aeration tanks represent a major energy consumer in municipal wastewater-treatment plants. To increase their efficiency, numerical investigations are conducted to capture the hydrodynamics, the mass transfer, and the biochemical reactions in the aeration tank. At first, the hydrodynamics of the bubble rise is computed separately to generate a reliable foundation for the mass-transfer problem.
The present work concentrates on numerical investigations of the hydrodynamics of rising air bubbles in water. Herein, the bubble-size distribution is assumed to be mono-disperse and the influence of this assumption on the specific mass-transfer area is discussed. To validate the numerical model, using experimental results from tomographic measurements, the specific mass-transfer area, the gas-volume fraction, and the velocity profiles are discussed. Furthermore, calculations using a poly-disperse bubble-size distribution are performed and compared to the mono-disperse model computations. These results are evaluated with respect to the mass-transfer problem and calculation time.

Numerical simulation of compressible multiphase flows using the new T-ENO scheme with a sharp-interface level-set method

Josef Winter (*Lehrstuhl für Aerodynamik und Strömungsmechanik, TUM Fakultät für Maschinenwesen*), Stefan Adami (*Lehrstuhl für Aerodynamik und Strömungsmechanik, TUM Fakultät für Maschinenwesen*), Nikolaus A. Adams (*Lehrstuhl für Aerodynamik und Strömungsmechanik, TUM Fakultät für Maschinenwesen*)

18:10–18:30

Compressible multiphase flows are dominated by sharp gradients, material interfaces and small-scale flow structures. Resolving these effects poses challenges on the numerical scheme, that requires to stably capture the effects of discontinuities while minimizing numerical dissipation to preserve small-scale flow structures. To address these high demands, we present a new combination of a targeted essentially non-oscillatory scheme (T-ENO) with a conservative sharp-interface level-set method. We use the recently developed fifth-order targeted-ENO (T-ENO) scheme for spatial reconstruction within our finite-volume based multiresolution two-phase flow solver. The material interface is modeled with the conservative level-set method. Interface-exchange terms are solved by a two-material Riemann problem. An explicit second-order TVD Runge-Kutta

integration is performed to evolve the conservative variables and advect the level-set field. Various one- and two-dimensional examples demonstrate the stability and accuracy of the proposed method. If available, we compare the results with analytical solutions or literature results. We also present more complex two-phase flow problems including shock-bubble interaction and validate our results with experimental data. Overall, T-ENO shows improved stability and less numerical dissipation as compared to classical WENO schemes.

S12 | Waves and acoustics

Organiser Sabine Christine Langer (*Institute for Engineering Design, Technische Universität Braunschweig*)
Martin Schanz (*Institute of Applied Mechanics, Graz University of Technology*)

S12.01 | Waves and acoustics

Date 22.03.2018
Room 0601

Wavelets and Lubich convolution quadrature for a time domain boundary integral formulation of the wave equation

Silvia Falletta (*Dep. of Mathematical Sciences (DISMA), Politecnico di Torino*), Silvia Bertoluzza (*IMATI-CNR*), Letizia Scuderi (*Dep. of Mathematical Sciences (DISMA), Politecnico di Torino*) 08:30–08:50

We consider a wave propagation problem, reformulated in terms of a BIE in the space-time domain. For its solution, we propose a numerical scheme which is based on a second order Lubich discrete convolution quadrature formula for the discretization of the time integral, coupled with a classical Galerkin method in space.
It is known that the main advantage of the Lubich formula is the use of the FFT algorithm to retrieve the discretization in time of the integral operators with a computational complexity of order $N \log N$, being N the total number of time steps performed. On the other hand, the discretization in space leads in general to a quadratic complexity in space and the global required working storage is M^2N, where M is the number of grid points chosen on the domain boundary. To reduce the complexity in space, we consider here approximant functions of wavelet type. According to the properties of the wavelet basis, it results that the integral operators have a rapid decay to zero with respect to time, and many of the associated matrix entries assume negligible values.
By taking advantage of this property, we apply a *time downsampling strategy* that allows to retrieve only those matrix entries which are significant with respect to a prescribed tolerance. Such a compression strategy allows to obtain highly sparse matrices by preserving the efficiency of the FFT algorithm.
This numerical approach allows to obtain a considerable reduction of the computational spatial complexity without affecting the accuracy of the solution.

Generalised Convolution Quadrature with Runge-Kutta method for Acoustic Boundary Elements

Martin Schanz (*Institute of Applied Mechanics, Graz University of Technology*) 08:50–09:10

Wave propagation problems can be treated well with the Boundary Element Method (BE) as long as the underlying partial differential equation is linear. For hyperbolic problems like acoustics the respective integral equation consists of an convolution integral in time over the retarded potentials. Further, a convolution in the space has to be computed as in all BE formulations. The latter is not the focus of this presentation but the evaluation of the convolution in time.
Several approaches exist varying from analytical integration up to transformation methods. The Convolution Quadrature (CQ) is used frequently but restricted to a constant time step size.

The generalisation to a non-uniform time mesh has been done by M. Lopez-Fernandez et al. This generalised CQ is used here for the single and double layer approach but also for a direct formulation for mixed boundary value problems. Essentially, the performance of the Runge-Kutta based generalized CQ is studied with respect to its convergence behaviour. As usual, the convergence order of the formulation is restricted by either the order of the Runge-Kutta method or by the spatial convergence order. In the presentation only a low order spatial discretisation is used. Examples are given for acoustics for Dirichlet and Neumann boundary conditions as well as for absorbing boundary conditions.

Adaptive cross approximation based boundary elements in elastodynamics

Anita Maria Haider (*Institute of Applied Mechanics, Graz University of Technology*), Martin Schanz (*Institute of Applied Mechanics, Graz University of Technology*) 09:10–09:30

The study of wave propagation in elastic bodies is of interest in many fields of engineering. Such problems can be treated by the boundary element method in an elegant manner. However, the boundary element method suffers from fully populated system matrices, which causes excessive requirements of memory and computing time. To overcome this drawback we carry out a low rank approximation by means of the adaptive cross approximation (ACA). This approximation has already been applied successfully to scalar-valued problems such as the scalar wave equation. The extension of the ACA to vector-valued problems, like elastodynamics or thermoelasticity, involves some difficulties. The crucial point of this algorithm is to find a suitable pivot element. In particular, the pivot strategy has to ensure that the inverse of the pivot element exists.
This talk addresses the approximation of boundary element matrices via adaptive cross approximation. First, a model problem of linear elasticity is introduced. We recall the principles of the adaptive cross approximation and turn our attention to finding a suitable pivot element. Finally, the results of numerical experiments are presented and discussed. They show that the occurring matrices can indeed be compressed significantly while retaining a good quality of the solution of the underlying problem.

On classical and novel mass lumping schemes for higher-order Serendipity-type finite elements

Sascha Duczek (*Otto-von-Guericke-Universität Magdeburg*), Hauke Gravenkamp (*Universität Duisburg-Essen*) 09:30–09:50

The solution of complex dynamic problems is even today a very challenging task. Besides a fine spatial discretization using (higher-order) finite elements also a fine temporal discretization is needed. Therefore, problems such as wave propagation or impact analysis are computationally very demanding. To alleviate the computational burden, it is common practice to diagonalize the mass matrix. Consequently, efficient and accurate mass lumping algorithms for different types of finite elements are indispensable. By employing a diagonal mass matrix, the advantages of explicit time integration methods can fully be exploited. In comparison to implicit time stepping schemes, where a linear system of equations needs to be solved in each time step, only matrix-vector products are computed in explicit methods to advance in time. In the contribution at hand, a novel numerical manifold method-based mass lumping scheme for higher-order finite elements using a trunk space formulation (Serendipity-type finite elements) is proposed. By means of conventional mass lumping techniques such as nodal quadrature or row summing, it was heretofore impossible to diagonalize the mass matrix of higher-order Serendipity-type finite elements. These methods gave rise to zero or negative entries in the lumped mass matrix which in turn resulted in an impaired convergence or even in divergence of explicit time integration

schemes. The only available alternative is the HRZ method (diagonal scaling) proposed by Hinton, Rock, and Zienkiewicz. Therefore, the results of dynamic benchmark problems are compared for the proposed algorithm and the HRZ method, and finally important conclusions are provided.

A fluid model for the simulation of fluid-structure interaction in the Scaled Boundary Finite Element Method for prismatic structures

Paul Wasmer (*Fachbereich 8.4 Akustische und elektromagnetische Verfahren, Bundesanstalt für Materialforschung und -prüfung (BAM)*) 09:50–10:10

The Scaled Boundary Finite Element Method (SBFEM) for prismatic structures is an efficient method for the simulation of acoustic behavior. Hence a further development of the method is of great interest. The wave propagation can be calculated for isotropic and anisotropic materials in solids. As for many applications the acoustic behavior in fluids and the behavior in case of fluid-structure interaction (FSI) is subject of research, the implementation of a fluid model in SBFEM for prismatic structures is needed. In case of FSI the coupling between fluid and solid domains can be performed without additional effort when describing both domains in the same variables. Hence a displacement-based fluid description is used. As the discretized formulation leads to spurious modes, a penalty method to suppress the unphysical behavior is chosen. To validate the derived model a comparison with analytical solutions of purely fluid domains is made. As to verify that in case of FSI the model shows the right behavior, dispersion curves of water-filled pipes are calculated and compared to results obtained with Comsol.

S12.02 | Waves and acoustics

Date 22.03.2018
Room 0601

Retarded potentials for wave propagation in elastic trusses

Dominik Pölz (*Graz University of Technology*), Michael Gfrerer (*University of Kaiserslautern*), Martin Schanz (*Institute of Applied Mechanics, Graz University of Technology*) 14:00–14:20

Truss structures play a central role in various fields of engineering and naturally there exist numerous different approaches for simulating elastodynamic trusses. Methods based on time domain boundary integral equations are a promising, yet hardly explored, alternative to such classical procedures. In this talk, we consider truss structures which consist of several elastic rods. In each of these members, the longitudinal displacement is governed by the 1D wave equation. We present an equivalent retarded potential equation based on an explicit and computable representation of the Dirichlet-to-Neumann map of the wave equation. The Bubnov-Galerkin discretization of the associated variational formulation is discussed and we provide a criterion on the time step size which is sufficient for its stability. Adaptive mesh refinement is enabled by a heuristic a posteriori error indicator. A truss system typically encountered in structural engineering is simulated, illustrating the potential of the proposed method.

Comparison of a numerical versus an analytical approach to calculate 1D impact problems of non-uniform cross section

Jens Burgert (*Institute of Engineering Mechanics, KIT - Karlsruhe Institute of Technology*), Wolfgang Seemann (*Institute of Engineering Mechanics, KIT - Karlsruhe Institute of Technology*) 14:20–14:40

Impacting rods are used in various devices in practical life but also for scientific experiments such as the split Hopkinson pressure bar. For another example, the percussion drilling process, researchers revealed, that the efficiency of the drilling process strongly depends on the longitudinal wave that is transmitted through the drill rod to the drill bit. Since it is a well-known fact that the geometry of the impacting piston is shaping the stress wave, the idea is to adjust the impacting piston for an optimized shape of the stress wave. Analytical solutions for the wave propagation on the impacting partners can only be found for certain shapes of the cross section by applying a modified exponential approach. For arbitrary cross sections, numerical methods have to be chosen. Therefore, the geometry of the impacting partners is discretized by a large number of piecewise constant cross sections. On a constant cross section, the solution of the governing partial differential equation is given by the well-known D'Alembert solution. At each change of cross section, the incoming wave is partly reflected and partly transmitted which is considered by transition conditions. The introduced numerical approach is applied and presented in the field of rock drilling. It is shown that the comparison of the numerical and analytical solutions yields very good agreement.

Guided wave-based damage detection in solids using computational intelligence

Daniel Hesser (*RWTH Aachen University, Institute of General Mechanics*), Bernd Markert (*RWTH Aachen University, Institute of General Mechanics*) 14:40–15:00

The field of structural health monitoring (SHM) focuses on the non-destructive evaluation of structures during on-going operation. In this paper, the application of elastic guided waves in solids is discussed and applied to monitor an aluminium plate. The interaction of waves with structural features and uncertainties results into a unique wave field, which can be achieved by bonding piezoelectric sensors on the surface. These sensors allow a controlled excitation and acquisition of waves in structural components. In this study, the acquired data is processed by the help of computational intelligence. Computational intelligence enables the ability to learn wave behaviours from data of undamaged as well as damaged structures. Once the training process is completed, the trained system can be applied under operational conditions and will continuously monitor the structure and detect the location of damage.

[1] Hesser, D.F., Markert, B.:*Excitation strategies for vibration based damage detection using piezoelectric transducers and machine learning*, PAMM, 16: 141–142, 2016, doi:10.1002/pamm.201610059

Frequency Dependence of Amplitude Properties of Guided Waves in Fibre-Metal-Laminates

Tobias Losch (*Maschinenbau, Helmut-Schmidt-Universität - Universität der Bundeswehr Hamburg*), Artem Eremin (*Kuban State University, Krasnodar, Russia and Helmut-Schmidt-Universität - Universität der Bundeswehr Hamburg*), Rolf Lammering (*Helmut-Schmidt-Universität - Universität der Bundeswehr Hamburg*) 15:00–15:20

The rising demands of modern lightweight constructions led to new complex materials. Fibre-Metal-Laminates (FML), composites from multiple thin metallic and fibre-reinforced plastics (FRP) sublayers, are already utilized in aerospace and wind-power industries. To continuously assess the integrity of thin-walled plate like structures, active Structural-Health-Monitoring (SHM) Systems are a potential solution [1]. Physically, they are based on ultrasonic elastic guided waves (GWs), which could propagate along the waveguide for long distances. This type of waves (Lamb

waves for isotropic plates) is known to be highly dispersive and possesses complex amplitude distribution through structure thickness. The latter is especially pronounced for anisotropic multilayered composites. In the current work dispersion and amplitude characteristics of GWs in FML are thoroughly investigated. Using the example of FML, the displacement fields of wave modes are reviewed in detail. A parametrization of the elliptical movement of particles in a harmonic solution reveals the proportion of in-plane and out-of-plane motion and thereby the direction of particle-rotation beeing depend on the frequency. This can be of practical intresset whenever a certain particle-motion within an ultrasonic wave is desired. For example, minimizing the out-of-plane motion at water-loaded surfaces by choosing the right frequency of an ultrasonic wave results in a lower energy loss into the water [2].

[1] Lammering; Gabbert; Sinapius; Schuster; Wierach (2018): Lamb-wave based structural health monitoring in polymer composites. Cham: Springer.

[2] Rose (2014): Ultrasonic guided waves in solid media. Cambridge: Cambridge University Press.

Parameter Estimation and Damage Detection using Stochastic Fourier Integral Operators

Martin Schwarz (*AB Technische Mathematik, Universität Innsbruck*), Michael Oberguggenberger (*Universität Innsbruck*) 15:20–15:40

This talk addresses a novel for wave propagation in material with spatially varying random properties. Possible applications are reliability analysis, damage detection and system identification. The novelty of our method is of a top-down approach, where the randomness included into the solution operator rather than in the coefficients of the model. The solution can be represented by stochastic Fourier integral operators (sFIO), which have nice computational properties for (numeric) simulations. Our model predicts the fully time dependent dynamic response of the structure, and its stochastic properties. Calibrating the sFIO to measurements can be used for both parameter estimation and damage detection.
We present

1. the deterministic solution operator,
2. the inclusion of random parameters of the sFIO,
3. a parameter estimation for a stochastic structure,
4. damage detection using the sFIO.

S12.03 | Waves and acoustics

Date 23.03.2018
Room 1601

Weak shock reflection in steady transonic dense gas flow

Alfred Kluwick (*Institute of Fluid Mechanics and Heat Transfer, Technische Universität Wien*), Ted Cox (*Mathematics and Statistics, University College Dublin*) 08:30–08:50

Flows of dense gases may exhibit a number of phenomena which are impossible in the case of perfect gases and thus are of considerable theoretical interest. These include, among others, the formation of rarefaction shock waves which accelerate rather than decelerate the gas and a substantial increase of the lower critical Mach number. As a consequence there is no danger of flow separation if rarefaction shocks interact with boundary layers in high Reynolds number flow.
Experimental work is needed to clarify whether these phenomena predicted by theory can be realised in a technical environment and be used to increase the efficiency of turbomachines in Organic Rankine Cycles for decentralised power plants in low popularised areas. Special interest here is for steady transonic flow. The present work is intended to support such experimental efforts. As a first step the most simple but canonical case of slightly supersonic flow past compression/compression ramps was considered in (1). The present study is intended to complete the understanding of such flows by investigating the reflection problem arising from the presence of an opposing solid wall in confined geometries.

(1) Kluwick, A. and Cox, E.A. (2017). Steady transonic dense gas flow past two – dimensional compression/expansion ramps. PAMM, in press.

Near-critical turbulent open-channel flow over wavy bottom

Markus Müllner (*AIA - Aerodynamisches Institut, RWTH Aachen University, AIA - Institute of Aerodynamics Aachen*) 08:50–09:10

Steady two-dimensional turbulent free-surface flow in a channel with mild baseline slope is considered. The shape of the channel bottom is assumed to be undular with a very small amplitude. The bottom roughness is constant. Asymptotic expansions for large Reynolds numbers and Froude numbers slightly above the critical value 1, respectively, give for the surface elevation a differential equation of KdV-type, with the additional terms representing turbulent dissipation and forcing due to the wavy bottom, respectively. No turbulence modelling is required. This asymptotic approach was successful in previous works [1−3] in describing stationary solitary waves in a channel with plane bottom and small variations in the bottom friction coefficient. Besides, it was shown recently [4, 5] that stationary single-wave solutions with smaller amplitudes, denoted as solutions of the second kind, can exist.
In the talk, we present stationary periodic solutions for the surface height. First, cnoidal-wave solutions for a family of particular bottom shapes are discussed. Remarkably, these particular solutions exist only in a narrow parameter range. The solutions are then used to verify the results obtained with a numerical solver. When different starting values are used in the numerical solver, we find new periodic solutions with smaller amplitude, which we denote as solutions of the second kind. Finally, we modify the shape of the bottom to a sine function. Again, numerical solutions of the first and second kind, respectively, are obtained. For the latter, a simple analytical solution for the surface height is also presented.

[1] W. Schneider. JFM 726, 137–159 (2013)

[2] M. Müllner, W. Schneider. PAMM 15(1), 491–492 (2015).

[3] W. Schneider, Y. Yasuda. J. Hydr. Eng. 142(1) (2016)

[4] M. Müllner. ZAMM 1–24 (2017)

[5] M. Müllner, W. Schneider. PAMM 17(1) (2017), to appear.

A method for filtering Galbrun's equation to identify acoustically relevant modes in complex flows

Marcus Maeder (*Chair of Vibroacoustics of Vehicles and Machines, Technische Universität München*), Steffen Marburg (*Chair of Vibroacoustics of Vehicles and Machines, Technische Universität München*) 09:10–09:30

Analyzing acoustic wave propagation within complex flow situations has been a challenging task for engineers in the field of aero-acoustics. Especially the automotive and aeronautical industry deals with full size models that, despite the significant increase in computational power, still exceed an acceptable time range to compute results. In analogy to structural dynamics where the solution due to a harmonic excitation can be reproduced by superimposing modal contributions, the authors seek to apply the same concept to aero-acoustic problems represented by Galbrun's equation. Galbrun's equation models the wave propagation phenomena within a complex flow through a mixed Eulerian-Lagrangian frame where the particle displacement represents the unknown to solve for. However, utilizing an eigenvalue extraction procedure results in spurious modes that are able to pollute the final solution. This paper presents a possible filtering procedure applied to Galbrun's equation before extracting the eigenvalues. This way, spurious modes are nicely distinguishable from acoustic relevant modes as a preparation for modal superposition.

Modelling of constrained layer damping for bending waves in frequency domain using finite shell elements

Matthias Dorn (*Institute for Engineering Design, Technische Universität Braunschweig*), Sabine Christine Langer (*Institute for Engineering Design, Technische Universität Braunschweig*) 09:30–09:50

Constrained layer damping (CLD) is a damping principle which utilizes a viscoelastic layer in between two elastic covering layers. A bending of the resulting plate structure leads to mainly shear deformation in the viscoelastic layer which in theory is more efficient dissipation-wise than damping due to pure strain deformation. This principle is typically used in application by applying damping tape to the surface of a metallic base plate. Because extensive use of such damping tape is economically expensive, one wants to achieve maximum dissipation with a limited amount of modified area. Therefore there is an interest in predicting the optimal distribution of a given amount of damping tape by numerical simulations. In most applications using the Finite Element Method (FEM), shell elements are prefered over volume elements, because the shell elements are computationally more efficient. To be able to use CLD in shell based FEM-applications an effective material model has to be derived first. In this contribution, FEM is used to model CLD in two different ways: First, an explicit volume model of a CLD-structure and second, an effective material model using shell elements. The frequency responses of both models are compared.

Characterization of the frequency dependent properties of damping materials

Fabian Duvigneau (*Institute of Mechanics, Otto-von-Guericke-University Magdeburg*), Lars Spannan (*Otto-von-Guericke-University Magdeburg*), Maria Gavila Lloret (*BMW Group*), Elmar Woschke (*Otto-von-Guericke-University Magdeburg*), Ulrich Gabbert (*Otto-von-Guericke-University Magdeburg*) 09:50–10:10

The comfort of modern passenger cars becomes more and more important. One main focus of the design process is on the acoustical behavior of the automobiles. The application of damping materials is one major treatment to improve the acoustic behavior significantly, which is additionally advantageous due to its simplicity, robustness and effectiveness. Moreover, damping materials can be added if unexpected acoustical problems occur in the prototype stage. In parallel, the product development process in automobile industry progressively bases on virtual engineering methods like advanced simulation techniques. Unfortunately, the modeling of damping materials within numerical vibration and acoustic analysis is very challenging. The reason is that in most cases neither sufficient material data for describing the damping behavior nor a suitable knowledge about the material behavior is available. In this paper different experimental methods for determining the frequency dependent stiffness and damping properties are compared in terms of their required effort and accuracy. Exemplarily different soft foams as typical damping materials in automotive applications are used. The results of the investigated methods are evaluated by comparing numerical simulations with acoustic measurements. As reference for the validation measured insertion loss functions of the sound power are used. The insertion loss functions are obtained in an acoustic transmission test bench consisting of an echo chamber and an anechoic room, which are connected via a window in that the samples are placed. With the help of simulations the experimentally determined frequency dependent material properties are tested in order to identify the best method to characterize damping materials from an acoustical point of view.

S13 | Flow control

Organiser Steven L. Brunton (*Department of Mechanical Engineering, University of Washington*)
Bernd R. Noack (*Mechanics, LIMSI-CNRS*)

S13.01 | Flow control

Date 21.03.2018
Room N1095

Closed-loop control of turbulent boundary layers using spanwise traveling surface waves

Marian Albers (*Institute of Aerodynamics, RWTH Aachen*), Pascal Sylvain Meysonnat (*Institute of Aerodynamics, RWTH Aachen*), Wolfgang Schröder (*Institute of Aerodynamics, RWTH Aachen*) 08:30–08:50

Drag reduction in turbulent boundary layer flows is one of the key methods for substantial energy savings in aerodynamics. Large parts of the flow over the wing of modern aircraft is turbulent, thus even net energy savings of a few percent can lead to high cost savings. In active flow control, it was shown that spanwise oscillating walls can decrease the friction drag up to 50 percent in turbulent channel flows [1]. Another promising approach are spanwise transversal traveling surface waves which impose a secondary flow field in the spanwise direction. Studies in channel flows have shown drag reductions of 30 percent [2], while the effect in turbulent boundary layers is in the range of 10 percent [3].
One advantage of active methods over passive methods, such as shark-skin surfaces, so-called riblets [4], is the possibility to quickly adapt the actuation parameters to the varying flow conditions. For instance, the amplitude or the wave speed of a spanwise traveling surface wave can be changed in response to a changed Reynolds number. Coupled with a suitable sensor the control-loop can then be closed and the controller chooses the parameter settings that leads to the highest drag reduction. Therefore, we consider in this numerical study a closed-loop control of a spanwise traveling surface wave in a turbulent boundary layer flow with a Reynolds number of $Re_\theta = 2000$ and a Mach number of $Ma = 0.2$. It is shown that the controller, together with a wall-shear stress sensor, autonomously chooses the wave amplitude that gains the highest drag reduction. Detailed results of the investigation will be presented at the conference.

[1] Quadrio M. Drag reduction in turbulent boundary layers by in-plane wall motion. Philosophical Transactions of the Royal Society of London A: Mathematical, Physical and Engineering Sciences 2011;1940:1428–1442.

[2] Zhao H, Wu JZ, and Luo JS. Turbulent drag reduction by traveling wave of flexible wall. Fluid Dynamics Research 2004;34(3):175-198

[3] Koh SR, Meysonnat P, Statnikov V, Meinke M, Schröder W. Dependence of turbulent wall-shear stress on the amplitude of spanwise transversal surface waves. Computers & Fluids 2015;119:261–275.

[4] Bechert DW, Bruse M, Hage W, and Van der Hoeven JG Th, Hoppe G. Experiments on drag-reducing surfaces and their optimization with an adjustable geometry. Journal of fluid mechanics 1997;338:59–87.

Aerodynamic forcing and vortex evolution in large-disturbance flows

Anya Jones (*Aerospace Engineering, University of Maryland*) 08:50–09:10

Highly unsteady flows often result in large force transients due to flow separation and the formation of large-scale vortices. The growth and motion of these vortices can have a large impact on the resulting force transient and recovery. In the current work, we focus on wind gusts and wing maneuvers that result in changes to the relative flow that are of the same order of magnitude as the freestream flow. In these cases, flow separation is significant, so the classical linear solution for the flow does not apply. Separated shear layers tend to roll up into leading and trailing edge vortices that are shed into the wake. The formation and motion of these vortices are characterized in an attempt to better understand their contribution to aerodynamic forcing and their relative importance as compared to other sources of airloads (e.g., added mass and virtual camber). We also explore a physics-based low order model of highly separated flows, and gain insight as to where flow control might be used most effectively to mitigate force transients and/or hasten flow recovery.

Numerical Experiments on the Response of Separating Boundary Layer to Zero-Net Mass Flux Actuation

Wen Wu (*Mechanical Engineering, Johns Hopkins University*), Jung Hee Seo (*Johns Hopkins University*), Charles Meneveau (*Johns Hopkins University*), Louis Cattafesta (*Florida State University*), Rajat Mittal (*Johns Hopkins University*) 09:10–09:30

Zero-net mass flux (ZNMF) devices have been shown to be effective for control of flow separation. Despite significant work on this topic, many fundamental questions regarding the response of the separation bubble to ZNMF forcing have not been answered. In particular the effect of actuator frequency, duty cycle, amplitude as well as the actuator slot geometry are not well characterized and universal principles that could help predict the performance of these actuators are missing. To investigate how the ZNMF jet perturbations can change the characteristics and dynamics of flow separation, we employ high-fidelity numerical simulations of separating boundary layer with ZNMF actuators. A suction-blowing velocity profile is applied at the top boundary of the computational domain to produce an adverse- pressure gradient and create a closed separation bubble. The ZNMF jets are placed at the bottom boundary upstream of the separation region. Various jet configurations as well as frequencies and duty-cycles are employed to probe the underlying flow physics. The characteristics of the separation bubble response vary significantly for these case. The size of the separation bubble, embedded vortical structures, and physical mechanisms behind the observations are documented and discussed for both the transient as well as the statistical steady states. Implications of the results for new actuator design tools as well as effective modulation/forcing schemes are discussed.

S13.02 | Flow control

Date 21.03.2018
Room N1095

Turbulent jet under the manipulation of unsteady minijets

Yu Zhou (*Institute for Turbulence-Noise-Vibration Interactions and Control, Harbin Intitute of Technology, Shenzhen*) 14:00–14:40

A turbulent round jet is experimentally manipulatedusing1-6 unsteady radial minijetsinjected prior to the issue of main jet.The decay rate of the jet centerline mean velocity under manipulation may reach more than 11 times that in the natural jet and is found to depend strongly onthe minijet configuration,the ratio of the minijet excitation frequency to the main jet preferred-mode frequency,the mass flow rate ratio of each minijet to the main jet, and the nozzle diameter ratio of the minijet to the main jet.Four mechanisms behind the highly effective manipulation are identified from extensive flow visualization data captured in three orthogonal planes, along with the PIV data. One is the jet column flapping associated with asymmetric minijet injection, which increases dramatically the spread along the flapping direction. The second is identified for symmetric minijet injection, characterized by rapidly and sequentially 'tossed-out' mushroom-like structures along the mid plane between minijets.The third and fourth are the rotating and oscillating jet columns, respectively, about the jet axis.Conceptual models of the corresponding flow structures are proposed. An empirical scaling analysis isalso conducted, along with a discussion onthe Reynolds number effect on the jet control.

Closed-loop turbulence control: From human to machine learning (and retour)

Bernd R. Noack (*LIMSI-CNRS*), Guy Y. Cornejo Maceda (*LIMSI-CNRS*), Luc Pastur (*LIMSI-CNRS*), Francois Lusseyran (*LIMSI-CNRS*), Ruiying Li (*Institute PPRIME*), Laurent Cordier (*Institut PPRIME*), Jacques Borée (*ENSMA*), Fabien Harambat (*Centre Technique de Velizy, PSA Peugeot Citroën*), Dewei Fan (*Institute for Turbulence-Noise-Vibration Interactions and Control, Harbin Intitute of Technology*), Zhi Wu (*Institute for Turbulence-Noise-Vibration Interactions and Control, Harbin Intitute of Technology*), Yu Zhou (*Institute for Turbulence-Noise-Vibration Interactions and Control, Harbin Intitute of Technology*), Marek Morzynski (*Chair of Virtual Engineering, Poznan University of Technology*), Eurika Kaiser (*Department of Mechanical Engineering, University of Washington*), Steven L. Brunton (*Department of Mechanical Engineering, University of Washington*) 14:40–15:00

Closed-loop turbulence control is a rapidly evolving, interdisciplinary field of research. The range of current and future engineering applications has truly epic proportions, including cars, trains, airplanes, noise, air conditioning, medical applications, wind turbines, combustors, and energy systems. A key feature, opportunity and technical challenge of closed-loop turbulence control is the inherent nonlinearity of the actuation response. For instance, excitation at a given frequency will affect also other frequencies. This frequency crosstalk is not accessible in any linear control framework. This talk will address these nonlinear actuation mechanisms. First, success stories of 'human learning' in turbulence control are presented, i.e. cases in which the nonlinear actuation mechanism has been modelled and understood. A large class of literature studies can be categorized in terms of surprisingly few mechanisms. Second, we discuss model-free machine learning control (MLC) and selected applications. MLC detects and exploits the

winning actuation mechanisms in the experiment in an unsupervised manner. Recent examples include the stabilization of the fluidic pinball, drag reduction of a car model at high Reynolds numbers and mixing optimization of a turbulent jet. In all studies, MLC has reproduced or outperformed existing optimized control strategies, as will also be elaborated in other talks at this Minisymposium. Finally, future directions of turbulence control are outlined. Methods of machine learning are a disruptive technology will contribute to rapidly accelerating progress in turbulence control—both for actuation performance and for physical understanding.

Experimental control of a fluidic pinball using genetic programming

Robert Martinuzzi (*Mechanical and Manufacturing Engineering, University of Calgary*), Cedric Raidbaudo (*Mechanical and Manufacturing Engineering, University of Calgary*), Bernd R. Noack (*LIMSI-CNRS*) 15:00–15:20

The wake stabilization of a triangular cluster of three rotating cylinders was investigated in the present study. Experiments were performed at Reynolds number 6000, and compared with URANS-2D simulations at same flow conditions. 2D2C PIV measurements and constant temperature anemometry were used to characterize the flow without and with actuation. Open-loop actuation was first considered for the identification of particular control strategies. Machine learning control was also implemented for the experimental study. Linear genetic programming has been used for the optimization of open-loop parameters and closed-loop controllers. Considering a cost function based on the fluctuations of the velocity measured by the hot-wire sensor, significant performances were achieved using the machine learning approach.

About MIMO control efficiency for fluidic pinball using MLC

Francois Lusseyran (*Mechanics, LIMSI-CNRS*), Guy Cornejo Maceda (*Mechanics, LIMSI-CNRS*), Bernd R. Noack (*Mechanics, LIMSI-CNRS*) 15:20–15:40

We are looking for wake stabilization in a multi input multi output (MIMO) configuration. The wake results from an obstacle made by three cylinders in an incoming flow. The means of action are the cylinders rotation and the output is the velocity taken downstream. Previous studies have shown that high and low frequency forcing stabilize the wake, revealing the nonlinear interactions. Linear control being not applicable in our case we are looking for an optimal control law regarding drag reduction using genetic programming, a model free MLC approach. Genetic programming can explore a broad spectrum of laws, exploiting the nonlinearities, ranging from open loop control to closed loop control.

Reduced-order modeling of the "fluidic pinball"

Nan Deng (*LIMSI-CNRS*), Luc Pastur (*Fluid Dynamics, IMSIA*), Marek Morzynski (*Institute of Combustion Engines and Basics of Machine Design, Poznan University of Technology*), Bernd R. Noack (*LIMSI-CNRS*) 15:40–16:00

The *fluidic pinball* is a geometrically simple configuration with three rotating cylinders on the vertex of an equilateral triangle. Yet, it remains physically rich enough to host a range of interacting frequencies and to allow testing of control laws within minutes on a laptop. The system has multiple inputs (the three cylinders can independently rotate around their axis) and multiple outputs (downstream velocity sensors). Investigating the natural flow dynamics, we found that the first unsteady transition undergone by the wake flow, when increasing the Reynolds number, is a Hopf bifurcation leading to the usual time-periodic vortex shedding phenomenon, typical of cylinder wake flows, in which the mean flow field preserves axial symmetry. The second bifurcation breaks the symmetry of the mean flow field, and results from a secondary pitchfork bifurcation.

In this work, we propose reduced-order models (ROMs) for both bifurcations. We have extracted dynamically consistent modes from the flow data in order to built our ROMs. The main dynamical features of the primary Hopf bifurcation can be described by three degrees of freedom. For the secondary bifurcation, at least five degrees of freedom are expected to be required in order to model the flow dynamics. Beyond their ability to identify the main physical features of the flow dynamics, ROMs also provide a simplified (and therefore faster) framework to train machine learning (flow) control.

S13.03 | Flow control

Date 21.03.2018
Room N1095

Data-driven discovery of Koopman eigenfunctions for control

Eurika Kaiser (*Mechanical Engineering, University of Washington*), Nathan Kutz (*University of Washington*), Steven L. Brunton (*University of Washington*) 16:30–17:10

Koopman operator theory has emerged as a principled framework to obtain linear embeddings of nonlinear dynamics, enabling the estimation, prediction and control of strongly nonlinear systems using standard linear techniques. Here, we present a data-driven control architecture that utilizes Koopman eigenfunctions to manipulate nonlinear systems using linear control theory. We approximate these eigenfunctions with data-driven regression and power series expansions, based on the partial differential equation governing the infinitesimal generator of the Koopman operator. In particular, we show that lightly damped eigenfunctions may be faithfully extracted using sparse regression. These lightly damped eigenfunctions are particularly relevant for control, as they correspond to nearly conserved quantities that are associated with persistent dynamics, such as the Hamiltonian. We formulate the control problem in these intrinsic eigenfunction coordinates and design nonlinear controllers using standard linear optimal control theory. The architecture is demonstrated on a variety of Hamiltonian systems and the double-gyre model for ocean mixing.

Sparse sensor placement in dynamical systems

Steven L. Brunton (*Mechanical Engineering, University of Washington*), Krithika Manohar (*Applied Mathematics, University of Washington*), Eurika Kaiser (*Mechanical Engineering, University of Washington*), Nathan Kutz (*Applied Mathematics, University of Washington*), Steven L. Brunton (*Biology, University of Washington*) 17:10–17:30

Understanding and controlling complex fluid flows is of central importance to a vast array of engineering and scientific applications, including drag reduction for fuel efficient transportation, lift increase for advanced aircraft and energy systems, and mixing enhancement for clean combustion and chemical synthesis. Put simply, flow control will be a critical enabler to address technological challenges in energy, defense, transportation, and many other endeavors. Sensors and actuators are the workhorses of active flow control.
Optimal sensor and actuator placement is one of the most challenging unsolved problems in flow control. Many competing factors impact control design, and a chief considerations is the latency, with larger latency imposing limitations on robust performance. As flow speeds increase and flow structures become more complex, it is increasingly important to make fast control decisions based on efficient low-order models, with sensors and actuators placed strategically

to gather information and exploit flow sensitivities. Nearly every downstream control decision is affected by these sensor/actuator locations, although determining optimal locations amounts to an intractable brute force search among the combinatorial possibilities. This optimization is computationally intractable for even moderately large problems. Therefore, the placement of sensors and actuators are typically chosen according to heuristics and intuition. The objective of this work is the leverage recent advances in machine learning and sparse optimization to design optimal sensor and actuator locations for closed-loop flow control in a framework that scales to arbitrarily large problems. Several approaches will be presented, based on matrix factorizations and sparse optimization.

Zonal Galerkin-free POD model for incompressible flows

Angelo Iollo (*Université de Bordeaux et Inria Bordeaux Sud - Ouest*) 17:30–17:50

Model-based flow control/optimization needs a fast and accurate representation of the input/output map between the parameter space and the flow response.The main steps to build such reduced model are i) sampling of the full model in parameter space; ii) definition of the reduced approximation space; iii) definition of the reduced model. In this talk we detail how these three steps are combined to obtain a domain decomposition method which couples a high and a low-fidelity model. This approach requires to solve the high-fidelity model in a small portion of the computational domain while the external field is described by a Galerkin-free Proper Orthogonal Decomposition (POD) model. We propose an error indicator to determine the extent of the interior domain and to perform an optimal coupling between the two models. This zonal approach can be used to study multi-body configurations or to perform detailed local analyses in the framework of control/shape optimization problems.

On the shape of resolvent modes in wall-bounded turbulence

Scott Dawson (*Graduate Aerospace Laboratories, California Institute of Technology*), Beverley McKeon (*Graduate Aerospace Laboratories, California Institute of Technology*) 17:50–18:10

A promising approach for reduced-order modeling and control of wall-bounded turbulence utilizes low-rank approximations of the resolvent operator corresponding to the Reynolds-decomposed Navier-Stokes equations. This work seeks to characterize and explain the shape of optimal response modes (i.e., singular vectors) of this resolvent operator. We show that the shape of wall-detached modes can be explained through consideration of the pseudospectra of Airy-type operators, which approximate the full dynamics within this regime. In particular, this characterization explains the approximately Gaussian envelope and linear variation in phase that are typical of such modes. Using this insight, we present several methods to approximate both the shape and amplification (i.e., corresponding singular values) of resolvent modes across a range of spatial wavenumbers and temporal frequencies. This approach allows for rapid estimation of dominant resolvent mode characteristics without the need for large numerical computations. We will discuss the implications of these findings for a number of possible applications, including real-time estimation and control.
This work is supported by AFOSR grant FA9550-16-1-0232.

Model reduction for transport dominated reactive flows

Julius Reiss (*TU Berlin*) 18:10–18:30

Mode-based model-reduction is effective when the system dynamics can be described by a small number of spatial modes. For transport dominated phenomena often a large number of modes is needed to reproduce the full solution.
Here, an approach is discussed, which decomposes a flow field into several co-moving frames, where each can be approximated by a low-rank field. The method of decomposition is formulated as an optimization problem.
This allows to include boundary condition in a simple manner. We apply the method to the description of a pulse detonation combustion chamber, where the description is obtained from experimental data by a data assimilation technique.

S13.04 | Flow control

Date 22.03.2018
Room N1095

Nonlinear Feedback Design for the Stabilization of Incompressible Flows via Updated Riccati-based Gains

Peter Benner (*Max-Planck-Institut für Dynamik komplexer technischer Systeme Magdeburg*), Jan Heiland (*Max-Planck-Institut für Dynamik komplexer technischer Systeme Magdeburg*) 08:30–08:50

The feedback stabilization of incompressible laminar flows has been under vivid investigation since long. Among the many different approaches, Riccati-based controllers have been proven successful in the cancellation and suppression of instabilities both in theory and in numerical experiments. However, like all linearization-based approaches, these controllers suffer from the conceptual shortcoming of a possibly small domain of attraction meaning that the unwanted dynamics must be small for the controller to work. To really steer a system from a developed unsteady state into a steady working point, nonlinear control laws are needed.
In this talk, we propose a scheme that continuously updates an initial feedback [1] and how it extends to models of incompressible flows [2]. This approach comes with theoretical and locally checkable sufficient conditions that guarantee the decay of the controlled state towards the working point. We discuss the numerical realization of this update scheme and illustrate its performance in the cancellation of vortex shedding in the flow past a cylinder.

[1]: PB & JH: *Exponential Stability and Stabilization of Extended Linearizations via Continuous Updates of Riccati Based Feedback*, Internat. J. Robust Nonlinear Control, 2017.

[2]: PB & JH: *Nonlinear Stabilizing Feedback Design for Incompressible Flows via Updated Riccati-Based Gains*, Proceedings of the IEEE Conference on Decision and Control, 2017.

Control of nonsmooth Cahn-Hilliard/Navier-Stokes systems

Michael Hinze (*Mathematik, Universität Hamburg*), Harald Garcke (*Universität Regensburg*), Christian Kahle (*Technische Universität München*) 08:50–09:10

We consider the optimal control of a two-phase fluid that is described by the thermodynamically consistent diffuse interface model proposed in 2012 by Abels/Garcke/Grün [1]. As key ingredient

we present an energy stable simulation scheme proposed by the authors in 2016 [2]. It allows us to simulate two-phase fluids in an energy stable way and provides enough regularity to apply classic theory from optimal control [3]. We prove existence of solutions to a semi-discrete in time optimal control problem, and present a convergence analysis for its finite element discretization. We illustrate the performance of our approach with some numerical examples.

This is joint work with Harald Garcke, Universität Regensburg, Germany, and Christian Kahle, Technische Universität München, Germany.

[1] H. Abels, H. Garcke, and G. Grün. Thermodynamically consistent, frame indifferent diffuse interface models for incompressible two-phase flows with different densities. Mathematical Models and Methods in Applied Sciences, 22(3):40 (2012).

[2] H. Garcke, M. Hinze, C. Kahle: A stable and linear time discretization for a thermodynamically consistent model for two-phase incompressible flow. Applied Numerical Mathematics 99:151-171 (2016). arXiv:1612.02283 (2016).

[3] H. Garcke, M. Hinze, C. Kahle: Optimal Control of time-discrete two-phase flow driven by a diffuse-interface model. arXiv:1612.02283 (2016).

Nonlinear Model Predictive Control of an Innovative Gasoline Engine

Thivaharan Albin (*Mechanical Engineering, Institute for Dynamic Systems and Control, ETH Zurich*)
 09:10–09:30

Reduction of CO2 emissions is a major goal of recent development of automotive propulsion systems. For this purpose, combustion engines with innovative combustion modes, such as Gasoline Controlled Auto Ignition (GCAI), are investigated currently. Compared to conventional gasoline engines, GCAI allows lowering CO2 emissions by up to 30 % in part load operation. However, for practical application of GCAI several challenges have to be tackled such as the process control. The GCAI process is nonlinear, instable and highly sensitive to disturbances such as temperature conditions. Additionally several manipulated variables have to be handled simultaneously for appropriate control.
The talk focuses on the control of the so-called late phasing combustion, a challenging GCAI process characteristic. Late phasing combustion arises for certain operating conditions and leads to a bifurcative cycle-to-cycle behavior. This behavior comprises a characteristic limit cycle for certain output values such as the center of combustion. Viable process control has to be capable of attenuating this dynamic behavior. The talk presents the investigation of an optimization based control strategy. Basis of the developed control algorithm is a physically motivated mathematical model. The derived state-space model consists of a set of Differential-Algebraic-Equations with three system states. As control algorithm, Nonlinear Model Predictive Control with Real-Time Iterations Scheme is applied. To yield a suitable nonlinear program, the optimization problem is discretized using a Multiple Shooting scheme. The implemented controller shows the capability of stabilizing the process and suitable reference tracking.

Optimal open-loop control of a periodic flow: application to the bifurcating jet

Léopold Shaabani Ardali (*LadHyX, Ecole polytechnique-CNRS & DAAA, ONERA, Université Paris-Saclay*), Lutz Lesshafft (*LadHyX, Ecole polytechnique-CNRS*), Denis Sipp (*DAAA, ONERA, Université Paris-Saclay*)
 09:30–09:50

Experiments and numerical simulations have shown that a round jet, excited with a forcing combining both axisymmetric and helical components, undergoes a global *bifurcation* which significantly increases the jet spreading and its mixing properties. Axisymmetric forcing alone, at frequency f_a, leads to the formation of vortex rings, that may undergo subsequent pairing. When an additional helical forcing at frequency f_h is superposed, these vortex rings are eccentrically displaced. The mutual interaction causes the vortices to further depart from the jet axis in opposite directions, which leads to a spectacular flaring of the flow, and to a large enhancement of its mixing with the outer flow when turbulence develops. The final flow behaviour depends on the ratio $r_f = f_a/f_h$. If $r_f = 2$, vortices move to opposite sides of the jet axis in an alternating fashion, leading to a jet with huge spreading in this direction. This case is called a bifurcating jet.
In our study, a time-periodic axisymmetric state is computed first, with the aid of a stabilisation routine that inhibits pairing. We then identify the linear optimal inlet forcing that triggers the bifurcation of vortices. The resulting optimal conditions are then imposed in non-linear simulations and the results are compared with traditional bifurcating jet forcings. Using an optimal control increases the band of Strouhal where the bifurcation phenomenon can be encountered.

A multi-scale tool for flow control via surface manipulation

Giuseppe Antonio Zampogna (*IMFT*), Jacques Magnaudet (*CNRS - IMFT*), Alessandro Bottaro (*Università degli Studi di Genova*) 09:50–10:10

It is well-known in the literature that certain types of rough walls are able to modify the characteristics of a fluid flowing above them, possibly reducing turbulent drag [1]. A reduced model to simulate fluids interacting with macroscopic bodies equipped with a surface rough layer has been developed. This model applies a double-sided procedure: in the first instance, microscopic problems must be solved in a representative elementary domain. This reduced domain is geometrically determined by identifying a periodic sample structure in the rough layer. The solutions of these problems are the surface permeability tensor, K_{ij}, and the slip tensor, L_{ijk}, and represent the microscopic behaviour of the fluid. A macroscopic boundary condition in the second instance is applied over a fictitious, smooth surface to simulate the fluid flowing above it. This boundary condition includes the macroscopic counterpart of K_{ij} and L_{ijk}, calculated with the introduction of an averaging operator. The present multi-scale approach allows to associate the microscopic characteristics of the surface to the macroscopic behaviour of the fluid in order to potentially understand how, where and when the microscopic geometry must be modified to, for example, yield drag reduction or delay turbulent transition. After a validation of the condition, a sample configuration is considered, to understand how the variation of the fundamental geometrical parameters which characterise the roughness, influences the macroscopic flow. One of the strengths of the model is its computational cost, if compared with that of a DNS which accounts for all surface features; this renders it a tool to furnish real time responses in real flow control applications.

[1] L. Sirovich and S. Karlsson (1997) Turbulent drag reduction by passive mechanisms. Nature, vol. 388, pp. 753-755

Numerical Study of Long Separation Bubble on Slotted Thick Airfoil

Mdouki Ramzi (*Mechanical engineering, University of Tebessa*) 10:10–10:30

Low Reynolds number flows over airfoils are generally accompanied with the transitional boundary layer and laminar separation bubble. The formation of laminar separation bubble for both types long bubble LoSB and short bubble ShSB contributes negatively on aerodynamic performances of airfoil. This work is aimed to testify the potential of double slot to control the LoSBs

developed on the suction side of the thick symmetric NACA0021 airfoil. Two dimensional simulations are carried out under steady state and incompressible regime with the correlation-based intermittency turbulent model γ-ReΘ in order to predict the boundary layer transition aspect. With clean airfoil, tests are performed for Reynolds number of 1.2 105 and freestream turbulent intensity of 7.5

S13.05 | Flow control

Date 22.03.2018
Room N1095

Force production from vortex shedding characterized by FTLE

Melissa Green (*Mechanical and Aerospace Engineering, Syracuse University*) 14:00–14:20

We study the formation and shedding of vortices in three vortex-dominated flows in order to detect the formation of coherent structures objectively (i.e., in a frame invariant fashion), and to determine how the formation and shedding of those structures relates to pressure and forces in the different applications. We specifically employ the Lagrangian technique of the finite-time Lyapunov exponent (FTLE). The FTLE analysis yields ridges of Lagrangian repulsion and attraction that have been shown to identify transport barriers in a range of flow fields, and vortex boundary features in vortex-dominated flows. In recent work, we have shown that using FTLE to identify and track material trajectories associated with forming and shedding vortices can indicate a shedding time that correlates well to surface pressure and body force extrema on a stationary circular cylinder in cross-flow and dynamic stall on a 2D flat plate undergoing a pitch-up maneuver. In bio-inspired flow, specifically the wake structure generated by a pitching caudal fin model, the release of material trajectories from the trailing edge also correlates well with thrust extrema. These results prompt us to question whether robust control of performance metrics (force, efficiency) may be accessible by exploiting the evolving flow structure available from the FTLE results. More simply, can we be more successful at flow control by targeting FTLE ridges?

Turbulent flows over superhydrophobic surfaces and LIS

Edoardo Alinovi (*DICCA, Scuola Politecnica, University of Genova*), Alessandro Bottaro (*DICCA, Scuola Politecnica, University of Genova*) 14:20–14:40

Superhydrophobic (SH) and liquid-impregnated surfaces (LIS) represent an interesting technique for the possible reduction of drag in applications involving the flow of liquids over solid surfaces, for a wide range of Reynolds number, from laminar to turbulent conditions [1]. Such coatings work by the interposition of a gas/oil layer between the liquid and the solid wall, trapped by distributed microscopic roughness elements present at the wall; over the gas layer the liquid can flow with negligible friction. The present activity is focused on the numerical modeling of the slippage over such coatings and on their drag reduction performance in the turbulent regime. The problem is subdivided into two parts: a microscopic problem, accounting for the flow in the proximity of the roughness elements and a macroscopic problem, accounting for the turbulent flow over SHs/LIS, where the effect of the slippage at the wall is modeled through a proper boundary condition. The near-wall, microscopic problem, governed by the Stokes equation [2], is recast into an integral form and then solved using a boundary element method. The aim of the microscopic calculations, performed by varying the viscosity ratio between the fluids, is to obtain the values of the slip lengths, used to quantify slippage. The slip length are then used in the definition of Navier boundary condition, applied at the walls of a turbulent channel flow at

moderate Reynolds number, solved by direct numerical simulations. The results are in excellent agreement with a theoretical model available in the literature [3].

[1] Bottaro, A. 2014 Superhydrophobic surfaces for drag reduction, Rendiconti Classe di Scienze Matematiche e Naturali, 148, 239-268.

[2] Luchini, P., Manzo, F., Pozzi, A. 1991 Resistance of a grooved surface to parallel flow and cross-flow. J. Fluid Mech. 228, 87-109.

[3] Luchini, P. 1996 Reducing the turbulent skin friction. In: Dèsidèri et al. (eds) Computational Methods in Applied Sciences '96. J. Wiley & Sons, Chichester, England, 466-470.

Magnetically induced movement of NdFeB particles in magnetorheological elastomers

Malte Schümann (*Chair of Magnetofluiddynamics, Measuring and Automation Technology, TU Dresden*), Stefan Odenbach (*Chair of Magnetofluiddynamics, Measuring and Automation Technology, TU Dresden*) 14:40–15:00

A key to gain a deeper understanding of magnetorheological elastomers is the analysis of the internal particle structure which determines the macroscopic material behavior to a great extent. For this study a soft magnetorheological elastomer with 40 wt% of highly anisotropically shaped NdFeB particles was synthesized. The internal particle structure and the magnetically induced mo-tion of the particles was evaluated by means of X-ray microtomography. The sample was gradually magnetized up to an external field of 2 T. This leads to a transition from the initial isotropic and homogeneous particle distribution to fully formed particle chains. At each point of magnetization the application of a 240 mT field during tomography results in a distinct rotation of the individual particles. This is a result of the tendency of the particles to align their magnetically strong axis to the direction of the magnetic field.
The results show a reversible material behavior at low magnetizations. At higher magnetization the increasing remanent magnetization of the particles leads to a non-reversible chain formation. A particle tracking was performed to evaluate the chain formation process and the translation of the particles in detail.
An accompanying mechanical characterization shows a significant magnetorheological effect, an increase of the Young's modulus, in presence of a 240 mT magnetic field. This fully reversible effect increases with progressing magnetization and chain formation.

The effect of magnetic field advection on turbulent magnetohydrodynamic flow in a square duct

Vinodh Bandaru (*Max-Planck-Institut für Plasmaphysik*), Thomas Boeck (*Mechanical Engineering, TU Ilmenau*), Jörg Schumacher (*Mechanical Engineering, TU Ilmenau*) 15:00–15:20

We report three-dimensional simulations of pressure-driven Shercliff flow in a square duct with insulating walls in a homogeneous external field that is parallel to one set of the walls. The complete induction equation for the magnetic field is solved consistently by coupling the interior of the duct with the external magnetic field through a boundary-element procedure. The relative importance of advection to diffusion of the magnetic field is characterized by the magnetic Reynolds number Rm. For comparison, we solve the flow problem also in the quasistatic limit Rm=0, where the induced magnetic field is a linear functional of the velocity field. We find that the Hartmann- and Shercliff layers on the walls perpendicular and parallel to the magnetic field

are affected differently by a finite value of Rm. Large-scale properties are not drastically different between cases of zero and finite Rm but the small-scale anisotropy increases.

Influence of the temperature gradient of the syntheses of monodisperse magnetic nanoparticles by thermal decomposition on the magnetically active particle volume

Erik Siebert (*Chair of Magnetofluiddynamics, Measurement- and Automation Technology, TU Dresden*), Stefan Odenbach (*Chair of Magnetofluiddynamics, Measurement- and Automation Technology, TU Dresden*) 15:20–15:40

The synthesis of monodisperse magnetic nanoparticles is of key-importance for un-derstanding the interaction processes between different fractions of nanoparticles, by varying their size ratios and volume por-tions. It has been observed that the magnetically active particle volume can strongly differ from the hydrodynamic size of the particles and thus, leading to strongly decreased interactions among them. This could be examined by the decrease of the magnetoviscous effects in ferrofluids accordingly. In contribution to the conference it will be shown how the temperature gradient of the synthesis of monodisperse magnetic nanoparticles has an influence on the magnetically active particle volume.
Iron oxide nanocrystals has been obtained by a thermal decomposition reaction using the reaction pattern for 12 nm particles by Park et al..
The controlling parameters of a temperature controller have been optimized so that the temperature gradient can be hold constant over the whole reaction process. Hence, while the heating-up process for the first reaction has just been executed by full power heating until reaching the boiling point of the solution at approximately 320°C the second process has been set to a constant temperature gradient of 3.3°C/min.
The obtained results lead to the assumption that the high temperature gradient of the uncontrolled heating up process is leading to a smaller magnetically active particle volume, while the constant slow heating is providing the possibility for the particles to grow magnetically "healthy".

New Strategies and Insights for Transient Growth Suppression using Dynamic Mode Shaping Control

Maziar Hemati (*Aerospace Engineering and Mechanics, University of Minnesota*), Huaijin Yao (*Aerospace Engineering and Mechanics, University of Minnesota*) 15:40–16:00

Sub-critical transition to turbulence is often attributed to the growth in transient energy of perturbations resulting from the high-degree of non-normality exhibited by the linearized Navier-Stokes operator. In this talk, we introduce a dynamic mode shaping approach for delaying transition to turbulence by aiming to reduce non-normality via feedback control. Dynamic mode shaping control allows for spectral specification of the closed-loop system, which provides several new strategies for transient growth reduction. We also present extensions of the dynamic mode shaping approach to address various practical challenges of fluid flow control, including high dimensionality, nonlinearity, and robustness to uncertainties. Lastly, these new controller synthesis approaches reveal fundamental performance limitations of more commonly invoked observer-based feedback strategies—e.g., linear quadratic Gaussian (LQR) control—in the context of transient growth suppression and transition delay. These various techniques and results are demonstrated on a set of illustrative examples.

S14 | Applied analysis

Organiser Marco Cicalese (*M7, Technische Universität München*)
Daniel Matthes (*Mathematics, Technische Universität München*)

S14.01 | Applied analysis

Date 20.03.2018
Room 1260

EDP-convergence: Gamma-convergence for gradient systems in the sense of the energy-dissipation principle

Alexander Mielke (*Weierstrass Institute for Applied Analysis and Stochastics*) 08:30–09:10

We study the general question of convergence for a family of gradient systems $(Q, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon)$ with a small parameter $\varepsilon > 0$. Because the evolution of gradient systems is driven by an energy functional $\mathcal{E}_\varepsilon$ and a dissipation potential $\mathcal{R}_\varepsilon$ the Γ-convergence of these to functionals seems to be natural at first sight. However, for some situations the nature of the dissipation can change dramatically, so the question is whether there is a method to derive the limiting gradient structure of a family of gradient systems, where in general the effective dissipation $\mathcal{R}_{\text{eff}}$ is not the limit of the dissipations $\mathcal{R}_\varepsilon$.
The theory was started by the fundamental work of Sandier-Serfaty in 2004, where the De Giorgi's energy-dissipation principle (EDP) was exploited for gradient systems with quadratic dissipation potentials. The EDP formulation features a dissipation functional over the relevant time interval

$$\mathfrak{D}_\varepsilon(u) = \int_0^T \Big(\mathcal{R}_\varepsilon(u(t), \dot{u}(t)) + \mathcal{R}_\varepsilon^*\big(u(t), -\mathrm{D}\mathcal{E}_\varepsilon(t, u(t))\big) \Big) \mathrm{d}t$$

that contains the interaction of the dissipation and the energy landscape. The point is now to understand the Γ-limit of $\mathfrak{D}_\varepsilon$ on curves $u : [0, T] \to Q$.
We report on recent progress that highlights the appearance of nonquadratic dissipation potentials as limit of quadratic ones. The theory will be explained along with applications in Fokker-Planck equations as well as for a scalar wiggly-energy problem.
This work is partly joint research with P. Dondl, Th. Frenzel, M. Liero, M. Peletier, and M. Renger. (M. Liero, A. Mielke, M. Peletier, D.R.M. Renger. On microscopic origins of generalized gradient structures. Discrete Contin. Dyn. Syst. S 10, 1-35, 2017)

Reverse approximation of gradient flows as Minimizing Movements: a conjecture by De Giorgi

Florentine Fleißner (*Mathematics, Technische Universität München*), Giuseppe Savaré (*Università di Pavia*) 09:10–09:30

We consider the Cauchy problem for the gradient flow

$$u'(t) = -\nabla\phi(u(t)), \quad t \geq 0; \quad u(0) = u_0, \tag{$\star$}$$

generated by a continuously differentiable function $\phi : \mathbb{H} \to \mathbb{R}$ in a Hilbert space $\mathbb{H}$ and study the reverse approximation of solutions to $(\star)$ by the De Giorgi Minimizing Movement approach. We prove that if $\mathbb{H}$ has finite dimension and ϕ is quadratically bounded from below (in particular if ϕ is Lipschitz) then for every solution u to $(\star)$ (which may have an infinite number of solutions)

there exist perturbations $\phi_\tau : \mathbb{H} \to \mathbb{R}$ ($\tau > 0$) converging to ϕ in the Lipschitz norm such that u can be approximated by the Minimizing Movement scheme generated by the recursive minimization of $\Phi(\tau, U, V) := \frac{1}{2\tau}|V - U|^2 + \phi_\tau(V)$:

$$U_\tau^n \in \operatorname{argmin}_{V \in \mathbb{H}} \Phi(\tau, U_\tau^{n-1}, V) \quad n \in \mathbb{N}, \quad U_\tau^0 := u_0. \tag{$\star\star$}$$

We show that the piecewise constant interpolations with time step $\tau > 0$ of all possible selections of solutions $(U_\tau^n)_{n\in\mathbb{N}}$ to ($\star\star$) will converge to u as $\tau \downarrow 0$. This result solves a question raised by Ennio De Giorgi.
We also show that even if $\mathbb{H}$ has infinite dimension the above approximation holds for the distinguished class of minimal solutions to ($\star$), that generate all the other solutions to ($\star$) by time reparametrization.
(arXiv 1711.07256)

A stabilized Weighted-Inertia-Dissipation-Energy approach to the incompressible Navier-Stokes system

Bernd Schmidt (*Institut f. Mathematik, Universität Augsburg*) 09:30–09:50

We present a variational resolution of the incompressible Navier-Stokes system by means of stabilized Weighted-Inertia-Dissipation-Energy (WIDE) functionals. The minimization of these parameter-dependent functionals corresponds to an elliptic-in-time regularization of the system. By passing to the limit in the regularization parameter along subsequences of WIDE minimizers one recovers a classical Leray-Hopf weak solution. (Joint work with M. Ortiz (Bonn / Pasadena) and U. Stefanelli (Vienna).)

Construction of Gradient Flows in Abstract Metric Spaces via BDF2

Simon Plazotta (*Zentrum Mathematik / M8, Technische Universität München*), Daniel Matthes (*Zentrum Mathematik / M8, Technische Universität München*) 09:50–10:10

In this talk I will discuss the construction of λ-contractive gradient flows in abstract metric spaces by means of a semi discretization of second order in time. In the smooth setting, our scheme is simply a variational formulation of the BDF2 method; in the metric setting, it can be considered as the natural second order analogue of the Minimizing Movement or JKO scheme. In difference to the JKO method, our scheme does not necessarily decrease the energy of the discrete solution in each time step, but we can still prove a suitable *almost diminishing* property.

It is well-know that in smooth situations, the BDF2 method converges to order τ^2. We prove that our variational scheme converges at least to order $\tau^{1/2}$ in the general non-smooth setting, provided a certain convexity hypothesis is satisfied. Specifically, that hypothesis is equivalent to λ-uniform convexity in the flat case, and is implied by λ-convexity along generalized geodesics in the L^2-Wasserstein case. The key element in the convergence proof is the derivation of step-size independent bounds on potential and kinetic energy of the discrete solution. The combination of the local bounds and a discrete Gronwall type argument into a global error estimate is significantly harder than for the Minimizing Movement scheme.

A Reshetnyak-type lower semicontinuity result for linearised elasto-plasticity coupled with damage

Gianluca Orlando (*Mathematics, TUM Technische Universität München*), Vito Crismale (*Ecole Polytechnique*) 10:10–10:30

In this talk I will present a lower semicontinuity result of Reshetnyak type for a class of functionals which appear in models for small-strain elasto-plasticity coupled with damage. The proof of the result is based on a precise characterisation of the limit of measures $\alpha_k \, \mathrm{E}u_k$ with respect to the weak convergence $\alpha_k \rightharpoonup \alpha$ in $W^{1,n}(\Omega)$ and the weak* convergence $u_k \overset{*}{\rightharpoonup} u$ in $BD(\Omega)$, E denoting the symmetrised gradient. A concentration compactness argument shows that the limit has the form $\alpha \, \mathrm{E}u + \eta$, with η supported on an at most countable set.

S14.02 | Applied analysis

Date 20.03.2018
Room 1260

A corrected Sadowsky functional for inextensible elastic ribbons

Peter Hornung (*TU Dresden*) 16:30–16:50

In the 1930's Sadowsky showed the existence of a developable Moebius strip. He proposed that the configuration assumed by such a strip can be computed by minimizing the bending energy. He further argued that the bending energy density is proportional to the square of the mean curvature of the surface, i.e., its Willmore energy density.
Wunderlich later formally justified the energy functional proposed by Sadowsky. His analysis showed that the Sadowsky functional can be recovered under an assumption of non vanishing curvature of the centerline of the strip.
We re-examine, by means of Gamma convergence, the derivation of the limit energy of such an inextensible, isotropic, elastic strip as the strip width goes to zero. Our analysis makes no a priori assumptions on the curvature of the centerline. The functional obtained in this rigorous way agrees with the classical Sadowsky functional, provided that the curvature of the centerline of the strip is large enough.
This is joint work with L. Freddi, M.G. Mora and R. Paroni.

Hyperelastic bodies under homogeneous Cauchy stress induced by non-homogeneous finite deformations

Patrizio Neff (*Mathematik / Nonlinear Analysis, Universität Duisburg-Essen*), Angela Mihai (*Cardiff University*), Eva Schweickert (*Universität Duisburg-Essen*) 16:50–17:10

We discuss whether homogeneous Cauchy stress implies homogeneous strain in isotropic nonlinear elasticity. While for linear elasticity the positive answer is clear, we exhibit, through detailed calculations, an example with inhomogeneous continuous deformation but constant Cauchy stress. The example is derived from a non rank-one convex elastic energy.

Analytical validation of the Young-Dupré law for epitaxially-strained thin films

Elisa Davoli (*Faculty of Mathematics, Universität Wien*), Paolo Piovano (*Faculty of Mathematics, Universität Wien*) 17:10–17:30

A variational model for epitaxially-strained thin films on substrates is derived both by Γ-convergence from a transition-layer setting, and by relaxation of a sharp-interface description. The model is characterized by a configurational energy that accounts for possibly different elastic properties for the film and the substrate, as well as for the surface tensions of all three involved interfaces: film/gas, substrate/gas, and film/substrate. Minimal configurations of this energy are then shown to exist and their regularity and geometrical properties are studied. The Young-Dupré law is shown to be satisfied by the angle that energetically-optimal profiles form at contact points with the substrate.

Calibrations for minimal networks in a covering space setting

Marcello Carioni (*Mathematik, Karl-Franzens-Universität Graz*), Alessandra Pluda (*Mathematik, Universität Regensburg*) 17:30–17:50

We define calibrations for the Steiner problem within the framework of covering space and we give some examples. Then we introduce the notion of calibration in families: we divide the set of competitors in suitable classes, where we define an appropriate (and weaker) notion of calibration. Calibrating the candidate minimizers in each family and comparing their energy, one finds the global minimizers of the problem. Thanks to this procedure we prove the minimality of the Steiner configurations spanning the vertices of a regular pentagon and hexagon.

Exact periodic stripes for minimizers of a local/non-local interaction functional in general dimension

Eris Runa (*Mathematics, Max Planck Institute for Mathematics*), Sara Daneri (*Mathematics, FAU Erlangen-Nürnberg*) 17:50–18:10

In this talk we will consider a functional consisting of a perimeter term and a non-local term which are in competition. In the discrete setting such functional was introduced by Giuliani, Lebowitz, Lieb and Seiringer. We show that the minimizers of such functional are optimal periodic stripes for both the discrete and continuous setting. In the discrete setting, such behaviour has been shown by Giuliani and Seiringer using different techniques for a smaller range of exponents. One striking feature of the functionals is that the minimizers are invariant under a smaller group of symmetries than the functional itself. In the continuous setting, to our knowledge this is the first example of a model with local/nonlocal terms in competition such that the functional is invariant under permutation of coordinates and the minimizers display a pattern formation which is one dimensional. This model has many similarities with the celebrated Ohta-Kawasaki functional. In particular for Ohta-Kawasaki functional, the minimality of periodic stripes is conjectured. This work is in collaboration with Sara Daneri.

Regularisation and Γ-convergence for a non-convex model of single-crystal elasto-plasticity with infinite cross-hardening

Keith Anguige (*Angewandte Mathematik, Albert-Ludwigs-Universität Freiburg*) 18:10–18:30

I will consider the numerical implementation of a non-convex model of single-crystal elasto-plasticity, where the non-convexity arises through the imposition of a hard 'single-plane' side condition on the plastic deformation. This well-posed variational model arises as the relaxation of a more fundamental 'single-slip' model in which at most one slip system can be activated at each spatial point. The relaxation procedure is motivated by the desire for efficient, oscillation-free simulation of single-crystal plasticity, but it is not immediately obvious how to implement the hard side-condition (that at most one slip-plane may be activated at each point) numerically. Our approach to this problem is to regularise the side-condition by introducing a large, but finite, integral cross-hardening penalty into the plastic energy, such that the cross-hardening matrix has a factor of $\frac{1}{\epsilon}$ on the front. The regularised model is then amenable to implementation with standard finite-element methods, and, with the aid of div-curl arguments, one can show that it Γ-converges to the single-plane model as $\epsilon \to 0$.

S14.03 | Applied analysis

Date 21.03.2018
Room 1260

Dispersive effective equations for lattice dynamics

Ben Schweizer (*Fakultät für Mathematik, TU Dortmund*) 08:30–08:50

Dispersion occurs in media in which waves with different wave-length travel with different speed. A linear wave equation with constant coefficients does not show dispersion. A linear wave equation with periodic coefficients and a small periodicity can be replaced, in the homogenization limit, by a linear wave equation with constant coefficients, we hence do not expect dispersive effects. On the other hand, numerical experiments show that solutions have a dispersive behavior, at least after long time. We discuss this effect and derive dispersive effective equations. We furthermore investigate the wave equation in a discrete spring-mass model. The discrete character of the model introduces small-scale oscillations, which result in a dispersive long time behavior. We derive the dispersive effective wave equations for the discrete model.
We present joint work, obtained with A. Lamacz, T. Dohnal, and F. Theil.

Coexistence of Hamiltonian-like and dissipative dynamics in chains of coupled oscillators with skew-symmetric coupling

Serhiy Yanchuk (*Technische Universität Berlin*), Oleksandr Burylko (*Institute of Mathematics, National Academy of Sciences of Ukraine*), Alexander Mielke (*Weierstrass Institute for Applied Analysis and Stochastics*), Matthias Wolfrum (*Weierstrass Institute for Applied Analysis and Stochastics*) 08:50–09:10

We consider rings of coupled phase oscillators with anisotropic coupling. When the coupling is skew-symmetric, i.e. when the anisotropy is balanced in a specific way, the system shows robustly a coexistence of Hamiltonian-like and dissipative regions in the phase space. We relate this phenomenon to the time-reversibility property of the system. The geometry of low-dimensional systems up to five oscillators is described in detail. In particular, we show that the boundary between the dissipative and Hamiltonian-like regions consists of families of heteroclinic connections. For larger chains with skew-symmetric coupling, some sufficient conditions for the coexistence are provided, and in the limit of $N \to \infty$ oscillators, we derive an amplitude equation for solutions in the neighborhood of the synchronous solution. It has the form of a nonlinear Schrödinger equation and describes the Hamiltonian-like region existing around the synchronous state similarly to the case of finite rings.

Infinite pinning of interfaces in a random elastic medium

Martin Jesenko (*Mathematisches Institut, Abteilung für Angewandte Mathematik, Albert-Ludwigs-Universität Freiburg*), Patrick Dondl (*Mathematisches Institut, Abteilung für Angewandte Mathematik, Albert-Ludwigs-Universität Freiburg*) 09:10–09:30

Moving of interfaces in a field of obstacles is modelled by the semilinear parabolic equation

$$\frac{\partial u}{\partial t} = \triangle u - f(x,u) + F$$

where $F > 0$ is a constant driving force and $f \geq 0$ gives the strength and position of obstacles. In [2] the authors considered the periodic setting. They showed existence of a critical force F^* such that for $0 \leq F \leq F^*$ there exist stationary solutions whereas for $F > F^*$ there are spatially periodic solutions with positive mean velocity. Hence, at F^* there is a border between the pinning and the depinning behaviour.

In [1] a random environment of obstacles was considered. It was shown that under some conditions on the distribution of positions and strengths again pinning takes place for small $F > 0$. Conversely, in [3] the depinning behaviour was explored. The authors found a lower bound for the average propagation velocity even if only the exponential moments of strengths of obstacles are finite.

In our contribution we will relate to these two works. We will explore the question of infinite pinning, i.e., the environment in which for any driving force $F > 0$ the interface gets pinned. We will present a construction of suitable stationary supersolutions and determine a necessary lower bound on the distribution of strengths of obstacles.

[1] Dirr, N.; Dondl, P. W.; Scheutzow, M. Pinning of interfaces in random media. Interfaces Free Bound. 13 (2011), no. 3, 411–421

[2] Dirr, N.; Yip, N. K. Pinning and de-pinning phenomena in front propagation in heterogeneous media. Interfaces Free Bound. 8 (2006), no. 1, 79–109.

[3] Dondl, P. W.; Scheutzow, M. Positive speed of propagation in a semilinear parabolic interface model with unbounded random coefficients. Netw. Heterog. Media 7 (2012), no. 1, 137–150

S14.04 | Applied analysis

Date 21.03.2018
Room 1260

Curve Diffusion Flow with a Contact Angle

Helmut Abels (*Fakultät für Mathematik, Universität Regensburg*), Julia Butz (*Fakultät für Mathematik, Universität Regensburg*)
 14:00–14:20

We consider the evolution of a curve due to the curve diffusion in two dimensions. This geometric evolution equation arises in problems of phase separation in material science and is the two-dimensional version of the surface diffusion flow. We consider the flow subject to boundary conditions that prescribe the position of the end point to be on a fixed line and a fixed angle with that line. First we will discuss a result on well-posedness locally in time for initial curves of low regularity. Then we will discuss how this result can be used to obtain a blow-up criterion in term of on L^2-bound of the curvature. This is a joint work with Julia Butz.

A coupled bulk-surface model for lipid raft formation in cell membranes and its connection to the Ohta-Kawasaki model

Johannes Kampmann (*Fakultät für Mathematik, Universität Regensburg*)
 14:20–14:40

We investigate a model for lipid raft formation and dynamics in biological membranes which was proposed in [1]. The model includes an cholesterol exchange between cytosol and cell membrane and takes lipid-cholesterol interaction energy into account. From a mathematical point of

view, we couple a bulk-diffusion to a surface PDE on the membrane. In particular, the surface evolution describes a relaxation dynamics for an energy which includes lipid-phase separation and lipid-cholesterol interaction energy. By allowing different constitutive laws for the exchange bet- ween cell membrane and cytosol, the resulting model can include nonequilibrium processes. The resulting equation on the surface takes the form of an extended Cahn-Hilliard equation. We discuss mathematical properties of the model, in particular the existence of stationary solutions. In the nonequilibrium case, we highlight a connection to the Ohta-Kawasaki equation by showing that weak solutions to this model converge to the solutions to the Ohta-Kawasaki equation if certain parameters in the model tend to zero. This is joint work with H. Abels, H. Garcke, A. Rätz and M. Röger.

[1] H. Garcke, J. Kampmann, A. Rätz, M. Röger, A coupled surface-Cahn-Hilliard bulk-diffusion system modeling lipid raft formation in cell membranes, Math. Models Methods Appl. Sci. 26 (2016), no. 6, 1149-1189. DOI: 10.1142/S0218202516500275

Recent results on self-similarity in Smoluchowski's coagulation equation

Marco Bonacini (*University of Bonn*), Barbara Niethammer (*University of Bonn*), Juan Velázquez (*University of Bonn*) 14:40–15:00

Smoluchowski's coagulation equation serves as a classical mean-field model to describe cluster formation and growth in irreversible mass aggregation phenomena, and is used in a large variety of applications. A central question is whether solutions exhibit a universal self-similar form in the large time limit. In this talk I will focus on the problem of existence of scale-invariant solutions. In particular, I will discuss some recent results establishing the existence of one-parameter families of self-similar solutions with finite mass and time-dependent tails, for some classes of rate kernels homogeneous of degree smaller than or equal to one, for which the equation preserves the total mass during the evolution. I will also show an existence result in the so-called gelation case, that is when solutions lose mass at some finite time, for the special case of the diagonal kernel (for which only particles with the same mass coagulate).

Viscosity and conductivity formulas for dilute suspensions

Richard Schubert (*Mathematics/ PDE and appications, University Bonn*) 15:00–15:20

Einstein's formula for the viscosity of dilute suspensions describes how rigid particles immersed in a Stokes-fluid increase its macroscopic viscosity. However, up to now, a rigorous justification has only been obtained for dissipation functionals of the flow field. In this talk, I will discuss ideas for the investigation of many-particle Stokes systems, e.g. the so-called method of reflections and dipole approximations. I will thereby obtain a rigorous result for the number of particles tending to infinity. Namely, in the limit, the suspension behaves like a fluid with increased viscosity that satisfies Einstein's formula. We will also show how the discussed methods lead to a similar result regarding Maxwell's formula for the conductivity of suspensions.

Analysis of an Anisotropic Interaction Model for Simulating Fingerprint Patterns

Lisa Maria Kreusser (*Department of Applied Mathematics and Theoretical Physics, University of Cambridge*) 15:20–15:40

Motivated by the formation of fingerprint patterns we consider a class of interacting particle models with anisotropic, repulsive-attractive interaction forces whose orientations depend on an underlying tensor field. This class of models can be regarded as a generalization of a gradient

flow of a nonlocal interaction potential which has a local repulsion and a long-range attraction structure. In contrast to isotropic interaction models the anisotropic forces in our class of models cannot be derived from a potential. However, most of the analysis of the interaction models in the literature relies on the existence of an interaction potential. In addition, the underlying tensor field introduces an anisotropy leading to complex patterns which do not occur in isotropic models. This anisotropy is characterized by one parameter in the model and depending on its value ring, ellipse and stripe patterns occur as stationary solutions. We study these stationary solutions both analytically and numerically. For the mathematical analysis we consider the associated mean-field partial differential equation. We analyze the equilibria and their stability and investigate the transition between the isotropic and the anisotropic model.

S14.05 | Applied analysis

Date 21.03.2018
Room 1260

Stochastic Modulation equations on unbounded domains

Dirk Blömker (*Institut für Mathematik, Universität Augsburg*), Luigi Amedeo Bianchi (*Universität Konstanz*), Guido Schneider (*Universität Stuttgart*) 16:30–16:50

We consider the approximation via modulation or amplitude equations for nonlinear stochastic PDEs on unbounded domains with additive space time white noise. Close to a bifurcation an infinite band of eigenvalues changes stability, and the solutions are well approximated by the slowly modulated amplitude of the dominating pattern that satisfies a Ginzburg-Landau PDE. We study the impact of small space-time white noise on this bifurcation.
In the talk present results for the stochastic Swift-Hohenberg equation on the whole real line. We use the mild formulation to split the result into a stochastic one for the linearized equation, and a deterministic pathwise estimate. The main problem in the final result is that due to the weak regularity of solutions all the standard methods for modulation equations fail, and we need to develop new tools to prove the approximation. It is necessary to consider weighted spaces that allow for unboundedness at infinity of solutions, which is natural for translation invariant noise like space-time white noise.

Homogenization of the time-harmonic Maxwell equations in general periodic microstructures

Maik Urban (*TU Dortmund University*), Ben Schweizer (*TU Dortmund University*) 16:50–17:10

Inspired by new experimental observations, homogenization of the time-harmonic Maxwell equations in periodic meta-materials has been an active field of research in the last 20 years. We contribute with a study of periodic meta-materials with period $\eta > 0$ consisting of perfectly conducting microstructures and void space. Most of the known results treat a microstructure with a particular topology. By contrast, we discuss the homogenization of Maxwell's equations for a general class of microstructures. The topological characteristics of the medium determine the structure of the macroscopic equations as well as the transmission properties of the effective medium.

From a non-Markovian system to the Landau equation

Raphael Winter (*Institut für angewandte Mathematik, University of Bonn*) 17:10–17:30

We consider the weak-coupling scaling limit, which models the evolution of particles in a plasma. An open problem in kinetic theory is to prove the convergence of the macroscopic evolution to a solution of the Landau equation. In this talk, we take as a starting point the (formal) leading order behavior of the system in the scaling limit, that can be derived under the assumption of propagation of chaos. We prove the well-posedness of this system on the macroscopic timescale, and the convergence to a solution of the Landau equation. The limit shows the transition from an evolution with memory effects and finite speed of propagation to a dissipative, parabolic limit.

Generalized Play Hysteresis Operators in Limits of Fast-Slow Systems

Christian Kuehn (*Mathematics, Technical University of Munich*), Christian Münch (*Technical University of Munich*) 17:30–17:50

Hysteresis operators appear in many applications, such as elasto-plasticity and micromagnetics, and can be used for a wider class of systems, where rate-independent memory plays a role. A natural approximation for systems of evolution equations with hysteresis operators are fast-slow dynamical systems, which—in their used approximation form—do not involve any memory effects. Hence, viewing differential equations with hysteresis operators in the nonlinearity as a limit of approximating fast-slow dynamics involves subtle limit procedures. In this talk, I am going to outline a proof of Netushil's "observation" that broad classes of planar fast-slow systems with a two-dimensional critical manifold are expected to yield generalized play operators in the singular limit. We also provide an illustration of our results in the context of oscillations in forced planar nonautonomous fast-slow systems. The study of this example also strongly suggests that new canard-type mechanisms can occur for two-dimensional critical manifolds in planar systems. The results can be found in detail in the paper: "Generalized play hysteresis operators as limits of fast-slow systems", C. Kuehn and C. Münch, SIAM Journal on Applied Dynamical Systems, Vol. 16, No. 3, pp. 1650-1685, 2017

On G-convergence and stochastic two-scale convergences of the squareroot approximation scheme to the Fokker-Planck operator

Martin Heida (*WIAS Berlin*) 17:50–18:10

We study the qualitative convergence properties of a finite volume scheme that recently was proposed by Lie, Fackeldey and Weber [2013] in the context of conformation dynamics. The scheme was derived from physical principles and is called the squareroot approximation (SQRA) scheme:

$$\partial_t u_i^\varepsilon = \frac{1}{\varepsilon^2} \sum_{(i,j)\in E^\varepsilon} \left(u_j^\varepsilon \frac{v_i^\varepsilon}{v_j^\varepsilon} - u_i^\varepsilon \frac{v_j^\varepsilon}{v_i^\varepsilon} \right), \quad v_i^\varepsilon = \exp\left(-\frac{\beta}{2} V_i^\varepsilon \right).$$

We show that solutions to the SQRA equation converge to solutions of the Fokker-Planck equation as $\varepsilon \to 0$ using a discrete notion of G-convergence. As an example, in the special case of stationary Voronoi tessellations we use stochastic two-scale convergence to prove that this setting satisfies the G-convergence property. In particular, the class of tessellations for which the G-convergence result holds is not empty.

A multiscale approximation of a Cahn–Larché system with phase separation on the microscale

Lisa Reischmann (*Universität Augsburg*), Malte Peter (*Universität Augsburg*) 18:10–18:30

We consider the process of phase separation of a binary system under the influence of mechanical deformation and we derive a mathematical multiscale model, which describes the evolving microstructure taking into account the elastic properties of the involved materials. Motivated by phase-separation processes observed in lipid monolayers in film-balance experiments, the starting point of the model is the Cahn–Hilliard equation coupled with the equations of linear elasticity, the so-called Cahn–Larché system. Owing to the fact that the mechanical deformation takes place on a macrosopic scale whereas the phase separation happens on a microscopic level, a multiscale approach is imperative. We assume the pattern of the evolving microstructure to have an intrinsic length scale associated with it, which, after nondimensionalisation, leads to a scaled model involving a small parameter $\epsilon > 0$, which is suitable for periodic-homogenisation techniques. For the full nonlinear problem the so-called homogenised problem is then obtained by letting ϵ tend to zero using the formal method of asymptotic expansion. Furthermore, we present a linearised Cahn–Larché system and use the method of two-scale convergence to obtain the associated limit problem, which turns out to have the same structure as in the nonlinear case, in a mathematically rigorous way. Properties of the limit model will be discussed.

S14.06 | Applied analysis

Date 22.03.2018
Room 1260

Recent developments in relaxation theory and its applications

Sergio Conti (*Institut für Angewandte Mathematik, Universität Bonn*) 08:30–09:10

Relaxation theory permits to study the macroscopic consequences of microstructure in materials without kinematically resolving the details. The general framework within nonlinear elasticity is well established and has been demonstrated to be very successful in selected prototype problems. Its applicability is limited on the theoretical side by the difficulty of dealing with nonlinear constraints, such as positivity of the determinant, and on the pratical side by the difficulty of explicitly determining the quasiconvex envelope of a given energy density. Recently a different approach has been proposed, which puts the equilibrium equations at the center, and which can be theoretically studied within the framework of A-quasiconvexity. It permits to deal with a data-driven formulation of nonlinear elasticity and yields a different effective macroscopic model. The difference can be realated to history dependence and hysteresis. Based on joint work with Georg Dolzmann, Stefan Müller and Michael Ortiz.

A Compactness and Structure Result for a Discrete Multi-Well Problem with SO(n) Symmetry in Arbitrary Dimension

Angkana Rüland (*Max-Planck-Institute for Mathematics in the Sciences*) 09:10–09:30

In this talk I will discuss a compactness and structure result for a quite general class of phase transformations with SO(n) symmetry in the regime of surface energy scaling. This includes for instance martensitic transformations but also phase-antiphase transformations, whose limiting structures are described. Mathematically the argument relies on a combination of a "spin-argument" with a reduction of the multi-well problem to an incompatible one well-problem. This is joint work with G. Kitavtsev, G. Lauteri and S. Luckhaus.

Stochastic homogenization revisited via stochastic unfolding

Martin Heida (*WIAS Berlin*), Stefan Neukamm (*Faculty of Mathematics, TU Dresden*), Mario Varga (*TU Dresden*) 09:30–09:50

In this talk we introduce a stochastic unfolding method that shares many similarities to the periodic unfolding and periodic two-scale convergence. We illustrate the method at the classical example of homogenization of convex integral functionals, and disucss homogenization of an evolutionary gradient system. We also discuss its relation to different (established) notions of stochastic two-scale convergence (in the mean and the quenched form).

Linearization for solid-solid phase transition

Manuel Friedrich (*Universität Wien*), Elisa Davoli (*Universität Wien*) 09:50–10:10

We establish a quantitative rigidity estimate for two-well nonlinear elastic energies, in the case in which the two wells have exactly one rank-one connection. We analyze the linearization around a laminate in the setting of two-dimensional solid-solid phase transition. We identify an effective limiting model by Gamma-convergence given by the sum of a quadratic linearized elastic energy and two surface terms, corresponding to the total length of interfaces created by jumps of the deformation gradient and the displacement field, respectively.

Stochastic homogenization of free-discontinuity problems

Caterina Ida Zeppieri (*Applied Mathematics, University of Muenster*), Filippo Cagnetti (*University of Sussex*), Gianni Dal Maso (*SISSA International School for Advanced Studies*), Lucia Scardia (*University of Bath*) 10:10–10:30

Motivated by applications to Fracture Mechanics in this talk I will present some recent results concerning the homogenization of a class of random free-discontinuity functionals depending on vector-valued functions u which can be discontinuous across hypersurfaces depending on u. We will show that, under the usual assumptions of stationarity and ergodicity, the homogenization procedure gives rise to a (homogeneous) deterministic free-discontinuity functional belonging to the same class.

S14.07 | Applied analysis

Date 22.03.2018
Room 1260

The choice of representative volumes for random materials

Julian Fischer (*Institute of Science and Technology Austria*) 14:00–14:20

The most widely employed method for determining the effective large-scale properties of random materials is the representative volume element (RVE) method: It basically proceeds by choosing a sample of the random medium - the representative volume element - and computing its properties. To obtain an accurate approximation for the effective material properties, the RVE should reflect the statistical properties of the material well. Hence, it is desirable to choose a large sample of the random medium as an RVE. However, an increased size of the RVE comes with an increased computation cost; for this reason, there have been attempts in material science and mechanics towards capturing the statistical properties of the material in a better way in an RVE of a fixed size. We provide an analysis of an approach by Le Bris, Legoll, and Minvielle, which has been capable of improving the computational efficiency by a factor of 10-50 in some numerical examples by such an ansatz.

POD-Galerkin modeling of a heated pool.

Jorge Yanez (*KIT - Karlsruhe Institute of Technology*), Andreas Class (*KIT - Karlsruhe Institute of Technology*) 14:20–14:40

Spent nuclear fuel elements contain a significant amount of fissile materials that decompose releasing residual heat over a long term. This decomposition occurs inside of the so-called spent fuel pool where spent elements are cooled by natural convection.
CFD calculation of all operating conditions of the pool including accident scenarios is unaffordable. Nevertheless, a light, fast and accurate model of this convection problem can be obtained utilizing Proper Orthogonal Decomposition (POD) and Galerkin Projection methods.
Thus, we carry our reduced order modeling as follows.
Firstly, the high fidelity solver Star-CCM+ is utilized to resolve the incompressible Boussinesq formulation of the pool. The results obtained constitute a set of solutions available at discrete times for each variable.
Subsequently, these solutions are utilized to build a distinct basis. The basis constitutes the POD. This is built considering an optimal linear combination of the solutions at different times. Notably, reduced sets of components of the basis allow for the reproduction of a maximum of the dynamics of the variables.
Thirdly, the system of equations is projected onto this basis (Galerkin Projection). A reduced order model can be created using a small amount of the components, sufficient for the required accuracy. Thus our simplified model is derived from first principles.
Finally, the results of the model are compared with high fidelity solutions. The assessment includes the capabilities of the model to reproduce transients and to approach the final steady state. Additionally, we evaluate the performance of the MPI-parallelized software generated.

Gamma-Convergence Analysis of a Generalized XY Model: Fractional Vortices and String Defects

Rufat Badal (*M7, Technische Universität München*), Marco Cicalese (*M7, Technische Universität München*), Lucia De Luca (*SISSA International School for Advanced Studies*), Marcello Ponsiglione (*Sapienza Università di Roma*) 14:40–15:00

We propose and analyze a generalized two dimensional XY model, whose interaction potential has n weighted wells, describing corresponding symmetries of the system. As the lattice spacing vanishes, we derive by Γ-convergence the discrete-to-continuum limit of this model. In the energy regime we deal with, the asymptotic ground states exhibit fractional vortices, connected by string defects. The Γ-limit takes into account both contributions, through a renormalized energy, depending on the configuration of fractional vortices, and a surface energy, proportional to the length of the strings. Our model describes in a simple way several topological singularities arising in Physics and Materials Science. Among them, disclinations and string defects in liquid crystals, fractional vortices and domain walls in micromagnetics, partial dislocations and stacking faults in crystal plasticity. Time permitting we investigate the dynamics of the model in the simple setting of two repelling half-vortices connected by a curve γ. Employing a curvature regularization technique and a minimizing movement scheme we derive equations governing the evolution of the regularized problem and show the existence of a global in time solution.

Convergence analysis of time-discretization schemes for rate-independent systems

Dorothee Knees (*Institute for Mathematics, University of Kassel*) 15:00–15:20

It is well known that rate-independent systems involving nonconvex stored energy functionals in general do not allow for time-continuous solutions even if the given data are smooth in time. Several solution concepts are proposed to deal with these discontinuities, among them the meanwhile classical global energetic approach and the more recent vanishing viscosity approach. Both approaches generate solutions with a well characterized jump behavior. However, the solution concepts are not equivalent. In this context, numerical discretization schemes are needed that efficiently and reliably approximate directly that type of solution that one is interested in. For instance, in the vanishing viscosity context it is reasonable to couple the viscosity parameter with the time-step size. Other approaches rely on different versions of local minimization or on alternate minimization strategies. The aim of this lecture is to discuss different time-discretization schemes proposed in literature, to present convergence results and to characterize as detailed as possible the limit curves as the discretization parameters tend to zero.

Particle sedimentation in Stokes flows

Richard Höfer (*Institute for Applied Mathematics, University of Bonn*) 15:20–15:40

In this talk, we will consider the N-particle dynamics of spheres immersed in a fluid subject to gravitation and study the limit of many small particles. We will discuss the physical relevant quantities that determine the macroscopic behavior of the cloud of particles. A rigorous convergence result is presented for the inertialess dynamics. The limit equations resemble the equations for a Stokes fluid of variable density.

Γ-convergence of an entropic regularized and discrete entropic regularized minimizing movement scheme with relativistic cost

Benjamin Söllner (*Mathematik, Technische Universität München*), Daniel Matthes (*Mathematics, Technische Universität München*) 15:40–16:00

In this talk, we consider minimizing movement schemes in the framework of optimal transport with a particular cost function c for linear or porous medium diffusion type internal energies, where the included optimal transport problem will be additionally regularized by means of an entropic energy functional. The cost function, $c(x, y) = \sqrt{1 - |x - y|^2}$ inside the closed unit ball and infinite outside, enforces an upper bound on the transportation distance, hence the term "relativistic". In addition we consider a spatial discretization of the above minimizing movement scheme.
Regularizing entropically in an optimal transport problem to approximate solutions has been used successfully to solve optimal transport problems in fields such as imaging sciences and machine learning. Especially algorithms that include calculating a solution to an optimal transport problem benefit from the possibility to highly parallelize the calculation.
We will show Γ-convergence of a regularized and a discrete regularized minimizing movement functional to the unregularized functional and therefore receive weak convergence of the corresponding minimizers.

S14.08 | Applied analysis

Date 22.03.2018
Room 1260

Stability of Hamiltonian lattice waves in the high-energy limit

Michael Herrmann (*Mathematics, Technische Universität Braunschweig*) 17:30–17:50

The dynamical stability of travling waves in FPU lattices is a longstanding open problem and the only available results are provided by the Friesecke-Pego theory of near-sonic waves with small energies. In this talk we consider the complementary high-energy limit and sketch an asymptotic stability proof. The key ingredient is to replace the nonlinear advance-delay-differential equation by a planar shape ODE and to control the approximation error in the corresponding eigenvalue problems.
Joint work with Karsten Matthies (University of Bath).

Michell trusses in two dimensions as a Gamma-limit of optimal design problems in linear elasticity

Heiner Olbermann (*Mathematics, Leipzig University*) 17:50–18:10

We reconsider the minimization of the compliance of a two dimensional elastic body with traction boundary conditions for a given weight. It is well known how to rewrite this optimal design problem as a nonlinear variational problem. The limit of vanishing weight is taken by sending a suitable Lagrange multiplier to infinity in the variational formulation. We show that the limit, in the sense of Γ-convergence, is a certain Michell truss problem. This proves a conjecture by Kohn and Allaire.

Willmore Flow of Networks

Harald Garcke (*Mathematik, Universität Regensburg*), Julia Menzel (*Mathematik, Universität Regensburg*), Alessandra Pluda (*Mathematik, Universität Regensburg*) 18:10–18:30

We consider networks Γ of curves in the plane moving according to the L^2-gradient flow of the elastic energy

$$\int_\Gamma \left(k^2 + \lambda\right) \, \mathrm{d}s \,, \quad \lambda > 0 \,.$$

We prove short time existence in the case of networks composed by three curves that are required to meet in one or two triple junctions. As a variation of the result we additionally impose that they form angles of 120 degrees at the triple junction(s).
We give some outlook on our expectations concerning the long time behaviour based on numerical work by Barrett, Garcke and Nürnberg.

S14.09 | Applied analysis

Date 23.03.2018
Room 1260

Conjecture on minimization of asymptotic energy of Müller's functional with nonlocal singular lower-order term

Andrija Raguz (*Department of Mathematics and Statistics, Zagreb School of Economics and Management*) 08:30–08:50

We conjecture the formula for Gamma-limit of generalized Müller's functional (cf. G. Alberti, S. Müller: A new approach to variational problems with multiple scales, Comm. Pure Appl. Math. 54, 761-825 (2001)) endowed with nonlocal singular lower-order term and we compute the minimal value attained by such Gamma-limit.

Pulses in FitzHugh-Nagumo systems with rapidly oscillating coefficients

Sina Reichelt (*Partielle Differentialgleichungen, Weierstraß-Institut (WIAS Berlin) für Angewandte Analysis und Stochastik*), Pavel Gurevich 08:50–09:10

This talk is devoted to pulse solutions in FitzHugh-Nagumo systems that are coupled parabolic equations with rapidly periodically oscillating coefficients. In the limit of vanishing periods, there arises a two-scale FitzHugh-Nagumo system, which qualitatively and quantitatively captures the dynamics of the original system. We prove existence and stability of pulses in the limit system and show their proximity on any finite time interval to pulse-like solutions of the original system.

New thoughts on the anti plane shear problem

Jendrik Voss (*Mathematics, Universität Duisburg-Essen*), Patrizio Neff (*Universität Duisburg-Essen*), Herbert Baaser (*Technische Hochschule Bingen*) 09:10–09:30

We study anti-plane shear deformations $\varphi(x) = (x_1, x_2, x_3 + u(x_1, x_2))^T$ based on the prior work of Knowles and relate existence of APS-deformations with fundamental concepts of elasticity like polyconvexity, rank-one convexity and tension-compression symmetry. In addition, we do some numerical calculations to prove and visualize these relations.

Modified semi-analytic calculation for the prediction of the volume flow rate in the Reverse Roll Coating Process

Zia Jang (*CBI, Lehrstuhl für Strömungsmechanik, FAU*), Oliver Litfin (*Technische Fakultät, Lehrstuhl für Strömungsmechanik, FAU*), Antonio Delgado (*Technische Fakultät, Lehrstuhl für Strömungsmechanik, FAU*) 09:30–09:50

Reverse roll coating (RRC) is one of the most widely adopted coating techniques for industries owing to versatility and precision of the process. (Coyle, Macosko, & Scriven, 1990) The coating bead consists of two counter-rotating cylinders with a defined gap, whose upstream side is fed by the nip-reservoir. The volume flow rate and the film separation point are, however, previously unknown. This is why the simplified Navier-Stokes equations, by the lubrication approximation, are not fully analytically solvable. In this work, it is intended to present the simplified Navier-Stokes equations with the presence of the gravity. The volume flows of the RRC process is

solved by substituting the results of the pressure gradient and the film separation point from the computational fluid dynamics calculations for the unknowns in the equations. This 'semi-analytic' approach is demonstrated, as a result, to reflect the non-linearity of the volume flow rate in the practical nip-fed RRC process better. This study especially covers the process range of the capillary number 1 leqCa $\leq$ 10 with the use of a virtual Newtonian coating fluid.

Computational modelling of fretting wear of Ti-6Al-4V incorporating cyclic plastic deformations and the debris evolution

Le Zhang (*Institut für Allgemeine Mechanik (IAM), RWTH Aachen University*), Songyun Ma (*Institut für Allgemeine Mechanik (IAM), RWTH Aachen University*), Bernd Markert (*Institut für Allgemeine Mechanik (IAM), RWTH Aachen University*) 09:50–10:10

Fretting wear characterizes a contacting behaviour under small oscillated slips[1]. Generally, complex wear mechanisms include adhesion, abrasion and oxidation in the wear process. In the wear process, wear particles referred to as the third-body flow from inside of the contact to outside[2]. Furthermore, the thin layer on the subsurface with a modified metallographic structure, which is named as the tribologically transformed structure (TTS), is formulated due to the local high plastic deformation and interactions with the environment [3]. Since the ductility is exhausted by the accumulation of plastic ratcheting, cracks parallel to the surface leading to delamination wear[4]. Hence, an accurate modelling of the fretting wear process have to account for the plastic ratcheting and different wear mechanisms.
In the present work, the wear model incorporating the plastic dissipation and the debris evolution is proposed to simulate the fretting wear profile of Ti-6Al-4V under cyclic loadings. In the proposed model, the wear depth from plastic deformation area is evaluated. The ejected rate of the debris is computed to estimate the accumulation of the debris volume. In addition, the contribution of the TTS to the wear is taken into account by relating the thickness of TTS with the highly stressed volume of the material undergoing the plastic deformation. Different wear configurations are considered in the simulations to validate the predictive ability of the proposed wear model. The computational results are compared to the experimental data from [5]. The results show that the proposed approach provides a reasonable prediction of the wear profiles for different wear configurations.

[1] Gallego, L.,Nélias, D.: *Modeling of fretting wear under gross slip and partial slip conditions*, Journal of tribology (2007) 129: 528-535.

[2] Godet, M.: *The third-body approach: a mechanical view of wear*, Wear (1984) 437-452.

[3] Sauger, E., Fouvry, S., Ponsonnet, L., Martin, J. M., Vincent, L.: *Tribologically transformed structure in fretting*, Wear (2000) 245: 39-52.

[4] Kapoor, A.: *Wear by plastic ratchetting*, Wear (2001) 212: 119-130.

[5] Ding, J., Bandaka, G., Leen, S.B., Williams, E.J., Shipway, P.H.: *Experimental characterisation and numerical simulation of contact evolution effect on fretting crack nucleation for Ti–6Al–4V*, Tribology International (2009) 42: 1651-1662.

S15 | Uncertainty quantification

Organiser Claudia Schillings (*University of Mannheim*)
Tim Sullivan (*Freie Universität Berlin and Zuse Institute Berlin*)

S15.01 | Uncertainty quantification

Date 20.03.2018
Room 1180

Multilevel and multifidelity estimators in Uncertainty Quantification

Elisabeth Ullmann (*Mathematik, Lehrstuhl für Numerische Mathematik, TU München*) 08:30–09:10

Uncertainty quantification (UQ) is a fast growing research area which deals with the impact of parameter, data and model uncertainties in complex systems. We focus on models which are based on partial differential equations (PDEs) with random inputs. For deterministic PDEs there are many classical analytical results and numerical tools available. The treatment of PDEs with random inputs, however, requires novel ideas and tools. We illustrate the mathematical and algorithmic challenges of UQ for Bayesian inverse problems arising from geotechnical engineering and medicine, and an optimal control problem with uncertain PDE constraints.

Fast sampling of parameterised Gaussian random fields

Jonas Latz (*Mathematics, TUM*), Elisabeth Ullmann (*Mathematik, Lehrstuhl für Numerische Mathematik, Technische Universität München*) 09:10–09:30

Gaussian random fields are popular models for spatially varying uncertainties, arising for instance in geotechnical engineering, hydrology or image processing. A Gaussian random field is fully characterised by its mean function and covariance operator. In more complex models these can also be partially unknown. Then we need to handle a family of Gaussian random fields indexed with hyperparameters. Sampling for a fixed configuration of hyperparameters is already very expensive, as it requires a Cholesky or spectral decomposition of the discretised covariance operator, which is in general a large dense matrix. Sampling from multiple configurations increases the total computational cost severely.
In this report we construct a reduced basis surrogate for parameterised Karhunen-Lo\'eve expansions - upon which our sampling procedure relies. The reduced basis is built using snapshots of Karhunen-Loève eigenvectors. In particular, we consider Matern type covariance operators with unknown correlation length and standard deviation. We suggest a linearisation of the covariance function and describe the associated online-offline decomposition. In numerical experiments, we investigate the approximation error of the reduced eigenpairs. As an application, we consider forward uncertainty propagation and Bayesian inversion in an elliptic PDE, where the log of the diffusion coefficient is a parameterised Gaussian random field. We discretise PDE operators and covariance operators with finite elements. In the Bayesian inverse problem we employ a Markov Chain Monte Carlo method on the reduced space to generate samples from the posterior distribution. All numerical experiments are done in 2D space with non-separable covariance operators on finite element grids with tens of thousands of degrees of freedom.

Variance robust Metropolis-Hastings algorithms for Bayesian inference with highly informative data

Björn Sprungk (*Institute of Mathematics, University of Mannheim*) 09:30–09:50

We consider Bayesian inverse problems with small observational noise, i.e., highly informative data. This represents a desirable setting in practice, since the resulting posterior distribution will be highly concentrated and less uncertainty remains. However, if we would like to sample from such concentrated posterior distributions by Markov chain Monte Carlo methods, we often observe a decreasing efficiency of these algorithms when the target distribution becomes more concentrated. In this talk we present a first analysis of the performance of Metropolis-Hastings algorithms in the limit of decreasing noise variance. In particular, we show that Metropolis-Hastings algorithms which use approximations of the posterior covariance for proposing new states can perform independently of the noise variance. Combined with the construction principles for dimension-independent Metropolis-Hastings algorithms, e.g., the pCN or gpCN Metropolis algorithm, this yields a Markov chain Monte Carlo method suited for exploring high-dimensional and highly concentrated posterior measures.

Simple Bayesian parameter estimation using functional approximation of random fields

Jaroslav Vondřejc (*Institute of Scientific Computing, Technische Universität Braunschweig*), Hermann Matthies (*Institute of Scientific Computing, Technische Universität Braunschweig*) 09:50–10:10

This contribution is focused on inverse problems, which are generally ill-posed problems to identify parameters of the system by observing its response. The probabilistic formulation using Bayes theorem overcomes the difficulties and leads to a unique solution describing the stochastic distribution of the parameters with incorporated information from measurements. Most of the Bayesian approaches are formulated in terms of probability measures, which are usually computationally realised using sampling methods such as Markov-chain Monte Carlo. Here, we focus on a sampling-free non-linear Bayesian update of random fields, which naturally arises in the computational framework of functional or spectral approximations such as stochastic Galerkin methods using polynomial chaos expansion. This variational formulation corresponding to conditional expectation gives rise to the well-known Kalman filter when it is linearised. The full non-linear version that is also suited for the general non-linear forward problems is investigated here. Our approach builds on an approximation with simple functions leading to an approximation of the conditional expectation in a simpler form, which can be efficiently treated by a numerical algorithm. The effectiveness of the method is demonstrated by numerical examples.

Efficient Conditional Reliability Updating with Polynomial Expansion Surrogates

Max Ehre (*TU München, Ingenieurfakultät Bau Geo Umwelt*), Iason Papaioannou (*TU München, Ingenieurfakultät Bau Geo Umwelt*), Daniel Straub (*TU München, Ingenieurfakultät Bau Geo Umwelt*) 10:10–10:30

Data on the performance of engineering systems can and should be used to learn system parameters and update the system reliability estimate. In a Bayesian framework, the updated probability of failure is obtained by integrating the joint posterior over the failure domain. This representation conceals a substantial amount of information on the uncertainty present in the probability

of failure estimate, which is associated with the fact that the updating relies on a finite and often small amount of data (epistemic uncertainty).

To reveal this information in the analysis one may consider the probability of failure conditional on the updating variables. The resulting expression is a conditional expectation whose measure carries information on the epistemic uncertainty, and hence can be used to assess the information gain from gathering additional data. In practice, evaluation of the conditional probability of failure requires solving a reliability problem at each possible outcome from the posterior distribution of the updating variables. This leads to a considerable increase in the required computational effort.

Our approach to enhance computational efficiency is two-fold: On the one hand, we perform updating using surrogate models based on polynomial bases (polynomial chaos expansions and canonical decompositions). Secondly, we devise a procedure for the fast re-computation of failure probabilities with sequential sampling methods (Papaioannou et al.). We exploit the similarity of reliability problems with small distance in a suitable norm by sequentially initializing computations with failure samples of similar problem solutions.

Papaioannou, I., C. Papadimitriou, and D. Straub (2016). Sequential importance sampling for structural reliability analysis. *Structural Safety* 62, 66 – 75.

S15.02 | Uncertainty quantification

Date 20.03.2018
Room 1180

A Statistical Learning View on Random PDEs

Martin Eigel (*WIAS*), Reinhold Schneider (*Mathematics, TU Berlin*), Philipp Trunschke (*Mathematics, HU Berlin*) 16:50–17:10

An obvious similarity of Machine Learning and UQ with random PDEs is the task to determine an appropriate mapping which relates some usually high-dimensional input (stochastic parameters, images, etc.) to some output (classes, representation coefficients, etc.). However, while the data set for learning problems usually is determined a priori, in UQ an essentially unlimited amount of "training data'" can be generated on the fly if required. In case that a functional approximation of the forward model is generated, additional data can be evaluated with very low computational cost. We pursue this notion in the context of statistical learning theory and employ hierarchical tensor product approximations for the stochastic solution representation. For approximations based on the minimization of (empirical) risk functionals, convergence results can be derived in probability based on concentration of measure estimates.

Statistical Methods for Parameter Identification of Temperature Dependent Viscoelastic Models

Hugo-Fernando Rosero-Velásquez (*Risk Analysis Engineering, Technische Universität München*), Giulio Cottone (*Università degli Studi di Palermo*), Natalia Colinas-Armijo (*Università degli Studi di Palermo*) 17:10–17:30

A fractional stochastic model for viscoelastic materials is proposed. Time dependent stress-strain response for creep and relaxation tests is described through Langevin equation, which results in a Zener's model. Main assumptions are constant friction coefficient between microscopic

entanglements and random effects modelled by a Continuous Time Random Walk (CTRW) whose propagator solves a subdiffusion Fractional Differential Equation. Such CTRW is simulated with alpha-stable waiting time distribution and jump length probability density function with nonzero mean and finite variance. Under those assumptions, the model follows in average a power-law asymptotic behavior, which coincides with the so called fractional model of viscoelasticity. Temperature dependency is explained through changes in friction coefficient, as well as through the randomness in waiting time and jump length distribution parameters. Simulated CTRWs are compared with experimental data for creep-recovery tests performed in different temperatures.

A probability-box approach on uncertain correlation lengths by stochastic finite element method

Mona Madlen Dannert (*Institute of Mechanics and Computational Mechanics, Leibniz Universität Hannover*), Amelie Fau (*Institute of Mechanics and Computational Mechanics, Leibniz Universität Hannover*), Rodolfo M. N. Fleury (*Institute of Mechanics and Computational Mechanics, Leibniz Universität Hannover*), Matteo Broggi (*Institute for Risk and Reliability, Leibniz Universität Hannover*), Udo Nackenhorst (*Institute of Mechanics and Computational Mechanics, Leibniz Universität Hannover*), Michael Beer (*Institute for Risk and Reliability, Leibniz Universität Hannover*) 17:30–17:50

Uncertainties, e.g. due to load, material or geometric properties, are inevitable in engineering applications. For this reason, providing finite element approaches considering uncertain input variables will increase the reliability of non-linear structural analysis.
In theory, there are two types to distinguish, aleatory uncertainties as a consequence of randomness, and epistemic uncertainties describing lack of knowledge. In practice, however, input parameter usually involve a mixture of both kind and thus demand for appropriate approaches. Regarding random fields, the influence of the values at two different points is described by the correlation length. As this parameter is difficult to determine, it may be considered to be epistemically uncertain. In addition to the aleatory character of the random field itself, a mixed uncertain random field occurs.
This work investigates how constitutive parameters described by mixed uncertain random fields influence the inelastic material response of a finite element simulation. While the Karhunen-Loève expansion is used for random field discretisation, the mixed uncertainties are modelled by a probability-box (p-box) approach. To cover the random space, a nested collocation algorithm is proposed. The computational efficiency will be demonstrated on elasto-plastic computations.

Duality Based Estimation of Linearization Errors in Stochastic Computations

Ulrich Römer (*TU Braunschweig*), Stéphane Clénet (*Arts et Métiers ParisTech*), Sebastian Schöps (*TU Darmstadt*) 17:50–18:10

A variety of numerical methods are available nowadays to quantify uncertainties in the simulation of technical systems. In particular, stochastic spectral methods are increasingly popular as they can efficiently handle large variations in input parameters. They can also be applied to high-dimensional problems using sparsity and adaptivity. However, when the uncertainties in the inputs are small, the well-known first order second moment analysis may still be an appealing alternative. Moreover, such a perturbation approach may be crucial to ensure tractability in the context of robust optimization.
In this work, we present a technique to control the linearization error in first order second moment analysis without computing higher order derivatives. The key ingredient is a Prager-Synge type estimate which holds in a stochastic setting. This estimate is used to derive error bounds for

statistical moments. Instead of a higher order derivative, the solution of a dual problem is required in this case. We will discuss different examples of dual formulations and give numerical examples for the error estimators.

Efficient computation of upper probabilities of failure using Monte Carlo simulation and reweighting techniques

Thomas Fetz (*Department of Basic Sciences in Engineering Science, Unit for Engineering Mathematics, University of Innsbruck*) 18:10–18:30

Let $(X_\lambda)_{\lambda\in\Lambda}$ be a family of random variables. The upper probability $\overline{p}_f$ of failure is the solution of the optimization problem

$$\overline{p}_f = \max_{\lambda\in\Lambda} \int_D \mathbf{1}_{g(x)\le 0}\, f_{X_\lambda}(x)\,\mathrm{d}x.$$

The function f_{X_λ} is the probability density of the random variable X_λ and $g : D \to \mathbb{R}$ a limit state function where $g(x) \le 0$ means failure of the underlying engineering structure. As an example, f_{X_λ} is the density of a multivariate Gaussian random variable $X_\lambda \sim \mathcal{N}(\mu(\lambda), \Sigma(\lambda))$ with expectation vector μ and covariance matrix Σ parametrized by $\lambda = (\lambda_1, \ldots, \lambda_n) \in \Lambda$. The objective function

$$p(\lambda) = \int_D \mathbf{1}_{g(x)\le 0}\, f_{X_\lambda}(x)\,\mathrm{d}x$$

of the above optimization problem can be approximated using Monte Carlo simulation together with reweighting or importance sampling techniques using only one single sample $x_1, \ldots, x_N$ distributed according to a random variable X^0 with $f_{X^0} > 0$:

$$p(\lambda) = \int_D \mathbf{1}_{g(x)\le 0}\, \frac{f_{X_\lambda}(x)}{f_{X^0}(x)}\, f_{X^0}(x)\,\mathrm{d}x \approx \frac{1}{N}\sum_{k=1}^{N} \mathbf{1}_{g(x_k)\le 0}\, \frac{f_{X_\lambda}(x_k)}{f_{X^0}(x_k)} =: p^{X^0}_{x_1,\ldots,x_N}(\lambda),$$

cf. [1,2]. An approximation of the upper probability $\overline{p}_f$ is obtained by $\overline{p}_f \approx \max_{\lambda\in\Lambda} p^{X^0}_{x_1,\ldots,x_N}(\lambda)$. This method needs only N function evaluations $g(x_1), \ldots, g(x_N)$ of the limit state function which is an advantage in cases where the evaluation of g is time consuming. The purpose of the presentation is to discuss and compare variants of the above approach such as iterating and strategies for choosing the random variable X^0.

[1] T. Fetz and M. Oberguggenberger. *Imprecise random variables, random sets, and Monte Carlo simulation.* International Journal of Approximate Reasoning, 78: 252–264, 2016.

[2] T. Fetz. *Efficient Computation of Upper Probabilities of Failure* In: Safety, Reliability, Risk, Resilience and Sustainability of Structures and Infrastructure, Proceedings of the 12th International Conference on Structural Safety and Reliability, C. Bucher, B.R. Ellingwood, D.M. Frangopol (eds.), TU-Verlag Vienna, 493–502, 2017.

S15.03 | Uncertainty quantification

Date 21.03.2018
Room 1180

Darcy Flow Equations with Compound Poisson Distributed Input

Toni Kowalewitz (*TU Chemnitz*), Oliver Ernst (*Mathematics, TU Chemnitz*) 08:30–08:50

We discuss approaches for the computation of quantities of interest for the solution of flow equations in random media. The conductivity is obtained by smoothing or taking level cuts of a Lévy distributed random field, which may result in much rougher random fields than in the Gaussian case. For the special case of a compound Poisson distribution a product quadrature rule will be used and compared to Monte Carlo and Multilevel Monte Carlo simulations. We investigate confidence intervals for both Monte Carlo estimators and the computational effort needed to achieve a certain mean square error.

A data-driven model order reduction approach for Stokes flow through random porous media

Constantin Grigo (*Mechanical Engineering, Technical University of Munich*), Stelios Koutsourelakis (*Technical University of Munich*) 08:50–09:10

Direct numerical simulation of Stokes flow through a random, impermeable rigid body matrix by finite elements requires meshes fine enough to resolve the pore-size scale and is thus a computationally expensive task. It is well known that on a larger scale, Stokes flow is accurately approximated by Darcy's law with an effective diffusivity field depending on the fluid viscosity and the matrix phase topology. To find appropriate effective diffusion coefficients, homogenization schemes exist but are limited to moment-matching of the flow field over representative volume elements. We propose a fully probabilistic Darcy type reduced order model which, based on only a few tens of full order model (FOM) runs, is capable to learn a fine-scale topology to effective diffusion map which in turn is maximally predictive for reconstruction of the FOM response. By using sparsity enforcing priors, the model automatically reveals the topology features (e.g. volume fraction, n-point correlations) that are most predictive for the full order solution field. Moreover, it is possible to adaptively refine the reduced order model based on predictive capability metrics until a predefined level of accuracy is met. After training, the model provides sharp predictive distributions based only on repeated evaluation of the much cheaper Darcy type reduced order model.

An efficient reliability scheme for polymorphic cross-correlated random field material description of structural multi-field systems

Albrecht Schmidt (*Institute of Structural Mechanics, Bauhaus University Weimar*), Long Nguyen-Tuan (*Bauhaus University Weimar*), Carsten Könke (*Bauhaus University Weimar*), Tom Lahmer (*Civil Engineering, Bauhaus University Weimar*) 09:10–09:30

Many natural and technical materials show a heterogeneous material distribution in existing engineering constructions, like dams or dikes. Their material behavior during a reliability analysis can be modeled by multi-dimensional random fields (RF).

Stationary RFs are characterized by their mean, (point-wise) standard deviation and auto-correlation structure. Whereas values for mean and standard deviation of material parameters are often reported in literature, the auto-correlation structure, described by the correlation length, is only vaguely known. Additionally, in the case of multi-field situations there are a series of sensitive material properties which show certain cross-correlations (e.g. regions with increased permeability show a reduced mechanical stiffness and strength). As a polymorphic uncertainty approach, these vaguely known RF parameters (auto-correlation lengths and cross-correlation coefficients) are described by fuzzy sets.
Therefor, a new reliability analysis scheme is proposed. Cross-correlated RF are generated, while their auto-correlation length and cross-correlation coefficients are described by fuzzy sets. An α-level optimization yields failure probability fuzzy sets for given RF parameter fuzzy sets. A surrogate model, approximating the failure probability as a function of the RF parameters, is utilized to reduce the computational costs.
As an application example, a multi-field engineering system is used, which is implemented as a finite element model. The failure probability results obtained by the proposed scheme using the surrogate model show good agreement with results derived using the original model. The computational costs are reduced by a factor of ≈ 50.

[1] A. Schmidt, L. Nguyen-Tuan, C. Könke, and T. Lahmer. Application of polymorphic cross-correlated random fields to material parameters of heterogeneous hydro-mechanical coupled systems. In *A Proceedings of the 15th International Probabilitsic Workshop & 10th Dresdner Probablistik Workshop, Dresden*, 2017.

[2] L. Nguyen-Tuan, C. Könke, V. Bettzieche, and T. Lahmer. Numerical modeling and validation for 3d coupled-nonlinear thermo-hydro-mechanical problems in masonry dams. *Computers & Structures*, 178:143 – 154, 2017.

[3] S. Pannier, M. Waurick, W. Graf, and M. Kaliske. Solutions to problems with imprecise data—an engineering perspective to generalized uncertainty models. *Mechanical Systems and Signal Processing*, 37(1-2):105–120, may 2013.

S15.04 | Uncertainty quantification

Date 21.03.2018
Room 1180

Assessment of the Karhunen-Loève expansion for Bayesian reliability updating with random fields

Felipe Uribe (*Engineering Risk Analysis Group, Technische Universität München*), Iason Papaioannou (*Engineering Risk Analysis group, Technische Universität München*), Wolfgang Betz (*Engineering Risk Analysis group, Technische Universität München*), Daniel Straub (*Engineering Risk Analysis group, Technische Universität München*)

14:00–14:20

Quantification of uncertainties and the estimation of rare event probabilities are tasks of fundamental interest in science and engineering. On the one hand, one aims at retrieving information about mathematical models of physical systems based on observational data; a type of inference known as an *inverse problem*. On the other hand, one is interested in evaluating probabilities of unacceptable system performance (rare events) based on the updated model; this task is also known as *reliability updating*. Bayesian statistical methods provide a tool to approach this type

of problems by incorporating a probabilistic description of the model parameters that combines prior information with observations. The inference process will also lead to an updated estimate of the system reliability, which is quantified in terms of updated rare event probabilities [1].
The complexity of the Bayesian inverse problem is increased when the spatial variation of the parameters is considered. Spatially variable quantities are modeled by random fields that are typically represented with a large number of random variables. In particular, the Karhunen-Loève expansion expresses a random field as a linear combination of orthogonal functions, chosen as the eigenfunctions resulting from the spectral decomposition of the autocovariance function of the field. This property allows us to reduce the dimensionality and efficiently parametrize the random field so that the inference can be performed directly on the random vector arising from this discretization.
In this paper, we focus on the analysis of the implications of different choices in the parametrization of the prior random field, on the solution of the Bayesian inverse problem and on the estimation of updated rare event probabilities. We demonstrate those effects by carrying out a parametric study on a 2D linear elasticity example problem, whose material properties are modeled as random fields with the Karhunen-Loève expansion.

[1] Straub, Daniel, Iason Papaioannou, and Wolfgang Betz."Bayesian analysis of rare events". *Journal of Computational Physics*, 314:538-556, 2016

Surrogate model adaption by explicit Bayesian inversion in tensor train format

Martin Eigel (*WIAS Berlin*), Manuel Marschall (*WIAS Berlin*), Reinhold Schneider (*TU Berlin*) 14:20–14:40

The statistical Bayesian approach is a natural setting to alleviate the inherent ill-posedness of inverse problems by assigning probability densities to the considered calibration parameters. Based on a parametrized coefficient in the forward model, a sampling-free approach to Bayesian inversion with an explicit representation of the parameter densities is developed to adjust the surrogate model.
The proposed sampling-free approach is discussed in the context of tensor trains, which are employed for the adaptive evaluation of the random PDE in orthogonal chaos polynomials and the subsequent high-dimensional quadrature of the log-likelihood. This modern compression technique alleviates the curse of dimensionality by hierarchical subspace approximations of the respective low-rank (solution) manifolds. All required computations can then be carried out efficiently in the low-rank format and discretization parameters are adjusted adaptively based on a posteriori error estimators or indicators.
Numerical experiments, involving affine and log-normal diffusion as examples of a more general framework, demonstrate the performance and confirm the theoretical results.

A probabilistic white-box model for PDE constrained inverse problems

Maximilian Koschade (*Technical University of Munich*), Stelios Koutsourelakis (*Technical University of Munich*) 14:40–15:00

Instead of employing deterministic solvers in a black-box fashion, we seek to address the inherent challenges of uncertainty quantification by restating the solution of a PDE as a problem of probabilistic inference. In doing so, state variables are treated as random fields, constrained or mutually entangled by underlying physical laws. The resulting fully probabilistic white-box model facilitates the seamless incorporation of epistemic uncertainty and allows the solution of the PDE-constrained inverse problem simply by introducing the observational data as an additional source of information into the posterior. We demonstrate the proposed framework for the solution

of PDE-constrained inverse problems in a solid mechanics setting and employ adjoint-free second-order methods to infer the joint posterior over the Hilbert space of displacement, stress and unknown material parameters. The method generalizes to nonlinear problems and higher-order function spaces, while the Maximum-A-Posteriori estimate recovers the results obtained by the mixed Finite Element method derived from the Hellinger-Reissner variational principle.

A Data-Driven Possibilistic Approach to the Identification of Uncertain Stability Lobe Diagrams

Dominik Hose (*Institute of Engineering and Computational Mechanics, University of Stuttgart*), Dominik Hamann (*Institute of Engineering and Computational Mechanics, University of Stuttgart*), Michael Hanss (*Institute of Engineering and Computational Mechanics, University of Stuttgart*), Peter Eberhard (*Institute of Engineering and Computational Mechanics, University of Stuttgart*) 15:00–15:20

Regression analysis is a powerful tool in a vast variety of scientific disciplines. In the context of multi-fidelity methods, it can be used to capture correlations between the outputs of time-consuming high-fidelity simulations or experiments and cost-efficient low-fidelity simulations in order to predict the output of the high-fidelity model from the output of the low-fidelity model. This is typically accomplished by assuming that the error between the two outputs is of some sort of stochastic noise. However, this assumption is often not plausible, especially when two deterministic models are compared, so that alternatives for a preferably better description of this type of uncertainty are worth to be considered.
Machining processes are optimized with respect to material removal rates. High removal rates, however, involve the regenerative effect, which may lead to chatter. In order to avoid this, stability lobe diagrams are used in the design process to predict stable regions. They can be obtained by experiment or by simulations requiring high-fidelity models. However, computational effort and the limited availability of suitable stability-analysis methods limit the application of high-fidelity models, and consequently, one often has to revert back to low-fidelity models. In order to successfully employ these surrogate models, the correlation between the two models has to be taken into account.
In this paper, an alternative approach to the classical regression analysis is explored which allows to identify fuzzy-valued regression models yielding a possibilistic interpretation of the uncertainties as opposed to e.g. the frequentist interpretation in probability. In a first step, it identifies a minimal set of possible regression parameters to reproduce the high-fidelity output from the low-fidelity output. Subsequently, it encodes their degree of possibility, i.e. the confidence in the respective parameter values, in their distribution functions, ultimately permitting a possibilistic identification of uncertain stability lobe diagrams.

Bayesian Estimation of Steel Material Properties and Damage Parameters under Cyclic Loading Conditions

Ehsan Adeli (*Institute of Scientific Computing*), Bojana Rosic (*Institute of Scientific Computing*), Hermann G. Matthies (*Institute of Scientific Computing*) 15:20–15:40

The state of materials and accordingly the properties of structures are changing over the period of use, which may influence the reliability and quality of the structure during its life-time. Therefore identification of the model parameters and states of the system is a topic which has attracted attention in the content of structural health monitoring.
In this work the focus is on identification of material parameters and states of an elasto-viscoplastic damaging material. It is proposed to use Bayesian inverse methods for this. To do so, two steps are considered, solving the forward and inverse problem. Therefore, first the

propagation of the a priori parametric uncertainty through a visco-plastic model including damage describing the behaviour of a steel structure is studied. A non-intrusive Stochastic Finite Element Method (SFEM) based on polynomial chaos is applied for the cyclic test.
From the forward model, material parameters and interval unobservable state variables can be identified using measurement data such as displacement/strain via Bayesian approaches. In this study, a Polynomial chaos based update method which is a modification of Kalman filter as an approximation of Bayes' theorem is employed.

Addressing Global Sensitivity in Chemical Kinetic Models Using Adaptive Sparse Grids

Sandra Doepking (*Institute for Mathematics, Freie Universität Berlin*), 15:40–16:00
Sebastian Matera (*Institute for Mathematics, Freie Universität Berlin*)

Chemical kinetic models often carry very large parameter uncertainties and show a strongly non-linear response with rapid changes over relatively small parameter ranges. In addition, the dimensionality of the parameter space can grow to a large number, without a priori known structure between the dimensions. Using a first principle model as a prototypical example, we demonstrate an adaptive sparse grid strategy (ASG) for the global sensitivity analysis of such models based on the Analysis Of Variances. The ASG utilizes local adaptivity, to address the rapid changes, as well as dimension adaptivity, to exploit the typical intrinsic low dimensional parameter dependence in reaction networks. This significantly reduces the number of points compared to a non-adaptive Sparse Grid (SG). In addition, we will discuss how ASG can be extended to a multilevel strategy in the case of a costly stochastic model. Besides the reduction of points by the adaptivity, the multilevel structure of the Sparse Grid allows to lower the sampling accuracy and therefore the CPU-time spent for the model evaluation in each refinement step. We find that the multilevel approach reduces the computational cost by one to two orders of magnitude compared to non-adaptive, single level SGâ€"without compromising the accuracy of the results. We find that parameter uncertainties can have a tremendous impact on the simulation output and that the predictions of the model have to be interpreted carefully.

S15.05 | Uncertainty quantification

Date 21.03.2018
Room 1180

Fully discrete approximations and adaptive solvers for random PDEs

Markus Bachmayr (*Hausdorff Center for Mathematics & Institut für Numerische Simulation, Universität Bonn*) 16:30–17:10

We consider the approximation of PDEs with parameter-dependent coefficients by sparse polynomial approximations in the parametric variables combined with suitable discretizations in the spatial domain. Here we are especially interested in problems with countably many parameters, as they arise when coefficients with uncertainties are modelled as random fields. For the resulting fully discrete approximations of the corresponding solution maps, we obtain convergence rates in terms of the total number of degrees of freedom. In particular, in the case of affine parametrizations, we find that independent adaptive spatial approximation for each term in the polynomial expansion yields improved convergence rates. Moreover, we give an overview of a construction of near-optimal adaptive solvers for finding such approximations. This talk is based on joint works with Albert Cohen, Wolfgang Dahmen, Ron DeVore, Dinh Dũng, Giovanni Migliorati, and Christoph Schwab.

Surrogate models for dynamic substructuring with geometric uncertainties

Maxime Koebele (*Institute of Engineering Mechanics, Karlsruhe Institue of Technology (KIT)*), Carsten Proppe (*Institute of Engineering Mechanics, Karlsruhe Institue of Technology (KIT)*) 17:10–17:30

Geometric uncertainties may influence the dynamical behavior of many industrial systems in a non-negligible proportion. Taking them into account in a realistic way is an important challenge in engineering mechanics. Indeed, discretization of stochastic fields representing the random geometry leads to a large number of uncertain parameters and to high dimensional problems. Such problems can be solved using Monte-Carlo simulations where computational effort is not much impacted by the stochastic dimension, but usually Monte-Carlo simulations are not directly suitable since they lead due to the complexity of the dynamical system to unreasonable computational cost. One possibility is then to reduce the system. Classical component mode synthesis (CMS) methods divide the system into several coupled substructures and approximate the dynamic response on each substructure as a finite combination of modes. In case of systems with geometric uncertainties, it may be necessary to make these modes dependent on the random geometry of the substructure in order to reach an acceptable convergence. This constitutes again a random problem. However, the stochastic dimension may be smaller and the response more regular than initially. Surrogate models can then be used in order to approximate the random modes. In our contribution, we compare different surrogate models (sparse polynomial chaos approximations, low-rank approximations, ...) for simple substructures as beams or plates and we analyze how they can exploit the specific structure of CMS random modes induced by the random geometry (low effective dimensionality, low-order interaction).

A Multi Level Monte Carlo approach for stochastic analysis of Fluid-Structure Interaction (FSI) problems

Anoop Kodakkal (*Civil, Geo and Environmental Engineering, Technische Universität München*), Roland Wüchner (*Department of civil, geo and environmental engineering, Technical University of Munich*), Kai-Uwe Bletzinger (*Department of civil, geo and environmental engineering, Technical University of Munich*) 17:30–17:50

With availability of increased computational power, computational modeling and numerical simulation is used as a method to tackle structural civil engineering problems. Unlike the conventional deterministic analysis, a stochastic analysis takes into consideration the uncertainties in the structural parameters, boundary/initial conditions, and loading to make realistic predictions. Monte Carlo (MC) methods, based on sampling from the input distribution and evaluating the Quantities of Interest (QoI) at each sampling points are the most commonly used approaches for uncertainty quantification. MC methods have gained universal acceptance for its robustness and simplicity. However, for computationally expensive problems, like fluid-structure interaction (FSI), uncertainty quantification using MC methods becomes computationally challenging and even infeasible in many cases. Multilevel Monte Carlo (MLMC) method is an improvement of standard MC method where the sampling is carried out from different approximations (i.e. levels) of QoI. This approach reduces the computational cost by evaluating most samples from low fidelity and low cost simulations. Only few samples are evaluated from high accuracy, expensive simulations. In this contribution, for the low levels the sampling is carried out from a low fidelity surrogate model resulting in a reduced computational cost. An overall reduction in computational cost is achieved by variance reduction in MLMC method. The efficacy of MLMC algorithm for expensive problems like FSI is compared in this study with classical MC. A set of

benchmark test cases of FSI are used for the study. The possibility of uncertainty quantification for FSI problems with a plausible computational cost using MLMC is demonstrated.

A Third Order Hierarchical Basis WENO Interpolation for Sparse Grids with Application to Conservation Laws with Uncertain Data

Oliver Kolb (*University of Mannheim*) 17:50–18:10

We present a third order hierarchical basis WENO interpolation, which possesses similar accuracy and stability properties as usual WENO interpolations. The main motivation for the hierarchical approach is the direct applicability on sparse grids. This is for instance of large practical interest in the numerical solution of conservation laws with uncertain data, where discontinuities in the physical domain often carry over to the (potentially high-dimensional) stochastic domain. For this, we apply the introduced hierarchical basis WENO interpolation within a non-intrusive collocation method and present some results on 2- and 3-dimensional sparse grids.

Hyperbolicity-preserving stochastic Galerkin method for hyperbolic systems with uncertainties

Florian Schneider (*Mathematik, TU Kaiserslautern*), Louisa Schlachter (*Mathematik, TU Kaiserslautern*) 18:10–18:30

Uncertainty Quantification through stochastic spectral methods is rising in popularity. We derive a modification of the classical stochastic Galerkin method, that ensures the hyperbolicity of the underlying hyperbolic system of partial differential equations. The modification is done using a suitable linear scaling limiter, based on similar ideas in the context of kinetic moment models. This limiter exploits the assumed convexity of the hyperbolicity set to dampen the oscillations of the stochastic Galerkin polynomial in such a way that hyperbolicity is always preserved. We demonstrate the applicability of the limiting process using the simple Lax-Friedrichs scheme in space and time and provide an outlook of extensions to high-order methods.
We apply the resulting modified stochastic Galerkin method to the compressible Euler equations and the M_1 model of radiative transfer. Our numerical results show that it can compete with other UQ methods like the intrusive polynomial moment method while being computationally inexpensive and easy to implement.

S15.06 | Uncertainty quantification

Date 22.03.2018
Room 2370

Imprecise probability models for uncertainty quantification in engineering

Michael Oberguggenberger (*Unit of Engineering Mathematics, University of Innsbruck*) 08:30–09:10

Engineering structures are usually modeled as input-output maps: the response Y is a function Y = F(X,D) of input parameters X (material properties, geometry, boundary conditions) and driving forces D (dynamic or distributed loads, noise). As a rule, knowledge about these parameters is incomplete, i.e., both X and D are nondeterministic and uncertain. While the forces and the noise terms can usually be modeled by means of stochastic processes, the available information about X might be best described by random variables, intervals, or random variables with set-valued distribution prameters, in short, by an imprecise probability model. The theory of random sets permits to combine interval methods, probability assessments and stochastic processes for quantifying the uncertainties and making predictions.

The goal of the talk is to present the concepts of random sets, to address questions of modelling and simulating the uncertain structural response by means of random sets, and to demonstrate selected engineering applications to sensitivity analyis and reliability.

Domain decomposition and Multi-scale failure analysis with polymorphic uncertainties for optimal design of rotor blades

Robert Gruhlke (*WIAS Berlin*), Martin Drieschner (*TU Berlin*) 09:10–09:30

Wind turbine blades are thin-walled spatial structures typically consisting of two composite shells and one or two shear webs assembled with adhesive bonds. Full-size mechanical tests of rotor blades are mandatory for certification but very costly. The definition of representative sub-components typically involves expert knowledge on one hand and is impeded by limited information on specific physical parameters on the other hand, leading to polymorphic uncertainties.
As an important example of a sub-component, the Henkel beam has been developed for testing adhesive bonds, which play a keyrole in structural integrity and reliability of rotor blades. Small defects, *i.e.* voids and delaminations, are common in the bond lines due to manufacturing and application process and can cause multiple tensile cracks and thus lead to macroscopic separation between spar cap and shear web.
First, we study the structural failure of adhesive bonds in a fuzzy-stochastic finite element model. The identification and integration of polymorphic uncertainties is done from an engineering point of view. Due to the extended computational cost of non-deterministic simulations, a two scale model is developed and the results are compared to the one scale model.
Applying a transformation of stochastic microstructure to reference configuration, we build up a uncertain microscopic model in a UQ setting, that leads to a high dimensional problem. By numerical upscaling we construct a statistical surrogate model using modern reduction methods, adaptivity and low-rank compression via hierachical tensor representation to overcome the curse of dimensionality. Domain decomposition techniques are applied to obtain local lower dimensional problems in suitable stochastic coordinates.

A fuzzy-stochastic model for transversely fiber reinforced plastics

Ismail Caylak (*Chair of Engineering Mechanics, Paderborn University*), Eduard Penner (*Paderborn University*), Alex Dridger (*Paderborn University*), Rolf Mahnken (*Paderborn University*) 09:30–09:50

In recent years, lightweight structures became increasingly important due to their excellent mechanical and lightweight properties. As a special component fiber reinforced plastics (FRP) become prominent. It is well known that material properties of FRP are uncertain due to the manufacturing process. In addition, there are measurement errors and missing or incomplete information on material properties. While several sources of uncertainties exist, these are often distinguished into aleatoric and epistemic uncertainty. Aleatoric uncertainty is presumed to be the intrinsic randomness of a phenomenon and is also called statistical uncertainty that can be modeled with stochastic methods based on the polynomial chaos expansion (PCE). On the other hand, epistemic uncertainty is the vagueness in a system definition due to subjectivity, simplification and incomplete knowledge that can be modeled with fuzzy methods based on the fuzzy set theory.
This contribution presents a framework of a transversely isotropic elastic material model. As a key idea, the constitutive equation is modeled by a combination of fuzzy-stochastic methods. The stochastic material parameters are expanded with the multivariate PCE, whereas epistemic material parameters are defined as design variables and are modeled as fuzzy sets. An underlying optimization problem for the fuzzy analysis is approximated by α-level discretization

techniques, resulting into a separation of minimum and maximum problems. To become more universal, so-called quantities of interest are employed, which allow a general formulation for the target problem of interest. Finally, numerical results are compared with existing experimental observations.

Possibilistic and stochastich analysis of rubber like material

Eduard Penner (*Chair of Engineering Mechanics, Paderborn University*), Ismail Caylak (*Chair of Engineering Mechanics, Paderborn University*), Alex Dridger (*Chair of Engineering Mechanics, Paderborn University*), Rolf Mahnken (*Chair of Engineering Mechanics, Paderborn University*) 09:50–10:10

Components and structures, e.g. made of adhesives and composites, are heterogeneous. This heterogeneity leads to uncertainties in the system response, whereby various causes can be responsible for this. In this work, we restrict ourselves to uncertainties due to fluctuating material parameters. When assessing the reliability of components and structures, uncertainties are distinguished into aleatoric and epistemic uncertainty. In the case of aleatoric uncertainties, the statistical data are known for stochastic quantities. Epistemic uncertainties, on the other hand, arise due to a lack of knowledge, i.e. due to incomplete and/or imprecise information. The aim of this contribution is to compare both kinds of uncertainty. For the aleatoric uncertainty, the mechanical system must be described by stochastic partial differential equations (SPDEs). The epistemic uncertainty requires a non-stochastical, for example a possiblistic approach.
Our work describes the stochastic and possibilistic evaluation of the stochastic and possiblistic modeling of Ogden's material model at large deformations. The statistics for stochastic evaluation are given from experiments of rubber materials. For possibilistic evaluation only sparse experiments are available. The stochastic modeling is based on polynomial chaos expansion, which requires statistics of material parameters. In the possibilistic approach, material parameters are interpreted as possibility distributions, which may occur considering the sparse information of the experimental data. Furthermore, in this work the dependencies between material parameters for both methods will be considered. A comparison with real experimental data will show to what extent both methods agree with reality.

Uncertainty quantification of probability box random variables

Truong Vinh Hoang (*Institute of Scientific Computing, Technical University of Braunschweig*), Hermann G. Matthies (*Institute of Scientific Computing, Technical University of Braunschweig*) 10:10–10:30

Uncertainties are usually classified into aleatoric and epistemic uncertainties. While many methods have been developed in the probabilistic framework to deal with aleatoric uncertainties, the alternative frameworks required when dealing with epistemic uncertainties have been much less discussed. One way to characterize the uncertain variables consisting both aleatoric and epistemic uncertainties is to use a probability box (p-box) which consists of a lower bound and an upper bound of the probability distribution. The aim of this work is to develop the efficient methods for uncertainty quantification of p-box variables. Three probabilistic methods, the pure sampling method, the stochastic collocation method, and the spectral stochastic Galerkin method, are extended and then compared for the considered problem. As an illustration, these methods are applied for the condition assessment of a reinforce concrete bridge in which localised damages are detected using strain measurements as input data.

S15.07 | Uncertainty quantification

Date 22.03.2018
Room 1180

Uncertainty Quantification for Global Weather Forecasting

Roland Potthast (*Department of Mathematics and Statistics, University of Reading*) 14:00–14:40

National weather services and research institution around the globe are reacting to the increasing need to estimate risk and distributions of both standard variables of weather and climate such as temperatures or humidity and high-impact phenomena such as strong precipitation, wind gusts and storm, tornados, hurricanes or fog on all scales of the forecasting process from minutes to days, from days to month, from month to years and decades.
The agenda of weather and climate forecasting and projection today includes the development and operation of ensemble forecasting system (EPS) on all scales, which have the ability to model and describe the distribution of possible events and as such the variability of extreme weather, its variables and phenomena.
We describe the setup of the ensemble data assimilation (EDA) and forecasting systems which have been developed and are under development at the German Weather Service DWD, including the ICON global model with its hybrid ensemble variational data assimilation (LETKF+EnVAR) and ensemble prediction system ICON EPS as well as the high-resolution ensemble data assimilation system COSMO-KENDA (Kilometer Scale Ensemble Data Assimilation), which is the operational system at DWD and further members of the COSMO consortium (Germany, Switzerland, Italy, Russia, Poland, Romania, Greece and Israel) to drive their high-resolution ensemble forecasting system. We demonstrate the high quality of the systems.
We discuss basic questions of uncertainty, initialization and uncertainty in the forecasting process in a large-scale environment, both from a mathematical as well as applied and industrial perspective.

Uncertainty Quantification in Marine Ecosystem Models

Thomas Slawig (*Computer Science, Kiel University*) 14:40–15:00

In climate prediction models, uncertainty naturally plays an important role, since the results of climate projections into the future are basis of political discussions and decisions. On the other hand, climate simulations are often very expensive w. r. t. the needed computational effort. This is due to the complexity and variability of the system, but also because of the necessity to compute stable annual cycles, i.e. periodic solutions. We study the marine ecosystem model part of Earth System Models. Here often so-called emulators or reduced-order and simplified models are used to accelerate the computation of stable annual cycles of the system. Two sources of uncertainty are taken into account: On the one hand poorly known model parameters (as growth rates etc.) in the biogeochemistry, and on the other hand the pre-computed ocean circulation. A main question is how these two uncertainties influence the model results. We show different ways to study this question in a simplified 1-d and also the 3-d setting and present some numerical results.

Identifying Vehicular Systems Using Gaussian Process Regression

Michael Burger (*MDF, Fraunhofer ITWM*) 15:00–15:20

We consider a vehicular system, that is, for instance, a full vehicle which is excited at its spindles (using corresponding displacements). As a relevant quantity of interest, one can think of accelerations at inner chassis positions, at the driver's seat or at even other positions. One the one hand side, it is possible to directly measure these quantities of interest, which requires, however, a substantial effort and which is costly and time-consuming and, thus, only workable for a few specifically chosen and equipped measurement vehicles. It is, by contrast, not suited for application within customer fleets. On the other hand, there is the option to model the corresponding part of the vehicle, e.g., as mechanical multibody system model. However, also this strategy requires a large modelling effort and, in addition, the availability of physical parameters, nonlinear force characteristics and so on. In this contribution, we propose and discuss an approach to identify the relvant vehicle dynamics based on measurements and using Gaussian processes (GP) as underlying model structure. We introduce the needed GP framework and we discuss how this framework allows to predict and to qunatitfy uncertainty during the output prediction. We present some results and discuss benefits, drawbacks and potentials of that approach.

Bayesian inference for estimating model discrepancy of an electric drive model

David John (*Corporate Sector Research and Advance Engineering, Corporate Research, Robert Bosch GmbH, Heidelberg University*), Michael Schick (*Corporate Research, Robert Bosch GmbH*), Vincent Heuveline (*Heidelberg University*) 15:20–15:40

The exponential increase of available compute power allows to leverage the potential of uncertainty quantification (UQ) in new applications assuming an industrial setup. A main challenge is related to the fact that the considered computational models are rarely able to represent the true physics perfectly and demonstrate a discrepancy compared to measurement data. Further, an accurate knowledge of considered model parameters is usually not available. E.g. fluctuations in manufacturing processes of hardware components introduce uncertainties which must be quantified in an appropriate way. This requires efficient methods for UQ based on Bayesian inference. An important task related to Bayesian inference is to accurately estimate parameter distributions from measurement data in presence of simulation model inadequacy. As a first step, we address this challenge by investigating the influence of model discrepancies onto the calibration of model parameters and further consider a Bayesian inference framework including an attempt to correct for model discrepancy by an additional term. A Markov Chain Monte Carlo (MCMC) method is utilized to approximate the posterior distributions of the parameters. Synthetic measurement data from an industrial application is then used to evaluate the framework. First measurement data is created with an electric drive model and second another electric drive model containing an artificial model discrepancy is used to infer physical parameters and the model discrepancy term. The application shows a promising perspective of the framework by good approximation of discrepancy and parameters.

A Stochastic Model for Strong Wind Events in Central Europe based on Historical Wind Data

Dominik Brands (*Institut für Mechanik, Universität Duisburg-Essen*), Carina Götzen (*Meyerthole Siems Kohlruss*), Maria Kiseleva (*Meyerthole Siems Kohlruss*), Jana Niekamp (*Meyerthole Siems Kohlruss*), Rainer Niekamp (*Institut für Mechanik, Universität Duisburg-Essen*), Jörg Schröder (*Universität Duisburg-Essen*), Onnen Siems (*Meyerthole Siems Kohlruss*) 15:40–16:00

Due to the European directive 'Solvency II' insurance companies need to estimate the possible claims for their individual portefeuille for a 200 year event. The total loss amount includes estimations for losses suffered natural catastrophes such as windstorms. For this task there exist a couple of commercial tools. A lot of expert's knowledge is used as input for the expensive simulation codes. They are based on physical models of wind appearance or they just work with distortions of historical hazards. At the end these tools are quite intransparent and contain a lot of assumptions not visible to the users. In contrast to these approaches we present a purely data driven model. From the historical data available in suitable internet weather casting platforms we extracted the hourly wind peeks measured at approximately 400 weather stations in central Europe over the last two decades. After a normalization of these data, removing the geographical exposure of the measure points, we generate a set of uncorrelated wind fields. At this point we focus on the problem of missing data (we have a sparsity of 50%), and give an algorithm derived from the Singular Value Decomposition, which finds an optimal and orthogonal data decomposition. The generated wind fields are used to get a Polynomial Chaos approach of the stochastic wind field by a recombination of these fields with stochastic coefficients. The stochastic coefficients themselves are constructed by multi-variate Hermite-polynomials with unknown deterministic coefficients. The equations for these latter coefficients are found by forcing the identity of a suitable set of mixed moments of the wind history and the stochastic model. The Quasi-Newton method is used to solve the arising highly non-linear equations. The generation of the random wind-events with this stochastic model is computational very cheap. In the computational time of some hours we can, using the Monte Carlo method, simulate 10^9 years of insurance risk due to wind hazards. In order to measure the quality of the model, we compare Kendall's rank correlation coefficients between model and historical wind data. We give our thank to the company Meyerthole Siems Kohlruss, Gesellschaft für aktuarielle Beratung mbH, to render the possibility to work on this project and for their support.

S15.08 | Uncertainty quantification

Date 22.03.2018
Room 1180

Scale Switching Computations for Heterogeneous Inelastic Materials

Thilo Moshagen (*Wissenschaftliches Rechnen, TU Braunschweig*), Hermann Matthies (*Institut f. Wissenschaftliches Rechnen, TU Braunschweig*), Adnan Ibrahimbegović (*Lab. Mécanique Roberval, University Technology Compiègne*) 17:30–17:50

For computations involving heterogeneous inelastic materials it is often necessary to consider several scales, as it is not possible to compute the object of interest at the fine scale resolution required by the heterogeneity. For this purpose many proposals for multi-scale computations have been made. We will look at a two-scale transition in a general setting where both scales are also described probabilistically. We envision two computational modes, a cheaper one with a pre-identified "homogenised" material model, and one with a more expensive true two-scale computation when the "homogenised" model is insufficient. For this situation we seek computable criteria locally estimating the modelling error in the "homogenised" material model. In this way it is possible to adaptively decide – element by element – which computational path to use in that particular instance and location.

Distribution based global sensitivity analysis for electronic structure based kinetic models

Sandra Doepking (*Freie Universität Berlin/ Institute for Mathematics*), Sebastian Matera (*Institute for Mathematics, Freie Universität Berlin*) 17:50–18:10

The last years have seen an increasing interest in (chemical) kinetic models which have been parametrized using first principles electronic structure calculations. While these allow to access material properties without fitting the model to experimental data, commonly employed electronic structure theories rely on some approximations and thereby the estimated parameters carry an usually sizeable error. Using a first principles kinetic Monte Carlo model for the CO oxidation on the RuO2(110) surface as a example, I will address the propagation of these errors to the kinetic model's output. For this, I will employ a newly developed distribution based approach to global sensitivity analysis. This approach allows to estimate all sensitivity indices from a single set of sampling points of the parameter space and is also applicable to stochastic model outputs. Further, the resulting sensitivity indices might be interpreted as induced uncertainty by the respective uncertain parameter. For the model at hand, we find sizeable uncertainties but also that only a subset of all errors control this. That is, only nine of the initial 22 parameters show non-vanishing sensitivities. As the parameters have an atomistic interpretation, this allows to identify the key aspects in the reaction mechanism.

Data driven approach to elastic problems

Tim Fabian Korzeniowski (*Mechanical Engineering, Universität Siegen*), 18:10–18:30
Kerstin Weinberg (*Universität Siegen*)

This contribution focuses on a new data driven approach for computational mechanics proposed by Kirchdoerfer and Ortiz. Material models are often gained by experimental data and a following empirical analysis. This adds uncertainty and error to the solutions as one is dependent on scatter and noise. Also, there is no or limited knowledge about the functional form of the material model, which raises the question if it is possible to bypass the step of modeling the material. This is done in a data driven approach by using data in the simulation of a finite element analysis. To each material point a state from a stress-strain data set is assigned. To get this state, a minimization problem with respect to the conservation laws has to be solved.
In this talk we want to explore the data driven approach, show results for different elastic problems as well as list some advantages and disadvantages of this new approach.

S16 | Optimization

Organiser Florian Jarre (*Mathematisches Institut, Heinrich-Heine-Universität Düsseldorf*)
Moritz Diehl (*Department of Microsystems Engineering and Department of Mathematics, University of Freiburg*)

S16.01 | Optimization

Date 20.03.2018
Room N1070

Order through partition: A semidefinite Programming Approach

Franz Rendl (*Mathematik, Alpen-Adria Universität Klagenfurt*), Renata Sotirov (*Tilburg School of Economics and Management, Tilburg University*), Christian Truden (*Institut für Mathematik, Alpen-Adria Universität Klagenfurt*) 08:30–09:10

Ordering Problems on n objects involve pairwise comparison among all objects. This typically requires $\binom{n}{2}$ decision variables.
In this talk we investigate the idea of partitioning the objects into k groups (k-partition) and impose order only among the partition blocks.
We demonstrate the efficiency of this approach in connection with the bandwidth minimization on graphs. We consider relaxations of the partition model with the following characteristics:
1) The weakest model is formulated in the space of symmetric $n \times n$ matrices and has the Hoffman-Wielandt theorem in combination with eigenvalue optimization as a theoretical basis.
2) We also consider semidefinite relaxations in the space of $n \times n$ matrices, involving k semidefinite matrix variables. The idea here is to linearize the quadratic terms using eigenvalue decompositions.
3) Finally, the strongest model is formulated in the space of symmetric $nk \times nk$ matrices. It is based on the standard reformulation-linearization idea.
We present theoretical results for these relaxations, and also some preliminary computational experience in the context of bandwidth minimization.

Decomposition of matrix inequalities with application to topology optimization

Michal Kocvara (*School of Mathematics, University of Birmingham*) 09:10–09:30

We will present a new approach to the decomposition of a large matrix inequality into several smaller ones, with the goal to efficiently use existing SDP solvers. This is a strenghtening of the well-known decomposition of matrices with chordal graphs, that is numerically more efficient. The efficiency of the new approach will be demonstrated on an SDP problem arising in topology optimization of mechanical structures with constraints on vibrations.

Computing solution-compensation spaces using an enhanced Fourier-Motzkin algorithm

Marc Eric Vogt (*Department of Civil, Geo and Environmental Engineering, Technical University of Munich*), Fabian Duddeck (*Department of Civil, Geo and Environmental Engineering, Technical University of Munich*), Helmut Harbrecht (*Computer Science and Mathematics, University of Basel*), Florian Stutz (*Computer Science and Mathematics, University of Basel*), Martin Wahle (*Department of Preliminary Design for Vehicle Dynamics, BMW Group*), Markus Zimmermann (*Institute of product development and lightweight design, Technical University of Munich*)

09:30–09:50

In complex system design, design variables can be divided into two groups, *early-* and *late-decision variables*. Early-decision variables are equipped with tolerance regions which are specified during the early stages of the development process. Tolerance is necessary to account for changes of design variable values due to later, and therefore unknown, design restrictions. In this sense, early design variables are subject to lack-of-knowledge uncertainty. Tolerance regions for early-decision variables can be significantly increased by the use of late-decision variables. The latter are not equipped with tolerance regions and, by contrast, have to be arbitrarily well adjustable within their design intervals. The values of late-decision variables are chosen in a later development phase when design restrictions are known and may compensate for the choice of early-decision variables. *Solution-compensation spaces* are regions of early- and late-decision variables where for all values of early-decision variables there exist values for late-decision variables from their associated intervals such that all design requirements are satisfied.
A new approach to compute solution-compensation spaces for linear systems is introduced. It is based on an advanced Fourier-Motzkin algorithm which uses H-redundancy removal. The new algorithm is applied to a design problem from vehicle dynamics and shown to outperform the so called *basic projection algorithm* presented in [Vogt et al. 2017].

Structural optimisation on multiple scales based on numerical homogenisation techniques

Wojciech Kijanski (*Numerische Methoden und Informationsverarbeitung, TU Dortmund University*), Franz-Joseph Barthold (*Numerische Methoden und Informationsverarbeitung, TU Dortmund University*)

09:50–10:10

Structural optimisation has a long tradition and has been investigated for many years. Techniques for numerical homogenisation, i.e. FE^2 methods, allow investigations of the physical behaviour of complex heterogeneous materials and lead to a remarkable number of several applications and real world problems, see [2] and references therein for details. A combination of both established methods leads to a significant increase of possible fields of applications and justifies its eminent importance. Besides mathematical algorithms, sensitivity analysis is a fundamental topic within solution strategies for optimisation problems, especially within techniques based on gradient information. Its realisation is responsible for the efficiency and accuracy of used methods. In this context several works conclude that performing sensitivity analysis using variational methods is the most promising approach, see [1] and references therein. The resulting gradients contain sensitivity information about the given overall mechanical system and can be used for further purposes.
The essential steps and principal investigations for the sensitivity analysis for optimisation problems on multiple scales in order to design micro-structures will be outlined and accentuated by some illustrative examples. Consequently, descriptions for design variables, objective functions and constraints on different scales are necessary and have to be introduced.

[1] F.-J. Barthold, N. Gerzen, W. Kijanski, D. Materna. Efficient Variational Design Sensitivity Analysis, *In Book: Mathematical Modeling and Optimization of Complex Structures, Springer* (2016), 229-257.

[2] C. Miehe, C.G. Bayreuther. On multiscale FE analyses of heterogeneous structures: from homogenization to multigrid solvers. *Int. Jour. for Numerical Methods in Engineering* (2007, Vol. 71), 1135-1180.

The Max-Cut Polytope, the Unit Modulus Lifting, and their set-completely-positive representations

Florian Jarre (*Mathematisches Institut, Heinrich-Heine-Universität Düsseldorf*) 10:10–10:30

In this talk a generalization of the "max-cut-polytope" $\text{conv}\{xx^T | |x_k| = 1 \text{ for } 1 \le k \le n\}$ in the space of real symmetric $n \times n$-matrices with all-ones-diagonal is considered to a complex "unit modulus lifting" $\text{conv}\{xx^* | |x_k| = 1 \text{ for } 1 \le k \le n\}$ in the space of complex Hermitian $n \times n$-matrices with all-ones-diagonal. Set-completely positive representations of both sets are derived and the relation of the complex unit modulus lifting to its semidefinite relaxation is investigated in dimensions 3 and 4.

S16.02 | Optimization

Date 20.03.2018
Room N1070

Nonlinear Model Predicitive Control of Complex Articulated Robots using Efficient Multiple Shooting Algorithms

Markus Giftthaler (*ETH Zürich*), Jonas Buchli (*ETH Zurich*), Moritz Diehl (*University of Freiburg*) 16:30–16:50

In this contribution, we show the application of a class of efficient multiple shooting algorithms to solving full-body Nonlinear Model Predictive Control (NMPC) problems in robotics. We demonstrate NMPC on a quadrupedal robot, where the NMPC loop runs at rates greater 100 Hz.
In recent years, numerical optimal control has become a popular tool in robotics, which has led to great progress in motion planning and robot control. However, optimal control problems and NMPC including the full rigid body dynamics for complex articulated robots are often believed to be too difficult to be solved online. In this contribution, we point out that this shortcoming can be overcome by careful algorithmic and software engineering.
In the robotics community, two main trends have evolved for discretizing and solving optimal control problems:

1. Transcribing the problem into a nonlinear program (NLP) using multiple-shooting, single shooting or direct collocation and subsequently solving it using standard NLP solvers such as IPOPT or SNOPT.

2. Using iterative solvers directly derived from the Principle of Optimality such as DDP, or their Gauss-Newton counterparts. These methods are popular due to their overall efficiency and linear time complexity.

The robotics literature often describes those methods as two distinctively different approaches. In fact, this gap does not exist. For example, it has been shown that NLPs can be efficiently solved using Riccati based QP solvers which corresponds to the backward pass in iLQR/DDP. At the same time, iLQR and DDP can be 'lifted' to also add the state trajectory to the decision variables, which effectively results in multiple-shooting variants of iLQR and DDP. We highlight this development resulting in a new formulation, combining the best of both worlds. Such algorithms have linear time complexity, robust initialization properties, increased stability through feedback control and efficiency through multi-threading.
We show an application example of a Gauss-Newton multiple shooting algorithm for NMPC on a quadrupedal robot, which features 36 states and 12 control inputs. We run our solver at rates higher than 100 Hz. These frequencies can be achieved even for long time horizons over 500ms and for complicated locomotion tasks without pre-specified contact sequences, -locations or -timings.

Low latency output feedback predictive control based on optimality conditions

Markus Kögel (*Laboratory for Systems Theory and Automatic Control, Otto-von-Guericke University Magdeburg*), Rolf Findeisen (*Laboratory for Systems Theory and Automatic Control, Otto-von-Guericke University Magdeburg*) 16:50–17:10

State space model predictive control requires full state information. Often the state is estimated from the sensor information. Based on the estimated states, the input is calculated. Reducing the delay – latency -between the measurements and implementing the control action is important, as this avoids discrepancies in the predictions and allows counteracting disturbances fast. Delays might result from long computation times on embedded hardware to obtain the optimal input by solving the underlying optimization problem. We propose an approach which allows splitting the computation of the output feedback control law: First based on the last state estimate a set of control laws is determined. Those are parameterized by the future measurements and calculated using the Karush-Kuhn-Tucker conditions. Once new sensor data are available, the controller selects the corresponding control law to determine the optimal input. This can be achieved with an extremely low computational demand. Implementation aspects such as the control law computation and closed loop properties such as the input-to-state stability of the arising closed loop system are discussed. We furthermore outline an extension towards a cloud based control implementation: The embedded controller connected to the actuator and sensor is often computationally limited for economic reasons or its energy demand should be limited to allow for long battery powered operation. Thus, it is desired to calculate major parts of the optimal control problem on a cloud server or edge device. The embedded controller then uses the precomputed feedback to obtain the control action once new measurements become available.

Towards Optimization with Piecewise Linearization for Non-Smooth Semilinear Elliptic PDEs

Olga Ebel (*Mathematics and its Applications, Paderborn University*), Andrea Walther (*Mathematics and its Applications, Paderborn University*), Stephan Schmidt (*Department of Mathematics, University of Würzburg*) 17:10–17:30

We consider non-smooth PDE constrained problems, where all non-differentiabilities are assumed to be given by piecewise smooth functions such as abs(), min() and max().
The key idea of the optimization method under consideration is locating stationary points via piecewise linearization of the original problem. To this end, we introduce an appropriate decomposition into branch problems such that each of them is smooth and can be solved by classical means. In an outer loop, we use the respective dual variables to chose the next branch problem

for further decrease of the function value. Numerical results are shown for a test problem based on elliptic PDEs proposed by Clason [1].

[1] C. Christof, C. Clason, C. Meyer, and S. Walther, Optimal Control of a Non- Smooth Semilinear Elliptic Equation, submitted to Mathematical Control and Related Fields, 2017

On algorithms based on unions of nonexpansive maps

Matthew Tam (*Georg-August Universität Göttingen*) 17:30–17:50

In this talk, we consider a framework for the analysis of iterative algorithms which can described in terms of a structured set-valued operator. More precisely, at each point in the ambient space, we assume that the value of operator can be expressed as a finite union of values of single-valued nonexpansive-type operators. Structure of this kind arises, for instance, in sparsity optimisation problem. Our main result, which shows that the associated fixed point iteration is locally convergent around strong fixed points, generalises a theorem due to Bauschke and Noll (2014).

Optimization of Deep Drawing Processes by Optimal Control of Elastoplasticity Problems with Finite Deformations

Anna Walter (*Technische Universität Darmstadt*), Stefan Ulbrich (*Technische Universität Darmstadt*) 17:50–18:10

We consider elastoplasticity problems with frictional contact to simulate the deep drawing of sheet metals. Within this process the drawing depth is relatively high compared to the sheet thickness thus we have to deal with large deformations. As it is common we assume a hyperelastic material model where we use a multiplicative split of the deformation gradient into an elastic and a plastic part. For a numerical treatment we rewrite the model as a quasivariational inequality and deploy an implicit time discretization scheme. We reformulate the quasivariational inequalities for frictional contact and plasticity as a system of semismooth equations in order to apply a semismooth Newton method in each time step. In addition we will have a closer look at the energetic formulation stated by A. Mielke. Based on the derived system we formulate the optimal control problem of the deep drawing process in order to get an optimal die filling along with a failure free production. We use a bundle trust region method with an adjoint based subgradient computation to determine the optimal controls such as the internal pressure or the blankholder force.

Composite step method for optimization of equality constrained problems on manifolds

Julian Ortiz (*Department of Mathematics, University of Bayreuth*), Anton Schiela (*Department of Mathematics, University of Bayreuth*) 18:10–18:30

In order to exploit the specific structure of certain problems, we generalize the usual constrained optimization setting in which the involved spaces are linear to the setting where the spaces are manifolds. In the vector space setting, the composite step method deals with the problem of feasibility and optimality by splitting the full Lagrange-Newton correction into a normal step and a tangential step, the update iterates are done by adding these corrections to the actual iterate. We extend these ideas to manifolds by using local retractions, which can be thought as local charts of the manifold. First, we pullback the objective and the constraint mappings to linear spaces, there, we compute the normal and tangential corrections and finally the update of the iterates is done using the retractions defined on the manifolds. We test our method on

equilibrium problems in finite elasticity where the stable equilibrium position of an inextensible transversely isotropic elastic rod under dead load is searched. There, we minimize the total potential energy over the manifold of kinematically admissible configurations that enforce the inextensibility condition. The optimal control problem of Elastic Rods is also considered. Here we minimize the distance to a desired configuration. The constraint mapping is given by the Euler-Lagrange equation of the bending energy affected by the control term. Here the manifold of admissible configurations is also given by the inextensibility of the Rod.
These two examples are test cases for a wider class of problems in which our method can be used. One could, for example, consider torsional effects or contact obstacles giving rise to different manifolds where the optimization problem must be carried out.

S16.03 | Optimization

Date 21.03.2018
Room N1070

On the Confluence of Deep Learning and Proximal Methods

Daniel Cremers (*Informatics & Mathematics, TUM Technische Universität München*), Tim Meinhardt (*TUM*), Thomas Frerix (*TUM*), Thomas Moellenhoff (*TUM*), Caner Hazirbas (*TUM*), Michael Möller (*Universität Siegen*) 14:00–14:40

While numerous low-level computer vision problems such as denoising, deconvolution or optical flow estimation were traditionally tackled with optimization approaches such as proximal methods, recently deep learning approaches trained on numerous examples demonstrated impressive and sometimes superior performance on respective tasks.
In my presentation, I will discuss recent efforts to bring together these seemingly very different paradigms, showing how deep learning can profit from proximal methods and how proximal methods can profit from deep learning. This confluence allows to boost deep learning approaches both in terms of drastically faster training times (Proximal Backpropagation) as well as substantial generalization to novel problems that differ from the ones they were trained for (domain adaptation).
This is joint work with Tim Meinhardt, Thomas Frerix, Thomas Moellenhoff, Caner Hazirbas and Michael Moeller.

Adaptive FISTA

Peter Ochs (*Saarland University*), Thomas Pock (*TU Graz*) 14:40–15:00

An optimized extrapolated proximal gradient method is presented and relations to proximal quasi-Newton methods are revealed. The generic form of the proposed update scheme is related to the accelerated proximal gradient method (also known as FISTA), however we adapt the extrapolation parameter locally. Convergence is proved in a general non-convex setting. For convex functions two variants with $O(1/k^2)$-convergence rate where k is the iteration count are presented. Using the equivalence to proximal quasi-Newton methods, new convergence guarantees for these methods are obtained. In particular, the results apply to a class of zero memory SR1 proximal quasi-Newton methods (identity minus rank 1 method). The efficiency of the method is shown for several examples.

Optimal EPO dosing in hemodialysis patients using model predictive control

Sabrina Rogg (*Fresenius Medical Care Deutschland GmbH*), Doris Fürtinger (*Fresenius Medical Care Deutschland GmbH*), Stefan Volkwein (*Mathematics and Statistics, University of Konstanz*), Franz Kappel (*Karl Franzens Universität*), Peter Kotanko (*Renal Research Institute New York*) 15:00–15:20

Anemia management with erythropoiesis stimulating agents is a difficult task in hemodialysis patients since their response to treatment varies highly. The aim is to stabilize hemoglobin levels within a narrow target window while keeping drug doses low to mitigate side effects and further reduce costs. Based on a model of erythropoiesis, which contains a number of personalized parameters, we present a non-linear model predictive control (NMPC) algorithm for the individualized optimization of EPO (Epoetin alfa) doses. The optimal control problem is formulated for a continuous drug administration at a daily or multiple-day constant rate. In each step of the NMPC method the open loop problem is solved with a projected BFGS method. The controller is successfully tested on various patient data sets and it satisfactorily handles the following challenging problems: bleedings, missed treatments and wrongly administered doses. Moreover, we analyze the effect of restricting EPO administration rates to be constant over a number of weeks.

A sequential homotopy method for unconstrained optimization problems

Andreas Potschka (*Interdisciplinary Center for Scientific Computing, Heidelberg University*) 15:20–15:40

We consider the problem of finding a local minimum of a twice continuously differentiable function $f : D \subseteq \mathbb{R}^n \to \mathbb{R}$. The main challenge for efficient numerical solution methods of this standard problem is the appropriate treatment of nonconvexity, degeneracy, and large scale. We attack these challenges through the successive partial solution of nonlinear homotopies, which aim to drive a proximal-type regularization of f to zero. If one of the homotopies can be solved entirely, we obtain a local minimum of f after a finite number of steps. Otherwise, the sequential homotopy approach generates a sequence of iterates whose accumulation points are stationary points of f. For the numerical solution of each homotopy subproblem, we employ a corrector-free path-following method based on backward step control with inexact solution of the linearized problems with a preconditioned conjugate gradient method. Numerical results on the unconstrained problems of the CUTEst test set indicate that our method performs competitively with a state-of-the art trust-region method in terms of computational speed, but tends to deliver better local optima in terms of the attained objective values. We close the talk with an outlook on extensions to constrained optimization problems.

Open Source Nonlinear Optimization Algorithms for Embedded Model Predictive Control

Moritz Diehl (*Department of Microsystems Engineering and Department of Mathematics, University of Freiburg*) 15:40–16:00

When nonlinear optimization problems are solved in the context of embedded model predictive control, efficient memory and CPU usage are as important as tailored numerical methods. The basic algorithmic ingredients of all direct optimal control methods are (a) numerical simulation and derivative generation, and (b) the solution of sparse symmetric linear systems or, more general, sparse quadratic programs. In this talk, we review some progress that has been made

between 2012 and 2018 in the second field. Most of the algorithms that will be presented and compared in the talk are available as open source (LGPL) code in the C++ optimal control packages ACADO [1], CasADi [2], as well as in the upcoming plain C toolbox acados [3], which all have additional user interfaces to high level environments such as Python, MATLAB, or Octave.
The progress highlighted in this talk regards the efficient solution of sparse quadratic programs as they arise in the direct multiple shooting method. Here, numerical advances in Riccati-based interior point and active set methods were complemented by the development of dense linear algebra routines that are tailored to block sparse embedded optimization problems, which alone turned out to lead to speed-ups of a factor of 2-10, and that have recently be made publicly available in the BLASFEO package [4].
The talk presents joint work with Gianluca Frison, Dimitris Kouzoupis, Tommaso Sartor, Branimir Novoselnik, Yuning Jiang, Andrea Zanelli, and Robin Verschueren.

[1] B. Houska, H. J. Ferreau, M. Diehl: ACADO Toolkit - An Open Source Framework for Automatic Control and Dynamic Optimization. Optimal Control Applications and Methods (2011)

[2] J. Andersson, J. Gillis, G. Horn, J. B. Rawlings, and M. Diehl: CasADi–a software framework for nonlinear optimization and optimal control. Submitted for publication in Mathematical Programming, 2017

[3] www.acados.org

[4] G. Frison, D. Kouzoupis, A. Zanelli, M. Diehl: BLASFEO: Basic linear algebra subroutines for embedded optimization. arXiv preprint 1704.02457 (2017)

S16.04 | Optimization

Date 21.03.2018
Room N1070

Riemannian BFGS methods for low-rank matrix and tensor completion

Gennadij Heidel (*Universität Trier*), Wen Huang (*Rice University*), Volker Schulz (*Universität Trier*), Bart Vandereycken (*University of Geneva*) 16:30–16:50

The recovery of partially known matrices and tensors under a rank restriction has attracted considerable interest is recent research. Riemannian optimization has been shown to be a powerful paradigm for these problems, since it avoids explicitly building any large, full structures (matrices or tensors); Riemannian nonlinear CG and trust-region methods have been discussed in recent literature.
On the other hand, a practical generalization of the BFGS quasi-Newton scheme, one of the most popular methods from nonlinear optimiation, has long remained an open problem. Based on results from recent literature on efficient vector transports on Riemannian manifolds, we present a (limited-memory) Riemannian BFGS method on low-rank matrix and tensor manifolds, which is compitationally efficient and has advantegeous theoretical properties.

Newton-Secant type's method for solving the nonlinear least squares problem

Roman Iakymchuk (*Computational Science and Technology, KTH Royal Institute of Technology*), Halyna Yarmola (*Ivan Franko National University of Lviv*), Stepan Shakhno (*Ivan Franko National University of Lviv*) 16:50–17:10

We propose an iterative differential-difference method for solving the nonlinear least squares problem. This method is based on the Gauss-Newton method [1] and the Secant method [2] and it uses the sum of derivative of the differentiable part of the operator and divided difference of the nondifferentiable part instead of computing Jacobian. To note, this approach works well for solving nonlinear equations [3]. We prove local convergence of the studied method under the generalized and classical Lipschitz conditions. Furthermore, we conduct a set of experiments on test problems; present their numerical results; and show that the method is high performing, especially, compared to the Secant method and the Gauss-Newton type's method.

[1] J. M. Dennis and R. B. Schnabel. *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*. SIAM, Philadelphia, 1996.

[2] S. Shakhno and O. Gnatyshyn. *On an iterative algorithm of order 1.839... for solving the nonlinear least squares problems*. Appl. Math. Comp., 161, (2005), 253-264.

[3] S. Shakhno, I. Melnyk, and H. Yarmola. *Analysis of the convergence of a combined method for the solution of nonlinear equations*, J. Math. Sci., 212 (2014), 32-43.

Consensus-Based Global Optimization

Claudia Totzeck (*Mathematik, TU Kaiserslautern*)

17:10–17:30

We discuss a first-order stochastic swarm intelligence model in the spirit of consensus formation, namely a consensus-based optimization algorithm, which may be used for the global optimization of a function in multiple dimensions. The algorithm allows for passage to the mean-field limit resulting in a nonstandard, nonlocal, degenerate, parabolic PDE. Exploiting tools from PDE analysis we provide convergence results that help to understand the asymptotic behavior of the swarm intelligence model. In fact, under some assumptions it is possible to show the convergence of the algorithm to a state that lies arbitrarily close to the global minimum of the objective function. Further, one can obtain a convergence rate. Numerical results underline the feasibility of the approach.

Pareto Front Interpolation Based on Parametric Sensitivity Analysis in a Bi-Objective Setting

Arne Berger (*Center for Industrial Mathematics (ZeTeM), University of Bremen*), Matthias Knauer (*Center for Industrial Mathematics (ZeTeM), University of Bremen*), Christof Büskens (*Center for Industrial Mathematics (ZeTeM), University of Bremen*)

17:30–17:50

In order to solve non-linear multiobjective optimization problems, one usually solves multiple scalarized subproblems. This provides a discrete approximation of the Pareto front which gives usefull information for the decision maker who, in praxis, has to select one single solution. If the desired solution is not part of the precomputed discrete approximation one needs to apply interpolation techniques.
This contribution shows a method which uses information from parametric sensitivity analysis of the scalarized subproblems in order to obtain a better interpolation between precomputed solutions. The problems are solved with the NLP solver WORHP which provides sensitivity information in an efficient way by reusing the factorization of the KKT matrix of the last optimization iteration. We show the basic functionality of the presented method by applying it to several bi-objective optimization problems. The method can also be used for more than two objectives if one can identify the neighboring precomputed points which are than used for interpolation.

A stochastic semi-smooth Newton method for convex composite problems

Andre Milzarek (*Beijing International Center for Mathematical Research, Peking University*), Xiantao Xiao (*Dalian University of Technology*), Shicong Cen (*Peking University*), Zaiwen Wen (*Beijing International Center for Mathematical Research, Peking University*) 17:50–18:10

In this talk, we present a globalized semi-smooth Newton method for solving stochastic optimization problems involving smooth nonconvex and nonsmooth convex terms in the objective function. More specifically, we assume that the smooth part of the objective function can be written as the expectation of a given smooth loss function or that only noisy gradient and Hessian information is available. The resulting class of problems that can be solved with our algorithmic framework comprises a variety of interesting applications such as l1-logistic regression, structured dictionary learning, and other minimization problems arising in machine learning or statistics. The approach we investigate utilizes stochastic second order information and sub-sampled semi-smooth Newton steps for a prox-type fixed-point equation to accelerate the basic stochastic proximal gradient method for convex composite programming. Approximate growth conditions are introduced to monitor the quality and acceptance of the Newton steps and to combine the two different algorithms. We prove that the proposed approach converges globally to stationary points in expectation and almost surely. Moreover, under standard assumptions, the method can be shown to locally turn into a pure semi-smooth Newton method and fast local convergence can be established with high probability. Finally, we provide numerical experiments illustrating the efficiency of the stochastic semi-smooth Newton method.

A Nonconvex Primal-Dual Algorithm under Moreau-Yosida Regularization

Emanuel Laude (*Chair for Computer Vision & Artificial Intelligence, TUM Technische Universität München*), Tao Wu (*TUM Technische Universität München*), Daniel Cremers (*TUM Technische Universität München*) 18:10–18:30

We tackle composite optimization problems whose objectives are (highly) nonconvex and nonsmooth. Classical nonconvex proximal splitting algorithms, such as nonconvex ADMM, suffer from lack of convergence for such a problem class. In this work, we consider a Moreau-Yosida regularized variant of the original model and propose a novel multiblock primal-dual algorithm on the resulting lifted problem. We provide a complete convergence analysis of our algorithm, and identify respective optimality qualifications under which stationarity of the regularized problem is retrieved at convergence. Numerically, we demonstrate the relevance of our model and the efficiency of our algorithm on robust regression as well as joint variable selection and transductive learning.

S16.05 | Optimization

Date 22.03.2018
Room N1070

Multi-Disciplinary Design Optimization of Missile Fin Configuration

Bosko Rasuo (*Faculty of Mechanical Engineering, University of Belgrade*), Nenad Vidanovic (*Faculty of Transport and Traffic Engineering, University of Belgrade*), Gordana Kastratovic (*Faculty of Transport and Traffic Engineering, University of Belgrade*) 08:30–08:50

In this study, with respect to predefined critical multi-point exploitation regimes, objectives and constrains, multi-disciplinary design optimization (MDO) was carried out on a scaled ballistic missile wind tunnel model configuration, in order to achieve global improvement of initial aerodynamic-structural responses. This paper establishes and demonstrates significant capacity and performances of a well predictive monolithic, multi-modular and on commercial code-based numerical environment, developed for MDO purposes, which presents one more contribution in cases of fluid-structure interaction (FSI) numerical modelling. The accuracy of numerical prediction of the aerodynamic and structural modules and FSI sub-environment was established through validation and verification procedures with respect to conducted experimental results and available published results. The proposed environment with very good overall computational efficiency and accuracy enables achieving optimal structure, with improved performances and high exploitation reliability throughout critical multi-point regimes in boost phase.

Coupled Analysis for Pin-fin Optimization using RSM model

Xiang Wang (*Xi'an Jiaotong-Liverpool University*), Min Chen (*Xi'an Jiaotong-Liverpool University*), Derrick Tate (*Xi'an Jiaotong-Liverpool University*), Shunqi Zhang (*Shanghai University*) 08:50–09:10

Pin-fins are widely used in the heat sink of electronics cooling system to enhance the heat transfer efficiency. There are many factors, like material, geometry or distribution of pin-fins, influencing the cooling performance. Most available research focuses on single factor for heat transfer and head loss, such as inline and staggered arrangement, size and height. Meanwhile few researcher consider comprehensively the influence of multiple factors on heat transfer and pressure loss based on uniform design (UD). This study aims to find out the optimized solution for coupled effects of parameters. Different turbulence models were studied and RSM (Response Surface Methodology) was the most appropriate one to deal with analysis of variables relativity and reduction of error compared with UD. A pin-fin cooling structure for PCU (Power Control Unit) in electric vehicle was used as a validation case. Less head loss and better cooling efficiency are achieved from redesign of the cooling structure with optimal shape, dimensions and interval space.

Optimization Framework for Process and Shape Optimization in High-Pressure Die Casting

Markus Frings (*Chair for Computational Analysis of Technical Systems, RWTH Aachen University*), Marek Behr (*Chair for Computational Analysis of Technical Systems, RWTH Aachen University*), Stefanie Elgeti (*Chair for Computational Analysis of Technical Systems, RWTH Aachen University*) 09:10–09:30

High-pressure die casting (HPDC) is a manufacturing method for mass production. The main cost drivers for HPDC parts are the die and process design. In addition, the quality of the designs is largely influenced by the experience of the particular designer.
Since computing power becomes widespread, it is a straightforward step to assist the designer with numerical optimization. This contribution proposes an optimization framework that couples the optimization library Dakota with different flow solvers. The application of the framework is shown for the shot curve design and the flow channel design.
The shot curve describes the motion of the plunger. This mainly influences the first phase of the process. During this phase the plunger moves the molten metal inside the shot sleeve towards the cavity. Breaking waves that occur during this phase cause air entrapment which leads to defects in the resulting cast part. Therefore, the optimization aims to minimize this air entrapment.
As a second application, the temperature control channels are optimized. The die is equipped with flow channels that should remove the heat while the cast part solidifies. A good flow channel design enables a large heat transport, which results in short cycle times. In addition it is important that the cast part is cooled homogeneously to avoid residual stresses. The optimization tries to reach this goals by modifying the path of the flow channels inside the die.
The presentation will address the numerical optimization methods that are used to find optimal die and process designs.

Sensitivity Analysis of Nonlinear Structural Response regarding Geometry and External Loads

Jan Liedmann (*Numerical Methods and Information Processing, TU Dortmund University*), Franz-Joseph Barthold (*Numerical Methods and Information Processing, TU Dortmund University*) 09:30–09:50

In the field of structural design optimization, the term *design* is often used in an abstract manner, as it can stand for geometry, material, topology, etc. The combination and optimization of different design parameterizations within an optimization process is challenging. Utilizing gradient based optimization strategies, e.g. SQP, implies the computation of structural response sensitivities regarding all chosen design parameters.
In this context the variational approach to compute response sensitivities, proposed by Barthold [1] is advantageous, as it is based on an enhanced kinematic concept that offers a rigorous separation of structural and physical quantities. Additionally, it allows simultaneous determination of the structural response and response sensitivities within a finite element framework, c.f. [2].
The arising gradient information, especially the sensitivity and pseudo load matrices, can further be examined using *Singular Value Decomposition (SVD)*. The resulting *internal structures of sensitivities*, as introduced in [3] and incorporated in [4], that is the eigen- and singluar values and vectors of the gradient information, reveal minor and major influence of design parameters on the structural response. Hence, gradient information can be filtered and the optimization problem can be accurately redefined.
The above methods are applied to optimization problems considering the combination of geometry and external loads as design parameters. Nonlinear elastic-plastic material behavior is considered to widen the range of possible materials, as the approach might be of special interest in the context of forming processes and damage control. Numerical and algorithmic implementation is presented and demonstrated in selected numerical examples.

[1] Barthold, F.-J.: Zur Kontinuumsmechanik inverser Geometrieprobleme. Habilitation. Braunschweiger Schriften zur Mechanik 44-2002, TU Braunschweig (2002)

[2] Barthold, F.-J. et al.: Mathematical Modelling and Optimization of Complex Structures. Springer International Publishing. Chap. Efficient Variational Design Sensitivity Analysis, pp. 229-257. (2016)

[3] Gerzen, N.: Analysis and Applications of Variational Sensitivity Information in Structural Optimisation, Dissertation. TU Dortmund (2014)

[4] Liedmann, J. and Barthold, F.-J.: Exploration of Internal Response Sensitivities of Materially Nonlinear Structures, PAMM (2017)

An accurate and fast regularization approach to thermodynamic based topology optimization

Dustin Roman Jantos (*Ruhr-Universität Bochum*), Philipp Junker (*Ruhr-Universität Bochum*), Klaus Hackl (*Ruhr-Universität Bochum*) 09:50–10:10

Many methods for topology optimization with compliance minimization under volume constraint exist, most of them base on continuous density methods. In our previous work, we introduced a variational approach derived from thermodynamical principles, i.e. Hamilton's principle for dissipative processes. The Hamilton principle directly yields evolution equations providing an (non heuristic) iterative update scheme for the design variables of the problem, requiring no additional (mathematical) minimization algorithms.
We enhance our approach to reduce the calculation effort and improve the overall results. We introduce a regularization by penalizing the gradient of the density field, which gives us a well-posed optimization problem. The gradient is evaluated on the strong form of the mechanical equilibrium, which includes a Laplace operator. The resulting parabolic partial differential equation is solved by a finite difference method requiring minimal calculation effort. The regularization yields mesh-independent results without checkerboarding. No additional filtering techniques are introduced and the complexity of the structure can be controlled a priori by a numerical parameter introduced along with the gradient penalization.

S16.06 | Optimization

Date 22.03.2018
Room N1070

Optimal design of energy networks for settlements involving renewable energies

Kristina Janzen (*TU Darmstadt*) 14:00–14:20

The trend towards sustainable energy supply and the corresponding impact of environmental aspects lead to an increasing complexity in terms of energy utilization, implying major challenges for decentralized energy supply. We present an optimization model of a coupled energy network of multiple energy carrier systems as well as renewable energy sources for settlements to determine the optimal design of the energy network that minimizes the investment and operational costs. Modelling the acquisition and operation of different technologies and discrete sizes of equipment yields to discrete integer decision variables. The energy transmissions as well as the energy generation through renewable energies is modelled using nonlinear equations resulting in a mixed-integer nonlinear optimization problem (MINLP). We present representative problem instances of the MINLP, and model them using the algebraic modelling language AMPL. We show initial numerical results for specific settlements, and compare different energy production scenarios in terms of price and availability.

Double-stage optimization of frame structures

Alexander Keller (*Karlsruher Institut für Technologie (KIT) - Institut für Baustatik*), Ingo Münch (*Karlsruher Institut für Technologie (KIT) - Institut für Baustatik*), Werner Wagner (*Karlsruher Institut für Technologie (KIT) - Institut für Baustatik*) 14:20–14:40

For the design of structures in civil engineering we are interested in an approach to combine topology optimization and shape optimization. Therefore, we use a phase field model to generate topology first. Next, shape optimization with a genetic algorithm is performed. Thus, topology optimization generates the design concept and shape optimization tunes the structure.
The phase field model is a continuum model, where hinges, cross sections and other details are not under consideration. Therefore, it is meaningless to estimate the fitness of evolved topologies at this stage of the concept. An interface just uses the topology to proceed with the second step of our concept. Then, sophisticated criteria required from civil engineering are faced with metaheuristic shape optimization. A genetic algorithm considers all practical demands, e.g., the variation of hinges, details in the design space, stress conditions, displacement restrictions, position of connections, etc. The genetic algorithm does not guarantee a global optimum but generally succeeds in finding an optimized solution even for complex systems. Several runs with different initial populations estimate the variation of the obtained solutions. Then, a master run uses the solutions from several runs as initial population to judge the result. We present analytical solutions to prove our results. From our point of view, this is one of several general principles to enhance the double-stage optimization of frame structures. Our aim is to provide a software tool on a high level of automatization.

Stacking Sequence Optimization of Multilayer Composite Materials

Simon Loske (*Numerical Methods and Information Processing, Faculty of Architecture and Civil Engineering, TU Dortmund University*), Franz-Joseph Barthold (*Numerical Methods and Information Processing, Faculty of Architecture and Civil Engineering, TU Dortmund University*) 14:40–15:00

The use of composite materials in various types of devices has increased steadily in the past decades. Hence it is worth investigating into the structural behaviour of these materials. The optimization of stacking sequences in multilayer composite materials opens a large field of improvements in industrial applications of composite materials. The center of investigation is set on fiber reinforced laminate plies, which are examined in the case of linear anisotropic theory of elasticity. As element formulation a non-linear solid shell element based on a mixed variational formulation by Klinkel [1] is chosen. For these mechanical systems, the modeling approach using lamination parameters is consulted. Under application of these lamination parameters, an optimization problem is formulated which uses an optimization procedure based on the SQP algorithm that optimizes the material properties of laminates to maximize the stiffness of the considered system.
The material properties obtained by the optimization of the lamination parameters are converted into possible stacking sequences for laminates by using simplified approaches. The optimization of material based on lamination parameters is combined with the optimization of geometry on the basis of variational sensitivity analysis introduced by Gerzen [2]. The combination of these two optimization approaches yields an optimal design of devices made of laminated composite materials. Considering different examples of components, the results of the optimization are analysed and possible ways for the improvement of the quality of the results are revealed.

[1] S. Klinkel, F. Gruttmann, W. Wagner, A robust non-linear solid shell element based on a mixed variationalformulation, Comput. Methods Appl. Mech. Engrg. 195 (2006) 179–201.

[2] N. Gerzen, F. J. Barthold, S. Klinkel, W. Wagner, D. Materna, Variational sensitivity analysis of a nonlinear solid shell element, Int. J. Numer. Meth. Engng. 96, 29 – 42 (2013)

Sensitivity Analysis of a Non-Local, Gradient Enhanced Damage Model

Fabian Guhr (*Numerische Methoden und Informationsverarbeitung, TU Dortmund University*), Franz-Joseph Barthold (*Numerische Methoden und Informationsverarbeitung, TU Dortmund University*) 15:00–15:20

Forming and deformation of a material induces damage into the micro-structure with macroscopic effects. This results in a weakened final product or immediate failure during the forming process. Structural optimisation can be used to generate a structure, where the present damage is minimised or under a certain threshold.
Using the finite element method, the mesh is constructed by control points, which are the necessary quantities to define the geometric design of the structure. A minimisation of an objective function with respect to these design variables leads to the optimised solution. Using gradient based methods, e.g. SQP, the sensitivities of the structural response are required. These can be calculated by means of a variational approach, which allows a separation of the structural from the physical quantities. The resulting sensitivities can then be incorporated into the numerical framework. Choosing the damage as the objective function or including it as a constraint of the optimisation, the framework can be used to generate optimised structures with a reduced damage state.
The above method is applied to an isotropic, non-local damage model. The model is enhanced by the gradient of the damage to generate mesh-independent behaviour. Due to its formulation, no local calculations are necessary. Minimisation with respect to the control points is then used to generate an optimised structure, where reduced damage is present. First, a volume minimisation with the damage as constraint is presented and analysed and afterwards compared to a direct damage minimisation, showing the effect on the optimised structure.

Stochastic two-dimensional decomposition of high-dimensional solution spaces for robust design

Dennis Tröndle (*Universität Basel*) 15:20–15:40

In the early design process of a vehicle, we would like to save resources by reducing the need for the designers to check for compatibility of their proposed vehicle components. We do this by assigning each designer an interval wherein each design is admissible. The product over all these intervals forms a high-dimensional, axis-parallel box. Given a space of admissible desgins $\Omega_{\text{ds}} \subset \mathbb{R}^n$, a threshold value $c \in \mathbb{R}$, and a scalar function $f : \Omega_{\text{ds}} \to \mathbb{R}$, a semi-infinite optimization problem can be formulated as follows: Maximize the volume $\mu(\Omega_{\text{box}})$ over all axis-parallel boxes

$$\mu(\Omega_{\text{box}}) \to \max_{\Omega_{\text{box}} \subset \Omega_{\text{ds}}}$$

subject to

$$f(\mathbf{x}) \leq c \text{ for all } \mathbf{x} \in \Omega_{\text{box}}.$$

At first, we will give a survey of an algorithm that produces these boxes. Building up on this, we show two improved algorithms that replace the axis-parallel box by either a rotated box or a polygon.

Structural Optimisation Using Parametrised Level Set Methods and Extended Finite Element Method

Felix Wohlgemuth (*Faculty of Architecture and Civil Engineering, Numerical Methods and Information Processing, TU Dortmund University*), Franz-Joseph Barthold (*Faculty of Architecture and Civil Engineering, Numerical Methods and Information Processing, TU Dortmund University*) 15:40–16:00

In the framework of level-set-based optimisation, several approaches to solve bi-material and topological problems have been developed. In this study, a combined concept of different approaches is introduced, joining together a parametrised geometry description with superellipses as in the work of *Noel 2010* and a modified approach for the extended finite element method within an optimisation setup of topological and shape iterations as introduced by *Allaire 2004*. The parametrisation with superellipses allows us to reduce the number of design variables to a minimum which is six per introduced ellipse, whereas we hold up a sufficient precision in the geometrical description. Moreover, it simplifies the shape derivatives as we gain an implicit description for the moving interfaces. In order to solve the boundary value problem in structural mechanics we introduce a modified extended finite element c.f. *Barthold 2015* approach which uses a sub meshing technique that makes it possible to keep existing strategies from homogeneous structures and transform them on a discontinuous material using enriched shape functions provided by the standard extended finite element method. Shape sensitivities are evaluated on the sub elements and extrapolated to the element nodes. The topological derivative as developed by *Novotny 2007* is evaluated and prescribes the initiation of new discontinuities as inclusions or holes. The optimisation results are discussed regarding algorithmic difficulties and inaccuracies in the sensitivity analysis due to ill-conditioning of the system matrices and insufficient mapping assumptions.

S16.07 | Optimization

Date 22.03.2018
Room N1070

A Multi-fidelity Approach Using Physical and Mathematical Surrogates for Crash Optimization

Koushyar Komeilizadeh (*Computational Mechanics, TUM BGU*), Rafael Hefele (*Technical University of Munich*), Fabian Duddeck (*Technical University of Munich, Queen Mary University of London*) 17:30–17:50

In crashworthiness optimization, contradicting demands have to be met. While increasing safety requirements can lead to additional weight through reinforced structures, environmental protection calls for enhanced fuel efficiency and therefore reduced weight. The high fidelity FEM models used to process such optimizations are computationally expensive; therefore, a small number of required function evaluations is desirable. Surrogate models offer the possibility to optimize expensive functions through physical simplification or mathematical approximation of the systems behavior.
We propose to combine information from physical and mathematical surrogate models to exploit the advantages of both. In this regard, we include gradients from the ESL (Equivalent Static Loads) method into the infill sampling criteria of the 'Efficient Global Optimization' (EGO) approach. Since gradients from ESL are not accurate, the proposed method takes uncertainty into account using a formulation based on the Gaussian function. To prove the effectiveness of

the approach, three steps were made: (1) mathematical test-functions were optimized using FD (Finite Differences) with artificial Gaussian noise to simulate inaccurate ESL-gradients, (2) a five bar truss with linear materials and constant loads was optimized, again using FD with artificial noise, and last (3) we optimized the thicknesses of a side sill in the side pole impact using finite element analysis and ESL-gradients in combination with the 'Expected Improvement' criterion. The results show that the proposed approach can lead to faster improvement in all cases. For the five bar truss a significantly better result was reached, while for the side sill much faster improvement was achieved.

Nonsmooth Shape Optimization with Stress Constraints for Contact Problems based on Isogeometric Analysis

Benjamin Manfred Horn (*Technische Universität Darmstadt*), Stefan Ulbrich (*Technische Universität Darmstadt*) 17:50–18:10

We present an application of nonsmooth optimization techniques to a shape optimization problem for mechanical connectors including stress constraints. For this purpose, we follow the approach of an algorithm based product development, which couples the CAD system with the finite element simulation used by the mathematical optimization. To ensure a consistent model representation, we choose an isogeometric approach to model the contact problem within the optimization method. This leads to a shape optimization governed by an elastic contact problem with friction. The frictional contact problem itself is modeled by a mortar approach using dual basis functions and solved by a semismooth Newton method. Based on the damage parameter of Smith, Watson and Topper, also called PSWT, we include stress constraints to guarantee a predefined level of fatigue strength. To determine the PSWT we calculate approximated elasto-plastic strains and stresses using the von-Neuber hypothesis and the Ramberg-Osgood material law. The resulting shape optimization problem is nonconvex and due to the contact conditions and the chosen objective functions nonsmooth. We solve this optimization problem with a bundle trust region algorithm, which is modified to ensure a feasible shape in each iteration. The design subgradients required by the bundle method can be calculated efficiently with the adjoint approach.

Influence of Cruising Mach Number Over a Global Optimized Shape of Flying Configuration, in Supersonic Flow

Adriana Nastase (*LAF, RWTH Aachen*) 18:10–18:30

A global optimized (GO) shape of a flying configuation (FC) has its distributions of camber and twist and also of the similarity parameters of its planform, simultaneously optimized, in order to have a minimum drag, at cruising Mach number. The determination of the GO shape of FC leads to an enlarged variational problem with free boundaries. The author has proposed a special strategy, called optimum- optimorum theory, by introducing a lower limit hypersurface of the drag functional as function of the set of considered similarity parameters of the planform of some elitary FCs (with optimized shapes of their surface but with several fixed planforms), belonging to the same class. The shape of the elitary FC of the class, which corresponds to the position of the minimum of this lower limit hypersurface, is also the GO FC of this class. The author has designed three models with GO shapes namely: the delta wing alone ADELA and two fully-integrated wing-fuselage FCs FADET I and FADET II. These models,are GO at cruising Mach numbers 2 , 2.2 and respectively, 3. All these models have the same area of their planform. The models FADET I and FADET II satisfy the same constraints and are good suited for the determination of the influence of the change of cruising Mach number over the shape of the surface and of the planform of a GO model. If the cruising Mach number increases, the

camber and the twist of FC increase and an important increase of its aspect ratio is observed. A morphing of the shape of the wing of supersonic aircraft, by using small movable leading edge flaps (in retracted position by a higher cruising Mach number by the flight over the sea and in stretched position by start, by landing and by the flight over the land) is useful for the performing of a multipoint global optimal design.

S17 | Applied and numerical linear algebra

Organiser Iveta Hnetynkova (*Department of Numerical Mathematics, Charles University, Faculty of Mathematics and Physics*)
Robert Luce (*École polytechnique fédérale de Lausanne*)

S17.01 | Applied and numerical linear algebra

Date 20.03.2018
Room 1402

Numerical integrators for rank-constrained differential equations

Bart Vandereycken (*Mathematics, University of Geneva*) 08:30–09:10

We present discrete methods for computing low-rank approximations of time-dependent tensors that can be the solution of a differential equation. The format for the low-rank approximation can be Tucker, tensor trains, MPS or hierarchical tensors. We will consider two types of discrete integrators: projection methods based on quasi-optimal metric projection, and splitting methods based on inexact solutions of substeps. For both approaches we show numerically and theoretically that their behavior is superior compared to standard methods applied to the so-called gauged equations. In particular, the error bounds are robust in the presence of small singular values of the tensor matricisations. Based on joint work with Emil Kieri, Christian Lubich, and Hanna Walach.

Low-rank solvers for Isogeometric analysis in PDE-constrained optimization

Alexandra Buenger (*Faculty of Mathematics, TU Chemnitz*), Martin Stoll (*TU Chemnitz*) 09:10–09:30

Isogeometric analysis is an extremely popular method for the discretization of partial differential equations motivated by the use of NURBS for representing geometries in industry and science. The assembly of the mass and stiffness matrices is typically very costly. To reduce the computing time and storage requirements low-rank tensor methods have become a promising tool. We present a framework for the assembly of these matrices in low-rank form as the sum of a small number of Kronecker products. We then show that these can be used within a PDE-constrained optimization problem and present an efficient solver for the corresponding KKT system. We illustrate the performance of the method on various examples.

Low-Rank Fluid Structure Interaction Discretization

Roman Weinhandl (*Max-Planck-Institut für Dynamik komplexer technischer Systeme*), Peter Benner (*Max-Planck-Institut für Dynamik komplexer technischer Systeme*), Thomas Richter (*Otto-von-Guericke Universität Magdeburg*) 09:30–09:50

In my talk I present low-rank discretizations of a parameter dependent stationary fluid structure interaction problem [3]. The fluid structure interaction problem depends on many parameters, such as the shear modulus of the solid and the dynamic fluid viscosity. Assume $m \in \mathbb{N}$ samples of shear moduli combined with dynamic viscosities are of interest. Each sample pair yields a separate FSI problem. Finite element discretization with $n \in \mathbb{N}$ degrees of freedom results in systems of equations of the form

$$(A_0 + \mu_s^i A_1 + \eta_f^i A_2)x = b \text{ for } i \in \{1, ..., m\}, \tag{1}$$

where $A_0, A_1, A_2 \in \mathbb{R}^{n\times n}$, $b \in \mathbb{R}^n$ and the finite element solution $x \in \mathbb{R}^n$. The material parameters μ_s^i and $\eta_f^i \in \mathbb{R}$ correspond to the ith sample of the shear modulus of the solid and the dynamic fluid viscosity, respectively.

Problem (1) can be translated into the matrix equation

$$A_0X + A_1XD_1 + A_2XD_2 = B, \tag{2}$$

where D_1, $D_2 \in \mathbb{R}^{m\times m}$ and $B \in \mathbb{R}^{n\times m}$. (2) is much more feasible to compute than m systems of equations as in (1) since n is already very big in a typical fluid structure interaction setting. The goal is approximating $X \in \mathbb{R}^{n\times m}$, the solution to (2), by a low-rank representation. In contrast to [2] this will be done using a low-rank approach based on the GMRES method similar to [1] specialized to the fluid structure interaction.

[1] J. Ballani and L. Grasedyck. *A projection method to solve linear systems in tensor format*, Numerical Linear Algebra With Applications, (2012), pp. 27-43.

[2] D. Kressner and C. Tobler. *Low-rank tensor Krylov subspace methods for parametrized linear systems*, SIAM J. Matrix Anal. and Appl., (2011), pp. 1288-1316.

[3] T. Richter. *Fluid-Structure Interactions - Model, Analysis and Finite Elements*, Springer, 2017.

Low rank updates and a divide and conquer method for matrix equations

Stefano Massei (*Applied Mathematics, Ecole Polytechnique Fédérale de Lausanne (EPFL)*), Daniel Kressner (*Ecole Polytechnique Fédérale de Lausanne (EPFL)*), Leonardo Robol (*ISTI-CNR Pisa*)

09:50–10:10

In this work we study how the solutions of certain linear matrix equations behave when the original coefficients are modified with low-rank perturbations. More precisely, given the solution X of the Sylvester equation $AX + XB = C$, and 3 low-rank matrices $\delta A, \delta B$ and δC, we are interested in characterizing the update δX that verifies

$$(A + \delta A)(X + \delta X) + (X + \delta X)(B + \delta B) = C + \delta C.$$

Under assumptions often satisfied in applications, δX turns out to have a low numerical rank and allows to be efficiently approximated by means of either low-rank ADI or Krylov subspace techniques. We show how to exploit this property to design divide and conquer methods for solving large-scale Sylvester equations whose coefficients are represented in hierarchical formats such as HODLR and HSS. This comprises the case of banded and quasiseparable coefficients that recently has received some attention.

Efficient Preconditioning of hp-FEM Matrices by Hierarchical Low-Rank Approximations

Paolo Gatto (*RWTH Aachen University*), Jan Hesthaven (*Ecole Polytechnique Fédérale de Lausanne (EPFL)*)

10:10–10:30

In this talk I will introduce a preconditioner based on low-rank compression of Schur complements. The construction is inspired by the well-known nested dissection strategy, and relies on the assumption that the Schur complements that arise in the elimination process can be

approximated, to high precision, by compressible matrices. The preconditioner is built as an approximate LDM^t factorization of a given matrix A, and no knowledge of A in assembled form is required by the construction. The LDM^t factorization is amenable to fast inversion, and the inverse can be applied fast as well. I will present numerical experiments that investigate the behavior of the preconditioner in the context of Discontinuous Galerkin finite element approximations of positive-definite problems, as well as indefinite wave propagation problems.

S17.02 | Applied and numerical linear algebra

Date 20.03.2018
Room 1402

Inexact rational Krylov subspace methods for large matrix equations

Patrick Kürschner (*Computational Methods in Systems and Control Theory, Max-Planck-Institut für Dynamik komplexer technischer Systeme Magdeburg*), Melina Freitag (*University of Bath*) 16:30–16:50

Rational Krylov subspace (RKS) methods are a widely accepted and established tool for the numerical solution of large-scale matrix equations, like algebraic Lyapunov and Riccati equations. In RKS, the generation of the basis vectors of the subspace requires the solution of shifted linear systems. For very large systems this solves can be implemented by using iterative methods, leading to inexact solves. In this talk we will provide theory how the errors from these inexact solves influence the RKS methods and consider a relaxation strategy within these inexact solves. The results are illustrated by numerical experiments.
This is joint work with Melina Freitag (Uni Bath).

On GMRES for singular EP and GP systems

Keiichi Morikuni (*Division of Information Engineering, University of Tsukuba*), Miroslav Rozloznik (*Institute of Mathematics, Academy of Sciences of the Czech Republic*) 16:50–17:10

In this contribution we study the numerical behavior of the GMRES method for solving singular systems of linear equations. in particular we are interested in the cases when the coefficient matrix is range-symmetric (EP), or its range and null-space are disjoint (GP) and the system is consistent. We show in theory and experiments that the accuracy of GMRES iterates computed in finite precision arithmetic may deteriorate due to the inconsistency of the system; the distance of the initial residual to the null-space of the coefficient matrix; and the extremal principal angles between the range of the coefficient matrix and of its transpose. These factors lead to ill-conditioning of the upper Hessenberg matrix in the Arnoldi process and affect the accuracy of the least squared solution computed in the transformed Hessenberg problem. The behavior of GMRES is also compared to the behavior of the range-restricted GMRES (RR-GMRES).

The Field of Values Bounds on Ideal GMRES

Jörg Liesen (*Technische Universität Berlin*), Petr Tichý (*Department of Numerical Mathematics, Charles University, Prague*) 17:10–17:30

A widely known result of Elman, and its improvements due to Starke, Eiermann and Ernst, give a bound on the GMRES residual norm using quantities related to the field of values of the given matrix and of its inverse. In this talk we present a simple and direct proof that these bounds also hold for the ideal GMRES approximation. Moreover, we propose an improvement of the bound derived by Beckermann, Goreinov, and Tyrtyshnikov.

Relating computed and exact quantities in Krylov subspace methods based on short recurrences

Tomas Gergelits (*Department of Numerical Mathematics, Charles University, Faculty of Mathematics and Physics*), Iveta Hnetynkova (*Department of Numerical Mathematics, Charles University, Faculty of Mathematics and Physics*), Marie Kubinova (*Department of Numerical Mathematics, Charles University, Faculty of Mathematics and Physics*) 17:30–17:50

Krylov subspace methods such as CG or MINRES represent an attractive way of solving large and sparse systems of linear algebraic equations with a symmetric (positive definite) matrix. These methods rely mathematically on the computation of orthonormal bases of a sequence of Krylov subspaces by short recurrences. It is well-known that in practical computations rounding errors typically cause loss of the global orthogonality and the basis vectors eventually become even linearly dependent. Consequently, the computed Krylov subspaces can be rank-deficient which may cause a significant delay of convergence. Inspite of many significant results, especially by Paige and Greenbaum, the connection between finite precision and exact computations is still not fully understood.
In this contribution, we compare computed and exact entities (in particular error and residual vectors, and their norms) coming from CG and MINRES methods using their mutual relationships. We explore how the Krylov subspaces generated in finite precision arithmetic differ from their exact arithmetic counterparts. This allows us to study to which extent the approximation properties of the methods in practical computations resemble (up to the delay caused by rounding errors) the exact process.

Effective use of data for image reconstruction with a Krylov subspace method

Kirk Soodhalter (*School of Mathematics, Trinity College Dublin, the University of Dublin*) 17:50–18:10

In this talk, we explore some practical strategies of incorporating outside information into a Krylov subspace method for image reconstruction, focusing mainly on augmented Krylov subspace methods. Many variants of these methods have been been proposed by different authors for the improvement of the reconstruction and acceleration of the semiconvergence, particularly in the case where one augments with known sharp edge features and jumps. However, what can one do in a more practical setting, where one may not know where any of these features are? We discuss here the state-of-the-art in the literature and propose some new ideas in the case that one augments with data from multiple sources.

On the Accuracy of the Element-wise Jacobi Methods for PGEP

Josip Matejaš (*Faculty of Economics and Business*), Vjeran Hari (*Department of Mathematics, Faculty of Science*) 18:10–18:30

We analyse the accuracy of two element-wise methods for the positive definite generalized eigenvalue problem (PGEP) $Ax = \lambda Bx$, where A and B are symmetric matrices and B is positive definite. The main use of these methods is to serve as kernel algorithms for the associated block Jacobi methods which are suitable for large-scale CPU and GPU computing. When implemented as one-sided block methods for the generalized singular value problem, the block methods are very efficient and the numerical tests indicate their high relative accuracy on the well behaved pairs of matrices. The two considered methods are designed to operate on B which has ones

along the diagonal. The first one is the HZ (Hari-Zimmermann) method. It first uses the spectral decompositions of the pivot submatrix of B and then the spectral decompositions of the updated pivot submatrix of A. The second one is the CJ (Cholesky-Jacobi) method. It uses the Cholesky decompositions of the pivot submatrix of B and then the spectral decompositions of the updated pivot submatrix of A. In analysing the relative accuracy of these methods a very detailed and subtle error analysis has been used, together with numerical tests. The standard error analysis has been refined in the following way: the higher terms of the errors are not neglected and the signs of the errors are taken into account. Using such an approach the error bounds can be greatly improved because the suppression and cancelation of the initial and intermediate errors can be detected and taken into account. In general, there are several critical points in the algorithms where severe cancelation can take place and the appropriate relative errors can blow up. However, under certain conditions one can show the high relative accuracy of the methods.

S17.03 | Applied and numerical linear algebra

Date 21.03.2018
Room 1402

A new algorithm for the solution of alternating polynomial eigenproblems

Philip Saltenberger (*AG Numerik, TU Braunschweig / Institut Computational Mathematics*), Heike Faßbender (*AG Numerik, TU Braunschweig / Institut Computational Mathematics*) 14:00–14:20

The numerical solution of a special polynomial eigenvalue problem $A(\lambda)u = 0$ for

$$A(\lambda) = \sum_{k=0}^{d} A_k \lambda^k,\ A_k \in \mathbb{R}^{n\times n}$$

is considered. We assume that $A(\lambda)^T = A(-\lambda)$ holds; this implies $A_k = A_k^T$ if k is even and $A_k = -A_k^T$ otherwise. Such matrix polynomials have been named alternating or T-even.
The eigenvalues of such matrix polynomials $A(\lambda)$ have a Hamiltonian eigenstructure; that is, the spectrum is symmetric with respect to both the real and the imaginary axis. Numerical methods that take this symmetry into account are capable of preserving the eigenvalue pairings despite the presence of rounding errors and thus return physically meaningful results. Moreover, exploiting the structure usually leads to more efficient and sometimes more accurate algorithms. Employing a special structure-preserving linearization [1] we turn $A(\lambda)u = 0$ into an eigenproblem for $L(\lambda) = \lambda X + Y$ with $X = -X^T, Y = Y^T \in \mathbb{R}^{dn\times dn}$ which is almost as sparse as the usual companion form linearization. Our eigensolver is based on an implicitly-restarted Krylov subspace method applied to $L(\lambda)$ (Even-IRA, see [2]) that subtly exploits its Hamiltonian eigenstructure. The whole algorithm can implicitly be performed involving only $n \times n$ matrix computations on $A(\lambda)$ due to the structure of $L(\lambda)$. To this end, using a slightly modified nullspace method improves the speed of all intermediate steps. In this talk we present the basic ideas of our approach showing how Even-IRA - implicitly applied to $L(\lambda)$ - yields an efficient and effective eigenvalue algorithm for this type of polynomial eigenvalue problem.

[1] Heike Faßbender and Philip Saltenberger. *Block Kronecker ansatz spaces for matrix polynomials.* Accepted for publication in *Linear Algebra and its Applications*, 2017.

[2] V. Mehrmann, C. Schröder, and V. Simoncini. *An implicitly-restarted Krylov subspace method for real symmetric/skew-symmetric eigenproblems. Linear Algebra and its Applications*, 436(10):4070–4087, 2012.

Relative Perturbation Bounds for Hyperbolic Quadratic Eigenvalue Problem

Ninoslav Truhar (*Department of Mathematics, University of Osijek*), Suzana Miodragović (*Department of Mathematics, University of Osijek*) 14:20–14:40

We will present relative perturbation bounds for hyperbolic quadratic eigenvalue problem of the form $\lambda^2 Mx + \lambda Cx + Kx = 0$, where M and K are Hermitian positive definite matrices, and C is such that $(x^*Cx)^2 > 4(x^*Mx)(x^*Kx)$ for all $x \in \mathbb{C}^n$, $x \neq 0$. These bounds are obtained using a new results for equivalent definite matrix pair $A - \lambda B$, where both A and B are nonsingular Hermitian matrices. Our bound can be applied to the gyroscopic systems which will be also shown. The obtained bounds will be illustrated by numerical examples.

On the Complex Falk-Langemeyer Method

Vjeran Hari (*Mathematical department, University of Zagreb, Faculty of Science*) 14:40–15:00

This communication is devoted to the derivation of the complex Falk-Langemeyer (FL) method for the simultaneous diagonalization of two Hermitian matrices of which one is positive definite. There are several incentives for this work.
In the case of real matrices it has been proven that the FL method is well defined for the definite pair of symmetric matrices, i.e. for the pair (A, B) such that $\alpha A + \beta B$ is positive definite for some real scalars α and β. Furthermore, the real FL method is closely related to the Hari-Zimmermann (HZ) method. Namely, the FL method can be viewed as the HZ method with fast-scaled transformation matrices. This relationship is important because it enables us to understand the behavior (the global and quadratic convergence, the accuracy and the termination criteria) of the both methods. Any of these two algorithms makes an excellent choice for the kernel algorithm of the block Jacobi method for the generalized eigenvalue or singular value problem. On contemporary CPU and GPU computing machines, the one-sided block Jacobi method has proved to be very efficient and accurate solver for the complete eigenproblem when the both matrices are dense.
So, our goal is to derive the complex FL and HZ methods, to establish their relationship, to prove their global and quadratic convergence and also to prove their high relative accuracy on the pairs well-behaved positive definite matrices. We intend to communicate the first results.

Perturbation Bounds for Parameter Dependent Quadratic Eigenvalue Problem

Matea Puvaca (*Department of Mathematics, Department of Mathematics, University of Osijek*), Zoran Tomaljnovic (*Department of Mathematics, University of Osijek*), Ninoslav Truhar (*Department of Mathematics, University of Osijek*) 15:00–15:20

We consider a quadratic eigenvalue problem (QEP):

$$(\lambda^2 M + \lambda D + K)x = 0, \tag{1}$$

where matrices M and K are Hermitian semidefinite and at least one of them is positive definite. The most widely used approach for solving the polynomial (which includes QEP) eigenvalue problem is to linearize in order to produce a larger order pencil, whose eigensystem can be found by any method for generalized eigenproblems. This approach has been used, for example, in [1], [2].
To avoid linearizion (or simultaneous diagonalization of M and K, which is sometimes the preprocessing step, as in [3]), we propose two different types of bounds, the first is a simple first

order approximation of function of several variables while the second one considers structured perturbation.
Thus, let $X = [x_1, \ldots, x_n]$ be a nonsingular matrix which contains n linearly independent right eigenvectors, and similarly, let $Y = [y_1, \ldots, y_n]$ be nonsingular matrix which contains n linearly independent left eigenvectors of QEP (1).
The corresponding perturbed QEP (1) is given by:

$$(\widetilde{\lambda}^2(M + \delta M) + \widetilde{\lambda}(D + \delta D) + K + \delta K)\widetilde{x} = 0, \tag{2}$$

where $(\widetilde{\lambda}_i, \widetilde{x}_i)$ is perturbed eigenpair of (2).
The first bound is the upper bound for the first order approximation, based on Taylor's theorem, for the eigenvalues and the corresponding left and right eigenvectors of the following QEP

$$(\lambda^2(v)M(v) + \lambda(v)D(v) + K(v))x(v) = 0, \tag{3}$$

where all three matrices M, D and K depend on $v = [v_1, \ldots, v_s] \in \mathbb{R}^s$. In this way we are able to efficiently calculate approximation of perturbed eigenvalues.
The second bound is of the following form

$$|y_i^*(M + T_{ij})\widetilde{x}_j| \leq \frac{\|y_i^* \delta M\|}{RG1} + \frac{\|y_i^* \delta C\|}{RG2} + \frac{\|y_i^* \delta K\|}{RG3},$$

where y_i is i-th left eigenvector and

$$T_{ij} = \frac{D_{ij}}{\widetilde{\lambda}_j + \lambda_i}, \tag{4}$$

$$RG1 = \min_{\substack{i=i_1,\ldots,i_p \\ j=j_1,\ldots,j_q \\ i \neq j}} \frac{|\lambda_i^2 - \widetilde{\lambda}_j^2|}{|\widetilde{\lambda}_j^2|}, \tag{5}$$

$$RG2 = \min_{\substack{i=i_1,\ldots,i_p \\ j=j_1,\ldots,j_q \\ i \neq j}} \frac{|\lambda_i^2 - \widetilde{\lambda}_j^2|}{|\widetilde{\lambda}_j|}, \tag{6}$$

$$RG3 = \min_{\substack{i=i_1,\ldots,i_p \\ j=j_1,\ldots,j_q \\ i \neq j}} |\lambda_i^2 - \widetilde{\lambda}_j^2|. \tag{7}$$

Here we also have the bounds for relative gaps (5),(6),(7), which can be efficiently calculated.
As presented in [4], the derivatives of eigenvalues and eigenvectors with respect to v_i can be calculated, more or less efficiently, depending on the multiplicity of eigenvalues. Using these results, we will estimate the quality of the approximation for the eigenvalues and eigenvectors based on the algorithm from [3]. We will use optimization methods presented in [5], together with given approximations and upper bounds, in order to optimize damping efficiently.

[1] Y. Nakatsukasa, F. Tisseur; *Eigenvector error bound and perturbation for polynomial and rational eigenvalue problems.* technichal report METR 2016–04 at *http://www.keisu.t.u-tokyo.ac.jp/research/techrep/index.html*

[2] N. Truhar, S. Miodragovic; *Relative perturbation theory for definite matrix pairs and hyperbolic eigenvalue problem.* Applied Numerical Mathematics 98 (2015), 106-121

[3] N. Truhar, Z. Tomljanovic; *Dimension reduction approach for the parameter dependent quadratic eigenvalue problem.* (2016), technical report at the Department of Mathematics, University of Osijek, 2016.

[4] N. P. Van Der Aa, H. G. Ter Morsche, R. R. M. Mattheij; *Computation of Eigenvalue and Eigenvector Derivatives for a General Complex-Valued Eigensystem*. Electronic Journal of Linear Algebra ISSN 1081-3810 A publication of the International Linear Algebra Society Volume 16, 300-314, October 2007.

[5] F. E. Curtis, T. Mitchell, M. L. Overton; *A BFGS-SQP Method for Nonsmooth, Nonconvex, Constrained Optimization and its Evaluation using Relative Minimization Profiles*. preprint, 2016

Relating noise and residuals in LSQR, LSMR, and CRAIG regularization

Iveta Hnetynkova (*Dep. of Numerical Mathematics, Charles University, Faculty of Mathematics and Physics*), Marie Kubinova (*Charles University, Faculty of Mathematics and Physics*), Martin Plesinger (*Technical University of Liberec*) 15:20–15:40

LSQR, LSMR, and CRAIG represent iterative Krylov subspace methods often used to solve large linear inverse problems polluted with additive noise. The core algorithm behind is the Golub–Kahan iterative bidiagonalization whose regularization properties have been studied previously. In this contribution, we consider a general noise setting and derive explicit relations between (noise-contaminated) bidiagonalization vectors and the residuals of LSQR, LSMR, and CRAIG. This allows us to analyze regularization properties of the methods by studying the match between their residuals and the true noise vector. Validity of the results for large two-dimensional inverse problems is also discussed.

Linear algebra properties of dissipative Hamiltonian descriptor systems

Michal Wojtylak (*Jagiellonian University*) 15:40–16:00

The properties of regular and singular matrix pencils of the form

$$\lambda E - LQ, \quad \text{with } E^*Q \geq 0,\ L + L^* \leq 0$$

are investigated. (Such pencils arise from dissipative Hamiltonian descriptor systems.) In particular, the location of finite eigenvalues and index of the infinity eigenvalue are studied in detail. The singular case is considered as well. The main ingredient of the method is the analysis of the pencil $\lambda E - Q$.
The talk is based on joint work with C. Mehl and V. Mehrmann.

S17.04 | Applied and numerical linear algebra

Date 21.03.2018
Room 1402

Krylov subspace methods for low-rank updates of matrix functions

Daniel Kressner (*Institute for Mathematics, École polytechnique fédérale de Lausanne*) 16:30–16:50

This talk is concerned with the development and analysis of fast algorithms for updating a matrix function $f(A)$ if A undergoes a low-rank change $A + L$. For example, when A is the Laplacian of an undirected graph then removing one edge or vertex of the graph corresponds to a rank-one change of A. Our algorithms are based on the tensorization of polynomial or rational Krylov subspaces involving A and A^T. The choice of a suitable element from such a tensorized subspace for approximating $f(A+L) - f(A)$ is straightforward in the symmetric case but turns out to be more intricate in the nonsymmetric case. We show that the usual convergence results for Krylov subspace methods for matrix functions can be extended to our algorithms, but this extension is not straightforward.

Incremental computation of the block triangular matrix exponential

Francesco Statti (*École polytechnique fédérale de Lausanne*), Daniel Kressner (*École polytechnique fédérale de Lausanne*), Robert Luce (*École polytechnique fédérale de Lausanne*) 16:50–17:10

We study the problem of computing the matrix exponential of a block triangular matrix

$$G_n = \begin{bmatrix} G_{0,0} & G_{0,1} & \cdots & G_{0,n} \\ & G_{1,1} & \cdots & G_{1,n} \\ & & \ddots & \vdots \\ & & & G_{n,n} \end{bmatrix} \in \mathbb{R}^{N \times N},$$

(all diagonal matrices $G_{i,i}$ are diagonal) in a peculiar way: Block column by block column, from left to right. In other words, we wish to compute the sequence of matrix exponentials

$$\exp(G_0), \exp(G_1), \exp(G_2), \ldots, \tag{1}$$

which are the leading portions of $\exp(G_n)$, until some termination criterion is satisfied.
The need for such an evaluation scheme arises naturally in the context of option pricing in polynomial diffusion models. In this setting a discretization process produces a sequence of nested block triangular matrices, and their exponentials are to be computed at each stage, until a dynamically evaluated criterion allows to stop.
Our algorithm is based on *scaling and squaring*. By carefully reusing certain intermediate quantities from one step to the next, we can efficiently compute the sequence (1) of matrix exponentials. In our implementation the computational overhead induced by this peculiar evaluation order is very moderate: Asymptotically the number of operations for computing $\exp(G_n)$ increases only by a logarithmic factor from $O(\log(||G_n||)N^3)$ for the standard scaling and squaring algorithm to $O(\log(||G_n||)^2 N^3)$.

Stability of network indexes defined trough matrix functions

Stefano Pozza (*Department of Numerical Mathematics, Charles University, Faculty of Mathematics and Physics*), Francesco Tudisco (*Department of Mathematics & Statistics, University of Strathclyde*) 17:10–17:30

One of the major goals of network analysis is to identify important components in a network by exploiting the topological structure of connections between its nodes. To this end, recent years have seen the introduction of many new measures of importance of a node or a set of nodes, defined in terms of suitable entries of functions of matrices $f(A)$, for different choices of f and A. However, this approach requires a significant computational effort to address the entries of $f(A)$. This is particularly prohibitive when the network changes frequently and the important components have to be updated.
Given the adjacency matrix A of a graph $G = (V, E)$, in this work we address the problem of estimating the changes in the entries of $f(A)$ with respect to changes in the edge set E. Intuition suggests that, if the topology of connections in the new graph $\tilde{G} = (V, \tilde{E})$ is not significantly distorted, relevant components in G maintain their leading role in $\tilde{G}$. We propose a bound showing that the magnitude of the variation of the entry $f(A)_{u,v}$ decays exponentially with the distance in G that separates either u or v from the set of nodes touched by the edges that are perturbed.

Stability preservation in Galerkin-type projection-based model order reduction

Roland Pulch (*Institut für Mathematik und Informatik, Ernst-Moritz-Arndt Universität Greifswald*) 17:30–17:50

We consider linear dynamical systems consisting of ordinary differential equations with high dimensionality. The aim of model order reduction is to construct an approximating system of a much lower dimension. Therein, the reduced system may be unstable, even though the original system is asymptotically stable. We focus on projection-based model order reduction of Galerkin-type. Thus each scheme is defined by a single projection matrix. A transformation of the original system guarantees an asymptotically stable reduced system. This transformation requires the numerical solution of a high-dimensional Lyapunov equation. We specify an approximation of the solution, which allows for an efficient iterative treatment of the Lyapunov equation if the number of non-negative eigenvalues is relatively small in a symmetric part. For example, the alternating direction implicit (ADI) method yields an iterative solution. Furthermore, this strategy can be generalized to preserve the asymptotic stability of stationary solutions in model order reduction of nonlinear dynamical systems consisting of ordinary differential equations. We present numerical results for high-dimensional examples, which confirm the computational feasibility of the stability-preserving approach.

An optimal model order reduction approach for parametric linear time-invariant systems

Manuela Hund (*Computational Methods in Systems and Control Theory, Max Planck Institute for Dynamics of Complex Technical Systems*), Petar Mlinarić (*Computational Methods in Systems and Control Theory, Max Planck Institute for Dynamics of Complex Technical Systems*), Jens Saak (*Computational Methods in Systems and Control Theory, Max Planck Institute for Dynamics of Complex Technical Systems*) 17:50–18:10

We consider parametric linear time-invariant (LTI) systems

$$\begin{aligned} E(\mu)\dot{x}(t) &= A(\mu)x(t) + B(\mu)u(t), \\ y(t) &= C(\mu)x(t), \end{aligned} \tag{1}$$

with affine decomposable matrices $E(\mu) \in \mathbb{R}^{n\times n}$, $A(\mu) \in \mathbb{R}^{n\times n}$, $B(\mu) \in \mathbb{R}^{n\times p}$ and $C(\mu) \in \mathbb{R}^{q\times n}$, where $E(\mu)$ is assumed to be uniformly invertible, i.e. invertible for all parameters $\mu \in \Xi \subset \mathbb{R}^d$. In addition, we assume (1) to be uniformly asymptotically stable, i.e. for all $\mu \in \Xi$ the transfer function

$$H(s,\mu) = C(\mu)\left(sE(\mu) - A(\mu)\right)^{-1} B(\mu),$$

describing the relation between input and output in the Laplace domain, must have all poles in the open left half of the complex plane.
Our aim is to reduce (1), while preserving the affine decomposition, in the $\mathcal{H}_2 \otimes \mathcal{L}_2$-optimal sense meaning that the reduced order model (ROM) minimizes the $\mathcal{H}_2 \otimes \mathcal{L}_2$-error:

$$\|H - H_r\|^2_{\mathcal{H}_2\otimes\mathcal{L}_2} := \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{\Xi} \|H(\mathrm{i}\omega,\mu) - H_r(\mathrm{i}\omega,\mu)\|_F^2 \mathrm{d}\mu \ \mathrm{d}\omega,$$

where H and H_r are the transfer functions of the full order model and the ROM, respectively.
In our contribution, we will show how related Wilson-type optimality conditions can be derived for parametric systems (1). Further, we present a way to solve these conditions analytically if only the input and output matrices are parametrized.

A case study of data-driven approximation methods applied to irrational functions

Dimitrios Karachalios (*Max Planck Institute for Dynamics of Complex Technical Systems*), Ion Victor Gosea (*DRI (Data-Driven System Reduction and Identification Group), Max Planck Institute for Dynamics of Complex Technical Systems*), Athanasios Antoulas (*Rice University*) 18:10–18:30

One of the main approaches to model reduction of both linear and nonlinear dynamical systems is by means of interpolation. Such approaches seek reduced models whose transfer function matches that of the original system at selected interpolation points.
A special class is represented by data-driven methods which are the topic of interest in this work. We present a case study of three such methods that produce a rational function (as output), that matches certain interpolation conditions (as input).
The first method, which will be referred to as the Loewner framework, was originally developed by the third author. It constructs models from given data sets (pairs of sample points and samples values) in a natural and straightforward manner. Its main attribute is that it provides a trade-off between accuracy of fit and complexity of the model.
We will compare this approach against other approximation methods, such as vector fitting (VF) and the more recent adaptive Antoulas-Anderson (AAA) approach. These methods are iterative, while the Loewner approach is direct (no iteration involved). Nevertheless, we propose ways of comparing all three methods that take into consideration not only accuracy but also robustness of the procedure.
The first example for which we apply the aforementioned methods is given by the classical Euler-Bernoulli beam model with Rayleigh damping. No spatial discretization will be performed for the underlying PDE model. Instead, we will use samples of its irrational transfer function, to build linear models by means of interpolation. The sampling domain is one-dimensional, i.e. the imaginary axis.

Afterwards, we will turn our attention to a classical example from approximation theory, i.e. the Bessel function. By means of the three methods, rational interpolants are produced by matching the original sample values. The sampling domain is in this case two-dimensional, i.e. a rectangular symmetric grid.
The Loewner framework requires performing singular value decomposition (SVD) for matrices with dimension comparable to the size of the dataset. In the case of a large amount of data, this may result in increased processing time. We use stochastic procedures such as randomized singular value decomposition (r-SVD) instead of the full SVD, to reduce the computational cost. An apriori bound of the singular value decay of the Loewner matrix is also provided.

S17.05 | Applied and numerical linear algebra

Date 22.03.2018
Room 1402

Topical tropical linear algebra

Peter Butkovic (*School of Mathematics, University of Birmingham*) 08:30–09:10

Tropical linear algebra (originally called max-algebra) will soon celebrate its 60th birthday. Its creation was motivated by a number of models of industrial problems from job-shop scheduling and railway timetabling to network optimisation problems. The key ideas of max-algebra proved useful in a wide range of areas of mathematics, from formal languages and algebraic topology (Hilbert's 16th problem) to stochastic control and mathematical physics. "Critical mass" of research achievements was reached in the 1990s when the principal idea of considering the pair of operations (max, +) instead of the conventional pair (+, x) has triggered even more intensive research with a number of remarkable findings in areas as diverse as algebraic geometry, phylogenetics and modelling of the cellular protein production. Real-life applications range from providing tools for a financial decision of the Bank England at the time of the financial crisis in 2008 to a model of the Dutch railway network. In this talk we provide a survey of selected results in tropical linear algebra such as solution of systems of max-linear equations, tropical eigenproblem (including subeigenvectors, supereigenvectors and its generalised version), matrix orbit and reachability of eigenspaces. We will highlight the differences between problems that have been essentially fully resolved and those where fundamental questions remain unanswered. Special attention will be paid to the recently studied intriguing problem of supereigenvectors.

The Total Least Squares and the Core Problem within Linear Approximation Problems

Martin Plesinger (*Department of Mathematics, Technical University of Liberec*),
Iveta Hnetynkova (*Charles University, Faculty of Mathematics and Physics*),
Jana Zakova (*Department of Mathematics, Technical University of Liberec*) 09:10–09:30

This contribution recapitulates two standard total least squares (TLS) formulations dealing with linear approximation problems with vector and matrix right-hand sides (also called the single and the multiple right-hand side problems, respectively). We show how the core problem concept can be used to analyze solvability of the TLS, in particular in the single right-hand side case. Finally, we emphasize difficulties that appear in the analysis of the multiple right-hand side problems, that cannot be avoided by using the core problem concept.

Selected Tensor Generalizations of the Total Least Squares

Jana Zakova (*Department of Mathematics, Technical University of Liberec*), Iveta Hnetynkova (*Charles University, Faculty of Mathematics and Physics*), Martin Plesinger (*Department of Mathematics, Technical University of Liberec*) 09:30–09:50

Our contribution is focused on the total least squares (TLS) problem and its extension from matrix to tensor setting. First, we briefly recapitulate some basic notation and concepts of the multilinear algebra. Then we present a few possible generalizations of the TLS definition. We show that the core problem concept can be generalized as well, and it can be related to the Tucker decomposition of the right-hand side tensor. Finally, we focus on the differences between core problems originated in the matrix and tensor formulation.

Solution analysis and continuation algorithms for multilinear pagerank

Beatrice Meini (*Dept. of Mathematics, University of Pisa*), Federico Poloni (*Dept. of Computer Science, University of Pisa*) 09:50–10:10

We focus on the solution of the multivariate equation $x = \alpha R(x \otimes x) + (1 - \alpha v)$, where $\alpha \in \mathbb{R}$, $v, x \in \mathbb{R}^n$, $R \in \mathbb{R}^{n \times n^2}$ studied in [Gleich, Lim, Yu, *Multilinear Pagerank*]. We show that some constraints on the coefficients imply a special structure of the set of (non-necessarily stochastic) solutions, and we analyze a few algorithms based on continuation on the parameter α.

The Tensor-Train Format and Its Applications

Patrick Gelß (*Mathematics and Computer Science, Freie Universität Berlin*) 10:10–10:30

The simulation and analysis of high-dimensional problems is often infeasible due to the curse of dimensionality. In this talk, we discuss the potential of tensor decompositions for mitigating this curse when considering systems from several application areas. Using tensor-based solvers, we directly compute numerical solutions of master equations associated with Markov processes on extremely large state spaces. Furthermore, we exploit the tensor-train format to approximate eigenvalues and corresponding eigentensors of linear tensor operators. In order to analyze the dominant dynamics of high-dimensional stochastic processes, we propose several decomposition techniques for highly diverse problems. These include tensor representations for operators based on nearest-neighbor interactions, construction of pseudoinverses for tensor-based reformulations of dimensionality reduction methods, and the approximation of transfer operators of dynamical systems. The results show that the tensor-train format enables us to compute low-rank approximations for various numerical problems as well as to reduce the memory consumption and the computational costs compared to classical approaches significantly. We demonstrate that tensor decompositions are a powerful tool for solving high-dimensional problems from various application areas.

S17.06 | Applied and numerical linear algebra

Date 22.03.2018
Room 1402

Decomposition into subspaces and operator preconditioning

Jakub Hrncir (*Department of Numerical Mathematics, Charles University, Faculty of Mathematics and Physics*), Ivana Pultarova (*Czech Technical University in Prague, Faculty of Civil Engineering*), Zdenek Strakos (*Department of Numerical Mathematics, Charles University, Faculty of Mathematics and Physics*) 14:00–14:20

We will consider linear equations in the abstract infinite-dimensional Hilbert space setting with bounded, coercive and self-adjoint operators, which can represent, e.g., boundary value problems formulated via partial differential equations. Efficient numerical solution procedures often incorporate transformation of the original problem using preconditioning. Motivated, in particular, by the works of Faber, Manteuffel, Parter, Oswald, Dahmen, Kunoth and Rüde published in the early 90's, we will present an abstract formulation of operator preconditioning based on the idea of decomposition of a Hilbert space into a finite number of (infinite-dimensional) subspaces, by formulating the main results using the concepts of norm equivalence and spectral equivalence of infinite-dimensional operators. Its goal is to describe in a concise way the common principles behind various adaptive multilevel and domain decomposition techniques using infinite-dimensional function spaces.

Preconditioning for Time-Dependent PDE-Constrained Optimization

John Pearson (*School of Mathematics, University of Edinburgh*) 14:20–14:40

We consider the development of preconditioned iterative methods to tackle the large-scale matrix systems that arise from the discretization of a number of time-dependent PDE-constrained optimization problems. In particular, we discuss the use of interior point methods to handle additional inequality constraints on the state and control variables, the solution of problems involving fractional differential equation constraints, and the application of deferred correction schemes to reduce the discretization error in the time variable.

Convergence of the multiplicative Schwarz method for singularly perturbed convection-diffusion problems discretized on a Shishkin mesh

Jörg Liesen (*Institute of Mathematics, TU Berlin*) 14:40–15:00

In this talk we will present a convergence analysis of the multiplicative Schwarz method applied to upwind and central finite difference discretizations of one-dimensional singularly perturbed convection-diffusion model problems posed on a Shishkin mesh. The matrices that arise in this context are nonsymmetric, nonnormal, and usually ill-conditioned, so that standard iterative solvers like the (unpreconditioned) GMRES method converge very slowly. Since the Shishkin mesh divides the discretized domain into subdomains where the analytic solution is characterized by different behavior, an algebraic solve based on domain decomposition seems to be a natural approach.
Several authors have previously applied the alternating (or multiplicative) Schwarz method to the continuous problem based on the partitioning of the domain into overlapping subdomains, and subsequently discretized by introducing uniform meshes on each subdomain. However, significant

numerical problems including very slow convergence and accumulation of errors (up to the point of non-convergence of the numerical solution) can occur when layer-resolving mesh transition points are used in this setup. We avoid these problems since we first discretize and then apply the multiplicative Schwarz method to the linear algebraic system.
Our convergence analysis uses the algebraic structure of the Schwarz iteration matrices, and we obtain bounds on the infinity norm of the algebraic error that are descriptive from the first step of the iteration. Beyond these bounds and numerical illustrations for the one-dimensional model problems, we will discuss the relevance of our results for more challenging (higher-dimensional) problems and for using the multiplicative Schwarz method as a preconditioner for GMRES.
The talk is based on joint work with Carlos Echeverría (TU Berlin), Daniel B. Szyld (Temple University, Philadelphia), Petr Tichý (Charles University, Prague).

Selective algebraic multigrid for implicitly coupled pressure-velocity system

Tessa Uroic (*Department of Energy, Power and Environmental Engineering, University of Zagreb, Faculty of Mechanical Engineering and Naval Architecture*), Hrvoje Jasak (*Department of Energy, Power and Environmental Engineering, University of Zagreb, Faculty of Mechanical Engineering and Naval Architecture*) 15:00–15:20

Systems of equations are dominated by inter-equation coupling terms. The conventional methods solve the system in a sequential manner, solving each equation separately and explicit treatment of coupled variables. Modern High-Performance Computing clusters with substantial memory resources have enabled development of coupled algorithms which rely on linearisation of cross-coupling terms and solving the system in an implicit manner.
This study presents a selective algebraic multigrid for the implicitly coupled pressure-velocity system in the framework of Finite Volume Method. The solution of this system is a saddle point. To remedy the problem, the pressure equation is derived as a Schur complement. The resulting system is point-ordered. Single-unknown interpolation has been used, i.e. the interpolation formula is calculated from the pressure equation, excluding the cross-couplings from the momentum equation. Thus, interpolation formula is the same for all unknowns corresponding to a single point. Benefits of the implicit coupling of the pressure and velocity equations are shown and compared to the conventional segregated algorithm. Performance of the selective algebraic multigrid is compared to the aggregation-based algebraic multigrid.

Machine Learning in Adaptive Algebraic Multigrid

Karsten Kahl (*Faculty of Mathematics and Natural Sciences, Bergische Universität Wuppertal*), Matthias Rottmann (*Bergische Universität Wuppertal*) 15:20–15:40

In this talk we show that the adaptive algebraic multigrid setup can be seen as a machine learning problem. Starting with least squares interpolation

$$\sum_{\kappa} \omega_\kappa \left(v_i^{(\kappa)} - \sum_j p_{ij} v_j^{(\kappa)} \right)^2 \to \min,$$

which can be interpreted as a local regression problem, we develop a novel coarsening ansatz by introducing a kernel function K_η and an ℓ_1 penalty term for the least-squares coefficients

$$\sum_{\kappa} \omega_\kappa \left(v_i^{(\kappa)} - \sum_j p_{ij} K_\eta(i,j) v_j^{(\kappa)} \right)^2 + \lambda \cdot ||p_i||_1 \to \min,\ \lambda \in \mathbb{R}.$$

The resulting non-linear optimization problem can be efficiently solved by least-angle regression and yields sparse fits to the underlying regression problem. These coefficients can then be used to define a strength of connection measure, which allows for the fully adaptive selection of coarse variables.
We demonstrate that our coarsening scheme yields suitable coarse grids and can be seamlessly integrated in the bootstrap algebraic multigrid framework to obtain efficient multigrid methods for problems on unstructured meshes in the presence of anisotropy and also when using non-standard relaxation methods, e.g., block relaxation, where we obtain the appropriate longe range interpolation relations.

S17.07 | Applied and numerical linear algebra

Date 22.03.2018
Room 1402

Approximation of Hermitian Matrices by Positive (Semi-)Definite Matrices using Modified LDL* Decompositions

Joscha Reimer (*Christian-Albrechts-University Kiel*) 17:30–17:50

A new algorithm to approximate Hermitian matrices by positive (semi-)definite matrices is presented. The parameters of the algorithm can be used to control whether the approximation is invertible or not. Moreover the condition number of the approximation is controllable by these parameters. The algorithm tries to keep the difference between the original matrix and the approximation as small as possible.
The LDL^* decomposition of the approximation is calculated as by-product by the algorithm. As a result corresponding systems of linear equations can be solved very quickly.
The approximation algorithm has no significant overhead regarding needed computation time and needed memory compared to the computation of an unmodified LDL^* decomposition. Furthermore, the algorithm preserves the sparsity pattern of a sparse matrix. The original matrix can also be changed in place so that (almost) no additional memory is needed. Thus the algorithm is also applicable for very large matrices.
In addition, the diagonal entries of the approximation can be constrained by non-negative lower and upper bounds. Especially non-negative diagonal entries of the original matrix can be preserved by the algorithm.
Numerical optimization and statistics are two fields of application for the algorithm.

A fast Cholesky factorization for Toeplitz-plus-Hankel matrices

Robert Luce (*EPFL*), Daniel Kressner (*EPFL*) 17:50–18:10

We consider the problem of computing the Cholesky factorization of a symmetric positive definite Toeplitz-plus-Hankel (TpH) matrix. We give a simple and elementary derivation of a generalized displacement operator for such matrices, which yields a displacement rank of four. Hence the generalized Schur algorithm can be used to compute the Cholesky factor with quadratic operation complexity instead of a cubic one. We present an efficient implementation of this algorithm, as well as an extension to the block TpH case.

Fast and backward stable computations of roots of polynomials - backward error analysis

Jared L. Aurentz (*Instituto de Ciencias Matemáticas*), Thomas Mach (*Department of Mathematics, School of Science and Technology, Nazarbayev University*), Leonardo Robol (*Istituto di Scienza e Tecnologie dell Informazione 'A. Faedo' (ISTI), CNR*), Raf Vandebril (*Department of Computer Science, University of Leuven*), David S. Watkins (*Department of Mathematics, Washington State University*)

18:10–18:30

In our earlier work, *Fast and backward stable computation of roots of polynomials* by J.L. Aurentz, T. Mach, R. Vandebril, and D.S. Watkins, SIAM Journal on Matrix Analysis and Applications, 36(3): 942–973, 2015, we introduced a companion QR algorithm that finds the roots of a polynomial by computing the eigenvalues of the companion matrix in $O(n^2)$ time using $O(n)$ memory. Based on this we will introduce, as an alternative, a companion QZ algorithm that solves a generalized eigenvalue problem for a companion pencil.

More importantly, we provide an improved backward error analysis that takes advantage of the special structure of the problem. We prove that for the companion QR algorithm, the backward error on the polynomial coefficients varies linearly with the norm of the polynomial's vector of coefficients. Thus the companion QR algorithm is more accurate than the unstructured QR algorithm (used by MATLAB's `roots` command, for example), for which the backward error on the polynomial coefficients grows quadratically with the norm of the coefficient vector. The companion QZ algorithm has the same favorable backward error as companion QR, provided that the polynomial coefficients are properly scaled.

Numerical experiments will underpin the sharpness of the presented proofs.

S18 | Numerical methods of differential equations

Organiser Lars Grasedyck (*IGPM, RWTH Aachen*)
Daniel Peterseim (*Universität Augsburg*)

S18.01 | Numerical methods of differential equations

Date 20.03.2018
Room 2370

Numerical simulation of nonlinear Schrödinger equations with disorder potentials

Daniel Peterseim (*Universität Augsburg*) 08:30–08:50

This talk reviews some numerical methods for the simulation of Bose-Einstein-Condensates modelled by nonlinear Schrödinger equations. We consider both the computation of stationary states as well as the simulation of the dynamics. Among the methodological and mathematical novelties are variational multiscale spatial discretization schemes for the acceleration of non-linear eigenvalue solvers [2,3].
Moreover, the talk addresses the numerical analysis of classical time-stepping schemes in the presence of disorder potentials [3]. Under low regularity assumptions, that are compatible with discontinuous potentials, we prove convergence with rates for the mass- and energy conserving variant of the Crank-Nicolson time discretization scheme due to Sanz-Serna. While for sufficiently smooth potentials, the rates are optimal without any coupling condition between the time step size and the spatial mesh width, the sharpness of the rates and the necessity of some coupling condition is open in the non-smooth case and will be discussed in a sequence of numerical experiments.

[1] P. Henning and D. Peterseim. Crank-Nicolson Galerkin approximations to nonlinear Schrödinger equations with disorder potentials. Math. Models Methods Appl. Sci. 27, 2147, 2017.

[2] H. Alaeian, M. Schedensack, C. Bartels, D. Peterseim, and M. Weitz. Thermo-optical interactions in a dye-microcavity photon Bose-Einstein condensate. New J. Phys. 19, 115009, 2017.

[3] P. Henning, A. Målqvist, and D. Peterseim. Two-level discretization techniques for ground state computations of Bose-Einstein condensates. SIAM J. Numer. Anal. 52(4):1525-1550, 2014.

[4] A. Målqvist and D. Peterseim. Computation of eigenvalues by numerical upscaling. Numer. Math., 130(2):337-361, 2014.

Rayleigh–Ritz approximation of the inf-sup constant for the divergence

Dietmar Gallistl (*Karlsruher Institut für Technologie - KIT*) 08:50–09:10

This contribution proposes a compatible finite element discretization for the approximation of the inf-sup constant for the divergence. The new approximation replaces the H^{-1} norm of a gradient by a discrete H^{-1} norm which behaves monotonically under mesh-refinement. By discretizing the pressure space with piecewise polynomials, upper bounds to the inf-sup constant are obtained. The scheme enables an approximation with arbitrary polynomial degrees. It can be

viewed as a Rayleigh–Ritz method and it gives monotonically decreasing approximations of the inf-sup constant under mesh refinement. In particular, the computed approximations are guaranteed upper bounds for the inf-sup constant. The novel error estimates prove convergence rates for the approximation of the inf-sup constant provided it is an isolated eigenvalue of the corresponding non-compact eigenvalue problem; otherwise, plain convergence is achieved. Numerical computations on uniform and adaptive meshes are presented.

Randomized a posteriori error estimation

Kathrin Smetana (*University of Twente*), Anthony T Patera (*Massachusetts Institute of Technology*), Olivier Zahm (*Massachusetts Institute of Technology*) 09:10–09:30

During the last decades (numerical) simulations based on partial differential equations (PDEs) have considerably gained importance in engineering applications, life sciences, environmental issues, and finance. However, especially when multiple simulation requests or a real-time simulation response are desired, standard methods such as finite elements may be too expensive. Model order reduction approaches have been developed to tackle such situations. Here, the key concept is to prepare a problem-adapted low-dimensional subspace of the high-dimensional discretization space in a possibly expensive offline stage to realize a fast simulation response by Galerkin projection on that low-dimensional space in the subsequent online stage.
We propose a constant-free, randomized a posteriori error estimator for reduced order approximations such as the reduced basis approximation for parametrized PDEs. This error estimator does not require to estimate any stability constants and is both reliable and efficient at (given) high probability. Here, we rely on results similar to the restricted isometry property employed in compressed sensing [Vershynin 12]. In order to obtain an a posteriori error estimator that is computationally feasible in the online stage we employ the solution of a reduced dual problem with random right-hand side, exploiting the typically fast convergence of reduced order models.

Multi-index Monte Carlo for PDEs with random coefficients

Michael Feischl (*IANM, KIT - Karlsruhe Institute of Technology*) 09:30–09:50

We present the idea of multi-index Monte Carlo methods in the frame of PDEs with random coefficients. We show error estimates and prove that the multi-index approach can be more efficient than the multi-level approach. We give examples which connect the theory with fast random field generation by use of H-matrices.

Stability and Preconditioning of Elliptic PDEs with Low-Rank Multilevel Structure

Markus Bachmayr (*Hausdorff Center for Mathematics & Institut für Numerische Simulation, Universität Bonn*), Vladimir Kazeev (*Department of Mathematics, Stanford University*) 09:50–10:10

Folding grid value vectors of size 2^L into Lth order tensors of mode sizes $2 \times 2 \times \cdots \times 2$, combined with low-rank representation in the tensor train format, has been shown to lead to highly efficient approximations for various classes of functions. These include solutions of elliptic PDEs on nonsmooth domains or with oscillatory data. This tensor-structured approach is attractive because it leads to highly compressed, adaptive approximations based on simple discretizations. Straightforward choices of the underlying basis, such as piecewise multilinear finite elements on uniform tensor product grids, lead to the well-known *basis ill-conditioning* of discretized operators. We demonstrate that for low-rank representations, the use of tensor structure additionally

leads to *representation ill-conditioning*, a new effect specific to computations in tensor networks. We construct an explicit tensor-structured representation of a BPX preconditioner with ranks independent of the number L of discretization levels, which combined with a carefully chosen representation of its product with the stiffness matrix turns out to remove both basis and representation ill-conditioning. Numerical tests, including problems with highly oscillatory coefficients, show that one arrives at reliable and efficient solvers which remain numerically stable beyond $L > 50$.

Splitting-Based Structure Preserving Discretizations for Magnetohydrodynamics

Cecilia Pagliantini (*MATHICSE-MCSS, MCSS, Ecole Polytechnique Fédérale de Lausanne (EPFL)*), Ralf Hiptmair (*Seminar for Applied Mathematics, ETH Zurich*) 10:10–10:30

We consider the splitting of the equations of magnetohydrodynamics (MHD) into a magnetic induction part and a fluid part. Relying on an Eulerian method of lines, we design numerical methods based on the coupling of Galerkin schemes for the electromagnetic fields via finite element exterior calculus with finite volume methods for the conservation laws of fluid mechanics. The magnetic induction problem is viewed as an instance of a generalized transient advection problem of differential forms. For the latter, we design spatial upwind discretizations of the Lie derivative based on the duality between the contraction of differential forms and the extrusion of chains. The balance laws for the fluid constitute a system of conservation laws with the magnetic induction field as a space and time dependent coefficient. We derive finite volume schemes based on approximate Riemann solvers adapted to accommodate the electromagnetic contributions to the momentum and energy conservation. A set of benchmark tests for 2D planar ideal MHD provides numerical evidence that the resulting lowest order coupled scheme is first order accurate for smooth solutions, conservative and stable.

S18.02 | Numerical methods of differential equations

Date 20.03.2018
Room 2370

Boundary element methods for shape optimization problems

Olaf Steinbach (*Institut für Angewandte Mathematik, TU Graz*) 16:30–16:50

The shape derivative of cost functionals in shape optimization problems can be represented in the Hadamard–Zolesio form which implies the choice of the new search direction. We will recall the computation of the shape derivative, and we comment and discuss the choice of different cost functionals and search directions. Numerical results are given which illustrate the potential of the proposed approach.

Coupling of discontinuous Galerkin schemes for viscous flow in porous media with adsorption

Raimund Bürger (*CI2MA & Departamento de Ingeniería Matemática, Universidad de Concepción*), Sudarshan Kumar Kenettinkara (*Department of Mathematics, Indian Institute of Technology Guwahati*), Ricardo Ruiz Baier (*Mathematical Institute, Oxford University*), Héctor Torres (*Departamento de Matemáticas, Universidad de La Serena*) 16:50–17:10

Polymer flooding is an important stage of enhanced oil recovery in petroleum reservoir engineering. A model of this process is based on the study of multicomponent viscous flow in porous media with adsorption. This model can be expressed as a Brinkman-based model of flow in porous media coupled to a non-strictly hyperbolic system of conservation laws for multiple components (water and polymers) that form the aqueous phase. The discretisation proposed for this coupled flow-transport problem combines an **H**(div)-conforming discontinuous Galerkin (DG) method for the Brinkman flow problem with a classical DG method for the transport equations. The DG formulation of the transport problem is based on discontinuous numerical fluxes. An invariant region property is proved under the (mild) assumption that the underlying mesh is a **B**-triangulation [B. Cockburn, S. Hou, and C.-W. Shu, Math. Comp., 54 (1990), pp. 545–581]. This property states that only physically relevant (bounded and non-negative) saturation and concentration values are generated by the scheme. Numerical tests illustrate the accuracy and stability of the proposed method.

A non-symmetric FEM-BEM coupling method to solve a time-dependent interface problem for eddy currents

Christoph Erath (*Deparment of Mathematics, TU Darmstadt*), Herbert Egger (*TU Darmstadt*), Robert Schorr (*TU Darmstadt*) 17:10–17:30

In 1987 MacCamy and Suri [2] proposed a time-dependent interface problem for two-dimensional eddy currents with an unbounded exterior domain. They analyzed the model problem and provided a semi discretization in terms of a non-symmetric finite element (FEM) boundary element (BEM) coupling formulation. However, in their formulation the coupling boundary has to be smooth to apply a compactness argument. In our presentation of the work [1], we consider the same model problem and prove well-posedness also for Lipschitz interfaces. Furthermore, we apply a classical line method to get a fully discrete system. For the spatial discretization we use as well a non-symmetric FEM-BEM coupling approximation. We establish well-posedness of this formulation for problems with Lipschitz interfaces and prove quasi-optimality for this semi-discretization under minimal regularity assumptions. For the subsequent discretization in time we use a variant of the classical implicit Euler method. This allows us to prove well-posedness and quasi-optimality for the fully discrete scheme under minimal regularity assumptions on the solution without the not available duality argument for our non-symmetric system. Error estimates with optimal order follow directly for both, the semi- and the full discretization. Numerical examples illustrate the predicted (optimal) convergence rates and underline the potential for practical applications.

Acknowledgement: The research of the third author was supported by the *Excellence Initiative* of the German Federal and State Governments and the *Graduate School of Computational Engineering* at TU Darmstadt.

[1] H. Egger, C. Erath, and R. Schorr: On the non-symmetric coupling method for parabolic-elliptic interface problems. Preprint (2017), available online: http://arxiv.org/abs/1711.08487.

[2] R. C. MacCamy and M. Suri: A time-dependent interface problem for two-dimensional eddy currents. Quart. Appl. Math., 44:675–690, 1987.

Stable non-symmetric coupling of finite volume and boundary element method for convection-dominated parabolic-elliptic interface problems

Robert Schorr (*Graduate School of Computational Engineering, TU Darmstadt*), Christoph Erath (*Deparment of Mathematics, TU Darmstadt*) 17:30–17:50

Many problems in electrical engineering or fluid mechanics can be modelled by parabolic-elliptic interface problems, where the domain of the exterior elliptic problem might be unbounded. These problems can be solved by the non-symmetric coupling of finite elements (FEM) and boundary elements (BEM) analysed in [1]. For convection dominated problems in the interior this method is not necessarily stable anymore, i.e., strong oscillations can occur in the computed solution.
Thus we propose another approach that also relies on a non-symmetric coupling with the boundary element method, but uses the vertex-centered finite volume method (FVM) in the interior. This method allows us to use an upwind stabilisation to prevent these oscillations. Furthermore, it ensures the conservation of mass due to its formulation which is mandatory for computational fluid mechanics applications. For stationary problems, this type of coupling has already been analysed in [2], but not for time-dependent ones.
In this talk we will present the analysis of FVM-BEM coupling concerning convergence and error estimates. Some numerical examples illustrate the theoretical findings.

Acknowledgements: The work of the second author is supported by the 'Excellence Initiative' of the German Federal and State Governments and the Graduate School of Computational Engineering at Technische Universität Darmstadt.

[1] H. Egger, C. Erath and R. Schorr: On the non-symmetric coupling method for parabolic-elliptic interface problems. *Preprint*, arXiv:1711.08487, 2017.

[2] C. Erath, G. Of and F.J. Sayas: A non-symmetric coupling of the finite volume method and the boundary element method. Numer. Math. *135*(3), 895–922 (2017). SIAM J. Numer. Anal. 51(3), 1777–1804 (2013).

[3] C. Erath, and R. Schorr: Stable non-symmetric coupling of finite volume and boundary element method for convection-dominated parabolic-elliptic interface problems. *In preparation.*

On the smoothing property of linear PDEs with delay

Robert Altmann (*Universität Augsburg*), Christoph Zimmer (*TU Berlin*) 17:50–18:10

In the last decades, ODEs and PDEs with delay terms were used to model practical problems as in population dynamics, fluid dynamics, climate modeling, or in control problems. A special class are problems where only the state - and not the time derivatives - appears with a delay. It is well-known that in the ODE case the solutions of these systems become smoother over time. Note that this knowledge is important for the choice of an appropriate discretization scheme. In this talk we investigate corresponding PDEs with delay and discuss under which conditions smoothing takes place.

Differential Riccati Equations - A Projection Based Approach

Maximilian Behr (*Max-Planck-Institut für Dynamik komplexer technischer Systeme Magdeburg*), Jan Heiland (*Max-Planck-Institut für Dynamik komplexer technischer Systeme Magdeburg*), Peter Benner (*Max-Planck-Institut für Dynamik komplexer technischer Systeme Magdeburg*) 18:10–18:30

We consider the autonomous differential matrix Riccati equation $\dot{X} = A^T X + XA - XBB^T X + C^T C$. The differential Riccati equation as well as the algebraic Riccati equation play important roles in applied mathematics like system and control theory. In our talk, we focus on the large-scale case. The numerical solution of these equations is challenging, not least, because of the enormous amount of storage. A general approach, that has led to several algorithms, bases on a suitably identified invariant subspace $Q \subseteq \mathbb{R}^{n\times n}$ such that $X(t) \in Q$ for all t. The subspace Q is given as $Q = \{VSV^T \mid S \in \mathbb{R}^{p\times p}\}$ and $V \in \mathbb{R}^{n\times p}$ spans the Krylov subspace $\mathcal{K}(A^T, C^T) \subseteq \mathbb{R}^n$. We use a geometric argument to show that in fact $X(t) \in Q$ for all t and use the subspace Q to develop projection based approaches to the numerical solution. Also, we show that the same geometric argument allows for an extension from the autonomous differential Riccati equation to certain time-dependent cases.

S18.03 | Numerical methods of differential equations

Date 21.03.2018
Room 2370

Explicit computational wave propagation in micro-heterogeneous media

Roland Maier (*Numerical Mathematics, Universität Augsburg*), Daniel Peterseim (*Universität Augsburg*) 08:30–08:50

Explicit time stepping schemes are popular for linear acoustic and elastic wave propagation due to their simple nature. However, explicit schemes are only stable if the time step size is bounded by the mesh size in space subject to the so-called CFL condition. In micro-heterogeneous media, this condition is typically prohibitively restrictive because spatial oscillations of the medium need to be resolved by the discretization in space. This talk presents a way to reduce the spatial complexity in such a setting and, hence, also enable a relaxation of the CFL condition. This is done using the Localized Orthogonal Decomposition method as a tool for numerical homogenization.

A Mixed FEM with mass lumping for acoustic wave propagation

Herbert Egger (*Mathematik, TU Darmstadt*), Bogdan Radu (*Graduate School Computational Engineering, TU Darmstadt*) 08:50–09:10

We consider the numerical approximation of acoustic wave propagation in time domain by a mixed finite element method. A mass-lumping strategy, which was proposed by Wheeler and Yotov in the context of subsurface flow problems, is employed to enable the efficient time integration by explicit time integration schemes. By a careful analysis, we show that the numerical approximation, which is only first order accurate, actually carries second order information. This is expressed as super-convergence of the numerical approximations to certain projections of the true solution. Using these estimates, we are able to reconstruct improved approximations for the pressure and the velocity in a post-processing step. Together with the leapfrog scheme time-stepping scheme, we thus obtain fully explicit approximations of second order which can be computed very efficiently. Some numerical tests are presented to illustrate the efficiency of the proposed approach.

Space-Time Finite Element Methods for the Wave Equation

Marco Zank (*TU Graz*) 09:10–09:30

For the discretisation of time-dependent partial differential equations usually explicit or implicit time stepping schemes are used. An alternative approach is the usage of space-time methods, where the space-time domain is discretised and the resulting global linear system is solved at once. In this talk the model problem is the scalar wave equation. First, a brief overview of known results for the wave equation is presented. Second, a space-time formulation is motivated and discussed.
Finally, numerical examples for a one-dimensional spatial domain are presented.

S18.04 | Numerical methods of differential equations

Date 21.03.2018
Room 2370

Low-rank approximability of nearest neighbor interaction systems

Andre Uschmajew (*Max Planck Institute for Mathematics in the Sciences*) 14:00–14:40

Low-rank tensor techniques are an important tool for the numerical treatment of equations with a high-dimensional state space. Nearest neighbor interaction systems like the Ising model or some Chemical Master equations are examples for this, and the low-rank tensor train format has shown to be efficient for their computation in some cases. A challenging task is to provide theoretical justification for this, that is, to show that the exact solutions are well approximable by low-rank tensors. For ground states of 1D quantum spin systems such arguments have been found recently in the theoretical physics community, but it applies more generally. The idea is to the study rank-increasing properties of polynomials of the system operator. We will explain this idea and give numerical examples. Joint work with Patrick Gel\ss{}, Sebastian Matera and Reinhold Schneider.

The Hierarchical Tucker Format for a multi-dimensional Neo-Hookean partial differential equation

Dieter Moser (*RWTH Aachen, IGPM*) 14:40–15:00

The interest in high-dimensional or at least multi-dimensional problems arises in many fields of research, e.g. in plasma physics, represented by the Fokker-Planck equations, or in material science, represented by parametric PDE's. In recent years, the tensor numerical methods were recognized as the basic tool to tackle high-dimensional problems, where the general strategy is to reduce the problem onto a low parametric rank-structured manifold.
In this talk we establish a reduced model of a multi-dimensional Neo-Hookean PDE by using the Proper Orthogonal Decomposition (POD) method. This reduced model is then used to approximate a multivariate function, which maps a multidimensional parameter onto a quantity of interest, like the displacement in a certain direction. For this approximation the Hierarchical Tucker (HT) Format is employed. Furthermore, we will show how this HT approximation may be used to improve the underlying basis of the POD.

Parallel finite element discretization of PDEs with variable coefficients using sparse grids in arbitrary dimensions

Rainer Hartmann (*Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Christoph Pflaum (*Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*) 15:00–15:20

The number of unknowns of a Ritz-Galerkin discretization can be reduced using a sparse grid discretization for elliptic differential equations of second order on a d-dimensional cube. To reduce the complexity of the sparse grid discretization matrix, we apply prewavelets and a discretization with semi-orthogonally. Stability and optimal convergence of this discretization is proved with respect to the H^1 -norm for the Helmholtz equation with variable coefficients for arbitrary dimension d. The corresponding discretization error is $O\left(N^{-1}\left(\log N\right)^{d-1}\right)$ in the H^1 -norm.
The matrix-vector multiplication is decomposed into 2^d recursive calls of one dimensional operators for restriction and prolongation. Thus this algorithm can be perfectly distributed to parallel processes. The communication overhead is small due to the small number of unknowns of sparse grids. The simulation results up to level 10 for a 6-dimensional Helmholtz problem with variable coefficients show an optimal sparse grid convergence behavior. The computation can be allocated equally to 64 computing nodes of a cluster.

Parallel algorithms for arithmetic in the Hierarchical Tucker format

Christian Löbbert (*IGPM, RWTH Aachen*), Lars Grasedyck (*IGPM, RWTH Aachen*) 15:20–15:40

High-dimensional tensors of low rank can be represented in the Hierarchical Tucker Format (HT format) with a complexity which is linear in the dimension d of the tensor. We developed parallel algorithms which perform arithmetic operations between tensors in the HT format, where we assume the tensor data to be distributed among several compute nodes. The parallel runtime of our algorithms grows like $\log(d)$ with the tensor dimension d, due to the tree structure of the HT format. On each of the compute nodes one can use shared memory parallelization to accelerate the algorithms further. One application of our algorithms is parameter-dependent problems. Solutions of parameter-dependent problems can be approximated as tensors in the HT format if the parameter dependencies fulfill some low rank property. Our algorithms can then be used to perform post-processing on solution tensors, e.g. compute mean values, expected values or other quantities of interest, which is of interest in the field of uncertainty quantification. If the problem is of the form $Ax = b$ with a linear operator A as well in the HT format, we can compute the solution tensor directly in the HT format by means of iterative methods.

Stable ALS Approximation for Rank-Adaptive Tensor Completion

Sebastian Kraemer (*RWTH Aachen, IGPM*), Lars Grasedyck (*RWTH Aachen, IGPM*) 15:40–16:00

Low rank tensor completion is a highly ill-posed inverse problem, particularly when the data model is not accurate, and some sort of regularization is required in order to solve it. In this article we focus on the calibration of the data model. For alternating optimization, we observe that existing rank adaption methods do not enable a continuous transition between manifolds of different ranks. We denote this flaw as *instability (under truncation)*. As a consequence of this flaw, arbitrarily small changes in the singular values of an iterate can have arbitrarily large influence on the further reconstruction. We therefore introduce a singular value based

regularization to the standard alternating least squares (ALS), which is motivated by averaging in micro-steps. We prove its *stability* and derive a natural semi-implicit rank adaption strategy. We provide numerical examples that show improvements of the reconstruction quality up to orders of magnitude in the new Stable ALS Approximation (SALSA) compared to standard ALS.

S18.05 | Numerical methods of differential equations

Date 21.03.2018
Room 2370

Residual-based a posteriori error analysis for symmetric mixed Arnold-Winther FEM

Joscha Gedicke (*Fakultät für Mathematik, University of Vienna*), Dietmar Gallistl (*KIT - Karlsruhe Institute of Technology*), Carsten Carstensen (*HU Berlin*) 16:30–16:50

This talk introduces an explicit residual-based a posteriori error analysis for the symmetric mixed finite element method in linear elasticity after Arnold-Winther with pointwise symmetric and div-conforming stress approximation. Opposed to a previous publication, the residual-based a posteriori error estimator of this talk is reliable and efficient and truly explicit in that it solely depends on the symmetric stress and does neither need any additional information of some skew symmetric part of the gradient nor any efficient approximation thereof. Hence it is straightforward to implement an adaptive mesh-refining algorithm obligatory in practical computations. Numerical experiments verify the proven reliability and efficiency of the new a posteriori error estimator and illustrate the improved convergence rate in comparison to uniform mesh-refining. A higher convergence rate for piecewise affine data is observed in the stress error and reproduced in non-smooth situations by the adaptive mesh-refining strategy.

A posteriori error estimation in space and time for contact problems in linear viscoelasticity

Mirjam Walloth (*Fachbereich Mathematik, Technische Universität Darmstadt*) 16:50–17:10

We consider the Signorini contact problem of a linear viscoelastic body following the Kelvin-Voigt model. This model problem gives rise to a quasi-static variational inequality as the material is time-dependent. For the discretization in space we use finite elements and for the discretization in time the implicit Euler. In order to improve the accuracy of the numerical solution for given computational resources adaptivity in space and time is indispensable. Therefore, we present a residual-type a posteriori error estimator for the discrete solution and confirm our theoretical findings by numerical results.
The estimator is designed to control the error of the displacements, velocities and of a suitable approximation of the contact force. Distinguishing between full- and semi-contact while considering the time-dependency, the approximation of the contact force reflects the local properties of the solution. The starting point for the derivation of residual-type a posteriori estimators for linear problems without constraints is to establish a relation between the error measure and the linear residual. For parabolic problems the residual consists of a temporal and a spatial residual. For contact problems a so-called Galerkin functional replaces the role of the linear residuals. Combining ideas for linear parabolic [2] and contact problems [1] we propose a temporal and spatial Galerkin functional. On this basis the a posteriori estimator is derived. The estimator contributions addressing the nonlinearity are related to the contact stresses and the

complementarity condition. On the one hand, these contact-related contributions vanish in the so-called full-contact zone and, on the other hand, the critical region between the actual and non-actual contact zone can be well refined.

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[2] R. Verfürth, A posteriori error estimates for finite element discretizations of the heat equation. Calcolo. A Quarterly on Numerical Analysis and Theory of Computation, 40 (3), pp. 195–212, 2003.

Multi-Objective Goal Functional Error Estimates for Nonlinear Problems

Bernhard Endtmayer (*RICAM, Austrian Academy of Sciences*), Ulrich Langer (*RICAM, Austrian Academy of Sciences*), Thomas Wick (*Institut für Angewandte Mathematik, Leibniz Universität Hannover*)

17:10–17:30

In this presentation, we design a posteriori error estimates and mesh adaptivity for multiple goal functionals defined on the solutions to certain nonlinear problems based on results from [2] in the single-goal case. We use a dual-weighted residual approach in which localization is achieved in a variational form using a partition-of-unity. The key advantage is that the method is simple to implement. Backward integration by parts is not required. For the treatment of multiple goals, we use the ideas from [1] where linear problems are treated, but we do not have to solve an additional problem. Our adaptive algorithm has been developed for a wide class of non-linear problems such like the p-Laplace problem for which we run several numerical tests.

[1] Endtmayer, B. and Wick,T. A Partition-of-Unity Dual-Weighted Residual Approach for Multi-Objective Goal Functional Error Estimation Applied to Elliptic Problems. Comput. Methods Appl. Math. 17 (2017), no. 4, 575-599.

[2] Rannacher, R. and Vihharev, J.
Adaptive finite element analysis of nonlinear problems: balancing of discretization and iteration errors. J. Numer. Math. 21 (2013), no. 1, 23-61.

Stress-based finite element method for contact problems and a-posteriori error estimation

Bernhard Kober (*Fakultät für Mathematik, Universität Duisburg-Essen*), Gerhard Starke (*Fakultät für Mathematik, Universität Duisburg-Essen*)

17:30–17:50

The use of stress-based finite element methods for the treatment of contact problems admits direct access to the surface forces at the contact zone. Hence we are studying the application of the stress-based finite element method described in [1] featuring next-to-lowest order Raviart-Thomas-Elements to the Signorini contact problem using the dual variational formulation studied in [2].
Together with a H^1-conforming displacement reconstruction following the ideas from [3] and [4] and some additional post-processing of the stress-approximation, we construct a reliable a-posteriori error estimator using results from [5]. We will examine the quality of our approximation and the effectiveness of our error estimator by computational results.

[1] D. Boffi, F. Brezzi, and M. Fortin. Reduced symmetry elements in linear elasticity. *Commun. Pure Appl. Anal.*, 8:95–121, 2009.

[2] A. Capatina. Variational Inequalities and Frictional Contact Problems. Springer International Publishing, 2014.

[3] R. Stenberg. Postprocessing schemes for some mixed finite elements. *ESIAM: Math. Model. a. Num. Anal.*, 25:151–167, 1991.

[4] A. Ern and M. Vohralík. Polynomial-degree-robust a posteriori estimates in a unified setting for conforming, nonconforming, discontinuous Galerkin, and mixed discretizations. *SIAM J. Numer. Anal.*, 53:1058–1081, 2015.

[5] R. Krause, B. Müller and G. Starke. An Adaptive Least-Squares Mixed Finite Element Method for the Signorini Problem. *Numerical Methods Part. Diff. Eq.*, 33:276–289, 2017.

Mixed-primal finite element methods for stress-assisted diffusion problems

Bryan Gomez Vargas (*CI2MA and Departamento de Ingeniería Matemática, Universidad de Concepción*), Gabriel N. Gatica (*CI2MA and Departamento de Ingeniería Matemática, Universidad de Concepción*), Ricardo Ruiz Baier (*Mathematical Institute, University of Oxford*) 17:50–18:10

We analyse the solvability of a static coupled system of PDEs describing the diffusion of a solute into an elastic material, where the process is affected by the stresses generated by the solid motion. The problem is formulated in terms of solid stress, rotation tensor, solid displacement, and concentration of the solute. Existence and uniqueness of weak solutions follow from adapting a fixed-point strategy decoupling linear elasticity from a generalised Poisson equation. We then construct mixed-primal and augmented mixed-primal Galerkin discretisations based on adequate finite element spaces, for which we rigorously derive a priori error bounds. The convergence of these methods is confirmed through a set of computational tests in 2D and 3D.

An Accuracy Criterion for Galerkin Meshfree and Meshbased Solution Schemes

Christian Weißenfels (*Institute of Continuum Mechanics, Leibniz Universität Hannover*), Peter Wriggers (*Institute of Continuum Mechanics, Leibniz Universität Hannover*) 18:10–18:30

Meshfree methods open up new possibilities in the simulation of technical demanding processes, like chip formation or additive manufacturing. However, accuracy of meshfree solution schemes on arbitrary point clouds is still a challenge in computational mechanics. Here a criterion is presented which measures the unphysical error resulting from the inaccurate solution of the partial differential equation. Exemplary the Optimal Transportation Meshfree (OTM) method is selected which belongs to the class of Galerkin solution schemes. Several examples demonstrate the negative influence due to a violation of this criterion. A possible remedy to mitigate the error is also presented. Since a real surface is not defined in meshfree methods the imposition of surface loads on boundary nodes is another challenge in meshfree solution schemes. It will be shown that the accuracy criterion also computes the accurate value of the prescribed nodal force due to surface loads even in the case of an unknown boundary. Additionally, this accuracy criterion gives another indicator of reasons for underintegration. At the end some hints and improvements for the development of accurate meshfree solution schemes will be presented.

S18.06 | Numerical methods of differential equations

Date 22.03.2018
Room 2370

High-order Adaptive Mortar Finite Element Discretization for PDE Eigenvalue Problems in Quantum Chemistry

Kersten Schmidt (*Fachbereich Mathematik, Technische Universität Darmstadt*), Reinhold Schneider (*Institut für Mathematik, Technische Universität Berlin*), Lukas Drescher (*ETH Zurich*), Michael Götte (*Technische Universität Berlin*) 14:00–14:20

Mortar element methods use a decomposition of the computational domain and couple different discretization spaces in the subdomains weakly by a mortar condition. We introduce a high-order mortar element method for full-potential electronic structure calculations. For this we use a spherical discretization in spherical elements around each nucleus, which is adapted to resolve the core singularity due to an unbounded potential term. The spherical discretization is coupled with the mortar condition to a high order finite element discretization in between the nuclei. We discuss the error of the mortar element method in comparion with the hp-adaptive finite element method and show a residual error estimator. Numerical experiments have been performed using implementations in the C++ library Concepts (http://concepts.math.ethz.ch/).

Modeling and Simulation of Solid-State Lasers, From Mathematics to Industrial Application

Christoph Pflaum (*Informatik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*) 14:20–14:40

Solid-state lasers are widely used for different industrial applications ranging from material processing to medical applications. For designing and optimization of a solid-state laser an accurate simulation tool is need. Such a simulation tool has to be able to simulate different kind of physical effects like thermal effects, depolarization caused by stress inside a laser crystal, non-linear gain, and mode competition. In order to calculate output power and beam quality, we apply an extension of the dynamic mode analysis concept (DMA) (see [1]). This model is based on a 3-dimensional discretization of population inversion and a system of complex rate equations. The resulting mathematical equation system is a large system of ODE's, which has to be solved by a suitable method including time step control. The difficulty in such a simulation is the extreme change of parameters. As a consequence the output signal might be a pulsed signal with high output power of pulse width 1ns and time period 1ms. In order to solve such a system of ordinary differential equations accurately, we present a suitable numerical method. Simulation results with industrial applications are presented.
[1] M. Wohlmuth; C. Pflaum: K. Altmann; M. Paster; C. Hahn. Dynamic multimode analysis of Q-switched solid state laser cavities, Optics Express, 17(20), pp. 17303-17316, 2009.

Application of Finite Cell Method to Tunnel Engineering Simulation

Hoang-Giang Bui (*Statik & Dynamik, Ruhr-Universitaet Bochum*), Günther Meschke (*Ruhr-Universitaet Bochum*), Dominik Schillinger (*Department of Civil, Environmental, and Geo-Engineering University of Minnesota*) 14:40–15:00

Finite Cell Method (FCM) is an embedded domain method, in which the simulation domain is divided to the fictitious domain and the physical domain. The material in the fictitious is

penalized to restrict the computation of the virtual work in the physical domain. The accuracy of the integration is guaranteed by the use of the adaptive quadrature scheme. The adaptive quadrature scheme employs the quad-tree (oct-tree in 3D) data structure to generate the quadrature points up to the specified level around the material boundary. This scheme is simple and straightforward to implement in the numerical code, while providing the robustness over large range of geometries.
FCM is applied for the tunnel engineering simulation, a.k.a. the machine advancement process [1]. The geometry of the excavation volume is embedded into background mesh by employing the B-Rep concept. The mesh for the soil volume is structured and is fixed during the tunnel advancement. The tunnel lining is embedded in the soil mesh as a surface mesh, which incorporates the shell element formulation. In terms of the material description, the soil is represented as a saturated two-phase medium [4], which consists of the soil matrix and the pore water. The effective stress of the soil with regards to the displacement fields is governed by means of the Mohr-Coulomb constitutive model. Selected numerical benchmarks will be performed and validated against typical tunnel simulation using Lagrange finite element method.

Perfectly matched layers for linear Boltzmann equations

Herbert Egger (*TU Darmstadt*), Matthias Schlottbom (*Applied Mathematics, University of Twente*) 15:00–15:20

The linear Boltzmann equation is a hyperbolic integro-partial differential equation that describes the dynamics of a single-particle probability distribution in location-velocity phase space. The dynamics is governed by streaming, damping and scattering. The two main challenges in the numerical approximation of solutions to the linear Boltzmann equation are (i) the high dimensionality of the phase space, and (ii) the non-smoothness of the solution. The linear Boltzmann equation is equivalent to a mixed variational problem that incorporates boundary conditions naturally. However, the natural inclusion of boundary conditions introduces a non-smooth coupling of spatial and velocity variables, which is inconvenient for practical implementations. To overcome this difficulty, we introduce an absorbing layer and consider a perturbed problem with reflection boundary conditions such that the resulting variational problems lead to sparse linear systems that exhibit a tensor product structure.

Similarity of Field Quantities in Scaled Radiation Transfer Lattice Boltzmann Simulations (RT-LBM)

Christopher McHardy (*Fachgebiet Lebensmittelbiotechnologie und -prozesstechnik, TU Berlin*), Cornelia Rauh (*Fachgebiet Lebensmittelbiotechnologie und -prozesstechnik, TU Berlin*) 15:20–15:40

The lattice Boltzmann framework provides a powerful tool to solve radiation transfer problems in participating media. Recently, different formulations of Radiation Transfer lattice Boltzmann methods (RT-LBM) have been proposed [1, 2]. Thereby, tuning of the collision rate to the numerical time step is necessary to ensure accurate solutions. One way of doing this is to scale the radiation characteristics of the medium what can be done by means of the similarity relations [3]. These relations conserve the transport mean free path in the medium and were shown to ensure similarity of intensity, which is the zeroth angular moment of radiance. However, there is still a controversial whether higher order moments are conserved after scaling and alternative scaling procedures were proposed in literature.
In the present contribution radiation characteristics of participating media are scaled to the numerical grid by means of the similarity relations to tune the accuracy of the RT-LBM. Thereby, a free parameter was introduced and its effect on the solution is investigated. Also, the similarity

of higher order angular moments is studied. The results show that conservation of the transport mean free path ensures the similarity of solutions and that by accurate computation of scattering matrices an almost perfect similarity of higher order moments can be achieved.

1 C McHardy, T Horneber, C Rauh (2016). Optics Express, 24(15), 16999-17017.

2 A Mink, G Thäter, H Nirschl, MJ Krause (2016). Journal of Computational Science, 17(2), 431-437.

3 BHJ McKellar, MA Box (1981). Journal of the Atmospheric Sciences, 38, 1063-1068.

Application of Lie group theory in solving problems of elastoplastic materials

Li-Wei Liu (*Institute of Thermomechanics of the Czech Academy of Sciences*) 15:40–16:00

Lie group and its Lie algebra are very beautiful theory in the Mathematics. The application of Lie group and Lie algebra is well-known in classical mechanics, quantum mechanics or other physics. Thanks to Hong and Liu [1, 2] who opened a new era in the integration of the model for elastoplastic materials based on the property of Lie group. They discovered the underlying structure of the perfectly elastoplastic model with von Mises yield surface. This symmetry is the cone of Minkowski spacetime $\mathbb{M}^{5+1}$ on which the proper orthochronous Lorentz group $\mathrm{SO_o}(5,1)$, a sub group of the Lie group, left acts. Therefore, the developed integration updates the stress points to be automatically on the yield surface of von-Mises at every time increment of plastic phase. This indeed influences over the researcher in the field of computational mechanics for elastoplastic materials. Following the work of Hong and Liu, scholars explored the internal symmetry of several elastoplastic models and developed their so-called group-preserving integrations individually. In this paper we attempted to apply the theory of other subgroups inside Lie group to solve the problems of elastoplastic materials. We systematically classified elastoplastic model into two different sets $\mathcal{C}$ and $\bar{\mathcal{C}}$. The property of the proper orthochronous pseudo-orthogonal group $\mathrm{SO_o}(p,q)$ can be used to develop the return-free integration [3], which keeps the stress points on the field surface without any extra enforment during every time increment of plastic phase, to solve every model inside the set $\mathcal{C}$. On the other hand, models of set $\bar{\mathcal{C}}$ which do not belong to the set $\mathcal{C}$ can be solved by aid of the theory of Lie group $\mathrm{GL}(n)$ [4]. Based on the aid of the property of Lie-group $\mathrm{SO_o}(p,q)$ and $\mathrm{GL}(n)$, we designed the algorithm of integration of elastoplastic models including two part, one is the elastic module and the other is the plastic module, and demonstrated the performance of the integration for the material model belong to sets $\mathcal{C}$ and $\bar{\mathcal{C}}$.

Acknowledgement: This material is based upon work supported by the European Regional Development Fund under Grant No. CZ.02.1.01/0.0/0.0/15_003/0000493 (Centre of Excellence for Nonlinear Dynamic Behaviour of Advanced Materials in Engineering) and by the Ministry of Science and Technology of Taiwan (MOST 104-2218-E-002-026-MY3).

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[3] Chein-Shan Liu, Li-Wei Liu*, and Hong-Ki Hong, A scheme of automatic stress-updating on yield surfaces for a class of elastoplastic models, International Journal of Non- Linear Mechanics Vol. 85, pp. 6 - 22, 2016.

[4] Chein-Shan Liu, Wen Chen, and Li-Wei Liu*, Solving mechanical systems with nonholonomic constraints by the Lie-group differential algebraic equations method, Journal of Engineering Mechanics, Vol. 143, No. 9, 04017097.

S18.07 | Numerical methods of differential equations

Date 22.03.2018
Room 2370

Fundamental nonlinear wave equations in nonlinear acoustics: analytical and numerical aspects

Mechthild Thalhammer (*Department of Mathematics, University of Innsbruck*) 17:30–17:50

In this talk, fundamental models from nonlinear acoustics are considered. In particular, a hierarchy of nonlinear damped wave equations arising in the description of sound propagation in thermoviscous fluids is introduced. It is seen that two classical models, the Kuznetsov and Westervelt equations, are retained as limiting systems for consistent initial data. Numerical simulations confirm and complement the theoretical results.

Operator splitting for stiff differential equations

Axel Ariaan Lukassen (*AG Numerik und wissenschaftliches Rechnen, TU Darmstadt*), Martin Kiehl (*AG Numerik und Wissenschaftliches Rechnen, TU Darmstadt*) 17:50–18:10

Splitting methods are frequently used for large scale chemical reaction systems. The main reason is the reduced computational costs for solving the subproblems in comparison to the time integration of the full problem. However, a splitting error is introduced. The most popular splitting schemes are the first order Lie-Trotter splitting and the second order Strang splitting. Although, in case of stiff differential equations the Strang splitting suffers from order reduction and both schemes have order one for stiff differential equations. Therefore, the step size restrictions due to the low order can result in a prohibitive small step size. Hence, splitting schemes with order larger than one are necessary for stiff differential equations. We prove that the Richardson extrapolation of the Lie-Trotter splitting is a second order scheme, which has order two in the stiff case. As a result the extrapolated Lie-Trotter splitting results in much smaller step sizes than the Strang splitting for stiff differential equations.

A Species-clustered ODEs Solver for Chemical Kinetics Based on Diffusion Map/Optimal Partition

Jianhang Wang (*Technische Universität München*), Shucheng Pan (*Technische Universität München*), Xiangyu Hu (*Technische Universität München*), Nikolaus A. Adams (*Technische Universität München*) 18:10–18:30

In this study, a species-clustered ODEs solver for chemical kinetics with large detailed mechanisms based on operator-splitting is presented. The ODEs system will be split into clusters of species with dependencies by using the network/graph partition methods which has been intensively studied in areas of model reduction, parameterization and coarse-graining, etc. , such as the diffusion map based on the concept of Markov random walk. Since the similarity matrix is application-driven, different definitions of it in the scenario of chemical kinetics will be discussed. As the partition will involve eigenvalue problems and costly matrix treatments, it is preferable

to perform clustering of species on-the-fly according to the time-dependent pairwise relations of species in every a few timesteps to reduce the computational efforts. Each cluster of species will be integrated by traditional ODEs solvers such as the popular implicit VODE which is intractable for large systems of many species and reactions. Good gain in computational efficiency will be expected and numerical experiments including the zero-dimensional auto-ignition problem and the laminar flame case are to investigate, taking into account the detailed hydrocarbon/air combustion mechanisms, e.g. the GRI 3.0 mechanism with 53 species and 325 reactions.

S18.08 | Numerical methods of differential equations

Date 23.03.2018
Room 2370

An optimal order DG time discretization scheme for parabolic problems with non-homogeneous constraints

Igor Voulis (*IGPM, RWTH Aachen University*), Arnold Reusken (*IGPM, RWTH Aachen University*) 08:30–08:50

We consider parabolic problems with non-homogeneous constraints. Standard problems of this kind include the heat equation with a non-homogeneous Dirchlet boundary condition and the following Stokes problem with an non-homogeneous divergence condition and a non-homogeneous boundary condition (in $\Omega \times [0,T]$, $\Omega \subset \mathbb{R}^d$):

$$\begin{aligned} u' - \Delta u + \nabla p &= f \\ \mathrm{div} u &= g \\ u|_{\partial\Omega} &= h \\ u(0) &= u_0. \end{aligned}$$

This problem can be seen as a parabolic problem in (an affine coset of) the space of divergence free functions with a Lagrange multiplier p and two non-homogeneous conditions: $\mathrm{div} u = g$ and $u|_{\partial\Omega} = h$.
If one applies standard DG in time sub-optimal results are obtained (cf. Table below). We present an analysis which explains the cause of this sub-optimal behavior. Based on this analysis we introduce a modification which leads to an optimal convergence order, not only for the energy norm of u, but also for the L^2 norm of the Lagrange multiplier p. Furthermore, an optimal nodal superconvergence result for u is obtained.
Our theoretical results are confirmed by numerical results. In the table below one can see that the temporal convergence order for the Lagrange multiplier is 1 for the standard method (SM) and 2 for our modified method (MM). In this experiment we used a $\mathcal{P}_2 - \mathcal{P}_1$ Taylor-Hood pair in space and linear functions in time. For the modified method we see that the spatial error dominates after a few temporal refinements (N_T).

N_T	4	8	16	32	64	128
SM	1.36231	0.73455	0.37695	0.19011	0.09513	0.04755
EOC_T		0.89112	0.96248	0.98752	0.99894	1.00042
MM	0.30828	0.07813	0.01984	0.00589	0.00286	0.00261
EOC_T		1.98035	1.97707	1.75344	1.04000	0.13472

Error in L^2-norm between exact p and the solution of the discrete problem.

Numerical Analysis for the Regularization of a Parabolic Obstacle Problem

Dominik Hafemeyer (*M17, TUM*) 08:50–09:10

We consider a parabolic obstacle problem, which arises for example in the modelling of finances. Given a finite time intervall I and a sufficiently regular domain $\Omega \subset \mathbb{R}^N$ with $N \in \{2, 3\}$ it has the form

$$\begin{cases} \partial_t y - \Delta y + f(y) \geq u \text{ in } I \times \Omega, \\ y|_{I\times\partial\Omega} = 0,\ y(0) = y_0, \\ y \geq \Psi \text{ in } I \times \Omega, \\ (y - \Psi, \partial_t - \Delta y + f(y) - u)_{L^2(I\times\Omega)} \geq 0. \end{cases}$$

Here Ψ is an obstacle of the appropriate regularity, $u \in L^\infty(I \times \Omega)$ and f is a "sufficiently nice" nonlinearity.
We also consider a regularization of it by a family of appropriate semilinear parabolic differential equations, which penalize a violation of the obstacle. Then we discretize those equations by discontinuous finite elements in time and piecewise linear finite elements in space. We deduce a sharp L^∞ discretization error estimate, which is independent of the regularization parameter. In this step we use a result on an L^∞ discretization error estimate for linear parabolic differential equations and a duality argument.
We can now combine this discretization error estimate with an regularization error estimate to give a complete a priori error estimate between a solution of the variational inequality and a regularized, discretized solution. Numerical examples will be provided as well.

A time-space FCT finite element formulation for time-dependent advection-diffusion-reaction equation

Dianlei Feng (*Institute of Fluid Mechanics and Environmental Physics in Civil Engineering, Leibniz Universität Hannover*), Insa Neuweiler (*Institute of Fluid Mechanics and Environmental Physics in Civil Engineering, Leibniz Universität Hannover*), Udo Nackenhorst (*Institute of Mechanics and Computational Mechanics, Leibniz Universität Hannover*) 09:10–09:30

We present a time-space flux-corrected transport (FCT) finite element formulation for solving time-dependent advection-diffusion-reaction equations. Especially, we are interested in advection dominated transport problems. Solving advection dominated transport equations with standard finite element methods often suffers from drawbacks of excessive numerical dispersion which results in non-physical, non-monotonic solutions. The FCT algorithm is an effective method which can suppress the non-monotonic behavior of the solution by applying multi-dimensional flux limiters. Previous studies on the FCT method are mostly based on the method of lines which discretizes the system of equations in time with finite difference methods, such as the Euler scheme, the Runge-Kutta method and so the forth. To the best of our knowledge, a time-space FCT formulation has not been developed. Applying time-space formulations to solve the advection dominated transport equations allows adopting large Courant numbers as well as using higher order (more than the second order) time schemes at the same time. A comparative study of the time-space FCT method to the Runge-Kutta based FCT method is carried out. Our studies demonstrate that the presented time-space FCT formulation maintains those advantages.

Optimal parameters for a family of flux-correction methods strongly reducing overshoot in unsteady flow computation

Herbert Niessner (*NiMa*) 09:30–09:50

Flux-correction allows to reduce or even avoid overshoot occuring when Lax-Wendroff methods are used to calculate one-dimensional flow. There is a whole family of methods depending on two parameters, whose optimal values are derived. One controls the amount of diffusion to reduce overshoot, the other determines removal of this diffusion as far as overshoot does not reappear, thus largely retaining accuracy of the employed Lax-Wendroff method.

Investigation of the symmetry-breaking behavior of low dissipation WENO schemes

Nico Fleischmann (*Lehrstuhl für Aerodynamik und Strömungsmechanik, Technische Universität München*), Stefan Adami (*Lehrstuhl für Aerodynamik und Strömungsmechanik, Technische Universität München*), Nikolaus A. Adams (*Lehrstuhl für Aerodynamik und Strömungsmechanik, Technische Universität München*) 09:50–10:10

Compressible flow solvers used for the simulation of shock phenomena commonly apply finite volume methods using high-order spatial discretization schemes. Recent publications provide so-called WENO (weighted essentially non-oscillatory) stencils up to 17th order. As shown in detail by different authors these stencils come along with a remarkable decrease in numerical dissipation. Solving the inviscid and per se unstable Euler equations is subject to new challenges due the fact that numerical dissipation no longer suppresses numerical instabilities triggered e.g. by floating point inaccuracies. We have investigated this new challenge and noticed a significant impact of floating-point arithmetics on the outcome of a simulation, especially when studying symmetric problems. Therefore, the actual implementation of the numerical algorithm requires careful validation. Different from previous interpretations, we can show that e.g. the symmetry-breaking property of the Rayleigh-Taylor instability is purely caused by roundoff errors and not a physical effect that is observable only with lowest-dissipation schemes.

Parallelized space-time boundary element methods for the heat equation

Stefan Dohr (*Technische Universität Graz*), Olaf Steinbach (*Technische Universität Graz*) 10:10–10:30

The standard approach in space-time boundary element methods for discretizing variational formulations of boundary integral equations is using space-time tensor product spaces originating from a separate decomposition of the boundary $\partial\Omega$ and the time interval $(0,T)$. However, this approach does not allow adaptive refinement in space and time simultaneously. This motivates the use of an arbitrary decomposition of the whole space-time boundary $\Sigma = \partial\Omega \times (0,T)$ into boundary elements. In this talk we consider the heat equation as a model problem and compare these two discretization methods. Both methods allow us to parallelize the computation of the global solution of the whole space-time system. This also includes the assembling of the dense system matrices. Due to the structure of the matrices one has to design a suitable scheme for the distribution of the matrix blocks to the computational nodes using MPI in order to get an efficient parallel solver. We present numerical tests to confirm the theoretical results and evaluate the efficiency of the proposed parallelization approach. The presented parallel solver is based on joint work with G. Of from TU Graz and J. Zapletal from the Technical University of Ostrava.

S19 | Optimization of differential equations

Organiser Irwin Yousept (*University of Duisburg Essen*)
Antoine Laurain (*Mathematics, Instituto de Matemática e Estatística*)

S19.01 | Optimization of differential equations

Date 20.03.2018
Room N1095

The dual formulation of elastoplasticity: Inf-sup stability and semismooth Newton method

Gerhard Starke (*Fakultät für Mathematik, Universität Duisburg-Essen*) 08:30–08:50

The dual variational formulation of elastoplasticity consists in minimizing the free energy with respect to the stresses subject to constraints given by the conservation of momentum, stress symmetry and the plastic flow rule. We study a weakly symmetric stress-based mixed finite element formulation using Raviart-Thomas spaces of next-to-lowest order. For the case of a plastic flow rule of von Mises type with isotropic hardening, the validity of the discrete inf-sup stability is investigated. This is done in the context of a semismooth Newton iteration which, in the dual setting, possesses a particularly simple structure.

Discretization error for quadratic-approximations to phase-field fracture control

Masoumeh Mohammadi (*TU Darmstadt*), Ira Neitzel (*Universität Bonn*), Thomas Wick (*Universtiät Hannover*), Winnifried Wollner (*FB Mathematik, TU Darmstadt*) 08:50–09:10

Within this talk, we will briefly discuss the function-space setting for a class of optimization problems involving fracture processes modeled by a phase-field approach. Although this problem need not satisfy a constraint qualification a quadratic-approximation, as needed in SQP-type algorithms, admits a unique solution for the considered class. We will discuss the regularity of the linearized equations. Based on the regularity, convergence with rates of a finite element approximation will be shown.

Maximization of the variations of a pressure coupled with the elastodynamics system

Sebastien Court (*Institut für Mathematik und Wissenschaftliches Rechnen, Karl-Franzens-Universität Graz*) 09:10–09:30

We are interested in the nonlinear unsteady elastodynamics system coupled with a mechanical pressure, in dimension 2 or 3. This pressure is a Lagrange multiplier associated with the - nonlinear - constraint of constant global volume that we impose through the time. This a scalar function, depending only on the time variable, and which appears in a nonlinear Neumann-type boundary condition for the hyperbolic PDE system. Our goal is to maximize the time-derivative of this pressure, at a time which is left free, and so chosen optimally. Thus the time at which this maximum is reached is a parameter that has to be determined in the same way as the control function. Theoretical issues including wellposedness, derivation of optimality conditions as well

as numerical realization will be addressed in this talk. This problem occurs in the context of cardiac electrophysiology. The heart is seen as an hyperelastic tissue crossed by the blood (an incompressible fluid). Under electric impulse, the efficiency of the defibrillation is indeed related to the amplitude of variations of this pressure.

Optimal Control of Time Discretized Dynamic Contact Problems

Georg Müller (*Chair of Applied Mathematics, Universität Bayreuth*), Anton Schiela (*Chair of Applied Mathematics, Universität Bayreuth*) 09:30–09:50

We address optimal control problems with distributed control and time discretized dynamic contact problems in linear elasticity as side constraints, i.e.,

$$\begin{aligned} &\min\ J(y,u) \\ &s.t.\ (y,u) \in Y \times U \\ &\quad y \in K \\ &\quad Bu - Ay \in T_K(y)^\circ, \end{aligned} \tag{1}$$

for the closed, convex set of admissible displacements K, where the variational inequality (1) results from the application of a suitable time integrator for the time continuous form of the dynamic contact problem.

The discretized contact problem (1) admits a Lipschitz continuous and generally directionally differentiable solution operator and we show existence of minimizers to the optimal control problem under standard assumptions on the cost functional. For dense controls, we obtain a set of first order optimality conditions.

A pointwise interpretation of the biactive set allows for the introduction of local quadratic models whose optimality conditions can be solved using an adjoint time stepping scheme to provide search directions for iterative minimization algorithms. We compare the performance of *simple* gradient-type approaches with different line searche methods to *accelerated* gradient-type schemes with and without momentum restart for two numeric examples in two-dimensional one-body contact.

Adaptive trust-region POD for optimal control of the Cahn-Hilliard equation

Carmen Gräßle (*Department of Mathematics, University of Hamburg*), Michael Hinze (*Mathematics, University of Hamburg*), Nicolas Scharmacher (*Mathematics, University of Hamburg*) 09:50–10:10

We consider the optimal control of a Cahn-Hilliard system in a trust-region framework. For an efficient numerical solution, the expensive high dimensional PDE systems are replaced by reduced order models utilizing proper orthogonal decomposition (POD-ROM). Within the trust-region POD (TR-POD), the accuracy of the surrogate models is controlled in the course of the optimization. The POD modes are computed corresponding to snapshots of the governing equations which are discretized utilizing adaptive finite elements. In the numerical examples, the smooth as well as the double-obstacle free energy potential are considered.

Optimal Control of Thermoviscoplasticity

Ailyn Stötzner (*TU Chemnitz*), Roland Herzog (*TU Chemnitz*), Christian Meyer (*TU Dortmund*) 10:10–10:30

Elastoplastic deformations play a tremendous role in industrial forming. Many of these processes happen at non-isothermal conditions. Therefore, the optimization of such problems is of interest not only mathematically but also for applications.
Optimal control problems governed by a thermovisco(elasto)plastic model are nonsmooth and nonconvex. In this talks we will give an overview of the analysis of the existence of a global solution as well as of the differentiability properties. Finally, we will discuss some numerical results.

S19.02 | Optimization of differential equations

Date 20.03.2018
Room N1189

Optimal error estimates of fully discrete solutions for initial data identification of parabolic problems

Dmitriy Leykekhman (*math, University of Connecticut*), Boris Vexler (*TU Muenchen*) 08:30–08:50

We consider a inverse source identification problem for parabolic problem. We view the problem as optimal control problem where the control acts at initial data. We discretize the problem with continuous piecewise linear elements in space and discontinuous Galerkin methods in time. The convergence of the fully discrete solution were shown previously, however to obtain optimal convergence rates we require novel pointwise smoothing fully discrete error estimates for homogeneous parabolic problems. To obtain such results we employ a newly developed discrete maximal parabolic regularity results together with elliptic pointwise error estimate. In my talk I will discuss the above results and main ideas of the proof.

Ill-posed backward nonlinear Maxwell's equations

Dehan Chen (*University of Duisburg-Essen*), Irwin Yousept (*University of Duisburg-Essen*) 08:50–09:10

This talk is concerned with Tikhonov regularization and optimization for ill-posed backward nonlinear hyperbolic evolution Maxwell equations. Through the use of an appropriate Tikhonov regularization, we recover the exact initial data from the final observation data with L2-noisy. The well-posedness and convergence behavior of the regularized solutions are established. In particular, we verify the variational source condition for the inverse problem and derive Hölder type convergence rates under an appropriate parameter choice and Sobolev-type priori assumptions on initial values. It is worth mentioning that our results can be applied to the Bean's critical state model in type-II superconductivity. The major tools used here include regularization theory and mathematical theory for Maxwell's equations.

Identifying diffusion coefficients in nonlinear parabolic equations

Jan-Frederik Pietschmann (*Westfälische Wilhelms-Universität Münster*), Herbert Egger (*TU Darmstadt*), Matthias Schlottbom (*UT Twente*) 09:10–09:30

In this talk we consider the identification of nonlinear diffusion coefficients of the form $a(t,u)$ or $a(u)$ in quasi-linear parabolic and elliptic equations. Uniqueness for this inverse problem is established under very general assumptions using partial knowledge of the Dirichlet-to-Neumann map. The proof of our main result relies on the construction of a series of appropriate Dirichlet data and test functions with a particular singular behavior at the boundary. This allows us to

localize the analysis and to separate the principal part of the equation from the remaining terms. We therefore do not require specific knowledge of lower order terms or initial data which allows to apply our results to a variety of applications. This is illustrated by discussing some typical examples in detail.

Parameter Identification for a Phase Field Tumor Model

Christian Kahle (*Technische Universität München*), Kei-Fong Lam (*The Chinese University of Hong Kong*) 09:30–09:50

We consider the inverse problem of identifying parameters in a variant of the diffuse interface model for tumour growth model proposed by Garcke, Lam, Sitka and Styles (Math. Models Methods Appl. Sci. 2016). The model contains three constant parameters; namely the tumour growth rate, the chemotaxis parameter and the nutrient consumption rate. We study the inverse problem from the viewpoint of PDE-constrained optimal control theory and establish first order optimality conditions. A chief difficulty in the theoretical analysis lies in proving high order continuous dependence of the strong solutions on the parameters, in order to show the solution map is continuously Frechet differentiable when the model has a variable mobility. Due to technical restrictions, our results hold only in two dimensions for sufficiently smooth domains. Analogous results for polygonal domains are also shown for the case of constant mobilities. Finally, we propose a discrete scheme for the numerical simulation of the tumour model and solve the inverse problem using a trust-region Gauss–Newton approach.

Inverse point source location with the Helmholtz equation

Philip Trautmann (*Uni Graz*), Daniel Walter (*TU München*), Konstantin Pieper (*FSU*), Tang Quoc Bao (*Uni Graz*) 09:50–10:10

In this talk the reconstruction of a linear combination of acoustic monopoles from given noisy measurements of the acoustic pressure at M observation points is addressed. For the solution of this problem a family of regularized optimal control problems involving the Helmholtz equation is used. These optimization problems are posed in the space of measures and the regularization functional is given by a weighted version of the total variation norm for measures which is non-smooth and favors solutions with a sparse support. To prove well-posedness of these optimization problems in a general setting the weights in the regularization functional are chosen unbounded in the observation points. Moreover, optimality conditions and conditions for the recovery of the exact sources in the case of small noise are derived. The regularized problems are solved by an accelerated conditional gradient method. The Helmholtz equation is discretized by linear finite elements. Finally, numerical experiments are presented which suggest that an appropriate choice of the weighting function increases the quality of the reconstructions over the unweighted approach.

The Fréchet derivative of rational best approximations to the matrix exponential and it's application on inverse parabolic problems

Mario Helm (*Numerical Mathematics and Optimization, TU Bergakademie Freiberg*) 10:10–10:30

We consider an inverse problem, where a high dimensional parameter $\mathbf{c}$ has to be identified from measurements of some components of the solution of the parametric initial value problem $\mathbf{u}'(t) = A(\mathbf{c})\mathbf{u}(t)$, $\mathbf{u}(0) = \mathbf{b}$ at some given time points. Here $A(\mathbf{c})$ is a large sparse symmetric negative definite matrix.

Applying Gauß-Newton's method it is important to have information about the sensitivity of the forward solution with respect to the parameter $\mathbf{c}$. But due to the size of the problem, it is unfeasible to compute the dense and large Jacobian directly. Therefore we will solve the linearized least square problems iteratively (e.g., by LSQR) which requires algorithms to compute products of the form $J\mathbf{v}$ and $J^T\mathbf{w}$.
We present a new approach, where the forward solution is approximated using the rational best approximation of the exponential function. We will focus on the Fréchet derivatives of the corresponding rational matrix functions, their numerical evaluation and approximation errors with respect to the Fréchet derivative of the matrix exponential. We show how products with the Jacobian and its transpose can be implemented in an economic way, and present numerical examples.

S19.03 | Optimization of differential equations

Date 20.03.2018
Room N1095

Optimal control of resources for species survival

Yannick Privat (*Laboratoire Jacques-Louis Lions, Sorbonne Universités, UPMC Univ Paris 06*) 16:30–16:50

In this work, we are interested in the analysis of optimal resources configurations (typically foodstuff) necessary for a species to survive. For that purpose, we use a logistic equation to model the evolution of population density involving a term standing for the heterogeneous spreading (in space) of resources. The principal issue investigated in this talk writes:
How to spread in an optimal way resources in a closed habitat?
This problem can be recast as the one of minimizing the principal eigenvalue of an operator with respect to the domain occupied by resources, under a volume constraint. By using symmetrization techniques, as well as necessary optimality conditions, we prove new qualitative results on the solutions. In particular, we investigate the optimality of balls. This is a joint work with Jimmy Lamboley (univ. Paris Dauphine), Antoine Laurain (univ. Sao Paulo) and Grégoire Nadin (univ. Paris 6).

Towards optimal biological transportation networks

Giacomo Albi (*University of Verona*), Martin Burger (*WWU Münster*), Jan Haskovec (*KAUST*), Peter Markowich (*KAUST*), Matthias Schlottbom (*Applied Mathematics, University of Twente*) 16:50–17:10

A transportation network is a realization of a spatial structure that permits flow of some commodity. Transportation networks are ubiquitous in both social and biological systems, such as transportation of nutrition in blood vessels. In this talk we interpret optimal transportation networks as minimizers of an energy functional, which has been introduced by Hu and Cai. For minimization of the non-convex energy functional, splitting algorithms are considered. The potential of this approach is shown by numerical examples.

A shape optimization algorithm for interface identification allowing topological changes

Martin Siebenborn (*Universität Trier*) 17:10–17:30

In many applications, which are modeled by partial differential equations, there is a small number of materials or parameters distinguished by interfaces to be identified. While classical approaches in the field of optimal control yield continuous solutions, a spatially distributed, binary variable is closer to the desired application. It is thus favorable, to treat the shape of the interface between an active and inactive control as the variable. Moreover, since the involved materials may form complex contours, high resolutions are required in the underlying finite element discretizations. We investigate a combination of classical PDE constrained optimization methods and a rounding strategy based on shape optimization for the identification of interfaces. The goal is to identify radioactive regions in a groundwater flow represented by a control that is either active or inactive. We use a relaxation of the binary problem on a coarse grid as initial guess for the shape optimization with higher resolution. The result is a computationally cheap method that does not have to perform large shape deformations. We demonstrate that our algorithm is moreover able to change the topology of the initial guess.

Classical optimal design on annulus and numerical solution by shape derivative method

Marko Vrdoljak (*Department of Mathematics, Faculty of Science, University of Zagreb*), Petar Kunštek (*Department of Mathematics, Faculty of Science, University of Zagreb*) 17:30–17:50

We consider optimal design problems for stationary diffusion equation, seeking for the arrangement of two isotropic materials, with prescribed amounts, which maximizes the energy functional. The aim is to present some classes of problems on an annulus with classical solutions.
The first class is a single state equation problem with a constant right-hand side and homogenous Dirichlet boundary condition. By analysing the optimality conditions, we are able to show that there exists a unique (classical) solution. Depending on the amounts of given materials, we find two possible optimal configurations in two- and three-dimensional case.
The second class of problems deals with a two-state optimal design problem. The presence of classical solutions enables us to test different numerical methods i.e. compare rates of convergence, stability or check for possible errors. For demonstration, a shape gradient method was implemented in `FreeFem++` showing robust convergence to the calculated explicit solution. Based on shape derivative, method creates vector field which moves interface between phases in order to increase value of object function.

On an inverse problem for fatigue modeling

Barbara Pedretscher (*KAI Kompetenzzentrum Automobil- und Industrieelektronik GmbH*), Barbara Kaltenbacher (*Alpen-Adria-Universität Klagenfurt*), Olivia Bluder (*KAI Kompetenzzentrum Automobil- und Industrieelektronik GmbH*) 17:50–18:10

In semiconductor applications, thermo-mechanical fatigue and its effect on reliability are under regular investigation. Especially, modeling and efficient numerical simulation of fatigue induced degradation in metal films of semiconductor devices is of interest to gain reliable lifetime models. In this work, the degradation of a bi-layer test structure (metal film on substrate) under repetitively applied thermo-mechanical stress is studied. For degradation modeling, we use a State Space Model (SSM) in combination with stochastic differential equations to account for intrinsic fluctuations.
Parameter identification is performed by a Maximum Likelihood approach based on the system's Fokker-Planck equation (Dunker, Hohage, 2014). The well-posedness criteria of the forward problem include a no-flux boundary condition, the ellipticity condition (Lax-Milgram), as well

as a condition, which guarantees that diffusion dominates transport at the boundary (Carrillo, Cordier, Mancini, 2011). The definition of a stochastically consistent Likelihood function is challenging for two reasons: First, two sources of variation (stochastic process, measurement error) have to be considered and second, the observation operator is not necessarily bijective in a general setting.
Efficient numerical optimization requires the gradient of the Likelihood with respect to the parameters, for which purpose an adjoint approach is followed. For implementation, we use the MATLAB Toolbox AMICI, provided by the Helmholtz Zentrum Munich. Since AMICI supports ODE based SSMs, the Fokker-Planck equation is semi-discretized by the Chang-Cooper discretization scheme, assuring mass and positivity conservation. With the developed mathematical framework, parameter identification for different degradation models can be performed.

Algorithmic Differentiation used for increased sensitivity in parameter identification problems of piezoelectric ceramics

Benjamin Jurgelucks (*Institut für Mathematik, Universität Paderborn*) 18:10–18:30

A cost effective way to identify material parameters of piezoelectric ceramics is to fit the measured and simulated electrical impedance curve as part of an inverse problem. However, one substantial problem is that the sensitivity of impedance with respect to some material parameters usually is low or close to zero. Thus, in this case this inverse problem cannot be solved to full satisfaction for all material parameters using a single specimen.
In order to improve this situation we optimize the electrode configuration on the piezoelectric ceramic which is used for exciting the ceramic. This allows for increased sensitivity of impedance. Here, instead of applying electrodes fully covering top and bottom of the ceramic, two ring electrodes on the top and one ring electrode on the bottom of the ceramic are applied. Furthermore, through the use of Algorithmic Differentiation (AD) in the simulation software we can optimize the electrode ring radii for a higher sensitivity for all material parameters or specifically for just a select few material parameters.
Furthermore, AD gives precise derivative information we utilize in the solution process for the inverse problem. We will show some numerical results of the sensitivity optimization as well as solving the inverse problem using artificial and real data.

S19.04 | Optimization of differential equations

Date 20.03.2018
Room N1189

Optimal voltage control of non-stationary eddy current problems

Alberto Valli (*Department of Mathematics, University of Trento, Italy*), Fredi Tröltzsch (*Institut für Mathematik„ Technische Universität Berlin, Germany*) 16:30–16:50

We propose and analyze a mathematical model that can be useful for controlled voltage excitation in time-dependent electromagnetism. The well-posedness of the model is proved and an associated optimal control problem is investigated. Here, the control function is a transient voltage and the aim of the control is the best approximation of desired electric and magnetic fields in suitable L^2-norms. Special emphasis is laid on an adjoint calculus for first-order necessary optimality conditions. Moreover, a peculiar attention is devoted to devise a formulation for which the computational complexity of the finite element solution method is substantially reduced.

Staggered discontinuous Galerkin methods for wave propagation

Eric Chung (*Department of Mathematics, The Chinese University of Hong Kong*) 16:50–17:10

In this talk, we will present the staggered discontinuous Galerkin (SDG) methods for wave propagation. The method is based on piecewise polynomial approximation defined on some carefully constructed staggered meshes. The resulting scheme is explicit, energy conserving, optimally convergent and has a super-convergence in terms of dispersion. We will illustrate the performance of the method for the acoustic wave equation, elastic wave equation and the Maxwell's equation. Eric Chung's research is partially supported by the Hong Kong RGC General Research Fund (Project: 14301314) and the CUHK Direct Grant for Research 2015-16.

Effective electromagnetic properties of a metamaterial consisting of small split-ring resonators

Agnes Lamacz (*Mathematics, University of Duisburg Essen*), Ben Schweizer (*TU Dortmund*) 17:10–17:30

Propagation of light in heterogeneous media is a complex subject of research. It has received renewed interest in recent years, since technical progress allows for smaller devices and offers new possibilities. At the same time, theoretical ideas inspired further research. Key research areas are photonic crystals, negative index metamaterials, perfect imaging, and cloaking.
The mathematical analysis of negative index materials, which we want to focus on in this talk, is connected to a study of singular limits in Maxwell's equations. We present a result on homogenization of the time harmonic Maxwell's equations in a complex geometry. The homogenization process is performed in the case that many (order η^{-3}) small (order η^1), flat (order η^2) and highly conductive (order η^{-3}) metallic split-rings are distributed in a domain $\Omega \subset \mathbb{R}^3$. We determine the effective behavior of this metamaterial in the limit $\eta \searrow 0$. For $\eta > 0$, each single conductor occupies a simply connected domain, but the conductor closes to a ring in the limit $\eta \searrow 0$. This change of topology allows for an extra dimension in the solution space of the corresponding cell-problem. Even though both original materials (metal and void) have the same positive magnetic permeability $\mu_0 > 0$, we show that the effective Maxwell system exhibits, depending on the frequency, a negative magnetic response. Furthermore, we demonstrate that combining the split-ring array with thin, highly conducting wires can effectively provide a negative index metamaterial.

Fully discrete scheme for Bean's critical-state model in type-II superconductivity

Malte Winckler (*Faculty for mathematics, University of Duisburg Essen*), Irwin Yousept (*University of Duisburg Essen*) 17:30–17:50

This talk is devoted to the electromagnetic phenomenon in type-II superconductivity, which occurs in many technological applications nowadays. Focusing on the original formulation of Maxwell together with Bean's critical state constitutive law, we obtain a non-smooth hyperbolic Maxwell system. After deriving a suitable formulation, we adress the numerical analysis of hyperbolic mixed variational inequalities of the second kind for the governing evolutionary Maxwell's equations. At first, we present a discretization in time with an implicit Euler method and analyse the resulting elliptic problems. This, in combination with a Ritz-Galerkin approximation in space, leads us to the fully discrete scheme. As a main result, we prove strong convergence

for the proposed approximation and realize it by means of the lowest order edge elements of Nédélec's first family. We close our talk by presenting some numerical results, which confirm not only our theoretical findings but also the physical effects in type-II superconductivity.

Feedback Control for Hyperbolic Balance Laws

Stephan Gerster (*IGPM, RWTH Aachen University*) 17:50–18:10

Physical systems such as water and gas networks are usually operated in a state of equilibrium and feedback control is employed to damp small perturbations over time. We consider flow problems on networks, described by hyperbolic balance laws, and analyze the stabilization of steady states. Sufficient conditions for exponential stability in the continuous and discretized setting are presented. Computational experiments illustrate the theoretical findings.

[1] Gerster, Herty, *Discretized Feedback Control for Hyperbolic Balance Laws*, Preprint-No. 468 (2017), RWTH Aachen University

On the optimal control problem for non-smooth wave phenomena

André Maldonado (*Universität Duisburg-Essen*), Irwin Yousept (*Universität Duisburg-Essen*) 18:10–18:30

In this talk we discuss the optimal control problem for a non-smooth and nonlinear hyperbolic PDE that describes acoustic phenomena defined in an unbounded domain. At first, we put the PDE problem in a semi-group theory framework and show that the infinitesimal generator of the group associated to the PDE is skew-adjoint. Therefore we can apply Stone's theorem to get the control-to-state operator which is given by the variation of constants formula. Also due to the skew-adjoint property, we are able to use the energy balance equality which is our main tool in order to prove the existence of the solution for the optimal control problem. In this part, we also discuss the lack of compactness arising from the unboundedness of the spatial domain in the governing PDE. We tackle this problem by restricting both the optimization problem and the control source to a bounded domain. Finally, we obtain a necessary optimality condition of the strong stationarity type for the optimal control problem.

S19.05 | Optimization of differential equations

Date 21.03.2018
Room N1189

Total Variation Diminishing Schemes in Optimal Control of Scalar Conservation Laws

Michael Hintermüller (*WIAS Berlin*), Soheil Hajian (*Mathematics, Humboldt-Universität zu Berlin*), Stefan Ulbrich (*Mathematics, TU Darmstadt*) 14:00–14:20

Optimal control problems subject to a nonlinear scalar conservation law, the state system, are studied. Such problems are challenging both at the continuous and discrete level since the control-to-state operator poses difficulties such as non-differentiability. Therefore discretization of the control problem has to be designed with care to provide stability and convergence. Here, the discretize-then-optimize approach is pursued and the state is removed by the solution of the underlying state system, thus providing a reduced control problem. An adjoint calculus

is then applied for computing the reduced gradient in a gradient-related descent scheme for solving the optimization problem. The time discretization of the underlying state system relies on total variation diminishing Runge-Kutta (TVD-RK) schemes, which guarantee stability, best possible order and convergence of the discrete adjoint to its continuous counterpart. While interesting in its own right, it also influences the quality and accuracy of the numerical reduced gradient, and thus the accuracy of the numerical solution. In view of these demands, it is proven that providing a state scheme which is a strongly stable TVD-RK method is enough to ensure stability of the discrete adjoint state. It is also shown that requiring strong stability for both, the discrete state and adjoint, is too strong, confining one to a first-order method regardless of the number of stages employed in the TVD-RK scheme. Given such a discretization, we further study order conditions for the discrete adjoint such that the numerical approximation is of the best possible order. Also, convergence of the discrete adjoint state towards its continuous counterpart is studied. In particular, it is shown that such a convergence result hinges on a regularity assumption at final time for a tracking-type objective in the control problem. Finally, numerical experiments validate our theoretical findings.

Optimality conditions for a class of elliptic VIs of second kind involving unbounded operators

Livia Susu (*University of Duisburg-Essen*), Irwin Yousept (*University of Duisburg-Essen*) 14:20–14:40

The talk is concerned with an optimal control problem governed by an elliptic variational inequality of second kind involving an unbounded operator. After presenting the precise model, the bounded counterpart thereof is introduced, which is still a variational inequality of second kind. Thus, Gâteaux-differentiability of the associated solution operator is not to be expected and standard adjoint calculus is not applicable. The control-to-state mapping is however directional differentiable. By employing this property, a strong stationary optimality system is derived, without imposing any additional regularity assumptions. By means thereof, one obtains optimality conditions for the original problem. These are deduced not by employing the standard regularization technique, but by exploiting the Yosida approximation of the unbounded operator in the original VI. The talk ends with the application of the general results to the the elliptic version of the Maxwell's equations governed by Bean's critical state law.

Efficient path-following for an optimal control problem with BV functions

Florian Kruse (*Institute of Mathematics and Scientific Computing, University of Graz*), Dominik Hafemeyer (*Lehr- und Forschungseinheit für Optimalsteuerung (M17), Technische Universität München*) 14:40–15:00

In this talk we consider the optimal control problem

$$\min_{(y,u)\in H_0^1(\Omega)\times BV(\Omega)} \frac{1}{2}\|y-y_\Omega\|^2_{L^2(\Omega)} + \beta|u|_{BV(\Omega)} \quad \text{s.t.} \quad \begin{cases} -\Delta y = u & \text{in } \Omega, \\ y = 0 & \text{on } \partial\Omega. \end{cases} \tag{P}$$

Here, $\Omega \subset \mathbb{R}^n$, $n \in \{2,3\}$, is a bounded Lipschitz domain, $y_\Omega \in L^2(\Omega)$, $\beta > 0$, and $|\cdot|_{BV(\Omega)}$ denotes the isotropic total variation.
To handle the nonsmooth BV seminorm, we introduce for $\gamma, \delta > 0$ the regularization

$$\min_{(y,u)\in H_0^1(\Omega)\times H^1(\Omega)} \frac{1}{2}\|y-y_\Omega\|^2_{L^2(\Omega)} + \beta\int_\Omega \sqrt{\delta + |\nabla u|_2^2}\,dx + \frac{\gamma}{2}\|u\|^2_{H^1(\Omega)} \quad \text{s.t.} \quad \begin{cases} -\Delta y = u & \text{in } \Omega, \\ y = 0 & \text{on } \partial\Omega. \end{cases}$$

The optimality system of the regularized problem includes a regularized mean curvature equation – a highly nonlinear elliptic PDE whose numerical solution is challenging.

We establish optimality conditions and prove convergence of the solution of the regularized problem to the solution of (P). Moreover, we present an efficient path-following method; it is based on reducing the regularized optimality system to the state and the adjoint state. Numerical examples that illustrate structural properties of optimal controls for (P) and demonstrate the effectiveness of the algorithmic approach are included, too.

Subgradient Computation for the Solution Operator of the Obstacle Problem

Anne-Therese Rauls (*TU Darmstadt*), Stefan Ulbrich (*TU Darmstadt*) 15:00–15:20

The obstacle problem is an important prototype of an elliptic variational inequality and it appears in the mathematical formulation of applications from physics, finance and other fields. When dealing with constraints of obstacle type in optimization problems, the main difficulty is the nondifferentiability of the corresponding solution operator.
In this talk we determine and characterize a specific element of the Bouligand subdifferential respective to the solution operator of the obstacle problem.
Using a generalization of Rademacher's theorem to infinite dimensions, we construct an abstract sequence of differentiability points, whose Gâteaux derivatives converge to a subgradient. In order to show this convergence a precise analysis of the relevant set-valued mappings connected to the Gâteaux derivatives is necessary. The limit and thus the subgradient itself is determined by the solution of a variational equation, which is independent of the abstract approximating sequence.
The analysis indicates that also other elements in the subdifferential can be obtained by similar approaches. Moreover, discretization or approximation of the variational equation can serve as a basis for the numerical computation of inexact subgradients.

Optimal control of reaction-diffusion-systems with hysteresis

Christian Münch (*Mathematics, Technische Universität München*) 15:20–15:40

We discuss an optimal control problem, where the state equation is given by a reaction-diffusion system, with a reaction term that includes a hysteresis operator.
The memory effect of hysteresis complicates the proof of existence and uniqueness theorems for the state equation. Due to the non-smoothness of the system, it is also not clear, whether or in which sense the solution operator is differentiable. It turns out that the state equation has unique solutions and is Hadamard differentiable. Nevertheless, some additional work has to be done to derive first order optimality conditions in form of an adjoint system.
Our main focus lies on deriving the adjoint system for the special case, when the hysteresis is given by a scalar stop operator. We either consider a distributed control, or one which acts on the Neumann boundary part of the domain.

Accelerated conditional gradient methods for continuous sparse optimization problems

Daniel Walter (*Centre for Mathematical Sciences, M17, TUM*), Konstantin Pieper (*Florida State University*) 15:40–16:00

We consider a class of sparse minimization problems over a space of measures on a continuum, with solutions consisting of a finite sum of Dirac-delta functions. Such problems arise in inverse source location problems and in the context of optimal experimental design. For the algorithmic solution we consider a conditional gradient method, which iteratively inserts Dirac-delta functions and optimizes the corresponding coefficients. Under general assumptions, a sub-linear convergence rate in the objective functional is obtained, which is sharp in most cases. To improve

efficiency, one can fully resolve the finite-dimensional subproblems occurring in each step of the method. We provide an analysis for the resulting procedure: under a structural assumption on the optimal solution, a linear $C\lambda^k$ convergence rate is obtained locally. Numerical experiments confirm the theoretical findings and the practical efficiency of the method.

S19.06 | Optimization of differential equations

Date 21.03.2018
Room N1189

Turnpike in optimal control

Emmanuel Trélat (*Laboratoire Jacques-Louis Lions, Université Pierre et Marie Curie Paris VI*) 16:30–16:50

The turnpike property emerged in the 50's, after the works by the Nobel prize Samuelson in econometry. It stands for the general behavior of an optimal trajectory solution of an optimal control problem in large time. This trajectory trends to behave as the concatenation of three pieces: the first and the last arc being rapid transition arcs, and the middle one being in large time, almost stationary, close to the optimal value of an associated static optimal control problem. In recent works with Can Zhang and Enrique Zuazua, we have established the turnpike property in a very general framework in finite and infinite dimensional nonlinear optimal control. We prove that not only the optimal trajectory is exponentially close so some (optimal) stationary state, but also the control and the adjoint vector coming from the Pontryagin maximum principle. Our analysis shows an hyperbolicity phenomenon which is intrinsic to the symplectic feature of the extremal equations. We infer a very simple and efficient numerical method to compute optimal trajectories in that framework, in particular with an appropriate variant of the shooting method.

A phase field approach for optimal boundary control of viscous damage processes in 2D

Mohammad Hassan Farshbaf Shaker (*Mathematik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*) 16:50–17:10

Controlling the growth of material damage is an important engineering task with plenty of real world applications. In this talk we approach this topic from the mathematical point of view by investigating an optimal boundary control problem for a damage phase-field model for viscoelastic media. We consider non-homogeneous Neumann data for the displacement field which describe external boundary forces and act as control variable. The underlying hyberbolic-parabolic PDE system for the state variables exhibit highly nonlinear terms which emerge in context with damage processes. The cost functional is of tracking type, and constraints for the control variable are prescribed.

Optimal control of a time-dependent Kohn-Sham quantum model

Gabriele Ciaramella (*University of Konstanz*), Alfio Borzi (*University of Würzburg*), Martin Sprengel (*University of Würzburg*) 17:10–17:30

A viable way to develop optimal control strategies for multi-particle quantum systems is to consider the framework of time-dependent density functional theory (TDDFT), where low-dimensional nonlinear Schrödinger models are developed to compute the electronic density of related high-dimensional linear Schrödinger equations. Among these models, the Kohn-Sham

TDDFT system allows to accommodate control mechanisms in the same potentials that appear in the original multi-dimensional Schrödinger equations, thus allowing a physical interpretation and a laboratory implementation. The purpose of this talk is the analysis and the numerical solution of optimal control problems governed by the time-dependent Kohn-Sham (TDKS) equations including a control potential that has the purpose to drive the evolution of the electron density to achieve given tasks. Existence of optimal solutions of these optimal control problems is discussed and their characterization as solutions of TDKS optimality systems is investigated. An efficient optimization method based on robust numerical techniques and an operator splitting discretization of the optimality system is illustrated. Results of numerical experiments demonstrate the computational effectiveness of the proposed control framework.

(A) A theoretical investigation of time-dependent Kohn-Sham equations - G. Ciaramella, A. Borzi, M. Sprengel - SIAM Journal on Mathematical Analysis 49 (3), 1681-1704 - 2017.

(B) Investigation of optimal control problems governed by a time-dependent Kohn-Sham model - G. Ciaramella, A. Borzi, M. Sprengel - accepted for publication in Journal of Dynamical and Control Systems - 2017.

(C) A COKOSNUT for the control of the time-dependent Kohn-Sham model - G. Ciaramella, A. Borzi, M. Sprengel - Computer Physics Communications 214, 231-238 - 2017.

Compactness by coercivity for nonlinear evolutionary optimal control problems

Hannes Meinlschmidt (*RICAM*)

17:30–17:50

We consider optimal control problems subject to an evolution equation in which the control enters nonlinearly. Since nonlinear superposition operators are, in a sense, categorically not weakly continuous, compactness properties of (subsets of) the set of admissible controls play an important role when trying to establish existence of optimal solutions to the optimal control problem. In the setting of time-dependent controls, such compactness properties are widely researched and well available, but enforcing them naively in the optimal control problem may result in structural difficulties in the associated first-order necessary conditions. We propose a Tychonov term based on real interpolation for the objective function which is coercive on a family of function spaces admitting compact embeddings into many standard control spaces, and explore the resulting first-order necessary conditions. These turn out to be essentially Banach space-valued obstacle problems in time.

Optimal control of instationary gas transport

Thomas Kugler (*TU Darmstadt*), Herbert Egger (*TU Darmstadt*)

17:50–18:10

We consider the optimal control of instationary gas transport in a pipeline network. The well-posedness of the governing system of partial differential-algebraic equations is discussed and the existence of minimizers is established. For the numerical solution, we consider a Galerkin approximation of the state equation by mixed finite elements, we establish well-posedness of this discretization, and prove the existence of minimizers for the corresponding discretized optimal control problem. We further discuss the efficient numerical minimization via projected Newton-type algorithms and present computational test to illustrate the performance of the proposed algorithms and to demonstrate their viability for online control of typical situations arising during intraday operation of a gas network.

Optimal boundary control of hyperbolic balance laws with state constraints

Johann Michael Schmitt (*Technische Universität Darmstadt*), Stefan Ulbrich (*Technische Universität Darmstadt*) 18:10–18:30

This talk deals with the treatment of pointwise state constraints in the context of optimal boundary control of hyperbolic nonlinear scalar balance laws.
We study an optimal control problem governed by balance laws with initial and boundary conditions, where we suppose that the boundary data switch between smooth function at certain switching points. The smooth functions and the switching points are hereby considered as the control.
The appearance of state constraints presents a special challenge, since solutions of nonlinear hyperbolic balance laws develop discontinuities after finite time, which prohibits the use of standard methods. In this talk, we will build upon the recently developed sensitivity- and adjoint calculus by Pfaff and Ulbrich to derive necessary optimality conditions. In addition, we will use Moreau-Yosida regularization for the algorithmic treatment of the pointwise state constraints. Hereby, we will prove convergence of the optimal controls and weak convergence of the corresponding Lagrange multiplier estimates of the regularized problems.

S19.07 | Optimization of differential equations

Date 22.03.2018
Room N1189

Discrete Total Variation with Finite Elements and Applications in Imaging, Inverse Problems and Optimal Control

Roland Herzog (*Mathematics, TU Chemnitz*) 08:30–09:10

The total-variation (TV) seminorm is ubiquitous as a regularizing functional in image analysis, inverse problems and is also gaining popularity in optimal control. In this talk, we propose and analyze a discrete analog of the TV-seminorm for functions belonging to a space of globally discontinuous or continuous finite element functions, including spaces of higher order. We show that our discrete TV functional admits a convenient dual representation close to the continuous formulation and allows for efficient implementations of classical algorithms in image restoration, inverse problems and optimal control.

Interacting Particle Systems & Optimization

Rene Pinnau (*Mathematics, TU Kaiserslautern*) 09:10–09:30

In this talk we try to shed some light on the connection of dogs herding sheep and the optimization of interacting particle systems. Main goal is the control of a large crowd of individuals by a few external agents. This yields a high dimensional constrained optimization problem, which is solved by an instantaneous control approach. And since there are many individuals involved we will also study the corresponding mean-field limit to gain some insight in the respective asymptotic behavior of the optimal control problem.

Optimal control of the bilinear heat equation subject to state and control constraints

Axel Kröner (*Humboldt-University Berlin*), Frederic Bonnans (*INRIA Saclay / CMAP, Ecole polytechnique*), M. Soledad Aronna (*EMAp/FGV*) 09:30–09:50

In this talk we discuss optimality conditions for an optimal control problem governed by a semilinear heat equation with bilinear coupling of control and state and subject to state constraints. The control enters affine in the cost function. We derive first and second order optimality conditions, taking advantage of the Goh transform.

Multilevel Optimization of Fluid-Structure Interaction based on Reduced Order Models

Stefan Ulbrich (*Mathematik, TU Darmstadt*), Johanna Biehl (*Mathematik, TU Darmstadt*) 09:50–10:10

The interaction of fluid flows with elastic materials is part of many applications, for example in medicine, civil engineering or aerodynamics. Therefore it is of interest to control flow and the corresponding deformation of the structure.
In this talk, we introduce a derivative based multilevel optimization algorithm for fluid-structure interaction problems of incompressible flows and hyperelastic structures in a laminar regime.
Since the corresponding monolithic finite element discretization is nonlinear and high dimensional, we introduce a reduced order model based on proper orthogonal decomposition to reduce the cost of the optimization process. The existence and stability of solutions of the resulting reduced saddle point problem is ensured with the help of supremizers, which guarantee that the inf-sup condition is satisfied.
For the optimization we use an adaptive SQP method for PDE-constrained problems introduced in [1, 2] with adjoint based derivative computation and a posteriori error estimators for the finite element discretization and reduced order model. The presented method is applied to a Benchmark problem proposed by Turek and Hron [3].

[1] J. Ziems, S. Ulbrich, *Adaptive Multilevel Inexact SQP Methods for PDE-constrained Optimization*, SIAM J. Optim., 2011, 21, 1-40

[2] S. Bott, *Adaptive SQP Method with Reduced Order Models for Optimal Control Problems with Constraints on the State Applied to the Navier-Stokes Equations*, Technischen Universität Darmstadt, 2016, Dissertation

[3] S. Turek, J. Hron, *Proposal for Numerical Benchmarking of Fluid-Structure Interaction between an Elastic Object and Laminar Incompressible Flow*, Fluid-Structure Interaction, Springer Berlin Heidelberg, 2006, 53, 371-385

Improving thermal ablation of liver tumors

Matthias Andres (*Mathematics, University of Kaiserslautern*) 10:10–10:30

Laser-induced thermotherapy is a medical treatment which attempts to destroy liver tumors by thermal ablation. The heat transfer inside the liver can be described by a nonlinear coupling of the so-called bio-heat equation and a radiative transfer model. What makes a realistic real-time simulation challenging are high computational costs for solving the system of equations and the identification of patient-specific parameters. In this talk we discuss the influence of different parameters on the simulation and a first attempt to address this problem.

S19.08 | Optimization of differential equations

Date 22.03.2018
Room N1189

Numerical analysis for Dirichlet control problems

Thomas Apel (*Institut für Mathematik und Bauinformatik, Universität der Bundeswehr München*), Mariano Mateos (*Universidad de Oviedo*), Johannes Pfefferer (*TU München*), Arnd Rösch (*Universtät Duisburg-Essen*) 14:00–14:20

Discretization error estimates for Dirichlet control problems are presented. State and control are discretized by piecewise linear and continuous functions. Singularities of the solution at corners of the domain are taken into account by using graded finite element meshes. These singularities are different for unconstrained and control constrained problems. Without grading, the methods converge with optimal rate only if the maximal maximal angle of the domain is below $2\pi/3 = 120°$. With grading, the methods are shown to converge optimally for arbitrary polygonal domains.

Error estimates for an optimal control problem related to quasi-linear parabolic pdes

Konstantinos Chrysafinos (*Mathematics, National Technical University of Athens*), Eduardo Casas (*Universidad de Cantabria*) 14:20–14:40

An optimal control problem related to quasilinear parabolic pdes is considered where the coefficients of the elliptic part of the operator depend on the state function. Several issues related to existence, uniqueness and regularity for the solution of the state equation as well as to first and second order optimality conditions are discussed. The controls are of distributed type and satisfy pointwise constraints. The discretization scheme of the state and adjoint equations is based on a discontinuous time-stepping scheme combined with conforming finite elements (in space). Provided that the time and space discretization parameters, τ and h respectively, satisfy $\tau \leq Ch^2$, error estimates of order $\mathcal{O}(h)$ are discussed for the difference between the locally optimal controls and their discrete approximations, when the controls are discretized by piecewise constants functions,

Finite element error estimates for normal derivatives on boundary concentrated meshes

Johannes Pfefferer (*Chair of Optimal Control, Technische Universität München*), Max Winkler (*Technische Universität Chemnitz*) 14:40–15:00

This talk is concerned with finite element error estimates for the solution of linear elliptic equations. More precisely, we focus on approximations and related discretization error estimates for the normal derivative of the solution. In order to illustrate the ideas, we consider the Poisson equation with homogeneous Dirichlet boundary conditions and use standard linear finite elements for its discretization. The underlying domain is assumed to be polygonal but not necessarily convex. Approximations of the normal derivatives are introduced in a variational sense. On quasi-uniform meshes, one can show that these approximate normal derivatives possess a convergence rate close to one in $L^2(\partial\Omega)$ as long as the singularities due to the corners are mild enough. Using boundary concentrated meshes, we show that the order of convergence can even be doubled in terms of the mesh parameter.

As an application, we use these results for the numerical analysis of Dirichlet boundary control problems, where the control variable corresponds to the normal derivative of some adjoint variable. Finally, the predicted convergence rates are confirmed by numerical examples.

Error Estimates for Bilinear Boundary Control Problems

Max Winkler (*Fakultät für Mathematik, TU Chemnitz*) 15:00–15:20

In this talk we consider bilinear boundary control problems, this is, the (possibly non-constant) Robin coefficient of a reaction-diffusion equation with boundary conditions of third kind is the control variable. These kind of problems arise for instance in stem cell division which can be modeled by a reaction-diffusion system describing the concentration of proteins forming the cell plasma and the cell wall. To understand these chemical reactions in a better way one is mainly interested in the unknown reaction parameters which can be computed from a bilinear optimal control problem, where the desired state is a given measurement of the protein concentrations. In this talk necessary and sufficient optimality conditions for these optimal control problems are presented. Moreover, regularity of solutions and finite element approximations with corresponding error estimates are discussed. The approximate solutions are obtained by a full discretization of the optimality system with cell-wise constant controls and continuous and linear state variables. In addition, error estimates for an improved control obtained in a postprocessing step by a pointwise evaluation of the projection formula are derived.

Robust Error Estimates for Time-Optimal Control Problems with Bang-bang Controls

Lucas Bonifacius (*TU München*), Konstantin Pieper (*Florida State University*), Boris Vexler (*TU München*) 15:20–15:40

We consider the time-optimal control problem

$$\text{Minimize } j(T,q) := T + \frac{\alpha}{2}\int_0^T \|q(t)\|^2_{L^2(\Omega)}\mathrm{d}t,$$

$$\begin{aligned} T > 0,\ q \in Q_{ad}, & \\ \partial_t u + Au = Bq, & \quad \text{in } (0,T)\times\Omega, \\ u(0) = u_0, & \quad \text{in } \Omega, \\ \|u(T) - u_d\|_{L^2(\Omega)} \le \delta, & \end{aligned} \tag{P}$$

with desired terminal state $u_d \in L^2(\Omega)$ and given $\delta > 0$. Moreover, Q_{ad} denotes the set of admissible controls and $\alpha > 0$ the regularization parameter. Since in case of bang-bang controls the natural critical cone used in sufficient optimality conditions is trivial, a second order condition is vacuously true, and it is unlikely that this guarantees local optimality of a solution. Instead, we rely on a well-established structural assumption on the adjoint state. This assumption leads to robust discretization and regularization error estimates for the optimal time and the control variable in $L^1((0,1)\times\omega)$.

Numerical Analysis for Time-Dependent Electromagnetic Field Control

Vera Bommer (*Universität Duisburg-Essen*), Irwin Yousept (*Universität Duisburg-Essen*) 15:40–16:00

This presentation investigates the optimal control of the full time-dependent Maxwell equations. The treatment of electromagnetic fields is important for many modern applications and technologies. We are interested in finding an optimal current source and its time-dependent amplitude which steer the electromagnetic field to the desired one at the final time. In our case, the Maxwell equations, that feature a first-order hyperbolic coupled structure, are discretized by mixed finite elements based on piecewise constant elements for the electric field and lowest order edge elements of Nédélec's first family for the magnetic field. Then, a Crank-Nicolson scheme in time leads to a fully discrete approximation of the evolutionary Maxwell equations. Applying this discretization strategy to our optimal control problem, we are able to prove strong convergence and a priori error estimates for the finite element approximation depending on the regularity of the data. As a conclusion, we present some numerical examples which confirm our theoretical findings.

S19.09 | Optimization of differential equations

Date 22.03.2018
Room N1189

Fast generation of initial estimates for indirect optimal control

Rainer Callies (*Department of Mathematics M2, Technical University of Munich*) 17:30–17:50

For the numerical solution of optimal control problems governed by large systems of ordinary differential equations two basic approaches are successfully applied. In the direct approach, controls (and states) are first discretized to form a large finite-dimensional nonlinear optimization problem which is then solved by standard algorithms. In the indirect approach, using optimal control theory based on the Maximum Principle the problem is transformed into a boundary value problem which is then solved numerically. In addition to the equations of motion, a set of differential equations for the adjoint variables and algebraic expressions for the controls are derived from the so-called Hamiltonian. A main challenge for indirect methods was the automatic generation of initial estimates for the adjoint variables. A new approach is presented based on the estimated or experimentally observed controls of a suboptimal solution. These controls are interpreted as optimal controls of a modified problem. They are formally integrated backwards; together with the algebraic constraints on optimal solutions (optimality condition and constant Hamiltonian) an inverse problem is formulated and solved to obtain reliable estimates for the adjoint variables on a predefined grid. By homotopy techniques the so obtained optimal solution of a modified problem is transferred into the solution of the original problem. As an example optimal flight trajectories for aerobatic aircraft in the Red Bull Air Races are calculated. Competitors have to complete tight turns through a challenging slalom course in minimum time and subject to multiple constraints. The optimal solutions show extremely complicated control structures.

On an optimal control problem with quasilinear parabolic PDE

Lucas Bonifacius (*Centre for the Mathematical Sciences, Chair of Optimal Control, Technische Universität München*), Ira Neitzel (*Institute for Numerical Simulation, University of Bonn*) 17:50–18:10

This talk is concerned with the discussion of second order sufficient optimality conditions for an optimal control problem governed by quasilinear parabolic PDEs. We consider problems with distributed and certain types of boundary control, respectively, in two and three space dimensions. We arrive at a quadratic growth condition without two-norm-discrepancy. Stability results with respect to certain perturbations of the nonlinear operator are derived.

Optimal Control of Coupled Systems involving ODEs and PDEs

Sven-Joachim Kimmerle (*Fakultät für Luft- und Raumfahrttechnik, Universität der Bundeswehr München*), Matthias Gerdts (*Fakultät für Luft- und Raumfahrttechnik, Universität der Bundeswehr München*) 18:10–18:30

We consider several examples for optimal control problems subject to coupled systems of ordinary differential equations (ODEs) and partial differential equations (PDEs).
As a key example we focus on a vehicle transporting a fluid container as load. The fluid container is mounted to the vehicle by a spring-damper element. The motion of the fluid is modelled by the Saint-Venant equations while the vehicle dynamics are described by Newton's equations of motion. The system may be controlled by the acceleration of the vehicle. This leads to an optimal control problem with a fully coupled system of nonlinear hyperbolic first-order partial differential equations and ordinary differential equations.
We present further mathematical models involving coupled ODEs and PDEs, formulate the optimal control problems and discuss numerical and analytic approaches for optimal control. As numerical approaches, we consider first-discretize-then-optimize methods, first-optimize-then-discretize methods, and structure-exploiting optimisation algorithms of the sequential quadratic programming (SQP) type as well. The idea of exploiting the particular structure may be applied to other optimal control problems as well.

S19.10 | Optimization of differential equations

Date 23.03.2018
Room N1095

Projected CG onto an Inexact Kernel for PDE Constrained Optimization

Anton Schiela (*Universität Bayreuth*) 08:30–08:50

Projected cg methods are popular inner solvers in nonlinear equality constrained optimization. They solve quadratic problems on the kernel of the linearized constraints by projecting corrections onto this kernel, applying a so called constraint preconditioner. In this way they preserve the given problem structure, in contrast to other iterative solvers like MINRES.
In PDE constrained optimization, application of a constraint preconditioner amounts in solving adjoint equation and linearized state equation once. For very large scale problems one would like to replace these (exact) solves by application of a preconditioner for these equations. This, however, means that the given quadratic problem is solved on a different, an inexact kernel.
In our talk we present an algorithm, where such an inexact inner solver is augmented by an outer iteration that corrects the inexactness of the kernel and thus converges to the solution of the original problem. We describe this algorithm in detail, present a convergence result, and discuss its numerical behaviour.

Regularization Techniques for PDE-Constrained Optimization under Uncertainty

Thomas M. Surowiec (*Mathematics and Computer Science, Philipps-Universität Marburg*), Drew P. Kouri (*Optimization and Uncertainty Quantification, Sandia National Laboratories*) 08:50–09:10

The vast majority of real world problems in the engineering and physical sciences are laden with uncertainty. In optimization and optimal control, this leads to stochastic programming problems

with distributed parameters. In order to handle this uncertainty in the constraints and objective functionals, we exploit techniques from risk management and employ convex and coherent risk measures. Since many of the most popular risk measures, e.g., expected shortfall, are in fact non-smooth, we often need a suitable regularization scheme in order to take advantage of efficient numerical approximation techniques and optimization algorithms from PDE-constrained optimization. To this end, we propose a variational smoothing technique, which we call "epi-regularzation". Epi-regularization provides us with a comprehensive theoretical framework for studying the effects on the axioms of coherency and regularity, differentiability, variational convergence, and consistency of minimizers and first-order stationary points. Moreover, whenever there are sufficient local second-order growth properties of the objective, we can derive rigorous error estimates. The theoretical results are confirmed by several numerical experiments.

On the Barzilai-Borwein step-sizes in Hilbert spaces

Behzad Azmi (*Johann Radon Institute for Computational and Applied Mathematics (RICAM), Österreichische Akademie der Wissenschaften*) 09:10–09:30

The Barzilai and Borwein (BB) method, proposed by Barzilai and Borwein in 1988, has received extensive attention due to its simplicity and numerical efficiency. The key idea in BB method is to maintain a steepest descent framework by approximating the Hessian by a scalar multiple of the identity matrix in such a manner that the secant condition holds. In this talk, we discuss the convergence of this method for problems in infinite-dimensional Hilbert spaces. First, we investigate the convergence of BB method for bounded quadratic problems in Hilbert spaces. Then based on this result, we study the local convergence of this method for twice Fréchet differentiable functions. Next, results concerning the mesh-independence of BB method are presented and numerical examples are given.

Discretization error estimates for optimal control of phase-field fracture.

Masoumeh Mohammadi (*TU Darmstadt*), Winnifried Wollner (*TU Darmstadt*) 09:30–09:50

An optimal control problem for fracture propagation will be presented. The fracture is modeled by a phase-field approach, and the regularized fracture model is relaxed by a penalization term. The choice of the penalty function guarantees the irreversibility of the fracture as well as the differentiablity. The final regularized problem is then linearized and discretized by finite element method. The a priori error estimate will be discussed for the discretization scheme.

Nonlinear Robust Optimization of PDE-Constrained Problems using Second-Order Approximations

Philip Kolvenbach (*Mathematik, Technische Universität Darmstadt*), Stefan Ulbrich (*Mathematik, Technische Universität Darmstadt*) 09:50–10:10

We present an algorithm for the robust optimization of nonlinear PDE-constrained problems with ellipsoidal uncertainty sets. We follow a deterministic worst-case approach which leads to a difficult min–max formulation. Using second-order approximations of the involved objective and constraint functions, the evaluation of the worst-case functions reduces to solving trust-region subproblems. The worst-case functions are locally Lipschitz continuous and regular in the sense of Clarke with readily available subgradient information, so that methods for nonsmooth nonconvex optimization such as bundle methods can be applied to solve the approximated robust counterpart. We address high-dimensional uncertainties with matrix-free methods and nonlinearities of higher order with an optimization-based adjustment of the expansion points of the second-order approximations. We apply our method to the parametrized shape optimization of elastic bodies and present numerical results.

Stabilization of a time-dependent discrete adjoint solver for chaotic incompressible flows

Suneth Warnakulasuriya (*Lehrstuhl für Statik, Technische Universität München*), Michael Andre (*Chair of Structural Analysis, Technische Universität München*), Roland Wüchner (*Lehrstuhl für Statik, Technische Universität München*), Kai-Uwe Bletzinger (*Lehrstuhl für Statik, Technische Universität München*) 10:10–10:30

Following the growth of computational fluid dynamics in engineering applications, adjoint methods for sensitivity analysis are being applied to an increasing range of industrial problems. In recent years, growth in computational power has led to widespread use of high-fidelity, time-resolved techniques, such as large-eddy simulation, for applications, including bluff-body aerodynamics, where time-averaged equations may be less reliable. The solution of time-dependent adjoint equations, however, becomes unstable in time as the Reynolds number increases and the flow becomes chaotic. The source of this instability has been explained by analysis of the system's Lyapunov exponents and several solutions have been proposed in the literature based on least-squares shadowing. Currently, such techniques impose a higher computational cost compared to classical adjoint methods and may become infeasible when the number of unstable Lyapunov exponents is large. In this work, we explore a more recently proposed approach, which balances the adjoint energy source term with added artificial dissipation. The stability of this approach is investigated for a discrete adjoint solver based on the time-dependent incompressible Navier-Stokes equations. The accuracy of the resulting shape sensitivities is analyzed using a linear regression technique for the flow around a circular cylinder.

S19.11 | Optimization of differential equations

Date 23.03.2018
Room N1189

Exterior Shape Calculus

Ralf Hiptmair (*D-MATH, ETH Zurich*), Jingzhi Li (*Department of Mathematics, SUSTEC*) 08:30–09:10

We study shape derivatives of solutions of second-order boundary value and transmission problems from the perspective of differential forms, following [Ralf Hiptmair and Jingzhi Li, *Shape derivatives in differential forms I: an intrinsic perspective*, Annali di Matematica Pura ed Applicata, 192 (2013), pp. 1077–1098]. Relying on variational formulations, we present a unified framework for the derivation of strong and weak forms of derivatives with respect to variations of domain boundaries or interfaces. The notion of Lie derivative will play a key role. In 3D for degrees 0 and 1 of the forms we obtain known and new formulas for shape derivatives of solutions of Helmholtz and Maxwell equations. They can form the foundation for numerical approximation with finite elements or boundary elements.

Optimal actuator design based on shape calculus

Kevin Sturm (*TU Wien*) 09:10–09:30

In this talk an approach to the optimal actuator problem based on shape and topology optimization techniques is presented. It is illustrated for the specific case of linear diffusion equations.

Two types of scenarios are considered. For the first one, best actuators are determined which depend on a specific initial condition, for the second, the resulting best actuators are determined uniformly for a all initial conditions not exceeding a chosen norm. Shape and topological sensitivities of these cost functionals are determined. Together with a level-set method they are the basis for a numerical algorithm. Numerical results support the proposed methodology. This is joint work with K. Kunisch and D. Kalise.

Modeling, identification, and optimization of violin bridges

Sandra Marschke (*Institut für Mathematik und Wissenschaftliches Rechnen, Karl-Franzens-Universität Graz*) 09:30–09:50

Our goal is to optimize a violin bridge regarding its material parameters and its shape. The simulations therefore are based on isogeometric analysis techniques. A crucial point for successful and accurate computations is the assembly of a realistic NURBS geometry. Hence, we construct the B-splines of our geometry with a non-linear least squares fit to data gained from a μ-CT scan of the bridge. Based on this new 3D-geometry we solve the eigenvalue problem of elasticity for the orthotropic material law of the wooden bridge and implement simulations for the dynamical behaviour with a Newmark-β scheme. Furthermore, we determine material parameters by an inverse problem based on actual measurements and identify sensitivities of the solution with respect to shape and material parameters.

Adjoint shape optimization for fluid-structure interaction

Jan Heners (*Numerical Structural Analysis with Application in Ship Technology, Hamburg University of Technology (TU Hamburg-Harburg)*), Lars Radtke (*Numerical Structural Analysis with Application in Ship Technology, Hamburg University of Technology (TU Hamburg-Harburg)*), Alexander Düster (*Numerical Structural Analysis with Application in Ship Technology, Hamburg University of Technology (TU Hamburg-Harburg)*), Michael Hinze (*Center for Optimization and Approximation, Universität Hamburg*) 09:50–10:10

A partitioned approach for the solution of the adjoint associated to the coupled system of time-dependent fluid-structure interaction is presented. Following the idea presented in [1] an ALE formulation of the governing fluid equations is considered for the derivation of the adjoint system. Allowing for an efficient computation of sensitivity and gradient distributions relying on the adjoint solution, an optimization strategy based on the steepest descent algorithm is applied. In contrast to previous works [2], the behavior of both structure and fluid is affected by variation of the shape of the overflowed structure alone. The performance of the developed shape optimization process improving flow conditions and related cost functionals is demonstrated by application to ducted flow simulations and common fluid dynamic design tasks considering the interaction between fluid loads and structural deformations [3]. Both physical capability and feasibility are discussed in terms of theoretical and numerical aspects in order to evaluate the efficiency of the realized optimal control process.

[1] Helgason E, Krajnovic S (2015) Optimization Using Arbitrary Lagrangian-Eulerian Formulation of the Navier-Stokes Equations. J. Fluids Eng 137(6)

[2] Bazilevs Y, Hsu M-C, Bement MT (2013) Adjoint-based control of fluid-structure interaction for computational steering applications. Proc Comput Sci 18:1989-1998

[3] Heners JP, Radtke L, Hinze M, Düster, A (2017) Adjoint shape optimization for fluid-structure interaction of ducted flows. Computational Mechanics, DOI 10.1007/s00466-017-1465-5.

Shape optimization for laminar particulate flow problems

Raphael Hohmann (*Transport processes, Fraunhofer ITWM*), Christian Leithäuser (*Fraunhofer ITWM*) 10:10–10:30

The standard model for simulating transport processes in laminar flows with low particulate load is the Eulerian-Lagrangian setting. However, in industrial separation and mixing processes one is often more interested in volume-averaged quantities such as the particulate phase's mass flux than in individual trajectories. In order to perform shape optimization for such situations we investigate a volume-averaged model for inert particles and derive the corresponding adjoint equations and shape gradient following the optimize-then-discretize approach.
First numerical results are presented in the limit of massless particles in Stokes flow. We consider the optimal design of a liquid polymer distributor, where the residence time of the fluid should be minimized in order to avoid degradation of the material. We compare the ansatz of solving an additional transport equation for the volume-averaged residence time with previous results based on the indirect approach of controlling the wall shear stress of the fluid.

S20 | Dynamics and control

Organiser Timm Faulwasser (*Karlsruhe Institute of Technology - KIT*)
Oliver Junge (*TUM Technische Universität München*)

S20.01 | Dynamics and control

Date 20.03.2018
Room N1080

H2-model reduction for stabilizable systems

Tobias Breiten (*Institute for Mathematics and Scientific Computing, Karl-Franzens-Universität Graz*), Chris Beattie (*Virginia Tech*), Serkan Gugercin (*Virginia Tech*) 08:30–08:50

For an asymptotically stable linear time-invariant systems, locally H2-optimal reduced-order models are known to satisfy Hermite type interpolation conditions. A numerical approach for computing such minimizers is provided by the iterative rational Krylov algorithm (IRKA). While generalizations to unstable systems exist, they typically require an explicit decomposition of the spectrum and thus are not feasible in a large-scale setting. Inspired by the method of LQG-balanced truncation, for stabilizable systems, we define a generalized H2-error measure based on the solution of a Riccati equation. We discuss a modification of IRKA with respect to this generalized error measure and show that its computation is independent of the underlying Riccati equation. Based on numerical examples the performance of the method is studied.

Clustering Model Order Reduction for Water Networks

Sara Grundel (*Max Planck Institute for Dynamics of Complex Technical Systems*), Petar Mlinarić (*Max Planck Institute for Dynamics of Complex Technical Systems*), Marc Steinbach (*Leibniz Universität Hannover*) 08:50–09:10

Modelling and simulation of water trough a water transportation network leads to a Differential Algebraic Equation over a network. We would like to use clustering based model order reduction techniques such that the reduced model is a network system as well. Given a clustering π the clustering matrix $P(\pi)$ is defined as

$$P_{ki} = \begin{cases} \alpha_{ki}, & \pi(k) = i \text{ (node } k \text{ is in cluster } i), \\ 0, & \pi(k) \neq i \text{ (node } k \text{ is not in cluster } i). \end{cases} \tag{1}$$

In the standard version of this algorithm all the α_{ki} are 1. We will present an updated version, where this is no longer the case. This leads to more flexibility and a better approximation quality. This matrix clusters the nodes. A further clustering takes place on the edges. This clustering matrix is denoted by the matrix R. The following relation has to hold

$$R^T E P = \hat{E},$$

where E and $\hat{E}$ are the incidence matrix of the original and a reduced graph.
We will show how to compute such matrices and what properties they have. We furthermore analyse what the clusters means and compare them with clusterings that are done in order to run optimization algorithms on the water distribution network of Berlin.

Coarse graining of forced metastable systems

Péter Koltai (*Institute for Mathematics, Freie Universität Berlin*) 09:10–09:50

Applications require simulation of biomolecular systems on timescales that are far beyond the capacity of computer power currently available. The reason for this is that many of the processes that constitute molecular function are rare event processes appearing on timescales that are many orders of magnitude longer than the typical time steps of the numerical simulation. As a consequence, there is an increasing need for reduced models of the dynamical behavior of molecular systems that still allow describing the relevant dynamical properties. Most of the rare events mentioned above correspond to so-called conformation changes of the molecule. Conformations are "hard-to-leave" metastable states of the system's dynamics, which plays an important role in the reduction approach called Markov state modeling (MSM). We will review the basic constructions behind MSM, and discuss data-based estimation and recent advances for non-equilibrium forced systems.

Clustering-Based Model Order Reduction for Nonlinear Multi-Agent Systems

Peter Benner (*Max Planck Institute for Dynamics of Complex Technical Systems*), Sara Grundel (*Max Planck Institute for Dynamics of Complex Technical Systems*), Petar Mlinarić (*Computational Methods in Systems and Control Theory, Max Planck Institute for Dynamics of Complex Technical Systems*) 09:50–10:10

Multi-agent systems are network systems where the subsystems, called agents, have the same dynamics. Model order reduction (MOR) by clustering was proposed in the literature (see [1, 3]) for multi-agent systems as a way to preserve the network structure in the reduced order model (ROM), along with system properties such as synchronization. The basic idea is to partition the agents based on "similarity" and then to approximate each cluster of agents by a single agent. The clustering-based ROM is obtained by a Galerkin projection, where the projection matrix is a sparse matrix which encodes the partition. Since clustering is a difficult combinatorial optimization problem, we propose a heuristic methodology: applying any projection-based MOR method followed by clustering the rows of the projection matrix using any clustering method. We motivate this framework further for linear multi-agent systems (as in [2]) and show its effectiveness on examples of nonlinear multi-agent systems.

[1] T. Ishizaki, K. Kashima, J.-i. Imura, and K. Aihara. Model reduction and clusterization of large-scale bidirectional networks. *IEEE Trans. Autom. Control*, 59(1):48–63, Jan. 2014.

[2] P. Mlinarić, S. Grundel, and P. Benner. Efficient model order reduction for multi-agent systems using QR decomposition-based clustering. In *54th IEEE Conference on Decision and Control (CDC), Osaka, Japan*, pages 4794–4799, Dec. 2015.

[3] N. Monshizadeh, H. L. Trentelman, and M. K. Çamlibel. Projection-based model reduction of multi-agent systems using graph partitions. *IEEE Trans. Control Netw. Syst.*, 1(2):145–154, June 2014.

Generalized Gramians and balanced truncation for switched linear systems

Igor Pontes Duff Pereira (*Computational Methods in Systems and Control Theory, Max Planck Institute for Dynamics of Complex Technical Systems*), Sara Grundel (*Max Planck Institute for Dynamics of Complex Technical Systems*), Peter Benner (*Max Planck Institute for Dynamics of Complex Technical Systems*) 10:10–10:30

Balanced truncation is one of the most common model order reduction techniques. For linear dynamical systems, it relies on the computation of reachability and observability Gramians [3], which are the solution X of algebraic Lyapunov equations as

$$AX + XA^T + Q = 0.$$

Later, the concept of algebraic Gramians was extended to bilinear systems [1, 2]. In this context, they satisfy generalized Lyapunov equations as

$$AX + XA^T + \sum_{j=1}^{M} D_j X D_j^T + Q = 0.$$

As a result, these algebraic Gramians allow us to compute reduced-order systems for bilinear systems.
In this talk, we propose an extension of balanced truncation for model reduction of continuous time Switched Linear Systems (SLS), whose dynamics are governed by

$$\Sigma_{SLS} : \begin{cases} \dot{x}(t) = A_{\sigma(t)}x(t) + B_{\sigma(t)}u(t), \\ y(t) = C_{\sigma(t)}x(t), \;\; x(0) = x_0, \end{cases}$$

where $\Omega = \{1, \ldots, M\}$ is the set of modes, $\sigma(t) \in \Omega$ is the switching signal, $A_j \in \mathbb{R}^{n\times n}$, $B_j \in \mathbb{R}^{n\times m}$ and $C_j \in \mathbb{R}^{p\times n}$, where $j \in \Omega$. First, we recast a switched linear system as a bilinear system. Then, inspired by the bilinear theory [2], we propose algebraic Gramians for SLS, which satisfy generalized Lyapunov equations. Also, we prove that these Gramians encode the reachability and observability sets. This allows us to find those states that are hard to reach and hard to observe via an appropriate transformation. Truncating such states yields reduced-order systems. The efficiency of these approximations is, then, demonstrated in some numerical examples.

[1] S. A. Al-Baiyat and M. Bettayeb. A new model reduction scheme for k-power bilinear systems. In Proc. of the 32st IEEE Conf. on Decision and Control, San Antonio, TX, pages 22–27. IEEE, 1993.

[2] P. Benner and T. Damm. Lyapunov equations, energy functionals, and model order reduction of bilinear and stochastic systems. *SIAM journal on control and optimization*, 49(2):686–711, 2011.

[3] B. Moore. Principal component analysis in linear systems: Controllability, observability, and model reduction. *IEEE Trans. Autom. Control*, 26(1):17–32, 1981.

S20.02 | Dynamics and control

Date 20.03.2018
Room N1080

Variational Integrators for Parameter Identification of Mechanical Systems

Kathrin Flaßkamp (*Center for Industrial Mathematics, Universität Bremen*), Christof Büskens (*Center for Industrial Mathematics, Universität Bremen*) 16:30–16:50

Modern numerical tools for simulation, optimization, and optimal control of dynamical systems strongly rely on realistic models of the underlying systems or processes. Thus, system identification is a crucial preliminary step. Classically, for mechanical systems, model structures are well established, e.g. Newton-Euler, Euler-Lagrange, or Hamilton equations. However, model parameters have to be fitted to the real system's behavior. Typically, this requires not only static measurements, but data from dynamic motions. Parameter fitting can thus be formulated as an optimization problem which is constrained by the system dynamics. Numerical approaches apply transcription methods, as they are known from direct methods in optimal control, in order to discretize the dynamics.
In this presentation, we study the use of variational integrators (VI) to perform this transcription step. This leads to a high-dimensional optimization problem, since the discrete-time configurations are considered as optimization variables in addition to unknown parameters. However, the problem possesses a sparse structure which can be exploited by nonlinear optimization solvers such as WORHP.
VI are known to be structure-preserving and are therefore used in long-term simulation, optimization and model-based control of mechanical systems. Similarly, in parameter identification, the discrete-time system approximation still leads to a physically realistic model. This is in contrast to usually chosen Runge-Kutta methods. We illustrate this effect by examples of robotic systems.

A family of extremum seeking algorithms for the Lie bracket approximation approach

Victoria Grushkovskaya (*Institute for Systems Theory and Automatic Control, University of Stuttgart*), Alexander Zuyev (*Max Planck Institute for Dynamics of Complex Technical Systems*), Christian Ebenbauer (*Institute for Systems Theory and Automatic Control, University of Stuttgart*) 16:50–17:10

Extremum seeking problems appear in many practical applications, such as target tracking and consensus problems, maximization of the power output in wind turbines and photovoltaic systems, optimization of bioreactors, etc. We present a family of control algorithms for the solution of extremum seeking problems based on the Lie bracket approximation ideas. The proposed control laws depend only on the values of the cost function without exploiting its derivatives, so that they can be used in cases when the analytical expression of a possibly time-varying cost function is partially or completely unknown. Unlike many other extremum seeking algorithms possessing the practical asymptotical stability property only, we propose asymptotic (and exponential) stability conditions in the sense of Lyapunov and describe the convergence rate for trajectories corresponding to the obtained controls. Since some important representatives of the obtained family of controls are not continuously differentiable, we also present a relaxed regularity assumption for the Lie bracket approximation approach. The obtained results are illustrated by numerical simulations and experiments with a mobile robot, which show that the high flexibility of the proposed family of control laws can be utilized to improve significantly the tracking behavior.

Geometry-Inspired Control of the Brockett-Integrator in Cylinder Coordinates

Carsten Knoll (*Institut für Regelungs- und Steuerungstheorie, TU Dresden*), Yifan Xue (*Institut für Regelungs- und Steuerungstheorie, TU Dresden*), Klaus Röbenack (*Institut für Regelungs- und Steuerungstheorie, TU Dresden*) 17:10–17:30

The so called Heisenberg system or Brockett-Integrator is a famous control system. On one hand it has a very simple structure (second order polynomial, three state components, two affine inputs, no drift) and fulfills the Lie-Algebra-Rank-Condition for (strong) local accessibility. Nevertheless, it has the challenging control property, that it does not admit a continuously differentiable control law, which stabilizes the origin.
In this contribution we consider the system in cylinder coordinates. If the first time derivatives of the radius and the orientation are chosen as the new inputs, the transformed system dynamics is even simpler (in terms of expression length) than in usual Cartesian form. Moreover, the system can be decomposed into two subsystems and a differentially flat output can be easily read off. Based on this partially decoupled system dynamics we formulate a simple three-staged control law which drives the system into the origin by aiming for a minimal arc length in the (original) state space.
Compared to approaches proposed in the past, e. g., [1, Section 4.2], our control law, while involving distinction of cases, does not rely on additional discrete state components and is guaranteed to reach the origin in finite time for any initial state. Aspects of time discrete implementation and singularity handling are also considered.

[1]: Daniel Liberzon: *Switching in Systems and Control*, Birkhäuser 2003.

Mechanics with non-Leibniz derivatives

Vladimir Kobelev (*Natural Sciences, Universität Siegen*) 17:30–17:50

The generalized derivative based on a non- Leibniz formalism is introduced in this article. The generalized differentiation operator (D-operator) possesses a non-zero Leibniz defect. The Leibniz defect of the introduced operator linearly depends on one scaling parameter. In a special case, if the scaling parameter turns to one, the Leibniz defect vanishes and generalized differentiation operator reduces to the common differentiation operator. The D-operator allows the formulation of the variational principles and corresponding Lagrange and Hamiltonian equations in mechanics. The solutions of some generalized dynamical equations are provided closed form. With a positive Leibniz defect the amplitude of free vibration remains constant with time with the fading frequency ("red shift"). The negative Leibniz defect leads the opposite behavior, demonstrating the growing frequency ("blue shift"). Notably that the Hamiltonian remains constant in time in both cases. Thus the introduction of non-zero Leibniz defect leads to an alternative mathematical description of the conservative systems with some uncommon physical properties. Consider an ensemble of states that occupies a particular volume of phase space in the initial moment. The evolution of the volume of phase space is governed by Hamilton's equations. The flow of phase space may deform the shape of the ensemble but it does not change its volume. The conservation of phase space volume is is known as the Liouville's Theorem [Goldstein, Poole, Safko, 2000]. On the other hand it is well known, that for dissipative systems the phase-space volume is not conserved [Hand, Finch, 1998, §11.10]. This means the evolution of the system could be not described by Hamilton's equations in their ordinary formulation. The multiplication of the undamped Lagrangian by an increasing exponent of time leads to a formally correct Hamilton's equations [Sussman, Wisdom, 2014, §3.8]. Conversely, the modified Hamiltonian is not a sum of potential and kinetic energy of the system. It is shown in [Bloch et al, 1996] that the system on Lie algebras cannot have linear dissipative terms of Rayleigh dissipation type.

In the present lecture an alternative way is investigated. Instead of the modification of the Hamilton's function, we examine the alteration of the derivatives. The formalism is based on the generalized differentiation operator (kappa-operator) with a non-zero Leibniz defect. The Leibniz defect of the generalized differentiation operator linearly depends on one scaling parameter. In a special case, if the scaling parameter turns to one, the Leibniz defect vanishes and generalized differentiation operator reduces to the common differentiation operator. The generalized differentiation operator allows the formulation of the variational principles and corresponding Lagrange and Hamiltonian equations. The developed formalism allows the representation of the mechanical systems with the Lie group methods.
The analytical solution of the equations of non-Leibniz oscillator is found. As an example of the partial differential equation with the generalized derivatives the wave is studied.

Mixed Galerkin Structure-Preserving Discretization of Port-Hamiltonian Systems

Paul Kotyczka (*Department of Mechanical Engineering, Technische Universität München*), Bernhard Maschke (*LAGEP UMR 5007, Univ Lyon, Université Claude Bernard Lyon 1, CNRS*), Laurent Lefèvre (*LCIS Valence, Univ. Grenoble Alpes*) 17:50–18:10

We present the structure-preserving discretization of systems of two conservation laws in port-Hamiltonian form. The key ingredients are a weak formulation of the underlying Stokes-Dirac structure and the use of mixed approximation spaces for the power variables (efforts and flows) according to their physical nature. Mapping the discrete power variables onto an embedding of the original discrete bond space in a power-preserving way defines a finite-dimensional Dirac structure. Adding dynamics and a consistent approximation of the constitutive equations gives finally a family of port-Hamiltonian approximate models in explicit state space form, which are particularly suited for simulation and control. The degrees of freedom in the power-preserving mappings can be used to parametrize the conservative numerical scheme in the sense of upwinding. The approach is illustrated on the example of the linear wave equation in one and two spatial dimensions using Whitney finite elements on a simplicial triangulation.

A Fractional Variational Approach for Modelling and Simulating Dissipative Mechanical Systems

Sina Ober-Blöbaum (*Engineering Science, University of Oxford*), Fernando Jiménez (*University of Oxford*) 18:10–18:30

Variational principles are powerful tools for the modelling and simulation of conservative mechanical and electrical systems. As it is well-known, the fulfilment of a variational principle leads to the Euler-Lagrange equations of motion describing the dynamics of such systems. Furthermore, a variational discretisation directly yields unified numerical schemes with powerful structure-preserving properties. Since many years there have been several attempts to provide a variational description also for dissipative mechanical systems, a task that is addressed in the talk in order to construct both Lagrangian and Hamiltonian pictures of their dynamics.
Employing a phase space which includes the (Riemann-Liouville) fractional derivative of curves evolving on real space, a variational principle for Lagrangian systems is developed yielding the so-called restricted fractional Euler-Lagrange equations, which are invariant under linear change of variables. This variational principle relies on a particular restriction upon the admissible variation of the curves. In the case of the half-derivative and mechanical Lagrangians, i.e. kinetic minus potential energy, the restricted fractional Euler-Lagrange equations model a dissipative system in both directions of time, summing up to a set of equations that is invariant under

time reversal. After performing the usual Legendre transformation in the new phase space, we obtain the so-called restricted fractional Hamilton equations which are fully consistent with the Euler-Lagrange equations. Finally, a discrete fractional Lagrangian version is derived and used to construct fractional variational integrators for the structure-preserving integration of dissipative systems.

S20.03 | Dynamics and control

Date 21.03.2018
Room N1080

Parametric model order reduction for district heating networks

Markus Rein (*Technomathematics group, Technische Universität Kaiserslautern*), Jan Mohring (*Fraunhofer ITWM*), Axel Klar (*Technische Universität Kaiserslautern*), Tobias Damm (*Technische Universität Kaiserslautern*) 08:30–08:50

District heating networks are an important tool for carbon neutral urban heating due to their high flexibility towards the injection of energy. The variable energy mix combined with the dynamical thermal transport to the connected houses makes them an interesting but challenging subject of optimization. Approaches towards finding the optimal use of the power resources such as model predictive control require simulating the network dynamics multiple times. The high number of transport pipelines and junctions makes them large scale dynamical systems, explaining the need for model order reduction. Using incompressible Euler equations, we capture the advective transport of the thermal energy within the heating network. The mass-flow of the transport fluid is determined by both the power requirement of the houses and Kirchhoff's laws acting as nonlinear algebraic equations. Modeling the resulting mass-flow as a time varying parameter vector allows to describe the thermal dynamics as a linear parametric system challenging to reduce. We reduce the system dimension by projection using the iterative rational Krylov approximation (IRKA) applied to different parameter realizations. Formulating the network as a port-Hamiltonian system maintains the structure of the algebraic constraints and ensures local stability for every parameter. The resulting low dimensional approximation adequately describes the network dynamics and paves the way for optimization.

Kolmogorov n-widths and optimal Hankel norm approximation

Benjamin Unger (*Institut für Mathematik, Technische Universität Berlin*), Serkan Gugercin (*Virginia Tech*) 08:50–09:10

In the model order reduction (MOR) community, Hankel singular values and Kolmogorov n-widths are standard quantities for applicability of (standard) MOR methods and error estimators/bounds. Although both concepts are widely used in the literature, there seems only little understanding on the relation of both concepts. In this talk, we show that the greedy search - commonly used in the reduced basis community - applied to the Hankel operator of an LTI system resembles the minimizing subspace for the Kolmogorov n-width. Moreover the approximation error is given by the (n+1)-th Hankel singular value, which equals the error of optimal Hankel norm approximation. In addition the proof shows that the greedy-approach is the dual concept to the method of active subspaces.

Balancing Related Model Reduction with the MORLAB Toolbox

Peter Benner (*Computational Methods in Systems and Control Theory, Max Planck Institute for Dynamics of Complex Technical Systems*), Steffen W. R. Werner (*Computational Methods in Systems and Control Theory, Max Planck Institute for Dynamics of Complex Technical Systems*) 09:10–09:30

The modeling of many applications, like mechanical systems and fluid dynamics, results in linear time-invariant continuous-time systems of the form

$$\begin{aligned} E\dot{x}(t) &= Ax(t) + Bu(t), \\ y(t) &= Cx(t) + Du(t), \end{aligned} \tag{1}$$

with $E, A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m}$, $C \in \mathbb{R}^{p\times n}$ and $D \in \mathbb{R}^{p\times m}$. The aim of model reduction methods is to construct an easy-to-evaluate surrogate model for (1) of order $r \ll n$. Beside well approximating the original system (1), the special properties, e.g., stability, contractivity, or passivity, should be preserved in the reduced-order model. This can be done, using balancing related model reduction methods; see [2] for an overview. These methods are based on the classical balanced truncation method, but the definition of the system Gramians is replaced by different matrix equations, e.g., by the continuous-time algebraic Riccati equation

$$A^T XE + E^T XA + E^T XBB^T XE + C^T C = 0.$$

In MATLAB and OCTAVE, medium-scale dense systems of the form (1) can be reduced using the MORLAB (Model Order Reduction Laboratory) toolbox [1, 3]. Therein, several different balancing related model reduction techniques are implemented, e.g., the bounded-real balanced truncation, the positive-real balanced truncation, or the linear-quadratic Gaussian balanced truncation. The arising matrix equations are efficiently solved using Newton schemes and spectral projection methods, like the matrix disk and matrix sign function. We will demonstrate this using some benchmark examples from the literature.

[1] P. Benner. A MATLAB repository for model reduction based on spectral projection. In *2006 IEEE Conference on Computer Aided Control System Design, 2006 IEEE International Conference on Control Applications, 2006 IEEE International Symposium on Intelligent Control*, pages 19–24, October 2006.

[2] P. Benner and T. Stykel. Model order reduction for differential-algebraic equations: A survey. In Achim Ilchmann and Timo Reis, editors, *Surveys in Differential-Algebraic Equations IV*, Differential-Algebraic Equations Forum, pages 107–160. Springer International Publishing, Cham, March 2017.

[3] P. Benner and S. W. R. Werner. MORLAB-3.0 – model order reduction laboratory, September 2017. see also: `http://www.mpi-magdeburg.mpg.de/ projects/morlab`.

S20.04 | Dynamics and control

Date 21.03.2018
Room N1080

Vibration control of base-isolated structures using active tendons

Seyed Hadi Seyedpour (*Islamic azad university of Sarab, Iran*), Seyed Morteza Seyedpour (*Civil Engineering, Institute of Mechanics Statics Dynamics, TU Dortmund University*), Omolbanin Arasteh Khoshbin (*Institute of Mechanics Statics Dynamics, TU Dortmund University*), Tim Ricken (*Institute of Statics and Dynamics of Aerospace Structures, University of Stuttgart*) 14:00–14:20

The use of modern construction techniques has always been a concern for engineers. Researchers are still looking for methods and techniques that help the engineers to improve the engineering construction. One of the promising plans to deal with earthquakes is the use of structural control systems. They are categorized as the passive, active, semi-active and hybrid control systems Naeim and Kelly (1999); Kelly (1993). It is essential to reduce the force induced by the earthquake to the structure. The base isolation, due to their low horizontal stiffness, increases the structural periodicity, which leads to reducing the induced force from the earthquake to the structure. But if these separators are exposed to severe shocks, they can be torn and destroyed. Therefore, the use of methods that reduce separator deformation is critical. In this paper, active tendons are used to control the seismic base isolation at any moment. The results designate that the base-isolated structures responses are reduced with the hybrid control system.

Keywords: Active tendon, Base isolator, Hybrid control, Seismic isolated

Naeim, F., Kelly, J. M., 1999. Design of seismic isolated structures : from theory to practice. John Wiley, New York.
Kelly, J. M., 1996. Earthquake-Resistant Design with Rubber, 2nd ed., springer-Verlag, London.

Analytic Center for the Passivity LMI

Daniel Bankmann (*TU Berlin*), Volker Mehrmann (*TU Berlin*), Yurii Nesterov (*Université catholique de Louvain*), Paul van Dooren (*Université catholique de Louvain*) 14:20–14:40

Passivity is a desired property of a dynamical system, since physical systems without any external input do not produce energy, i. e., are passive. Sometimes, it might happen though, that the linear time-invariant system obtained from linearization and spatial discretization approaches applied to such passive and nonlinear partial differential equations are not passive anymore. Hence, one is interested in analyzing the distance to passivity of a non-passive system and the radius of passivity, i. e., robustness, of a passive system.
For linear systems, passivity can be characterized via non-negativity of Willems' passivity LMI. We propose to use a certain strictly positive solution of that LMI, that will have maximal distance to semi-positive solutions in some sense. This solution is called analytic center and indeed provides us with estimates for the radius of passivity.
In this talk we show, how this analytic center can be computed efficiently via Newton's method. We also show that, while one can also compute the analytic center in the discrete-time setting, the corresponding feedback matrices corresponding to the solutions are *not* preserved under bilinear transformations.

Fault tolerant funnel control

Thomas Berger (*Fachbereich Mathematik, Universität Hamburg*) 14:40–15:00

In this talk a new approach to adaptive fault tolerant tracking control for uncertain linear systems is presented. Based on recent results in funnel control and the time-varying Byrnes-Isidori form, we develop a low-complexity model-free controller which achieves prescribed performance of the tracking error for any given sufficiently smooth reference signal. Within the considered system class, we allow for more inputs than outputs as long as a certain redundancy of the actuators is satisfied. An important role in the controller design is played by the controller weight matrix, which is a rectangular input transformation chosen such that in the resulting system the zero dynamics, which are assumed to be uniformly exponentially stable, are independent of the new input. We illustrate the fault tolerant funnel controller by an example of a linearized model for the lateral motion of a Boeing 737 aircraft.

On the relation between the observer and controller form for hyperbolic distributed-parameter systems

Frank Woittennek (*Private University for Health Sciences, Medical Informatics and Technology (UMIT)*), Nicole Gehring (*Johannes Kepler University Linz*) 15:00–15:20

It is well known that the design of state feedback controllers and state observers for finite-dimensional dynamical systems is significantly facilitated by the use of particular coordinates. Over the last years, similar strategies have been proposed for linear distributed parameter systems of hyperbolic type [Woi13]. They rely on a representation of the infinite-dimensional system in the so-called hyperbolic controller form and the hyperbolic observer form. This talk focuses on the question, how the state estimate provided by the observer (in observer form coordinates) can be used in a state feedback (of the controller form coordinates). An intermediary transformation into hyperbolic observability form plays an essential role in this context.

[Woi13] F. Woittennek. On the hyperbolic observer canonical form. In *Proc. 8th Int. Workshop on Multidimensional Systems (nDS'13), Erlangen, Germany, Sep 9-11 2013*, 2013.

Flatness-based control of a rigid body carried by multiple heavy ropes

Abdurrahman Irscheid (*Chair of Systems Theory and Control Engineering, Universität des Saarlandes*), Daniel Gerbet (*Chair of Systems Theory and Control Engineering, Universität des Saarlandes*), Joachim Rudolph (*Chair of Systems Theory and Control Engineering, Universität des Saarlandes*) 15:20–15:40

Flatness-based trajectory planning for the distributed-parameter system consisting of a rigid body carried by multiple heavy ropes is discussed. The suspension points (controlled ends) of the ropes are assumed to be freely movable. The other ends of the ropes are parametrized by a flat output of the nonlinear boundary system at the load, which describes the motion of the rigid body. This is then used to parametrize the solution of the linearized partial differential equations for the heavy ropes under small angle approximations around a stable vertical position by the means of operational calculus. It is shown, that the system trajectories of the ropes depend on distributed delays and advances of the flat output trajectory at the load side boundary system. Evaluating the derived parametrization of the heavy ropes at the controllable ends will yield the desired open-loop controller by using a planned trajectory for the flat output. This control

can be used to realize a desired transition of the load position and orientation in finite time. In order to illustrate the introduced method, such a design is carried out on the example of a linear infinite-dimensional model of two heavy ropes carrying a rigid rod.

Time Optimal Path Tracking for Industrial Robots with Low Cost Computational Unit using Model Predictive Control

Matthias Jörgl (*Institute of Robotics, Johannes Kepler University Linz*), Hubert Gattringer (*Institute of Robotics, Johannes Kepler University Linz*), Andreas Müller (*Institute of Robotics, Johannes Kepler University Linz*) 15:40–16:00

This paper deals with time optimal path tracking along prescribed geometric paths for robotic systems, like computerized numerical control (CNC) machines. These machines are typically controlled by a low cost microcontroller computational unit (MCU). Such MCUs are commonly used in industrial applications but are limited in view of computational performance. In many cases, these robotic systems have not only a MCU on which e.g. a motion controller is implemented, but also an associated desktop computer that serves as input device and transmits raw data to the MCU. Therefore, the calculation of the time-optimal path following can be divided into two steps, where the paths are in our case defined as B-Splines. On the desktop computer, an approximation of the solution is recursively recalculated using a log-barrier method, which solves a convex reformulated path tracking problem with velocity and torque constraints. This log-barrier solution serves then as a reference generator for a model predictive controller (MPC), which is implemented as a trajectory tracking controller on the MCU. Due to the special formulation of the MPC, the continuity of the solution can be chosen arbitrarily. Thus the method is suitable for control of elastic systems, where C^4 continuity is required to avoid vibrations. Assuming that the MPC works well as tracking controller, it is possible to consider only input constraints for the MPC and thus to minimize the computational effort. At last, a validation by means of experimental results is shown, in which the *ACADO Toolkit* is used for the MPC implementation.

S20.05 | Dynamics and control

Date 21.03.2018
Room N1080

Funnel control for overhead crane model

Thomas Berger (*Mathematik, Universität Hamburg*), Huy Hoang Le (*Mathematik, Universität Hamburg*), Timo Reis (*Mathematik, Universität Hamburg*) 16:30–16:50

We consider an overhead crane whose control variables are the length of the rope and force/velocity at the gantry. The output consists of the position of the load. The objective is to design a closed-loop tracking controller which also takes into account the transient behavior. First we show that this system has no well-defined relative degree, which unfortunately does not allow to apply established methods for adaptive control to achieve the objective. To circumvent this problem, we design a dynamic state feedback which results in a system with relative degree four. Thereafter, we apply a funnel controller to this feedback system. We show that our approach can be used to move loads from one to another given position in the situation where there are several obstacles which have to be circumnavigated.

Optimal Power Flow Subject to Non-Gaussian Stochastic Uncertainties: An L2-based Approach

Tillmann Mühlpfordt (*Karlsruhe Institute of Technology - KIT*), Timm Faulwasser (*Karlsruhe Institute of Technology - KIT*), Veit Hagenmeyer (*Karlsruhe Institute of Technology - KIT*) 16:50–17:10

The need to de-carbonize the current energy infrastructure, and the increasing integration of renewables pose a number of difficult control problems. Among those, the optimal power flow (OPF) problem—i.e., the task to minimize power system operation costs while maintaining technical and network limitations—is key for operational planning of power systems. The influx of inherently volatile renewable energy sources calls for methods that allow to consider stochasticity directly in the OPF problem. Modeling uncertainties as second-order continuous random variables, we will show that the OPF problem subject to stochastic uncertainties can be posed as an infinite-dimensional L2-problem. A tractable and exact reformulation thereof can be obtained using polynomial chaos expansion (PCE), under mild assumptions. PCE as such is a Hilbert space series expansion for random variables that is employed for uncertainty propagation and uncertainty quantification. We will show that PCE offers several advantages for OPF subject to stochastic uncertainties. For example, multivariate non-Gaussian uncertainties can be considered easily. Also, the solutions from PCE are effectively feedback laws in terms of the realizations of the uncertainty that are determined in a single numerical run. We apply our findings to IEEE test cases and demonstrate the efficacy of PCE applied to OPF subject to non-Gaussian stochastic uncertainties.

A unified approach to ensemble controllability of linear parametric systems

Michael Schönlein (*University of Würzburg*) 17:10–17:30

We consider families of linear systems that are defined by matrix pairs $\big(A(\theta), B(\theta)\big)$ which depending continuously on a parameter θ that is varying over finite union of disjoint compact intervals $\mathbf{P}$. In this talk we consider reachability properties of the entire family of systems $\big(A(\theta), B(\theta)\big)$, i.e. the task is to steer a family of initial states $\{x(0,\theta) \,|\, \theta \in \mathbf{P}\}$ in finite time arbitrarily close to a family of desired terminal states $\{x^*(\theta) \,|\, \theta \in \mathbf{P}\}$ via a *parameter-independent* open-loop control input. In this case the pair $\big(A(\theta), B(\theta)\big)$ is called ensemble controllable. Using well-known characterizations of approximate controllability of systems in Banach spaces, ensemble controllability of $\big(A(\theta), B(\theta)\big)$ is equivalent to an infinite-dimensional extension of the Kalman rank condition. Applying methods from complex approximation, functional analysis and topology, this talk presents a unified approach to ensemble controllability. The analysis of the spectra of the family of matrices $A(\theta)$ provides structural insights to ensemble controllability and yields sufficient conditions that can be checked directly in terms of the matrix pair.

Instability in Power Grids Due to Switching

Tjorben Groß (*Fraunhofer ITWM*), Stephan Trenn (*Jan C. Willems Center for Systems and Control, University of Groningen*), Andreas Wirsen (*Fraunhofer ITWM*) 17:30–17:50

A common linear model of power grids based on the swing equation is presented. Failures of components can be modeled in the framework of switched systems. In general, stability is not preserved under switching; indeed, a simple example of a power grid shows that for a "bad" switching signal the overall system behavior becomes instable. Sufficient conditions in terms of the topology of the power grid are given, which ensure stability under arbitrary switching.

Prediction of Stability Limit for Rotor-Seal Systems Using Tangential Forces by Active Magnetic Bearings

Christian Wagner (*Chair of Applied Mechanics, Technical University of Munich*), Johannes Maierhofer (*Technical University of Munich, Chair of Applied Mechanics*), Mikael Eronen (*Technical University of Denmark*), Thomas Thümmel (*Technical University of Munich, Chair of Applied Mechanics*), Daniel Jean Rixen (*Technical University of Munich, Chair of Applied Mechanics*) 17:50–18:10

In high rotational speed turbomachinery, contactless seals in various layouts like labyrinth, brush, floating ring or usually liquid gap seals are used. However, the presence of a leakage flow through the clearance in the contactless seal can cause a rotor instability, which leads to large displacements and a breakdown of the system, similar to the 'oil-whip' phenomenon in journal bearings. This is due to unsymmetrical fluid velocity distribution for the vibrating or eccentered rotor. Further, the rotor-system or the seal condition can change during lifetime. Thus, an experimental diagnosis method is necessary to avoid rotor instability and to ensure safe and stable long-term operation.

This article presents an experimental methodology to determine the onset speed of instability –in the safe operating range- and the rotordynamic behavior of coupled rotor seal systems.

Therefore, two Active Magnetic Bearings (AMB) are used to generate an artificial cross-coupling stiffness matrix, which introduces additional exciting tangential forces. To apply this exact amount of force, a pre calibration of the AMB and an online measurement of the actual rotor position is needed. Using this enables to identify the destabilizing interaction of the seals and the stability margin of the system at several conditions of operation.

For presenting the analytical description of the rotordynamic effects, the test rig's behavior and the developed methodology, a simple Jeffcott-rotor model is applied. The seals are modeled using rotordynamic seal coefficients, calculated by models based on the bulk-flow theory from well-known literature. Thus, the experiment, theory and simulation show good conformity.

Control design for a 2x2 hyperbolic system with application to preferential crystallization

Alexander Zuyev (*Max Planck Institute for Dynamics of Complex Technical Systems*), Peter Benner (*Max Planck Institute for Dynamics of Complex Technical Systems*) 18:10–18:30

Consider the following system of quasilinear partial differential equations:

$$\frac{\partial w_k(x,t)}{\partial t} + G_k(x, w_1, w_2)\frac{\partial w_k(x,t)}{\partial x} + u_0 h(x) w_k(x,t) = 0, \quad x \in [0, L],\ t \geq 0, \tag{1}$$

subject to the boundary conditions

$$G_k w_k|_{x=0} = B_k(u_k, w_1(\cdot, t), w_2(\cdot, t)), \quad k = 1, 2, \tag{2}$$

where $w_k(x,t)$ are unknown functions, and the vector $u = (u_0, u_1, u_2)$ is treated as the control. The above control system corresponds to a population balance model for the preferential crystallization of enantiomers with fines dissolution (cf. [1]). In such models, $w_1(x,t)$ and $w_2(x,t)$

describe the crystal size distribution for the preferred ($k = 1$) and counter ($k = 2$) enantiomers, respectively, $h(x)$ describes the dissolution of particles below some critical value, u_0 corresponds to the possibility of controlling the flow-rate at the fines dissolution unit, the growth rate of the k-th enantiomer is represented by G_k, and the functionals B_k describe the nucleation rates of particles of minimum crystal size.
Assume that the functions $w_k(x,t) \equiv w_k^0(x)$ define a steady state solution of system (1)–(2) with some constant control $u \equiv u^0$. Our goal is to propose a control design scheme in order to stabilize the above steady state. For this purpose, we use the square of a weighted H^2-norm as a control Lyapunov function candidate:

$$V = \sum_{k=1}^{2} \int_0^L \left(\rho_{0k}(x)\tilde{w}_k^2 + \rho_{1k}(x) \left(\frac{\partial \tilde{w}_k}{\partial x} \right)^2 + \rho_{2k}(x) \left(\frac{\partial^2 \tilde{w}_k}{\partial x^2} \right)^2 \right) dx,$$

where $\tilde{w}_k(x,t) = w_k(x,t) - w_k^0(x)$ and $\rho_{jk}(x) > 0$, $j = 0,1,2$, $k = 1,2$. Under additional assumptions, we propose a feedback control for system (1)–(2) such that the above V is a strict Lyapunov function for the corresponding closed-loop system.
Our construction extends the idea of [2] for the case of hyperbolic systems with fluxes of the same sign ($G_1 \cdot G_2 > 0$) and functionals in the boundary conditions (2).

[1] S. Qamar, A. Ashfaq, I. Angelov, M.P. Elsner, G. Warnecke, and A. Seidel-Morgenstern, *Numerical solutions of population balance models in preferential crystallization*, Chemical Engineering Science, 63 (2008), pp. 1342–1352.

[2] G. Bastin and J.-M. Coron, *Stability and Boundary Stabilization of 1-D Hyperbolic Systems*, Birkhäuser (2016).

S20.06 | Dynamics and control

Date 22.03.2018
Room N1080

Variational Integrators and Optimal Control for a Hybrid Pendulum-on-Cart-System

Dominik Kern (*TU Chemnitz*), Michael Groß (*TU Chemnitz*)

08:30–08:50

Hybrid systems combine time continuous and time discrete dynamics. They emerge in mechanical systems, when collisions are modelled by an impulse-like contact force. During such a collision of two or more bodies, their positions go on continuously, but their velocities jump. On the one hand this non-smoothness complicates the optimal control problem significantly, on the other hand it opens up new horizons.
This contribution uses a nested optimization in order to swing up a hybrid pendulum-on-cart-system. Both, pendulum and cart, move in finite ranges which are bounded by limiters. While the inner loop optimizes the continuous motions from start to collision, from collision to collision and finally to the final state, the outer loop optimizes time and state of the collisions. The time discretization and the optimal control during continuous motions are based on the Discrete-Mechanics-and-Optimal-Control (DMOC) approach.

Sensitivity Analysis of Time Dependent Optimal Control Motivated by Model Predictive Control

Manuel Schaller (*University of Bayreuth*), Lars Grüne (*University of Bayreuth*), Anton Schiela (*University of Bayreuth*) 08:50–09:10

Model Predictive Control is a control method in which the solution of optimal control problems on infinite or indefinitely long horizons is split up into the successive solution of optimal control problems on relatively short finite time horizons. Only a first part with given length of this solution is implemented as a control for the longer, possibly infinite horizon.
Motivated by this application, we want to establish that the effect of perturbations and discretization errors near the end of the optimization horizon on the initial part of the control is negligible if the horizon is long enough. For finite dimensional systems, namely systems governed by ordinary differential equations, the above property can be shown by decoupling the dynamics using solutions of the Algebraic Riccati Equation. In the context of partial differential equations, a different, more functional analytic approach is considered, as the above mentioned can not be extended to infinite dimensional systems. These theoretical considerations will be accompanied by numerical results for the optimal control of ordinary as well as partial differential equations.

Noncooperative Model Predictive Control

Marleen Stieler (*Mathematisches Institut, University of Bayreuth*), Michael Heinrich Baumann (*University of Bayreuth*), Lars Grüne (*University of Bayreuth*) 09:10–09:30

Nash strategies are a natural solution concept in noncooperative game theory because of their 'stable' nature: If the other players stick to the Nash strategy it is never beneficial for one player to unilaterally change his or her strategy. In this sense, Nash strategies are the only reliable strategies.
The idea to perform and analyze Model Predictive Control based on Nash strategies instead of optimal control sequences is appealing because it allows for a systematic handling of noncooperative games, which are played in a receding horizon manner. However, existence and structure of Nash strategies heavily depend on the specific game under consideration. This is in contrast to solution concepts such as usual optimality and Pareto optimality, in which one can state very general existence results or, in the case of Pareto optima, one knows that they are to be found on the 'lower left' boundary of the set of admissible values in the value space. Moreover, the calculation of Nash strategies is, in general, a very difficult task.
In this talk we present a class of games for which the closed-loop trajectory of the Nash-based MPC scheme converges to an equilibrium of the system. This equilibrium turns out to be a Pareto-optimal steady state, i.e. a Pareto-optimal solution to the multiobjective problem of minimizing all players' stage costs restricted to the set of equilibria. We furthermore investigate the relation between the closed loop and open-loop Nash strategies on the infinite horizon in terms of the trajectories as well as of the performance.

Efficient Computation of Reachable Sets for Critical Space Mission Phases

Kai Wah Chan (*Center for Industrial Mathematics, University of Bremen*), David Seelbinder (*Navigation and Control Systems, German Aerospace Center (DLR), Institute of Space Systems*), Stephan Theil (*Navigation and Control Systems, German Aerospace Center (DLR), Institute of Space Systems*), Matthias Knauer (*Center for Industrial Mathematics, University of Bremen*), Christof Büskens (*Center for Industrial Mathematics, University of Bremen*) 09:30–09:50

To achieve true autonomy during critical mission phases in deep space, it is imperative to know which states are attainable from a given starting point, using only admissible control inputs. These attainable states form the reachable set. If the latter is computed in real time, this can provide a system for Guidance, Navigation and Control on-board of an autonomous spacecraft with knowledge of all the feasible and infeasible options in order to choose the correct course of action.
Though several means exist to compute reachable sets, the most promising ones are based on optimization techniques. We currently explore an approach, in which we approximate a reachable set with an altering polytope. The center of a selected face of the polytope is the starting point from which a new feasible vertex is placed in normal direction with the largest possible step size. This approximates the set's boundary successively. Simultaneously, the underlying equations of motion must be satisfied. We formulate these tasks as an optimal control problem (OCP).
Commonly approached with direct methods, we transcribe the OCP into a nonlinear program (NLP) by discretization which is then processed by an NLP solver. It is noted that this approach does not require any convexification as conducted in other works. Within the scope of our project we make use of the software package TRANSWORHP for transcription and WORHP to solve the NLP.

On the Interplay of Open and Closed Loop in Model Predictive Control Without Terminal Constraints or Costs

Karl Worthmann (*Technische Universität Ilmenau*) 09:50–10:10

A commonly used stability condition in nonlinear Model Predictive Control (MPC) is the relaxed Lyapunov inequalities, see, e.g. [1]. Indeed, summing up such a series of inequalities along the MPC closed loop even yields a degree of suboptimality. However, these conclusions remain valid even if the relaxed Lyapunov inequality only holds after every m steps of the MPC closed loop [2]. But can we exploit this observation to weaken the stability conditions in MPC while still maintaining its inherent robustness? To address this question, we present a novel MPC algorithm, which is based on a multi-step relaxed Lyapunov inequality, but checks whether the MPC closed loop can be closed prematurely without additional computational effort, see [3] for details.

[1] L. Grüne and J. Pannek: Nonlinear Model Predictive Control - Theory and Algorithms, Springer, London, 2nd edition, 2017.

[2] L. Grüne, J. Pannek, M. Seehafer, K. Worthmann: Analysis of unconstrained nonlinear MPC schemes with time varying control horizon, SIAM Journal on Control and Optimization 48 (8), 4938-4962, 2010.

[3] K. Worthmann, M.W. Mehrez, G.K.I. Mann, R.G. Gosine, and J. Pannek: Interaction of Open and Closed Loop Control in MPC, Automatica 82, 243-250, 2017.

S20.07 | Dynamics and control

Date 22.03.2018
Room N1080

Stability Issues in Hardware-in-The-Loop tests of Flexible Components

Andreas Bartl (*Lehrstuhl für Angewandte Mechanik*), Daniel Jean Rixen (*Lehrstuhl für Angewandte Mechanik*) 14:00–14:20

The well-known Hardware-In-The-Loop (HiL) paradigm can be applied to noise, vibration and harshness (NVH) problems to test components of complex systems and their effects under realistic boundary conditions. The system is split into a virtual component and a physical testbed. Coupling both with a control system makes it possible to replicate the full systems dynamics. However depending on dead times, actuator dynamics and dynamics properties of the test specimen, the system may exhibit stability problems. In this contribution, the characteristics of the system and their effects on stability and accuracy are investigated. In order to improve stability behavior, we recently proposed the use of an Adaptive Feed-Forward Cancellation approach with a Recursive Least Squares (RLS) or a gradient descent adaption law for interface synchronization of harmonically excited systems. The interface forces are generated from multiple harmonic components of the excitation force. This approach is compared to a conventional PID-Controller regarding stability and accuracy properties.

Parameter Identification for Micro Underwater Vehicles

Eugen Solowjow (*Siemens Corporation*), Daniel-André Dücker (*Hamburg University of Technology (TU Hamburg-Harburg)*), Edwin Kreuzer (*Hamburg University of Technology (TU Hamburg-Harburg)*), Gunnar Maerker (*Hamburg University of Technology (TU Hamburg-Harburg)*) 14:20–14:40

Detailed knowledge of model parameters is key for accurate dynamical forward simulations and control design. Determining these parameters is especially challenging for underwater vehicles, as hydrodynamic effects acting on the vehicles have to be taken into account. Thus, the equations of motion have to be supplemented by hydrodynamic effects. These parameters can be determined analytically, numerically with a computational fluid dynamic simulation, or experimentally. Often, analytical and numerical approaches are preferred because they do not require hardware realizations. However, both, analytical and numerical approaches are subject to simplifications and hence deviations between a vehicle model and the physical reality arise. Due to the small size and cost of micro underwater vehicles experiments with full-size vehicles are feasible. We present an experimental method for determining hydro-parameters of micro underwater vehicles and use the determined parameters for path following control synthesis. In order to determine hydro-parameters such as added mass and added damping, forces and moments of various known magnitudes are applied to the underwater vehicles. Moreover, the resulting translational and rotational velocities and accelerations are measured. The recorded data is used to determine the hydrodynamic parameters through regression techniques. We compare the vehicle's parameters, which are identified in the experiments with the analytically derived parameter set. Moreover, deviations between both parameter sets are analyzed. We show that the determined parameters are sufficient for control design.

A Filter-Based Motion Cueing Algorithm for a Redundant Driving Simulator

Felix Ellensohn (*Institute for Applied Mechanics, Technische Universität München*), Daniel Jean Rixen (*Institute of Applied Mechanics, Technical University of Munich*) 14:40–15:00

In times when automated driving is becoming increasingly relevant, dynamic simulators present an appropriate simulation environment to faithfully reproduce driving scenarios. A realistic replication of driving dynamics is an important criterion to immerse persons in the virtual environments provided by the simulator. Motion Cueing Algorithms (MCA) determine the simulator's input subject to the driving dynamics demands. The main limitations are due to technical restrictions of the simulator's actuators. Typical dynamic simulators consist of a hexapod with six degrees of freedom (DoF) to reproduce the vehicle motion in all dimensions. Since its workspace dimensions are limited, one significant improvement consists in expanding the simulator with redundant DoF by means of additional motion systems.
In our work, we introduce a filter-based MCA that is able to find a motion for a driving simulator with three redundant degrees of freedom. The simulator consists of a tripod with three DoF in a longitudinal-, lateral- and yaw direction as well as a hexapod mounted on top of the tripod's motion platform. The MCA is mainly based on linear transfer functions, like scaling and filters. The motion system's kinematics are included to estimate the resultant specific forces and angular velocities at the driver position. A parameter-optimization scheme estimates the unknown values of the filters subject to the actuators' limitations on position, velocity and acceleration level. Besides, the scheme minimizes deviations between the expected motions of a driver in a real car and in the simulator.

Model-based Identification of Injector Aging in Common Rail Fuel Systems

Oliver Hofmann (*Faculty of Mechanical Engineering, Technical University of Munich, Chair of Applied Mechanics*), Daniel Jean Rixen (*Technical University of Munich, Chair of Applied Mechanics*) 15:00–15:20

Common rail injectors with solenoid valves are complex dynamic systems that require a thorough understanding of the interaction between the coupled disciplines mechanics, electromagnetics, and hydraulics. In addition, the altered dynamical behavior due to aging effects such as erosive damage or coking phenomena further complicates the application of optimization and control strategies and is not yet fully understood. Consequently, we built up a control-oriented prediction model of the plant, which was validated with experimental data of differently modified injectors. In the present work, we discuss several identification strategies that are based on the feedback from either a high-frequency pressure sensor or an eddy current sensor for measuring the control piston displacement. All strategies have in common, that they use characteristic features of the simulative and experimental data at each cycle, and combine these features by using a state estimator of the Kalman filter type. The results of this work show the great potential in accurately predicting important injection characteristics that can be used to control performance and emissions over an engine's lifetime.

Semi-active Vibration Reduction based on a Sliding Mode Controlled Serial-Stiffness-Switch System

Chaoqing Min (*Fakultät für Maschinenbau, Fachgebiet Mechatronik, TU Ilmenau*), Martin Dahlmann (*Fakultät für Maschinenbau, Fachgebiet Mechatronik, TU Ilmenau*), Thomas Sattel (*Fakultät für Maschinenbau, Fachgebiet Mechatronik, TU Ilmenau*) 15:20–15:40

This research presents a concept for semi-active vibration control based on a serial-stiffness-switch system. The system is mainly composed of two serial elements, each of them consisting of one spring and one switch in parallel with each other and connected to a mass. It allows vibration energy harvesting by storing kinetic energy of the mass as potential energy in both springs. One spring acts as compression spring, the other as elongation spring. The stored potential energy is used for vibration control. In a previous work, a specified switching law based on the zero crossing of the velocity of mass was used for vibration reduction. This contribution investigates a sliding mode controller to improve system response and reduce the steady state error. The proposed controller uses a sliding mode surface so that the mass reaches a reference position. With the combination of the above two potential energy storages, the switching law is determined so that sliding mode motion of the system occurs. This control strategy is characterized, simulated, and proven to be more effective than the velocity controlled switching law.

Parameter Identification for the Optimal Control of Robotic Systems

Margareta Runge (*Center for Industrial Mathematics, University of Bremen*), Kathrin Flaßkamp (*University of Bremen*), Christof Büskens (*University of Bremen*) 15:40–16:00

Nowadays parameter identification is one of the main tasks inside many engineering applications, e.g. in robotic systems, where a model of the dynamic behavior is needed. Before we can operate our system, e.g. solve an optimal control problem to perform an assigned task, we have to identify not directly measurable parameters within the system model. Generally, system identification is a one-time job before system operation, but often there remain inaccuracies or the system changes over time, e.g. due to wear. Thus, the model has to be adapted during the process. So far, inexactness in the model is compensated under high energy effort with feedback control, e.g. Riccati control. The literature describes techniques such as adaptive control to compute online new parameter for the specific control law, but the underlaying model is not improved.
In order to model the dynamic behavior of an idealized robot (like a DENSO VS-050) we seek to numerically identify parameters arising in the corresponding Euler-Lagrange equations. Fitting the model to simulated data leads to an optimization problem with a system of ordinary differential equations as constraints, which encourages to use transcription methods from optimal control. This talk focusses on numerical results for the identification of an idealized robotic system, where the optimal control problem and the parameter identification problem of the system are solved alternatingly. One can expect to iteratively obtain better feedforward controls, which need less correction by a feedback controller and give better predictions on costs.

S20.08 | Dynamics and control

Date 22.03.2018
Room N1080

New results on dissipativity of linear-quadratic optimal control problems

Lars Grüne (*Mathematisches Institut, Universität Bayreuth*), Roberto Guglielmi (*Gran Sasso Science Institute*) 17:30–17:50

Dissipativity of linear quadratic optimal (LQ) control problems is a well studied topic since Jan Willems' pioneering work in the early 1970s. It may therefore seem surprising that there are still new results to be obtained. The reason for this is twofold: on the one hand, motivated by its importance for understanding the performance of model predictive control schemes, the stronger concept of *strict* dissipativity has attracted significant interest in recent years and for

this concept nothing much can be found in the classical literature. On the other hand, LQ problems with input and state constraints were not studied in the classical literature and require different approaches and concepts.
In this talk we will provide a comprehensive characterization of strict dissipativity for LQ problems with and without state constraints in terms of systems theoretic and spectral properties of the system matrices. We will also explain the relation of these new results to the turnpike property and its use in model predictive control.

Symmetry Groups and the Observability of PDEs

Bernd Kolar (*Institute of Automatic Control and Control Systems Technology, Johannes Kepler University Linz*), Markus Schöberl (*Institute of Automatic Control and Control Systems Technology, Johannes Kepler University Linz*) 17:50–18:10

Symmetry groups of PDEs are a well-studied topic with numerous applications. Roughly speaking, a symmetry group of a system of PDEs is a transformation group which acts on the space of independent and dependent variables in such a way that it transforms solutions onto solutions. In other words, a symmetry group allows to deform solutions continuously into other solutions. In the following, we restrict ourselves to symmetry groups that only affect the dependent variables. Symmetry groups of this type can be useful for studying the observability of systems of nonlinear PDEs with inputs and outputs. More precisely, with respect to observability it is of interest whether there exist symmetry groups that do not change the input and the output of the system. Such symmetry groups allow to construct solutions with the same input but different initial conditions, that generate the same output. Thus, the initial condition cannot be determined uniquely from the input and the output, which shows that the system is not observable.
In this contribution, we first recapitulate the basics of symmetry groups and discuss the application to the observability analysis of nonlinear PDEs. Then we show how the approach simplifies for a class of linear PDEs. Furthermore, we compare the symmetry group approach to the well-known concepts from infinite-dimensional linear systems theory.

Multiscale optimal control of collective behavior phenomena

Dante Kalise (*Mathematics, Imperial College London*) 18:10–18:30

In this talk we review different results in optimisation and optimal control of large-scale, agent-based models. We model the role of external interventions over a large population as a mean-field optimal control problem. Such control problems are constrained by a PDE of continuity-type, governing the dynamics of the probability distribution of the agent population. We show the existence of mean field optimal controls both in the stochastic and deterministic setting. We present a novel approximating hierarchy of sub-optimal controls based on a Boltzmann approach, whose computation requires a very moderate numerical complexity with respect to the one of the optimal control. We provide numerical experiments for models in opinion formation comparing the behavior of the control hierarchy.

S20.09 | Dynamics and control

Date 23.03.2018
Room N1080

A Comparison of Transcription Methods for Dynamic Parameter Identification Problems

Kai Schäfer (*University of Bremen*), Kathrin Flaßkamp (*University of Bremen*), Christof Büskens (*University of Bremen*) 08:30–08:50

A technical system's dynamic behavior is oftentimes qualitatively known such that a general model can be formulated, but parameter values within the model are unknown since they depend on system specifications. In this work we aim at simultaneously identifying the whole set of parameters in order to find a suitable model formulation. This task can be solved by means of nonlinear optimization.
More specifically, we formulate parameter identification problems governed by ordinary differential equations, in which the aim is to fit the model to given data in a least squares sense. Thanks to the similarity to optimal control problems, direct methods can be applied which lead to standard nonlinear optimization problems. We apply different transcription methods and analyze the resulting problem formulations regarding complexity and structural sparsity information. In order to model the dynamic behavior of a multi-link robot, we seek to numerically identify parameters arising in the corresponding Euler-Lagrange equations as well as parameters which model external forces. With the help of this application we compare the methods regarding robustness, efficiency, and quality of the calculated set of parameters and state trajectories.
We use the software package TransWORHP for the transcription into a nonlinear optimization problem. To find a local minimum, it uses the NLP solver WORHP.

Review and Perspectives of Magnetically Levivated Trains

Werner Schiehlen (*Institute of Eng. Comp. Mechanics, University of Stuttgart*) 08:50–09:10

MAGLEV vehicles are running on solid guideways propelled, guided and levitated by magnetic actuators without any contact forces. The first patents on MAGLEV trains were registered in first half of the 20th century and, due to the Second World War, an engineering design of MAGLEV's did start only after 1970.
The inventor era is characterized by the patents of Zehden (1902), Bachelet (1910) and Kemper (1934). The engineering design era started 1971 when the MBB company constructed the world's first demonstration vehicle after a personal meeting of Kemper and Bölkow. A detailed review of MAGLEV test and application vehicles is available from Meisinger and Shu Guangwei (2011). The scientific methods include ground vehicle dynamics by Popp and Schiehlen (2010) for the longitudinal, lateral and vertical motions. For the propulsion of MAGLEV's long or short stator versions are used. For the modeling of the magnet undercarriage the method of multibody systems is most appropriate. For the control of lateral and vertical motions electromagnetic (EMS) or electrodynamic (EDS) suspensions may be used where single magnet or degree of freedom control are at hand. A detailed analysis was performed by Gottzein (1984) denoted as "Magnetic Wheel". Finally, the guideway is modelled as a flexible structure of simply supported Bernoulli-Euler beams. It remains a periodically time-varying system with jumping states.
The perspectives of MAGLEV vehicles are still very challenging. The Shanghai MAGLEV, similar to the German Transrapid TR07, is successfully operating since 2004. Recently, Incheon Airport MAGLEV began its commercial operation with EMS suspension, too. Moreover, China

Railway Rolling Stock Corp. (CRRC) will develop a MAGLEV train that can reach 600 km/h.

[1] Zehden, A.: Patent US 782312 A (1902)

[2] Bachelet, E.: Patent US 1020942 A (1910)

[3] Kemper, H.: German Patent 643316 (1934)

[4] Meisinger, R.; Shu Guangwei: 40 Years of MAGLEV Vehicles in Germany. Georg- Simon-Ohm-Hochschule, Nürnberg (2011)

[5] Popp, K.; Schiehlen,W.: Ground Vehicle Dynamics. Springer, Berlin 2010.

[6] Gottzein, E.: Das „Magnetische Rad“ als autonome Funktionseinheit modularer Trag- und Führungssysteme für Magnetbahnen. VDI-Verlag, Düsseldorf 1984. (in German)

Sensitivity Analysis of a Two-Lens System for Positioning Feedback

Christopher Schindlbeck (*Institute of Measurement and Automatic Control, Leibniz Universität Hannover*), Christian Pape (*Institute of Measurement and Automatic Control, Leibniz Universität Hannover*), Eduard Reithmeier (*Leibniz Universität Hannover*) 09:10–09:30

Precise alignment of optical components is crucial for the assembly of optical system. Misaligned components (due to positioning tolerances) lead to a distorted wavefront that deviates from a desired wavefront given by the initial nominal design. Inferring the current poses of optical components solely from detector measurements is a difficult but necessary task in order to calculate correction terms for feedback control without using external measurement devices. In this paper, we aim at inferring the lens poses of a two-lens system solely from wavefront measurements. The wavefront can be decomposed into a finite sequence of polynomials which is weighted by coefficients. Since position deviations directly lead to deviations in the wavefront (and therefore in the wavefront coefficients), a sensitivity matrix can be established. The choice of lens positions and wavefront coefficients determines the sensitivity matrix which is often ill-conditioned and may potentially suffer from rank loss. We analyze the feasibility and show the limitations of this approach by conducting a sensitivity analysis. Experimental validation is conducted on an optical system consisting of a laser, two bi-convex lenses, and a wavefront sensor.

Parameter Optimization of a Reduced Model for Multi-Contact Locomotion of Humanoid Robots

Philipp Seiwald (*Mechanical Engineering, Technical University of Munich*), Anian Leyerer (*Technical University of Munich*), Felix Sygulla (*Mechanical Engineering, Technical University of Munich*), Daniel Jean Rixen (*Mechanical Engineering, Technical University of Munich*) 09:30–09:50

In the past decades there have been great advances concerning bipedal locomotion of humanoid robots. As typical applications of future service robots involve cluttered and dynamically changing environments, robust, safe and fast algorithms for planning and control have been developed recently. However, the stabilizing performance of humans remains unrivaled. A natural reason for the difference is the usage of arms to support against walls in order to reject disturbances. In contrast classical bipedal walking robots only use their legs to interact with the environment. At present various groups investigate methods for so called multi-contact locomotion, i. e. using additional robot-environment contacts. As hard real-time requirements have to be met for

planning and controlling those complex movements, reduced models which approximate the dynamics of the robot are necessary. Unfortunately the popular linear inverted pendulum model is not sufficient in this case, as the dynamics of fast moving arms are not taken into account. Within this contribution we present a multi-body model consisting of five masses, which can be used for real-time motion and stability analysis within the planning stage. Aside from explicitly considering arms and legs, the robot-environment interaction is modeled with unilateral contacts. Special focus lies on finding an optimal parameter set, which keeps the approximation error minimal. As the optimization problem involves many local minima, global optimization techniques like particle-swarm optimization and genetic algorithms are applied to find an optimal mass distribution of the reduced model.

S21 | Mathematical signal and image processing

Organiser Felix Krahmer (*Mathematics, Technische Universität München*)
Benedikt Wirth (*University of Muenster*)

S21.01 | Mathematical signal and image processing

Date 20.03.2018
Room N1179

Mathematical image processing in the age of deep learning

Michael Möller (*Visual Scene Analysis, University of Siegen*) 08:30–09:10

The concept of tackling ill-posed problems by defining an energy whose minimizer is the desired solution, has been among the most powerful tools to solve inverse problems in imaging. It gives rise to four fundamental lines of research: 1) Model design, i.e., the choice of energy which yields minimizers with desirable properties, 2) Model analysis, i.e., proving certain properties of the chosen model, 3) Optimization algorithms, i.e., finding numerical methods that allow to solve the proposed model efficiently, and 4) Applications, i.e., the demonstration that the minimizer of the proposed energy yields the desired state-of-the-art results on a particular problem. The latter has recently been challenged by deep learning methods that use a parameterized function to directly map the input to the desired output. In this introductory talk I will given an overview over the two methodologies, summarize their respective advantages and drawbacks, and review some recent approaches that try to combine their respective advantages.

Optimal Approximation of Classifiers by Sparse Deep Neural Networks

Philipp Petersen (*TU Berlin*) 09:10–09:30

In this talk, we present a fundamental lower bound on the sparsity of connectivity necessary to guarantee uniform approximation rates for arbitrary function classes in $L^2(\mathbf{R}^d)$. In other words, we establish a connection between the complexity of a function class and the necessary complexity of a neural network that is to approximate functions from this class up to a certain accuracy. Additionally, we study achievability of this lower bound, specifically for classes of functions that assume only finitely many values, i.e., piecewise constant functions. This analysis is motivated by the recent successful applications of deep neural networks in classification tasks, where complex and high-dimensional data is mapped to only a few classifying labels. For such function classes, we will demonstrate that approximation with neural networks is optimal concerning those fundamental lower bounds mentioned above. As an example, we demonstrate for $n, d \in \mathbf{N}$ arbitrary, the number of edges and the depth of a ReLU neural network approximating a piecewise C^n function on $\mathbf{R}^d$ with jump singularities along C^n curves, scale optimally with respect to the approximation quality.
This talk is based on joint work with Helmut Boelcskei, Philipp Grohs, Gitta Kutyniok, and Felix Voigtlaender.

Using deep neural networks to approximate the solution of the Black-Scholes equation

Dennis Elbrächter (*Faculty of Mathematics, University of Vienna*) 09:30–09:50

We show that deep neural networks (i.e. the depth of the network depends on the quality of the approximation) are capable of efficiently approximating the solution to the Black-Scholes equation for the european maximum option. In particular the number of nodes only has a polynomial dependence on the dimension (i.e. number of options) of the problem. To do so, we use results of D. Yarotsky, which show that deep networks can be used to implement an approximate multiplication, where the number of nodes and layers only has a logarithmic dependence on the accuracy. This can further be used to construct deep networks which can efficiently approximate a more general class of smooth functions.

Choosing specific orthogonal projections for dimension reducing preprocessing in learning tasks

Anna Breger (*Department of Mathematics, University of Vienna*), Martin Ehler (*Department of Mathematics, University of Vienna*) 09:50–10:10

Computation cost of data analysis methods, such as machine learning tools, depend highly on the dimension of the input data. When reducing the dimension as a preprocessing step we want to preserve as much information of the data as possible while representing the data in a more efficient way. If the projection preserves pairwise distances within the data set, we can expect that subsequent learning tools still perform well on the projected lower-dimensional data. The Johnson-Lindenstrauss Lemma states that with high probability a random orthogonal projector will preserve the distances well. We aim to replace random projections by specific sequences of deterministic projectors that cover the Grassmannian manifold in an optimal fashion.
Principal component analysis (PCA) is widely used for dimension reduction and noise suppression in applications. The method projects data in a lower dimensional space such that the total variance within the data is maximized. We will show, however, that maximizing the total variance can yield bad preservation of the pair-wise distances. Therefore we suggest to choose a deterministic orthogonal projector that balances those two values, always depending on the particular input data. Numerical experiments in classification learning tasks support our theoretical results.

Learned Reconstruction Methods for Photoacoustic Tomography

Christoph Brune (*University of Twente*), Yoeri E. Boink (*University of Twente*), Srirang Manohar (*University of Twente*) 10:10–10:30

Photoacoustic tomography is a hybrid imaging technique that combines high optical tissue contrast with high ultrasound resolution. Direct reconstruction methods such as filtered backprojection, time reversal and least squares suffer from curved line artefacts and blurring, especially in case of limited angles or strong noise. In recent years, there has been great interest in regularised iterative methods. These methods employ prior knowledge on the image to provide higher quality reconstructions. However, easy comparisons between regularisers and their properties are limited, since many tomography implementations heavily rely on the specific regulariser chosen. To overcome this bottleneck, we present a modular reconstruction framework for photoacoustic tomography where the regularisation can be learned from training data reflecting different a-priori assumptions. This enables comparisons with standard approaches, e.g. nonlinear, higher-order or directional regularisation. We solve the underlying minimisation problem with an efficient first-order primal-dual algorithm. Convergence rates are optimised by choosing an operator dependent preconditioning strategy. Our learned reconstruction methods are tested on challenging synthetic and experimental data sets. They outperform standard reconstruction approaches for strong noise levels and limited angle measurements, offering immediate benefits in terms of acquisition time and quality in biomedical imaging.

S21.02 | Mathematical signal and image processing

Date 20.03.2018
Room N1179

Stochastic proximal gradient algorithms for multi-source quantitative PAT

Simon Rabanser (*Mathematics, University of Innsbruck*) 16:30–16:50

We approch the image reconstruction problem in quantitative photoaoustic tomography by modelling light transport using the radiative transfer equation. We formulate the reconstruction problem as a single inverse problem to estimate tissue relevant parameters from measured photoacoustic data. To solve the inverse problem we use Tikhonov regularization in combination with the proximal gradient iteration for minimizing the Tikhonov functional and expand it to a stochastic version to incorporate multi-source data in our reconstruction method. Additionally, in this talk, we reformulate the image reconstruction problem in quantitative photoaoustic tomography as a multi-linear inverse problem avoiding the time consuming computation of the radiative transfer equation. We present numerical results and point out the differences of the two approaches.
This talk bases on joint work with Markus Haltmeier and Lukas Neumann.

ProxToolbox: Fixed Point iterations and their numerical investigation

Anna-Lena Martins (*Fakultät für Mathematik und Informatik, Georg-August Universität Göttingen*) 16:50–17:10

The tremendous amount of first-order methods for structured optimization or their relaxations which are published on a weekly basis do sometimes overwhelm us. Often this is not due to the new algorithmic strategies itself but to their classification and behavior in comparison to other (already existing) algorithms of their kind. A standard testbed of real-world problems for trustworthy comparisons is missing. The ProxToolbox started as an effort to establish reproducibility of numerical experiments. It has since developed into what I hope to convince you is a platform for testing and comparing prox-based methods on data sets, both simulated and experimental, from some of the more popular applications of first order methods.

Optimization by Non-convex Majorization-Minimization

Jonas Geiping (*Visuelle Szenenanalyse, University of Siegen*), Michael Möller (*Visual Scene Analysis, University of Siegen*) 17:10–17:30

Optimization algorithms can often be generalized into a majorization-minimization framework. The majorizing function is generally chosen to be convex and thus simple to solve in each step. This talk however will discuss non-convex majorizing functions, detailing some suitable classes of non-convex majorizing functions that still allow solving each sub-problem to near global optimality and furthermore provide a convergent optimization scheme. We show a numerical analysis of this optimization scheme and illustrate examples where the application of this scheme leads to superior local optima compared to descent methods, while being significantly more efficient than global methods. Further, we show some examples where we apply this scheme for imaging tasks, namely in the context of time-of-flight super-resolution.

On monotone and primal-dual active set schemes for l^p-type problems, p in (0,1]

Daria Ghilli (*mathematics, University of Graz*), Karl Kunisch (*University of Graz*) 17:30–17:50

Nonsmooth nonconvex optimization problems involving the ℓ^p quasi-norm, $p \in [0, 1)$, of a linear map are considered. A monotonically convergent scheme for a regularized version of the original problem is developed and necessary optimality conditions for the original problem in the form of a complementary system amenable for computation are given. Then an algorithm for solving the above mentioned necessary optimality conditions is proposed. It is based on a combination of the monotone scheme and a primal-dual active set strategy. The performance of the two schemes is studied and compared to other existing algorithms by means of a series of numerical tests in different cases, including optimal control problems, fracture mechanics and microscopy image reconstruction.

Computation of Optimal Transport on Discrete Metric Measure Spaces

Bernhard Schmitzer (*Angewandte Mathematik, WWU Münster*) 17:50–18:10

Optimal transport distances between probability measures are becoming increasingly popular as a numerical tool in image and data analysis. They are geometrically intuitive and robust to noise. In particular, the geodesic between two data points is given by the so-called displacement interpolation, which provides a more natural trajectory than simple pointwise interpolation. Unfortunately, such geodesics do not exist for optimal transport distances when the underlying base space is discrete. This includes metric graphs which are omnipresent in data analysis. As a remedy, Maas (2011) has proposed an adapted formulation for transport distances on discrete Markov kernels. While the original optimal transport problem on a graph can be written as finite-dimensional linear program, the new formulation involves a non-linear, non-smooth, infinite-dimensional, convex, spatio-temporal optimization problem. We give a discretization that is consistent in the sense of Gamma-convergence and an optimization algorithm for the discretized problem based on proximal splitting. This allows to numerically evaluate the new distance and its geodesics and provides a new tool for geometric data analysis for signals living on graphs.
Joint work with Matthias Erbar, Martin Rumpf and Stefan Simon.

Edge-Parallel Inference with Graphical Models using Wasserstein Messages and Geometric Assignments

Ruben Hühnerbein (*Heidelberg University*), Fabrizio Savarino (*Heidelberg University*), Freddie Åström (*Heidelberg University*), Christoph Schnörr (*Heidelberg University*) 18:10–18:30

A novel approach to Maximum A Posteriori inference based on discrete graphical models is introduced. The given discrete objective function is smoothly approximated by using regularized local Wasserstein distances in order to couple assignment measures across edges of the underlying graph. This approximation is restricted to the assignment manifold and optimized by a multiplicative update combining (i) geometric integration of the resulting Riemannian gradient flow and (ii) rounding to integral solutions that represent valid labelings.

S21.03 | Mathematical signal and image processing

Date 21.03.2018
Room N1179

Median filters for multivariate images: Concepts and relations to PDE filters

Martin Welk (*Department of Biomedical Computer Science and Mechatronics, Private University for Health Sciences, Medical Informatics and Technology (UMIT)*) 08:30–08:50

The median filter for grey-value images is a well-established tool for structure-preserving denoising. Besides the classical sliding-window setting it can also be combined with space-variant structuring elements for adaptive filtering.
Generalisations of median filters to multivariate images have frequently been based on the L1 median concept. Whereas the L1 median is the oldest concept of a median for multivariate data, there are interesting alternatives in the statistical literature, some of which also turn out advantageous in the context of image filtering. For example, some of these yield affine equivariance which is not true for the L1 median. Also, when generalising the well-known link between the univariate median filter and the curvature flow PDE to the multivariate case, alternative median concepts lead to simpler PDEs.
In the talk, selected multivariate median concepts and their applicability in image processing are discussed. Moreover, PDE approximation results are presented that also contribute to the understanding of the properties of these filters.

Bias Reduction in Variational Regularization

Julian Rasch (*Institute for Computational and Applied Mathematics, University of Münster*), Eva-Maria Brinkmann (*Insitute for Computational and Applied Mathematics, University of Münster*), Martin Burger (*Insitute for Computational and Applied Mathematics, University of Münster*), Camille Sutour (*MAP5, Université Paris Descartes*) 08:50–09:10

Variational methods suffer from inevitable bias. The simplest example is ℓ^1-regularization, which leads to sparse solutions, but however affects the quantitative peak values. We present a two-step method to reduce bias. After solving the standard variational problem, the key idea is to add a consecutive debiasing step minimizing the data fidelity on an appropriate convex set. Here, these so-called model manifolds are built up of the roots of a Bregman distance, using the subgradient appearing in the optimality condition of the variational method. All elements in a model manifold share the same regularity as the biased solution, which allows to choose a better (or "unbiased") candidate from this set while keeping the regularity. In particular, the model manifolds lead to a decomposition of the overall bias into two parts, model and method bias, which provide further insight into the systematic errors of variational regularization. While the former is shown to be intrinsic to the choice of regularization and hence inevitable, the latter is encoded in the proposed framework and can be entirely corrected for. We provide numerous examples and experiments to illustrate both the performance and the statistical behavior of the method.

Topological Analysis of Open-Pore-Structures

Lukas Bogunia (*Maschinenbau, Universität Siegen*), Kerstin Weinberg (*Maschinenbau, Universität Siegen*) 09:10–09:30

Open-cell structures like open-pore foams have several applications, e.g. as acoustic damping material in civil engineering. Most material models do not capture the dynamic and static behavior of theses structures correctly. In order to develope a model which is able to describe the dynamic and the static properties an analysis of the microstructure is required. Suitable methods summerized in [1] and [2] are used to determine the topological parameters of open-pore PUR foam. Simplified models based on the extracted structural parameters are studied.

[1] J. Ohser and K. Schladitz, 3D Images of Materials Structures: Processing and Analysis. Wiley-VCH, 2009.

[2] P. Soille, Morphological Image Analysis Principles and Applications. Springer, 2003.

S21.04 | Mathematical signal and image processing

Date 21.03.2018
Room N1179

Phase retrieval in infinite dimensions

Rima Alaifari (*Seminar for Applied Mathematics, Department of Mathematics, ETH Zurich*) 14:00–14:40

In phase retrieval problems, a signal is sought to be reconstructed from only the magnitudes of a set of complex measurements. The missing information of the phase of the measurements severely obstructs the signal reconstruction.
We study this problem in the setting where the signal belongs to an infinite-dimensional Hilbert space. This problem is inherently unstable, i.e. highly sensitive to noise in the measurements. We show that in some sense this property is independent of the redundancy of the measurements. However, the instabilities observed in practice are all of a certain type. Motivated by this observation, we introduce a new paradigm for stable phase retrieval.
We demonstrate that in audio processing applications this new notion of stability is natural and meaningful and that in this new setting stability can actually be achieved for certain measurement systems.
This is joint work with I. Daubechies (Duke University), P. Grohs (University of Vienna) and R. Yin (Duke University).

Stable Gabor Phase Retrieval and Spectral Clustering

Martin Rathmair (*Mathematics, University of Vienna*), Philipp Grohs (*University of Vienna*) 14:40–15:00

We consider the problem of reconstructing a signal f from its spectrogram, i.e., the magnitudes $|V_\varphi f|$ of its Gabor transform

$$V_\varphi f(x,y) := \int_{\mathbb{R}} f(t) e^{-\pi(t-x)^2} e^{-2\pi i y t} dt, \quad x, y \in \mathbb{R}.$$

Such problems occur in a wide range of applications, from optical imaging of nanoscale structures to audio processing and classification.
While it is well-known that the solution of the above Gabor phase retrieval problem is unique up to natural identifications, the stability of the reconstruction has remained wide open. Our work discovers a deep and surprising connection between phase retrieval, spectral clustering and spectral geometry. We show that the stability of the Gabor phase reconstruction is bounded by the inverse of the *Cheeger constant* of the flat metric on $\mathbb{R}^2$, conformally multiplied with $|V_\varphi f|$. The Cheeger constant, in turn, plays a prominent role in the field of spectral clustering, and it precisely quantifies the 'disconnectedness' of the measurements $|V_\varphi f|$.
It has long been known that a disconnected support of the measurements results in an instability - our result for the first time provides a converse result in the sense that there are no other sources of instabilities.

Time-Frequency Shift Invariance and the Balian-Low Theorem

Andrei Caragea (*Lehrstuhl Wissenschaftliches Rechnen, Katholische Universität Eichstätt-Ingolstadt*), Dae Gwan Lee (*Lehrstuhl Wissenschaftliches Rechnen, Katholische Universität Eichstätt-Ingolstadt*), Götz Pfander (*Lehrstuhl Wissenschaftliches Rechnen, Katholische Universität Eichstätt-Ingolstadt*), Friedrich Philipp (*Mathematik, Katholische Universität Eichstätt-Ingolstadt*) 15:00–15:20

Both the Balian-Low Theorem and the Amalgam-Balian-Low Theorem are well known facts in time-frequency analysis stating in two ways that a function generating a Gabor Riesz basis of $L^2(\mathbb{R})$ cannot be well localized in both time and frequency. In 2016, Cabrelli, Molter, and Pfander proved the following generalization of the Amalgam-Balian-Low Theorem.

Theorem 1. *Let $\Lambda \subset \mathbb{R}^2$ be a lattice with rational density and let $g \in \mathcal{S}_0(\mathbb{R})$ (the Feichtinger algebra) such that the Gabor system (g, Λ) generated by g and Λ is a Riesz basis of its closed linear span $\mathcal{G}$. Then for any $\mu \in \mathbb{R}^2$ whose time-frequency shift $\pi(\mu)g$ lies in $\mathcal{G}$ we have that $\mu \in \Lambda$.*

Using VMO methods, we prove that the same conclusion of Theorem 1 holds when $g \in \mathcal{S}_0(\mathbb{R})$ is replaced by $g \in H^{p/2}(\mathbb{R})$ and $\hat{g} \in H^{q/2}(\mathbb{R})$, where $\frac{1}{p} + \frac{1}{q} = 1$ and $1 < p < \infty$, i.e.,

$$\left(\int_{\mathbb{R}} |x|^p |g|^2 \, dx \right) \left(\int_{\mathbb{R}} |\omega|^q |\hat{g}|^2 \, d\omega \right) = \infty.$$

This can be seen as a generalization of the so-called (p, q)-Balian-Low-Theorem, which was proved in 2008 by Z. Gautam and itself generalizes the classical Balian-Low Theorem. The main difficulty to overcome in proving our theorem is that – unlike in the case where $g \in \mathcal{S}_0(\mathbb{R})$ – the assumptions on g do in general not imply that its Zak transform is continuous. However, it is locally VMO which turns out to be a good replacement for being continuous.

The talk is based on joint work with A. Caragea, D. Lee, and G. Pfander (all from KU Eichstätt).

Inhomogeneous shearlet coorbit spaces and their atomic decomposition

Lukas Sawatzki (*AG Numerik, Philipps-University Marburg*) 15:20–15:40

We establish inhomogeneous coorbit spaces related to the continuous shearlet transform and weighted Lebesgue spaces $L_{p,v}$. For the wavelet setting, inhomogeneous coorbit spaces have been obtained by Fornasier, Rauhut and Ulrich. Our construction is based on a generalization of this approach to the shearlet case. Furthermore, we present an atomic-like decomposition for these spaces which allows us to derive some properties. A major difficulty in our work is the integrability of the corresponding kernel function.

A Deterministic DCT Algorithm for Vectors with Short Support

Sina Bittens (*Institute for Numerical and Applied Mathematics, Georg-August Universität Göttingen*) 15:40–16:00

There are many well-known fast algorithms for the discrete Fourier transform (DFT) of sparse input signals or vectors, both deterministic and randomized ones. The fastest of the deterministic algorithms achieve runtimes of $\mathcal{O}\left(m^2 \log^{\mathcal{O}(1)} N\right)$ for a general m-sparse input signal of length N. If it is even known that the input signal has a short support of length m, the runtime can be reduced to $\mathcal{O}(m \log N)$.
For the closely related discrete cosine transform of type II (DCT-II), given by

$$\mathbf{x}^{\widehat{\mathrm{II}}} = \sqrt{\frac{2}{N}} \left(\varepsilon_N(j) \cos\left(\frac{j(2k+1)\pi}{2N} \right) \right)_{j,\,k=0}^{N-1} \mathbf{x}, \quad \mathbf{x} \in \mathbb{R}^N,$$

where $\varepsilon_N(0) = 1/\sqrt{N}$ and $\varepsilon_N(j) = 1$ for $j \neq 0$, no such algorithms are known so far. In this talk we present a new fast and deterministic DCT-II algorithm that reconstructs the input vector $\mathbf{x} \in \mathbb{R}^N_{\geq 0}$, $N = 2^J$, with short support of length m from $\mathbf{x}^{\widehat{\mathrm{II}}}$ by combining ideas from two sparse FFT algorithms for vectors with short support by Plonka and Wannenwetsch in Numerical Algorithms, 71(4):889-905, 2016, and Journal of Computational and Applied Mathematics, 321:532 – 539, 2017. The resulting algorithm has a runtime of $\mathcal{O}(m \log m \log N)$ and requires $\mathcal{O}(m \log N)$ samples of $\mathbf{x}^{\widehat{\mathrm{II}}}$.

S21.05 | Mathematical signal and image processing

Date 21.03.2018
Room N1179

Optimal convergence rates for variational regularization of inverse problems with Poisson and Bernoulli data

Yusufu Simayi (*University of Goettingen, Institute for Numerical and Applied Mathematics*) 16:30–16:50

We discuss Tikhonov-type regularization method for linear and nonlinear ill-posed inverse problems described by an operator equations $Tf^\dagger = g^\dagger$, where $g^\dagger$ is an integrable, non-negative function and the measured data are described either by a Poisson or by a Bernoulli process with density $g^\dagger$. Such inverse problems occur for example in photonic imaging and parameter identification problems in stochastic differential equations, and variational regularization methods for such problems have been studied intensively in recent years. However, known rates of convergence for mildly ill-posed problems are not optimal so far. For both noise models, Kullback-Leibler data fidelity terms appear naturally as negative log-likelihood functionals. We derive for the first time optimal convergence rates in the mildly ill-posed case. To achieve the optimal rates of convergence, the key tool of our analysis are deviation inequalities for Poisson and Bernoulli data in negative Besov norms.

On convergence of solutions of total variation regularized linear inverse problems

Jose A. Iglesias (*RICAM-OeAW*), Gwenael Mercier (*RICAM-OeAW*), Otmar Scherzer (*University of Vienna*) 16:50–17:10

In a recent paper by Chambolle, Duval, Peyre, and Poon (2017) it was proved that if the subgradient of the total variation at the true data is not empty, the level-sets of the total variation denoised solutions converge to the level-sets of the true solution with respect to the Hausdorff distance. We generalize that result to total variation regularization of general linear inverse problems and different boundary conditions on bounded domains, under the standard source condition for convex regularization functionals introduced by Burger and Osher (2004). Applications include deblurring, inversion of the circular Radon transform, and denoising in bounded domains.

Low-rank techniques for seismic data interpolation

Christian Kümmerle (*TU München*), Claudio Verdun (*TU München*) 17:10–17:30

In seismology, the problem of exploration of soil layers for oil and gas reservoirs is a procedure that involves the sampling of seismic data across a large spatial and temporal domain. Economical and physical constraints suggest subsampling of the data, giving rise to missing sensor traces that have to be interpolated before further processing.
In this talk, we survey approaches for the seismic data interpolation problem that make use of low-rank structures in suitable data domains. We discuss different transformations that expose low-rank structures in fully sampled data, making the use of low-rank matrix completion techniques feasible.
One modelling of particular interest requires the recovery of very high-dimensional low-rank Hankel or Toeplitz matrices. We argue for the use of optimization methods that combine statistical accuracy with computational efficiency in this context.

Regularization of bilinear and quadratic inverse problems by tensorial lifting

Robert Beinert (*Institut für Mathematik und Wissenschaftliches Rechnen, Karl-Franzens-Universität Graz*) 17:30–17:50

Considering the question: how non-linear may a non-linear operator be in order to extend the linear regularization theory, we introduce the class of dilinear and diconvex mappings. Using tensorial liftings, we generalize the concept of subgradients and Bregman distances from convex analysis to establish convergence rates under similar assumptions than in the linear setting. Finally, we apply our results to the deautoconvolution problem to derive satisfiable source conditions and numerically provable convergence rates.

Saturation Rates for Filtered Back Projection Reconstructions

Matthias Beckmann (*University of Hamburg*), Armin Iske (*University of Hamburg*) 17:50–18:10

The filtered back projection (FBP) formula allows us to reconstruct bivariate functions from given Radon samples, where low-pass filters with finite bandwidth and compactly supported window function are employed to make the reconstruction by FBP less sensitive to noise.
The aim of this talk is to analyse the intrinsic FBP reconstruction error which is incurred by the application of a low-pass filter. To this end, we present error estimates in Sobolev spaces of fractional order, where the obtained error bounds depend on the bandwidth of the utilized filter, on the flatness of the filter's window function at the origin, on the smoothness of the target function, and on the order of the considered Sobolev norm. Further, we prove convergence for the approximate FBP reconstruction in the treated Sobolev norms along with asymptotic convergence rates as the filter's bandwidth goes to infinity, where we observe saturation at fractional order depending on smoothness properties of the filter's window function.
The theoretical results are supported by numerical experiments.

Numerical Identification of Motor Units using an Optimal Control Approach

Tobias Sproll (*Lehrstuhl für Angewandte Mathematik, Universität Bayreuth*), Anton Schiela (*Universität Bayreuth*) 18:10–18:30

High density surface Electromyography (sEMG), is a non-invasive method of measuring the activity of muscle whereby an array of electrodes is placed above the skin and a spatially and temporally resolved measurement of the electric potential on the skin is obtained. Recent advances in high-density sEMG measurement have opened the possibility of extracting information about single motor units (groups of muscle fibers controlled by the same motor neuron) from the sEMG signal.
While significant advancements have been made in identifying the activity of individual motor units from the surface EMG signal through EMG decomposition methods, a reliable and accurate method to determine the position of the motor units from the sEMG signal is not yet available. Previous works consider spatial data only or use simple parametric models within a least squares approach.
In this talk we consider an approach to automate the identification of motor units using techniques from numerical simulation and non-linear optimization.

S21.06 | Mathematical signal and image processing

Date 22.03.2018
Room N1179

ATLAS: A Multi-Penalty Approach to Compressed Sensing of Low-Rank Matrices with Sparse Singular Vectors

Johannes Maly (*Technische Universität München*), Massimo Fornasier (*Technische Universität München*), Valeriya Naumova (*Simula Research Laboratory AS*) 08:30–08:50

Compressed Sensing is about recovering an unknown vector of dimension n from $m \ll n$ linear measurements. This task becomes possible, for instance, when few entries of the vectors have large magnitude and, hence, the vector is essentially of low intrinsic dimension. If one wishes to recover a $n_1 \times n_2$ matrix instead, low-rankness can be added as sparsity structure of low intrinsic dimensionality. For this purpose we propose a novel algorithm, which we call ***A**lternating **T**ikhonov regularization and **Las**so* (ATLAS). It is based on a multi-penalty regularization for recovery of low-rank matrices with approximately sparse singular vectors, which is able to leverage both structures (low-rankness and sparsity) simultaneously and effectively reduce further the number of necessary measurements with respect to the sole use of one of the two sparsity structures. We provide nearly-optimal recovery guarantees of ATLAS. The analysis is suprisingly relatively simple, e.g., compared to the one of other similar approaches such as *Sparse Power Factorization* (SPF). It relies on a cleaverly adapted restricted isometry property of measurements for low-rank and approximately sparse matrices, LASSO techniques, and results on proximal alternating minimization. We show that ATLAS is bound to be more efficient than convex relaxation and is as competitive as SPF, supersiding it in strong noise regimes and for matrices whose singular vectors do not possess exact (joint-) sparse support. Moreover, contrary to SPF, ATLAS is shown to converge even for measurements not fulfilling the restricted isometry property to matrices with some guaranteed sparsity and minimal discrepancy to data.

Variants of total generalized variation

Birgit Komander (*Institut für Analysis und Algebra, Technische Universität Braunschweig*), Dirk A. Lorenz (*Institut für Analysis und Algebra, Technische Universität Braunschweig*), Lena Vestweber (*Institut Computational Mathematics AG Numerik, Technische Universität Braunschweig*) 08:50–09:10

By revisiting the classical Rudin-Osher-Fatemi total variation denoising method [Rudin, L., Osher, S. and Fatemi, E., 1992], we first augment the model with an estimate of the image gradient. This is related to an approach by Lysaker et al. [Lysaker, M., Osher, S. and Tai, X., 2004], where they estimated image normals as a pre-step and used these for better image denoising. Further, we analyze, how an estimated gradient could be helpful for image denoising and combine this estimation process with the image denoising into one simultaneously working method. This, however, is very close to the total generalized variation denoising method from Bredies et al. [Bredies, K., Kunisch, K. and Pock, T., 2010]. This combination and analysis sheds more light on the motivation of the TGV model. Furthermore, we propose different versions of the TGV denoising method which have several advantages over the classical one: First, switching from penalties to constraints,in some cases, allows for a simple, clean and effective parameter choice. Second, other formulations lead to other dual problems and hence, different algorithms. Some of these turn out to be a little simpler regarding duality gaps and stopping criteria and show slightly different numerical performance.

Total Roto-translational Variation

Thomas Pock (*Institute of Computer Graphics and Vision, Graz University of Technology*), Antonin Chambolle (*Ecole polytechnique-CMAP*) 09:10–09:30

We investigate curvature depending variational models for image regularization, such as Euler's elastica. These models are known to provide strong priors for the continuity of edges and hence have important applications in shape- and image processing. We consider a lifted convex representation of these models in the roto-translation space: In this space, curvature depending variational energies are represented by means of a convex functional defined on divergence free vector fields. The line energies are then easily extended to any scalar function. It yields a natural generalization of the total variation to the roto-translation space. As our main result, we show that the proposed convex representation is tight for characteristic functions of smooth shapes. We also discuss cases where this representation fails. For numerical solution, we propose a staggered grid discretization based on an averaged Raviart-Thomas finite elements approximation. This discretization is consistent, up to minor details, with the underlying continuous model. The resulting non-smooth convex optimization problem is solved using a first-order primal-dual algorithm. We illustrate the results of our numerical algorithm on various problems from shape- and image processing.

Locally adaptive regularization parameter selection for total variation minimization

Andreas Langer (*Universität Stuttgart*) 09:30–09:50

A good approximation of the original image from an observed image may be obtained by minimizing a functional that consists of a data-fidelity term, a regularization term, and a parameter, which balances data-fidelity and regularization. The proper choice of the parameter is delicate. In fact, large weights not only remove noise but also details in images, while small weights retain

noise in homogeneous regions. However, since images consist of multiple objects of different scales, it is expected that a spatially varying weight would give better reconstructions than a scalar parameter. In this vein we present algorithms for computing a distributed weight. We study the convergence behaviour of the proposed algorithms and present numerical experiments for Gaussian noise removal, for impulsive noise removal, and for eliminating simultaneously mixed Gaussian-impulse noise.

Blind Image Fusion for Hyperspectral Imaging with Directional Total Variation

Rafael Reisenhofer (*Universität Bremen*), Leon Bungert (*Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), David A. Coomes (*University of Cambridge*), Matthias J. Ehrhardt (*University of Cambridge*), Jennifer Rasch (*Fraunhofer Heinrich Hertz Institute*), Carola-Bibiane Schönlieb (*University of Cambridge*) 09:50–10:10

We propose a method for increasing the spatial resolution of a hyperspectral image by fusing it with an image of higher spatial resolution that was obtained simultaneously with a different imaging modality. This is accomplished by solving a variational problem in which the regularization functional is the directional total variation. To accommodate for possible mis-registrations between the two images, we consider a non-convex blind super-resolution problem where both the fused image and the corresponding convolution kernel are estimated. Our experimental results indicate that the non-convexity is negligible in practice and that reliable solutions can be computed using a variety of different optimization algorithms. Numerical results on real remote sensing data from plant sciences and urban monitoring show the potential of the proposed method and suggests that it is robust with respect to the regularization parameters, mis-registrations and the shape of the kernel. This is joint work with Leon Bungert (Erlangen-Nürnberg), David A. Coomes (Cambridge), Matthias J. Ehrhardt (Cambridge), Jennifer Rasch (Fraunhofer HHI) and Carola-Bibiane Schönlieb (Cambridge).

Determining angular velocities of fast rotating objects based on motion blur to control an optomechanical derotator

Bettina Altmann (*Institut für Mess- und Regelungstechnik, Leibniz Universität Hannover*), Christian Pape (*Leibniz Universität Hannover*), Eduard Reithmeier (*Leibniz Universität Hannover*) 10:10–10:30

The investigation of machine component parts is important for a faultless functioning of the machine. Ideally, the components are investigated during operation. Thus, the real performance of the machine can be analyzed. However, measurements of fast rotating machine components can be quite challenging especially under bad illumination conditions leading to the necessity of high exposure times.
In case high-speed cameras reach their limits due to motion blur resulting of high exposure times, an optomechanical image derotator can still lead to sufficient results. This is due to its operating principle consisting of a rotating reflector assembly inspired by an Abbe-Koenig-prism which optically eliminates the rotational movement. To generate a stationary image the optomechanical image derotator containing the reflector assembly has to rotate exactly half as fast as the rotating object. Therefore, the angular velocity of the object has to be determined. A common way for this is the use of angular encoders although not every machine can be equipped with such a sensor. A flexible solution for this is to identify the angular position and thereby the velocity with a high speed camera capturing images of the rotating object. Using image processing algorithms the marker can be first detected and thus the velocity can be calculated from the image data.

However, due to the high rotational velocities and long exposure times motion blur of the marker can occur. Generally, motion blur can be treated as an artifact since it makes the image analysis more difficult. However, motion blur can be used to determine the velocity of the rotating objects in knowing the shutter speed as well as the length of the streaking of a blurred object. This work presents an approach which determines the rotational velocity from image blur for different exposure times and object speeds. The resulting information will be used as the input source for a velocity control of the derotator. Furthermore it will be discussed whether the velocity information is precise enough to control the derotator leading to a resting image of the rotating object.

S21.07 | Mathematical signal and image processing

Date 22.03.2018
Room N1179

Edge-Preserving Variational Methods for Regularizing Manifold-Valued Data and Images

Andreas Weinmann (*Mathematics and Natural Sciences, Hochschule Darmstadt*) 14:00–14:20

Nonlinear manifolds appear as data spaces in various applications in image processing. Important examples are spheres, the Euclidean motion group and the Riemannian manifold of positive matrices. Although very prominent for scalar and vector space valued data, algorithms for the variational regularization of manifold-valued data have been considered only recently. In this talk, we present algorithmic schemes for the variational regularization of manifold-valued data and, in particular, for TV and TGV denoising of manifold-valued data. The presentation includes joint work with K. Bredies, L. Demaret, M. Holler, and M. Storath.

A Graph Framework for Manifold-valued Data

Daniel Tenbrinck (*Institute for Analysis and Numerics, Westfälische Wilhelms-Universität Münster*), Ronny Bergmann (*Fachbereich Mathematik, Technische Universität Kaiserslautern*) 14:20–14:40

Novel imaging modalities may yield data whose values are not given in an Euclidean space but on a surface or a manifold. As typical image processing tasks still persist for this data it is important to generalize traditional processing methods for these new situations, e.g., variational methods or PDEs. In this talk we present a framework for processing discrete manifold-valued data, for which the underlying (sampling) topology is modeled by a graph. We introduce the notion of a manifold-valued derivative on a graph and based on this deduce a family of manifold-valued graph p-Laplace operators. We give simple numerical schemes to compute solutions to the related evolution equations and apply this algorithm to different manifold-valued data in denoising applications.

The Graph Infinity-Laplacian for Manifold-valued Data

Ronny Bergmann (*Fachbereich Mathematik, Technische Universität Kaiserslautern*), Daniel Tenbrinck (*Westfälische Wilhelms-Universität Münster*) 14:40–15:00

Due to recent technological advances in the development of modern sensors new imaging modalities have emerged for which the acquired data values are given on a Riemannian manifold,

e.g., in phase values in InSAR imaging or when dealing with diffusion tensors in DT-MRI. Furthermore, to process not only rectangular domains and regular grids, graphs can be employed to model both data on arbitrary (sampled) manifolds as well as nonlocal vicinity.
In this talk we extend a framework for processing discrete manifold-valued data to the task of inpainting missing values, such that the inpainted area nonlocally incorporates data into the reconstruction. We discuss a generalization of the graph infinity-Laplacian to manifold-valued data based on the min-max characterization of the local discrete Lipschitz constant. Finally, we present a numerical scheme to solve the obtained manifold-valued infinity-Laplace equation.

Image Extrapolation for the Time Discrete Metamorphosis Model – Existence and Applications

Alexander Effland (*Institute for Numerical Simulation, University of Bonn*), Martin Rumpf (*Institute for Numerical Simulation, University of Bonn*), Florian Schäfer (*California Institute of Technology*) 15:00–15:20

The space of images can be equipped with a Riemannian metric measuring both the cost of transport of image intensities and the variation of image intensities along motion lines. The resulting metamorphosis model was introduced and analyzed by Trouvé, Younes and coworkers and a variational time discretization for the geodesic interpolation was proposed by Berkels et al. In this talk, this time discrete model is expanded and an image extrapolation via a discrete exponential map is consistently derived for the variational time discretization. For a given weakly differentiable initial image and an initial image variation, the exponential map allows to compute a discrete geodesic extrapolation path in the space of images. It is shown that a time step of this shooting method can be formulated in the associated deformations only. For sufficiently small time steps local existence and uniqueness can be proven using a suitable fixed point formulation and the implicit function theorem. A spatial Galerkin discretization with cubic splines on coarse meshes for the deformations and piecewise bilinear finite elements on fine meshes for the image intensities are used to derive a fully practical algorithm. Different applications underline the efficiency and stability of the proposed approach.

Statistical Shape Modeling

Behrend Heeren (*Institute for Numerical Simulation, University of Bonn*), Martin Rumpf (*Institute for Numerical Simulation, University of Bonn*), William Smith (*Department of Computer Science, University of York*), Chao Zhang (*Department of Computer Science, University of York*) 15:20–15:40

We consider a novel formulation of Principal Geodesic Analysis (a nonlinear generalization of Principal Component Analysis) in general manifolds and shape spaces. Our model is described variationally and comes with an effective time discretization of underlying shortest paths (i.e. geodesics). This tool allows us to analyze important sources of shape variability in a given set of input shapes, compress large variations and fit a given model to measurements. We show applications in the manifold of triangle meshes equipped with a metric reflecting the physics of viscous dissipation. In particular, we demonstrate model-constrained mesh editing and the reconstruction of a dense animated mesh from sparse motion capture markers.

Describing Shapes by Numerical Integration of PDEs

Michael Breuß (*Mathematics, BTU Cottbus - Senftenberg*) 15:40–16:00

In this talk recent work on shape descriptors is presented that relies on the numerical solution of partial differential equations (PDEs) formulated on the surface of 3-D shapes.

S21.08 | Mathematical signal and image processing

Date 22.03.2018
Room N1179

Model-based geometry reconstruction of quantum dots from transmission electron microscopy (TEM)

Anieza Maltsi (*Weierstraß-Institut für Angewandte Analysis und Stochastik*), Thomas Koprucki (*Weierstrass Institute for Applied Analysis and Stochastics*), Karsten Tabelow (*Weierstrass Institute for Applied Analysis and Stochastics*), Tore Niermann (*TU Berlin Institut für Optik und Atomare Physik*) 17:30–17:50

The growth of semiconductor quantum dots (QDs) with desired electronic properties would highly benefit from the assessment of QD geometry, distribution, and strain profile in a feedback loop between growth and analysis of their properties. One approach to assist the optimization of QDs consists in imaging bulk-like samples (thickness 100-300 nm) by transmission electron microscopy (TEM) instead of high resolution (HR) TEM of thin samples (thickness 10 nm). For HRTEM the relaxation of the lamella-like samples may strongly modify the strain field or the preparation may potentially destroy the QDs. However, a direct 3D geometry reconstruction from TEM of bulk-like samples by solving the tomography problem is not feasible due to its limited resolution (0.5-1 nm), the highly nonlinear behaviour of the dynamic electron scattering and strong stochastic influences due to uncertainties in the experiment, e.g. excitation conditions. Here, we present a novel concept for 3D model-based geometry reconstruction (MBGR) of QDs from TEM images. The approach includes an appropriate model for the QD configuration in real space, a database of simulated TEM images and a statistical procedure for the estimation of QD properties and classification of QD types based on machine learning techniques. MBGR requires the simulation of TEM images by the numerical solution of partial differential equations for the propagation of the electron wave through the sample. The mapping of QD geometry to TEM images is governed by the relativistic Schrödinger equation for dynamic electron scattering. Together with the MBGR approach we will present preliminary results on the database of simulated TEM images.

Joint Exit Wave Reconstruction and Multimodal Registration of Transmission Electron Microscopy Image Series

Christian Doberstein (*Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University*), Benjamin Berkels (*Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University*) 17:50–18:10

The two main limitations inherent to transmission electron microscopy (TEM) imaging are the aberrations from the objective lens and the fact that in conventional TEM only the amplitude of the electron wave at the image plane is recorded. These limitations can be overcome by means of reconstructing the full complex-valued electron wave at the exit plane of the specimen, the so-called exit wave, from a series of TEM images recorded with varying focus of the objective lens. However, microscope instabilities and specimen movement demand for an accurate registration when working with a series of images, which has to be performed in addition to the exit wave reconstruction.
In this talk, a novel approach for simultaneous exit wave reconstruction and TEM image series registration is presented, which is based on the maximum-likelihood (MAL) method proposed

by Coene et al. in 1996. In TEM, the forward model of image simulation from known exit wave, instrument settings and lens aberrations is very well understood, but no explicit and accurate inverse is available. Therefore, the problem is formulated in a variational form, which essentially consists of minimizing the squared L^2-distance of simulated images to the registered experimental images. Here, image simulation and registration is done based on the current estimate for the exit wave and the registration.
The validity of this approach is evaluated on simulated input data and the minimization is done numerically using derivative based optimization algorithms.

Simultaneous Registration of Multiple Images - Measuring Similarity by Singular Values

Kai Brehmer (*Institute of Mathematics and Image Computing, Universität zu Lübeck*), Benjamin Wacker (*Institute of Mathematics and Image Computing, University of Lübeck*), Jan Modersitzki (*Institute of Mathematics and Image Computing, University of Lübeck*) 18:10–18:30

Image Registration is the task of aligning corresponding structures in images. A distance measure has to be set up to measure similarity between two images. In medical applications, we often face the problem of aligning images of the same patient taken at different time points. As distance measures are usually defined between two images, sequential approaches are normally used to register these images. Wanting to register all images simultaneously, we propose a new distance measure based on the singular values of the matrix which consists of the images' gradients. For the case of two images, we can relate our proposed distance measure to normalized gradient fields (NGF). To demonstrate the potential of our approach, we numerically apply it to dynamic contrast-enhanced magnetic resonance imaging data of the human kidney (data courtesy due to Jarle Rørvik, Haukeland University Hospital of Bergen).

S21.09 | Mathematical signal and image processing

Date 23.03.2018
Room N1070

Gelfand numbers related to structured sparsity

Tino Ullrich (*Institute for Numerical Simulation, Universität Bonn*), Sjoerd Dirksen (*RWTH Aachen University*) 08:30–08:50

We consider the problem of determining the asymptotic order of the Gelfand numbers of mixed-(quasi-)norm embeddings $\ell_p^b(\ell_q^d) \hookrightarrow \ell_r^b(\ell_u^d)$ given that $p \leq r$ and $q \leq u$, with emphasis on cases with $p \leq 1$ and/or $q \leq 1$. These cases turn out to be related to structured sparsity. We obtain sharp bounds in a number of interesting parameter constellations. Our new matching bounds for the Gelfand numbers of the embeddings of $\ell_1^b(\ell_2^d)$ and $\ell_2^b(\ell_1^d)$ into $\ell_2^b(\ell_2^d)$ imply optimality assertions for the recovery of block-sparse and sparse-in-levels vectors, respectively. In addition, we apply the sharp estimates for $\ell_p^b(\ell_q^d)$-spaces to obtain new two-sided estimates for the Gelfand numbers of multivariate Besov space embeddings in regimes of small mixed smoothness. It turns out that in some particular cases these estimates show the same asymptotic behaviour as in the univariate situation. In the remaining cases they differ at most by a $\log\log$ factor from the univariate bound.

On Unlimited Sampling

Ayush Bhandari (*MIT Media Lab, Massachusetts Institute of Technology*), Felix Krahmer (*Mathematics, Technische Universität München*), Ramesh Raskar (*MIT Media Lab, Massachusetts Institute of Technology*) 08:50–09:10

Shannon's sampling theorem provides a link between the continuous and the discrete realms stating that bandlimited signals are uniquely determined by its values on a discrete set. This theorem is realized in practice using so called analog–to–digital converters (ADCs). Unlike Shannon's sampling theorem, the ADCs are limited in dynamic range. Whenever a signal exceeds some preset threshold, the ADC saturates, resulting in aliasing due to clipping. The goal of this paper is to analyze an alternative approach that does not suffer from these problems. Our work is based on recent developments in ADC design, which allow for ADCs that reset rather than to saturate, thus producing modulo samples. An open problem that remains is: Given such modulo samples of a bandlimited function as well as the dynamic range of the ADC, how can the original signal be recovered and what are the sufficient conditions that guarantee perfect recovery? In this paper, we prove such sufficiency conditions and complement them with a stable recovery algorithm. Our results are not limited to certain amplitude ranges, in fact even the same circuit architecture allows for the recovery of arbitrary large amplitudes as long as some estimate of the signal norm is available when recovering. Numerical experiments that corroborate our theory indeed show that it is possible to perfectly recover function that takes values that are orders of magnitude higher than the ADC's threshold.

Estimation of structured signals from noisy 1-bit Gaussian observations via empirical risk minimization using the hinge loss

Sjoerd Dirksen (*RWTH Aachen University*), Martin Genzel (*Institut für Mathematik, Technische Universität Berlin*), Alexander Stollenwerk (*Lehrstuhl C für Mathematik (Analysis), RWTH Aachen University*) 09:10–09:30

We consider a memoryless 1-bit compressed sensing setup, where our goal is to estimate an unknown high-dimensional signal from finitely many noisy 1-bit Gaussian measurements. Assuming that the signal lies in a known low-dimensional signal set, our estimator will be any solution to a structured empirical risk minimization program, where we use the hinge loss to penalize wrong predictions. Under mild conditions on the 1-bit quantization model, the signal is well approximated as soon as the number of observations exceeds the effective dimension of the signal set.

Sparse Recovery From Superimposed Non-Linear Measurements

Martin Genzel (*Mathematik, Technische Universität Berlin*), Peter Jung (*Technische Universität Berlin*) 09:30–09:50

In this talk, we study the problem of sparse recovery from superimposed, non-linearly distorted measurements. This challenge is particularly relevant to wireless sensor networks that consist of autonomous and spatially distributed sensor units. Here, each of the M wireless sensors acquires m individual measurements of an s-sparse source vector $x_0 \in \mathbb{R}^n$. All devices transmit simultaneously to a central receiver, causing collisions. Since this process is imperfect, e.g., caused by low-quality sensors and the wireless channel, the receiver measures a superposition of corrupted signals. First, we will show that the source vector can be successfully recovered from $m = O(s \log(2n/s))$ coherently communicated measurements via the vanilla

Lasso. The more general situation of non-coherent communication can be approximated by a bilinear compressed sensing problem. Even in the non-linear setting, it will turn out that $m = O(s \cdot \max\{M, \log(2n/s)\})$ measurements are already sufficient for reconstruction using the (group) $\ell^{1,2}$-Lasso. In particular, as long as $M = O(\log(2n/s))$ sensors are used, there is no substantial increase in performance when building a coherently communicating network. Finally, we shall discuss several practical implications and extensions of our approach. This is joint work with Peter Jung (TU Berlin).

S21.10 | Mathematical signal and image processing

Date 23.03.2018
Room N1179

Estimating statistical parameters in PIV using the ensemble averaged correlation function

Claudia Strobl (*Fachgebiet Hydromechanik, Technische Universität München*), Michael Manhart (*Fachgebiet Hydromechanik, Technische Universität München*) 08:30–08:50

In optical measurement techniques the information of interest is often entrapped in a convolution of the function searched for and the so-called point spread function (psf). Examples are: (1) the optical flow measurement technique particle image velocimetry (PIV) where the probability density function (pdf) of the velocity is convolved with the autocorrelation function of the particle images forming the evaluated correlation function [2]; (2) the evaluation of star images which are convolved with the psf of the recording telescope [1]. One concept to determine parameters of these enclosed functions is to deconvolve the convolution function by the psf. Due to the presence of noise this is a mathematically ill-posed problem such that direct deconvolution is impossible [1]. Therefore, several algorithms are available which iteratively deconvolve the convolution function with the psf in order to determine the function of interest and its parameters, e.g. its standard deviation. At the conference we intend to introduce a different method to determine the statistical moments of the pdf stored in the ensemble averaged correlation function which has no need for deconvolution but simply depends on the moments of the correlation function and of the autocorrelation. Comparing this method to an iterative deconvolution routine we will furthermore show factors influencing the accuracy of this method.

[1] Starck, J.L. and Pantin, E. and Murtagh, F.:Deconvolution in astronomy: A review. Publications of the Astronomical Society of the Pacific 114 (2002)

[2] Adrian, R. J.:Double Exposure, Multiple-Field Particle Image Velocimetry for Turbulent Probability Density. Optics and Lasers in Engineering 9 (1988)

Time-dependent imaging problems in tomography and localization microscopy

Bernadette Hahn (*University of Würzburg*), Annika Richter (*University of Würzburg*) 08:50–09:10

Imaging structural and functional changes of a specimen, e.g. in biomedical applications or non-destructive testing, introduces analytical and numerical challenges. First, the additional time dimension results in a large amount of data which has to be processed efficiently. Furthermore, most imaging modalities record the data sequentially, such as in computerized tomography, magnetic resonance imaging or localization microscopy. Thus, the temporal resolution is in general limited by the acquisition time of the imaging system.

One possibility to circumvent this limitation consists in developing algorithms capable of reconstructing the searched-for quantity from undersampled data, for example via a compressive sensing strategy. Localization microscopy represents one potential application, where this approach allows faster imaging rates.
Another possibility is the development of motion compensation algorithms, which take information about the dynamic behavior of the object into account. This strategy will be illustrated at the examples of computerized tomography and magnetic resonance imaging.

Challenges in image reconstruction in 4D magnetic particle imaging

Christina Brandt (*Department of mathematics, Universität Hamburg*) 09:10–09:30

Magnetic particle imaging (MPI) is a novel imaging technique based on the nonlinear magnetization response of iron oxide particles. The linear reconstruction problem consists of the computation of the evolution of the 3D particle distribution given the induced voltage measured in the receive coils. In most applications, the linear operator, called system function, is measured in a time-consuming measurement process because model-based reconstructions do still not provide the same image quality as the measurement-based methods. Possible explanations are the simplifying assumptions in the model such as the lack of relaxation effects or ideal magnetic fields. Moreover, the real magnetic fields in the scanner, the particle size distribution, coils sensitivities etc. are only known approximately and the related model parameters are therefore only estimated. The measurement based approach leads to large scale linear equation systems with a non-sparse and non-structured system matrix.
Challenges in MPI image reconstruction are therefore the handling of model errors, model improvement, and efficient reconstruction methods which enable 4D online-reconstruction. We will present some recent results towards improved image reconstruction in MPI. We will illustrate the results with simulated as well as real experimental data.

Statistical multiscale processing for superresolution microscopy

Timo Aspelmeier (*Institute for Mathematical Stochastics, University of Göttingen*) 09:30–09:50

Superresolution microscopy offers unique images from, e.g., the interior of living cells. Due to the optical principles involved, the images are typically very noisy and blurred. Statistical multiresolution estimation, where a function is sought which minimizes a regularization functional under the contraint of being compatible with the noise on many different length scales, allows for accurate image reconstructions with statistical guarantees about the smoothness of the result. The corresponding optimization problem can be solved for instance by the Alternate Direction Method of Multipliers (ADMM), for which linear convergence can be shown even without strong convexity, which is necessary for the application of nonsmooth regularization functionals such as the L_1 or TV norms.

Super-resolution imaging and discrete tomography

Andreas Alpers (*Zentrum Mathematik, Technische Universität München*), Peter Gritzmann (*Zentrum Mathematik, Technische Universität München*) 09:50–10:10

Super-resolution imaging aims at improving the resolution of an image by enhancing it with other images or data that might have been acquired using different imaging techniques or modalities. Motivated by applications in plasma physics, we consider the task of doubling the resolution of tomographic grayscale images of binary objects by fusion with double-resolution tomographic data that has been acquired from two viewing angles.

We give a polynomial-time algorithm for the case that the gray levels have been reliably determined. The problem, however, becomes NP-hard if the gray levels of some pixels come with an error of ± 1 or larger. The NP-hardness persists for any larger resolution enhancement factor. This means that noise does not only affect the quality of a reconstructed image but, less expectedly, also the algorithmic tractability of the inverse problem itself.

Model-based Reconstruction for Quantitative Parameter Mapping in Magnetic Resonance Imaging

Martin Uecker (*Institut für Diagnostische und Interventionelle Radiologie, Universitätsmedizin Göttingen*), Xiaoqing Wang (*Institute for Diagnostic and Interventional Radiology, University Medical Center Goettingen*) 10:10–10:30

Magnetic resonance imaging (MRI) usually employs an inverse FFT to get an image from the acquired Fourier-space data. By exploiting the complementary information from multiple coils (i.e., parallel imaging), modern image reconstruction formulates the image estimation as an inverse problem. Model-based reconstruction techniques further introduce a physical signal model into the inverse problem. This enables highly accelerated quantitative mapping of relaxation times for tissue characterization, which has important clinical applications.
The MR signal obtained from multiple receiver coils can be written as

$$s_j(t) = \int M_t(\vec{r}) c_j(\vec{r}) e^{-i\vec{r}\cdot\vec{k}(t)} d\vec{r} \tag{1}$$

with $c_j(\vec{r})$ the jth coil, $\vec{r}$ the position in image space, $\vec{k}(t)$ the chosen k-space trajectory and $M_t(\vec{r})$ the magnetization signal which can be derived from the Bloch equations. Taking single-shot quantitative T_1 mapping for example, $M(\vec{r})$ at time t_k after inversion can be expressed as:

$$M_{t_k}(\vec{r}) = M_{ss}(\vec{r}) - \big(M_{ss}(\vec{r}) + M_0(\vec{r})\big) \cdot e^{-t_k \cdot R_1^*(\vec{r})} \tag{2}$$

where M_{ss} represents the steady-state magnetization, M_0 is the equilibrium magnetization, t_k the inversion time and R_1^* the effective relaxation rate.
Estimation of both the parameter maps and the coil sensitivity maps from the acquired k-space data can then be formulated as a nonlinear inverse problem, i.e.,

$$\hat{x} = \operatorname*{argmin}_x \|F(x) - y\|_2^2 + \alpha R(x_{\mathbf{p}}) + \beta Q(x_{\mathbf{c}}). \tag{3}$$

where $F(\cdot)$ is the nonlinear forward model mapping the unknows to the measured data y. In the above T_1 example, $x_{\mathbf{p}} = (M_{ss}, M_0, R_1^*)^T$ and $x_{\mathbf{c}} = (c_1 \dots c_N)^T$. $R(\cdot)$ and $Q(\cdot)$ are regularization terms on parameter maps and coil sensitivities respectively. $R(\cdot)$ can be chosen as a joint sparsity constraint and $Q(\cdot)$ is a Sobolev norm to enforce smoothness of coil sensitivites. α and β are the corresponding regularization parameters. Equation (3) is then solved by iteratively regularized Gauss-Newton method (IRGNM) where the nonlinear problem is linearized in each Gauss-Newton step.
An application of the above technique in quantitative T_1 mapping based on an inversion-recovery radial FLASH measurement demonstrates high-quality parameter maps from undersampled data acquired in a single shot (4 seconds).

S22 | Scientific computing

Organiser Matthias Bolten (*Mathematik, Bergische Universität Wuppertal*)
Hans-Joachim Bungartz (*Informatics, Technische Universität München*)

S22.01 | Scientific computing

Date 20.03.2018
Room 0534

Fast iterative solvers for an optimal transport problem

Martin Stoll (*Fakultät für Mathematik, TU Chemnitz*), Roland Herzog (*TU Chemnitz*), John Pearson (*University of Edinburgh*) 16:30–16:50

Optimal transport problems pose many challenges when considering their numerical treatment. We investigate the solution of a PDE-constrained optimization problem subject to a particular transport equation arising from the modelling of image metamorphosis. We present the nonlinear optimization problem, and discuss the discretization and treatment of the nonlinearity via a Gauss–Newton scheme. We then derive preconditioners that can be used to solve the linear systems at the heart of the (Gauss–)Newton method. With the optical flow in mind, we further propose the reduction of dimensionality by choosing a radial basis function discretization that uses the centres of superpixels as the collocation points. Again, we derive suitable preconditioners that can be used for this formulation.

FROSch - A Parallel Implementation of the GDSW Domain Decomposition Preconditioner in Trilinos

Alexander Heinlein (*Mathematical Institute, University of Cologne*), Axel Klawonn (*University of Cologne*), Oliver Rheinbach (*TU Bergakademie Freiberg*) 16:50–17:10

The FROSch (Fast and Robust Overlapping Schwarz) library, a parallel implementation of the GDSW (Generalized Dryja Smith Widlund) preconditioner, has recently been integrated into Trilinos as part of the package ShyLU. The GDSW preconditioner has been introduced by Dohrmann, Klawonn, and Widlund and is a two-level overlapping Schwarz preconditioner with an energy-minimizing coarse space that is inspired by non-overlapping domain decomposition methods, such as FETI-DP and BDDC methods. It is robust for a wide class of problems, e.g., solid or fluid mechanics, and can be constructed in an algebraic way. In particular, the coarse space can be constructed from the fully assembled matrix without an additional coarse triangulation, even for irregular subdomains. However, the preconditioner can benefit from additional information about the problem.
This talk gives an overview of the FROSch code, its features, and user-interface and shows the parallel scalability and robustness of the solver for several problems. In particular, FROSch is applied to scalar elliptic problems, linear elasticity, and nonlinear elasticity in fluid-structure interaction applications and as a monolithic preconditioner for saddle-point problems. Parallel scalability of the code is shown up to a maximum of 64K cores using a direct coarse solver on one core.

AMG smoothers for Maxwell's equations

Lisa Claus (*Mathematik, Bergische Universität Wuppertal*), Matthias Bolten (*Mathematik, Bergische Universität Wuppertal*) 17:10–17:30

Multigrid methods are efficient iterative solvers for the solution of partial differential equations (PDEs).
The efficiency of multigrid methods is due to the combination of suitable smoothers with a coarse grid correction. For geometric multigrid solvers, as one of the two key ingredients smoothers have a significant impact on the performance.
In contrast, the coarse grid correction has a considerable effect on algebraic multigrid (AMG) solvers, in general. For important new classes of problems it is necessary to merge geometric smoothers with AMG solvers.
In this talk, we concentrate on expanding AMG's applicability to Maxwell's equations, therefore we present adapted smoothing techniques for AMG. For example, we consider an adapted overlapping schwarz smoother for AMG. We rely on Nédélec's elements (edge elements) to discretize the problem.
First results regarding the smoothing quality of the AMG smoothers for Maxwell's equations will be presented.

Multigrid Methods for Variational Space-Time Elements

Marco Favino (*Institute of Computational Science, Institute of Computational Science, Università della Svizzera italiana*), Seif Ben Bader (*Institute of computational Science, Institute of Computational Science, Università della Svizzera italiana*), Pietro Benedusi (*Institute of computational Science, Institute of Computational Science, Università della Svizzera italiana*), Alessio Quaglino (*Institute of computational Science, Institute of Computational Science, Università della Svizzera italiana*), Stefan Schuß (*Chair of Computational Mechanics, Chair of Computational Mechanics, University of Siegen*), Maik Dittmann (*Chair of Computational Mechanics, Chair of Computational Mechanics, University of Siegen*), Simon Eugster (*Institute for Nonlinear Mechanics, Institute for Nonlinear Mechanics, University of Stuttgart*), Christian Hesch (*Chair of Computational Mechanics, Chair of Computational Mechanics, University of Siegen*), Rolf Krause (*Institute of computational Science, Institute of Computational Science, Università della Svizzera italiana*) 17:30–17:50

Finite element discretizations of space-time formulations are usually based on discontinuous Galerkin methods in time [1, 2]. This approach leads to lower triangular stiffness matrices for the complete space-time system to be solved and preserves *causality* of the information which flows always in the direction of positive time.
We present a multigrid solver for a novel space-time finite element discretisation presented in [3]. Differently from the standard space-time methods, it is based on a Bubnov-Galerkin approach (i.e. the same shape functions are employed for the solution as well as for the test functional space) using continuous finite elements in time and space-time, . This approach can be derived in a variationally consistent way and allows to transfer information in positive and negative time directions.
For two-dimensional problems in space, existing solvers for three-dimensional problems can be applied directly to solve the arising large-scale problem. The application of multigrid solvers is formally straightforward, since we only have to consider $\mathbb{R}^{n+1}$ dimensional space-time problems. However, certain modifications might be necessary as the differential operator in time behaves

differently than in space. The main difficulty is that the problem is purely convective in time, hence multigrid methods require suitable stabilizations in time in order to recover ellipticity in time direction [2, 4].
For the application of continuous Lagrangian finite elements in time and space-time, we construct the coarser approximation spaces using semi-geometric multigrid methods [5]. These methods create a nested hierarchy of finite element spaces based on a hierarchy of possibly non-nested meshes. Then, a discrete (pseudo-)L^2-projection operator between the finite element spaces is employed to restrict the residual from fine to coarse levels.
The proposed formulation is applied to thermal, fluid, and mono-domain system, this latter representing a highly non-linear system with sharp space-time gradients.

[1] Horton, G. and Vandewalle, S. *A space time multigrid method for parabolic partial differential equations* SIAM J. Sci. Comput., (1995).

[2] Gander, Martin J. and Neumüller, Martin *Analysis of a New Space-Time Parallel Multigrid Algorithm for Parabolic Problems*. SIAM Journal on Scientific Computing, 2016.

[3] C. Hesch, S. Schuß, M. Dittmann, S. R. Eugster, M. Favino and R. Krause *Variational Space-Time Elements for Large-Scale Systems*, CMAME, 2017.

[4] Krause, D. and Krause, R., *Enabling local time stepping in the parallel implicit solution of reaction-diffusion equations via space-time finite elements on shallow tree meshes*, Applied Mathematics and Computation, (2016).

[5] Krause, R. and Zulian, P. *A Parallel Approach to the Variational Transfer of Discrete Fields between Arbitrarily Distributed Unstructured Finite Element Meshes*, SIAM Journal on Scientific Computing, (2016).

Improving Time Stepping in Partitioned Multi-Physics

Benjamin Rüth (*Informatics, Technical University of Munich*), Benjamin Uekermann (*Informatics, Technical University of Munich*)

17:50–18:10

The partitioned approach is widely used for the simulation of multi-physics phenomena. Multiple single-physics problems are solved independently and then coupling is enforced either in a staggered fashion (weak coupling) or by iteratively solving a fixed-point problem (strong coupling). A minimal invasive, partitioned approach, where multiple black-box solvers (participants) are coupled allows reuse of existing single-physics solvers for multi-physics. For non-matching spatial meshes interpolation methods are provided. However, if state of the art coupling schemes are used, time-stepping is reduced to first order of convergence and stability problems arise.
In this talk the convergence order of time-stepping for a very simple 1D model problem is investigated: Two 1D heat transport equations are coupled using a Dirichlet-Neumann coupling at the interface. A monolithic solution is used as reference. Firstly, the aforementioned effects are reproduced and a specialized coupling scheme is developed. This specialized scheme maintains second order and unconditional stability of the trapezoidal rule when being applied to the model problem. Afterwards, a general order conserving scheme is introduced that allows to couple participants using arbitrary time stepping schemes and differing temporal meshes. This schemes uses a combination of dense output and waveform relaxation to achieve high order coupling in time.
We finally plan to solve complex multi-scale-multi-physics scenarios, such as turbulent fluid-structure interaction or fluid-structure-acoustics interaction. Currently very small time steps are needed in this area due to degradation of convergence order and stability properties of the time-stepping.

Simulation of Calcium Release in Heart Cells by Modified Patankar Schemes

Stefan Kopecz (*Universität Kassel*), Andreas Meister (*Universität Kassel*), Bradford E. Peercy (*University of Maryland Baltimore County*), Matthias K. Gobbert (*University of Maryland Baltimore County*) 18:10–18:30

Modified Patankar-Runge-Kutta (MPRK) schemes are numerical methods for the solution of positive and conservative production-destruction systems. The MPRK schemes adapt classical Runge-Kutta schemes to guarantee positivity and conservation irrespective of the chosen time step size.
We discuss the derivation of MPRK schemes for ordinary differential equations up to third order and also present numerical results of MPRK schemes applied to linear partial differential equations. In particular, we consider a model for the calcium dynamics in a heart cell, which is build on a linear diffusion-reaction equation.

S22.02 | Scientific computing

Date 21.03.2018
Room 0534

Running Waves Through Many Cores

Benjamin Hazelwood (*Computer Science, Durham university*), Tobias Weinzierl (*Computer Science, Durham University*) 14:00–14:20

ExaHyPE is a H2020 project where an international consortium of scientists writes a simulation engine for hyperbolic equation system solvers based upon the ADER-DG paradigm. Two grand challenges are tackled with this engine: long-range seismic risk assessment and the search for gravitational waves emitted by rotating binary neutron stars. The code itself is based upon a merger of flexible spacetree data structures with highly optimised compute kernels for the majority of the simulation cells. It provides a very simple and transparent domain specific language as front-end that allows to rapidly set up parallel PDE solvers discretised with ADER-DG or Finite Volumes on dynamically adaptive Cartesian meshes.
This talk starts with a brief overview of ExaHyPE, it demonstrates how ExaHyPE codes are programmed, and it sketches the algorithmic workflow of the underlying ADER-DG scheme. We rephrase steps of this workflow in the language of tasks. These tasks are rearranged such that they reduce accesses to the memory, i.e. weaken the pressure on the memory subsystem, the most expensive tasks are optimised semi-manually w.r.t. vectorisation, and we add an umbrella of autotuning around them, too. The main focus of this talk however is to discuss recent extensions of OpenMP w.r.t. task scheduling and loop traversals in this framework. Do modern task-based formalisms yield better throughput than old-fashioned, plain parallel for? Do modern task-based formalisms yield other execution patterns than we know them from classic linear algebra? Can we bring together our insights within the framework of such a complex application to exploit modern manycore systems?
This is joint work with groups from Frankfurt's FIAS, the University of Trento, as well as Ludwig-Maximilians-Universität München and Technische Universität München. We focus on results obtained on Intel Xeon Phi 7200 (codenamed KNL) nodes provided by the RSC Group as well as through CoolMUC3.
The authors appreciate support received from the European Union's Horizon 2020 research and innovation programme under grant agreement No 671698 (ExaHyPE).

Improving the Performance of Numerical Algorithms for the Bethe-Salpeter Eigenvalue Problem

Peter Benner (*Max Planck Institute for Dynamics of Complex Technical Systems*), Andreas Marek (*Max Planck Computing and Data Facility*), Carolin Penke (*Computational Methods in Systems and Control Theory, Max Planck Institute for Dynamics of Complex Technical Systems*) 14:20–14:40

The Bethe-Salpeter eigenvalue problem

$$H_{BS}x = \lambda x \tag{1}$$

arises in quantum chemistry. Eigenvalues of H_{BS} represent excitation energies and the eigenvectors can be used to compute the optical absorption spectrum of a system. When many atoms are involved, the matrix becomes very large such that parallel, efficient and well-scaling algorithms are of high relevance. H_{BS} is a complex block matrix with the structure

$$H_{BS} = \begin{bmatrix} A & -D^H \\ D & -A^T \end{bmatrix}, \quad \text{where } A = A^H,\ D = D^T, \tag{2}$$

where X^H denotes the conjugate transpose and X^T the transpose of a complex matrix. Eigenvalues appear in pairs $(\lambda, -\lambda)$ or in quadruples $(\lambda, -\lambda, \bar{\lambda}, -\bar{\lambda})$. We aim to solve the eigenvalue problem and preserve this structure. As a side effect, less memory and computations are required if the matrix structure can be preserved.
A state-of-the art implementation is given in the BSEPACK library[1]. Here, a purely imaginary Hamiltonian eigenvalue problem equivalent to (1) is considered. We measure and discuss the performance of the available software on a high performance distributed system. On an implementational level, the ELPA library[2] is used to improve performance, while keeping the basic algorithmic strategy. In order to achieve effects of a larger magnitude, algorithms have to be developed that are more aware of and exploit the present structure of the matrix. We point out further approaches which lead into this direction.

Sparsity pattern extraction for assembly of KKT-like matrices in multibody dynamics

Benedikt Hofmeister (*Institute of Structural Analysis, Leibniz Universität Hannover*), Cristian Guillermo Gebhardt (*Leibniz Universität Hannover*), Christian Hente (*Institute of Structural Analysis, Leibniz Universität Hannover*), Raimund Rolfes (*Leibniz Universität Hannover*) 14:40–15:00

The implicit dynamic solution of multibody and finite element simulations with kinematic constraints requires the assembly of KKT-like matrices, which are constant in structure, but unsymmetric in the most general case. Basically, the numerical solution is computed by means of a Newton-Raphson iterative scheme and applying a direct sparse solver in this context demands a reordering step prior to the actual iterative solution procedure. This means that the sparsity pattern of the KKT structure has to be known in advance for all possible configurations and loading patterns that are going to be employed along each stand along simulation step.
In this contribution, we present a scheme, in which the sparsity pattern is extracted dynamically from the assembly code of KKT-like matrices. The underlying sparse scheme is transparent to the element and constraint iteration matrix assembly. This is enabled by exploiting the structure

[1] https://sites.google.com/a/lbl.gov/bsepack/
[2] https://elpa.mpcdf.mpg.de/

and order of events during the element matrix assembly. The proposed strategy is implemented with an object oriented programming style in a modern Fortran 2008 environment.
First, we run an initial KKT matrix assembly routines with specially conditioned configuration and load inputs. Nonzero values are identified and the sparsity pattern is established. Secondly, a mapping from the element matrix to the sparse storage structure coordinates is established. The third step is the iterative solution procedure, where the mapping information is used to assemble element matrices directly into the sparse structure. Thus, a computationally efficient and easy-to-use system for a sparse Newton-Raphson scheme is established.

Computational Methods for Nondestructive Testing by Active Thermography

Sebastian Götschel (*Zuse Institute Berlin (ZIB)*) 15:00–15:20

Active thermography is a fast and contactless method for nondestructive testing of a wide range of structures. It is based on the generation of a non-stationary heat flux inside the object under investigation, and time-resolved measurements of its surface temperature by an infrared camera. Defects and inhomogeneities in the material with thermal properties differing from the surrounding material can be detected from spatial temperature differences within a particular time range.
In this talk, we present methods for the reconstruction of defects in carbon-fiber reinforced composites from such thermographic measurements, which should not only allow to locate defects, but also give a quantitative characterization of the defect properties. We discuss the efficient simulation of the measurement process using finite element methods, as well as computational techniques for the estimation of material parameters from experimental data. A special focus will be on the detection of delaminations, i.e., the separation of layers in composite materials, which amounts to identifying the anisotropic, piecewise constant thermal conductivity.
This is joint work with Martin Weiser (Zuse Institute Berlin) as well as Christiane Maierhofer and Jan P. Müller (BAM Federal Institute for Materials Research and Testing).

Modeling and efficient simulation of dry spinning processes in airflows

Manuel Wieland (*Mathematik, Universität Trier*), Walter Arne (*Fraunhofer ITWM*), Robert Feßler (*Fraunhofer ITWM*), Nicole Marheineke (*Universität Trier*), Raimund Wegener (*Fraunhofer ITWM*) 15:20–15:40

In dry spinning processes solvent evaporates out of the spun jet and leads to thinning and solidification of the produced fiber. We describe the fiber dynamics by a one-dimensional uniaxial viscous two phase flow resulting from cross-sectional averaging of underlying three-dimensional balance laws. To include radial effects, observable in experiments, we develop an iterative coupling algorithm with consistent two dimensional advection-diffusion-equations for polymer mass fraction and temperature, which can be solved very efficiently in terms of Green's functions and employing the product integration method. This efficiency allows further coupling with the surrounding air based on the action-reaction-principle and builds the basis for the simulation of industrial dry spinning set-ups.

Patient-specific cardiac parametrization from Eikonal simulations

Daniel Ganellari (*Institute for Mathematics and Scientific Computing, Karl Franzens University of Graz*), Gundolf Haase (*Institute for Mathematics and Scientific Computing, Karl Franzens University of Graz*) 15:40–16:00

Simulations in cardiac electrophysiology use the bidomain equations describing the intercellular and the extracellular electrical potential. Its difference, the trans-membrane potential, is responsible for the excitation of the heart and its steepest gradients form an excitation wavefront

propagating in time. This arrival time $\varphi(x)$ of the wavefront at some point $x \in \Omega$ can be approximated by the simpler Eikonal equation. The accuracy of these simulations is limited by unavailable patient specific conductivity data.
The human heart consists of various tissues with different conductivity parameters. We group these tissues into m different classes with its individual scaling parameter γ_k yielding to the modified Eikonal equation

$$\sqrt{\left(\nabla\varphi(x,\underline{\gamma})\right)^T \gamma_k \cdot M(x)\nabla\varphi(x,\underline{\gamma})} = 1 \qquad x \in \Omega_k$$

where the velocity information M(x) in each material domain Ω_k is scaled by the parameter $\gamma_k \in \mathbb{R}$. Now the activation time depends also on the scaling parameters $\underline{\gamma} \in \mathbb{R}^m$.
One chance to scale the scaling parameters suitably consists in comparing the Eikonal computed activation sequence on the heart surface with the measured ECG on the torso mapped onto this surface. It remains to minimize the functional

$$f(\underline{\gamma}) := \| \varphi^*(x) - \varphi(x,\underline{\gamma}) \|^2_{\ell_2(\omega_h)}$$

with respect to $\underline{\gamma}$. The vertices in the discretization on the surface of Ω_h are denoted by ω_h. By minimizing the squared distance between the measured solution ϕ^* and the Eikonal computed solution $\phi(\underline{\gamma},\underline{x})$ we are able to determine the scaling parameters $\gamma \in \mathbb{R}^m$.
The minimization problem is solved by the quasi-Newton method with BFGS update and adaptive step size control. The gradient $\nabla_\gamma f(\underline{\gamma})$ is computed via finite differences or via automatic differentiation using dco$\frac{1}{3}$++.
We present numerical examples demonstrating the parallel performance of our Eikonal solvers as well as of the optimization. Calculating the gradient via an analytic adjoint-state method is ongoing work.
Supported by the FWF project F32-N18.

S22.03 | Scientific computing

Date 21.03.2018
Room 0534

Nonlinear domain decomposition with Robin interface conditions for nonlinear dynamic systems arising in multibody dynamics

Eva-Maria Dewes (*Lehrstuhl für Angewandte Mechanik (TUM)*), Daniel Jean Rixen (*Lehrstuhl für Angewandte Mechanik (TUM)*) 16:30–16:50

In engineering applications, one can often assume that the deformations within flexible bodies of a multibody system remain small, but the overall motion of the system, which is typically described by a co-rotated floating frame, is highly non-linear. Applying domain decomposition methods to such a problem seems a natural approach, since each body can be considered as a subdomain. The challenge is then to solve the global non-linear system efficiently during time integration.
In order to decompose the system into substructures one has to choose wether the interface conditions are imposed via prescribed displacements, interface forces or a combination of the two (Robin conditions), leading to a primal, a dual or a mixed formulation.
In this contribution, we use the mixed formulation, leading to Robin interface condtions to ensure the nonlinear kinematic constraints of the mechanical system. This formulation leads to a linear combination of conditions, in which an additional optimizable interface parameter appears which is of the magnitude of a stiffness matrix and holds information from the neighbouring subdomains. With this, we introduce additional information about the overall system behaviour

into the local subdomain problems. Especially when solving the subdomain problems in parallel with a nonlinear system solver (i.e. independant of each other) we aim to accelerate convergence significantly via additional information about the neighbouring subdomains.
We validate our results numerically based on an academical test model.

[1] Negrello, Camille ; Gosselet, Pierre ; Rey, Christian: *A new impedance accounting for short and long range effects in mixed substructured formulations of nonlinear problems.* http://dx.doi.org/10.1002/nme.5195. Version: Februar 2017. – working paper or preprint

[2] In: Roux, François-Xavier: *A FETI-2LM Method for Non-Matching Grids.* Berlin, Heidelberg : Springer Berlin Heidelberg, 2009. – ISBN 978–3–642–02677–5, 121–128

Extension of Adaptive Multi-Preconditioned FETI to Multiple Right-Hand Sides.

Michael Leistner (*Mechanical Engineering, Technical University of Munich, Chair of Applied Mechanics*), Daniel Jean Rixen (*Mechanical Engineering, Technical University of Munich, Chair of Applied Mechanics*) 16:50–17:10

Finite element tearing and interconnecting algorithms are among the most scalable and powerful non-overlapping iterative domain decomposition algorithms. To make them robust against strong material heterogeneities, numerous coarse-gird corrections and a multi-preconditioned variant were published in the recent years. In this work, an extended version of the adaptive multi-preconditioned FETI algorithm to multiple right-hand sides is presented. We analyze and compare methods that are tailored to the efficient repeated solution of a constant operator of linear problems in structural mechanics in a multi-preconditioned environment. We focus on the decrease of computational cost in the local subdomain solvers and on the reduction of the necessary offline cost, which is a significant factor in the available coarse-grid based algorithms. The presented methods are compared against the state-of-the art for an academic example.

Finite volume based multigrid preconditioners for Discontinuous Galerkin methods

Lea Miko Versbach (*Centre for Mathematical Sciences, Lund University*), Philipp Birken (*Centre for Mathematical Sciences, Lund University*), Gregor Gassner (*Mathematisches Institut, Universität zu Köln*) 17:10–17:30

We consider compressible turbulent flow problems which arise for example in the design of next generation jet engines and air frames, wind turbines or star formation. These can have a 100 million unknowns, thus a fast low memory parallel solver is needed. An important ansatz for solving these problems are implicit Discontinuous Galerkin (DG) methods. In this talk I consider the DG spectral element method with Gauss-Lobatto-Legendre nodes (DGSEM-GL) for nonlinear conservation laws. It was recently proven that DGSEM-GL fulfills the discrete summation by parts property with a simultaneous approximation term (SBP-SAT) to take care of the boundary fluxes between the cells. This gives a finite difference scheme with diagonal norm operator for all polynomial degrees in 1D. Moreover, DGSEM-GL can be written as a finite volume (FV) method. This allows to apply known theory for these methods to the DGSEM-GL formulation. Our main interest is in multigrid methods for convection dominated problems. The aim is to have efficient preconditioners for very high order methods. Multigrid iterations for FV methods have a long history. Here, we take advantage of this by constructing multigrid methods for approximations to the FV discretization equivalent to DGSEM-GL. This will give us new and efficient preconditioned DG methods with improved speed of the method.

Using mixed precision in iterative eigensolvers

Sarah Huber (*Bergische Universität Wuppertal*), Martin Galgon (*Bergische Universität Wuppertal*), Bruno Lang (*Bergische Universität Wuppertal*) 17:30–17:50

We investigate the effects of mixed precision computation on several subspace iteration type eigensolvers for interior eigenvalue problems within our BEAST framework. Since several iterations of a selected eigensolver within BEAST are expected before convergence to a given tolerance is reached, the initial iterations may be performed in single precision, switching to double precision once the achievable single precision tolerance has been reached. We demonstrate that that this approach has only limited effect on the overall convergence and the final accuracy and that it generally requires no additional iterations if the switch to double precision is performed in a timely manner. This approach provides potential for substantial savings in time and energy without sacrificing overall accuracy or robustness. Furthermore, we investigate which components of the solver are most sensitive to a change in precision, illuminating opportunities for more targeted mixed precision approaches.

Profiling and Inspecting Linear Algebra Applications using FlexiBLAS

Christian Himpe (*Max Planck Institute for Dynamics of Complex Technical Systems*), Martin Köhler (*Max Planck Institute for Dynamics of Complex Technical Systems*), Jörn Papenbroock (*Max Planck Institute for Dynamics of Complex Technical Systems*), Jens Saak (*Max Planck Institute for Dynamics of Complex Technical Systems*) 17:50–18:10

The Basic Linear Algebra Subroutines (BLAS) and the Linear Algebra Package (LAPACK) are two of the most fundamental libraries in Scientific Computing. Since their NETLIB standard only defines the interfaces many implementation exists mostly developed by the CPU vendors to achieve high performance. The FlexiBLAS framework allows to switch between several implementations at runtime without the need to recompile any part of the software project. Due to the fact that many high level tools, like GNU Octave or MATLAB, are using BLAS and LAPACK as their computational backend it is not known which functions are actually called. The recording of all BLAS and LAPACK calls allows to clarify this situations and helps to improve the code in the high level language. Therefore, the FlexiBLAS framework provides a profiling tool which stores all meta data of the BLAS calls, like dimensions and scaling factors, in an easy to access database.
A possible application of this technique,besides performance profiling, is the detection of faulty BLAS implementations. Therefore, we use the recorded informations to redo all BLAS calls using NETLIB's reference implementation and compare them with the eventually corrupted implementation. We demonstrate this technique by the detection of a bug in Goto/OpenBLAS which exists for more than 10 years.

GPU-aware variants of the tangential IRKA for model order reduction of linear time-invariant systems

Jens Saak (*Computational Methods in Systems and Control, Max Planck Institute for Dynamics of Complex Technical Systems*), Georg Pauer (*Otto-von-Guericke-Universität Magdeburg*) 18:10–18:30

We consider the the $\mathcal{H}_2$-optimal model order reduction of linear time-invariant dynamical sys-

tems,

$$E\dot{x} = Ax + Bu,$$
$$y = Cx,$$

with sparse matrices $E, A \in \mathbb{R}^{n\times n}$, and possibly dense matrices $B \in \mathbb{R}^{n\times p}$, and $C \in \mathbb{R}^{q\times n}$, via the iterative rational Krylov algorithm (IRKA).
The use of inexact solves for the generation of the rational Krylov basis enables the use of optimized GPU-kernels together with techniques like Krylov subspace recycling, preconditioner realignment, and concurrent basis creation with reduced numbers of matrix sweeps.
In our contribution, we evaluate, compare and combine some of these approaches to derive an optimized GPU-aware IRKA implementation.

S22.04 | Scientific computing

Date 22.03.2018
Room 0534

An open-source FEM based simulation of a transient 3D model of a piezoelectric ceramic disk

Veronika Schulze (*Mathematics and its Applications, Paderborn University*), Kshitij Kulshreshtha (*Mathematics and its Applications, Paderborn University*), Andrea Walther (*Mathematics and its Applications, Paderborn University*), Benjamin Jurgelucks (*Mathematics and its Applications, Paderborn University*) 08:30–08:50

The behaviour of piezoelectric materials can be described by a coupled 2nd order partial differential equation system to calculate the mechanical displacement and the electric potential in the material. The underlying model is linear, includes Rayleigh damping but ignores thermal effects. We consider a transient 3D simulation of a piezoelectric disc with material parameters extracted from real measurements top and bottom surfaces. A brief overview of the well-posedness of the initial boundary value problem is given. With the aid of the software tool OPEN CASCADE the geometry is created and Gmsh is used to generate a grid for the spacial discretization.
Reference numerical 2D results already exist for the case of a disk with electrodes covering the full top and bottom surface and also a special triple-electrode ring configuration. Here segment-shaped electrodes on top and bottom at various angles are used to excite the disk using either a free charge or potential difference pulse, respectively. The variational formulation of the initial boundary value problem is solved with FEniCS. Numerical results are shown and further questions of interest are established.

Multi-physics simulations with OpenFOAM through preCICE

Gerasimos Chourdakis (*Informatics, Technische Universität München*), Hans-Joachim Bungartz (*Informatics, Technische Universität München*), Lucia Cheung Yau (*Informatics, Technische Universität München*), Benjamin Uekermann (*Informatics, Technische Universität München*) 08:50–09:10

A multi-physics simulation can be built by coupling pieces of single-physics simulation software with preCICE[3], a free library for black-box, partitioned surface coupling. We introduce an official adapter for OpenFOAM, adding it to the list of 10+ solvers supported by preCICE and

[3] http://www.precice.org/

eliminating the duplication of development effort we previously observed. This allows users to couple standard or in-house OpenFOAM solvers to any other solver for plug-and-play conjugate heat transfer, mechanical fluid-structure interaction, or other multi-physics simulations. The adapter is an OpenFOAM function object that can be loaded and configured at run-time, does not require any changes in the solvers, and supports all the features of preCICE. This talk will present the challenges we had to overcome in order to support any OpenFOAM solver with the same code in a non-invasive way and it will discuss typical application scenarios.

Parallelization of block-based preconditioners for fluid-structure interaction problems

Daniel Jodlbauer (*RICAM, Austrian Academy of Sciences*), Ulrich Langer (*RICAM, Austrian Academy of Sciences*), Thomas Wick (*Institut für Angewandte Mathematik Leibniz Universität Hannover*) 09:10–09:30

The efficient solution of fluid-structure interaction problems is still a challenging problem. In this paper, we present a preconditioner for the monolithic system based on an approximate block LDU-factorization for the solution of the linear systems. This splits the coupled system into its natural subproblems - the fluid, solid and mesh-motion equations - arising from the linearization using Newtons method. Application of this preconditioner shows similarities to partitioned methods. Hence, it allows the use of available solvers for the single subproblems. As shown in our previous work [1], this type of preconditioner shows robust behavior with respect to the mesh- and timestep-size and various material parameters. We conclude the paper with numerical experiments for two and three dimensional fluid-structure interaction problems. We present results regarding the parallel performance of our solver. The obtained scalability is comparable to the results reported in [2, 3], being the only references of parallel monolithic results to the best of our knowledge.

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[2] Crosetto, P., Deparis, S., Fourestey, G., and Quarteroni, A., Parallel Algorithms for Fluid-Structure Interactoin problems in Haemodynamics, SIAM Journal on Scientific Computing **33**, 1598-1622 (2011).

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Randomized nonlinear model order reduction methods for large dynamical problems with explicit time integration

C. Bach (*Technische Universität München; BMW Group Research and Innovation Centre*), D. Ceglia (*Technische Universität München; BMW Group Research and Innovation Centre; Politecnico di Torino*), L. Song (*BMW Group Research and Innovation Centre*), Fabian Duddeck (*Technische Universität München; Queen Mary University of London*) 09:30–09:50

Projection-based nonlinear model order reduction (MOR) reduces computing times for the solution of PDE-constrained problems, particularly for many-query and real-time applications. In case of computational structural and fluid mechanics, research has shown that the achieved speed-ups are due to:

- a reduced number of degrees of freedom, and nonlinear function evaluations when hyper-reduction is used,
- typically larger timesteps for explicit time integration [1, 5].

Most nonlinear MOR methods rely on a reduced basis approximation of some state variables $\mathbf{x}$, such as the displacements. A popular choice is the snapshot method. It involves a truncated singular value decomposition (SVD) of a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ computed from training simulations, and retains the k most significant vectors.

However, computing the SVD can be prohibitive for detailed models, as often encountered in the industry. This is particularly true for explicit integration, since strong nonlinearities and smaller timesteps require a larger number of snapshots for accurate approximations. Certain hyper-reduction methods entail further factorizations of large matrices. The main reason for this behavior is that the most widely used SVD algorithms [2, 3] have an overall computational complexity of $\mathcal{O}(mn^2)$. Based on the assumption that we only need to compute the most significant basis vectors, we propose the use of randomized algorithms to compute a reduced basis. Such methods only scale with $\mathcal{O}(mnk)$ or even $\mathcal{O}(mn \log(k))$ [4]. We then analyze their applicability to the field of nonlinear model order reduction using a structural mechanics example model, and present a modified algorithm for highly efficient reduced basis computation.

[1] C. Farhat, P. Avery, T. Chapman, and J. Cortial. Dimensional reduction of nonlinear finite element dynamic models with finite rotations and energy-based mesh sampling and weighting for computational efficiency. *International Journal for Numerical Methods in Engineering*, 98(9):625–662, 2014.

[2] G. H. Golub and C. F. Van Loan. *Matrix Computations*. The John Hopkins University Press, Baltimore and London, 3rd edition, 1996.

[3] M. Gu and S. C. Eisenstat. A Divide-and-Conquer Algorithm for the Bidiagonal SVD. *SIAM Journal on Matrix Analysis and Applications*, 16(1):79–92, 1995.

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Efficiency of parallel in time methods for coupled PDEs on moving domains

Andreas Naumann (*Institut für Wissenschaftliches Rechnen, TU Dresden*), Jörg Wensch (*Institut für Wissenschaftliches Rechnen, TU Dresden*)

09:50–10:10

In recent years, several parallel in time methods have been developed. Amongst them are ParaReal, ParaExp and PFASST. In this talk, we apply these methods on the heat conduction problem of a coupled machine tool, which consists of several parts and materials. Neighbouring parts are coupled at their common boundary with a robin type boundary condition. The challenging part comes from the fact that parts may move with respect to each other. We discretize this coupled PDE system on varying domains in space by finite elements. Due to the movement, we obtain a multiscale ODE containing the time scale of diffusion and the time scale of the movement. We will apply different parallel in time methods on the resulting multiscale ODE and compare their parallel efficiency in numerical experiments.

Variational space-time formulations for non-linear large-scale problems

Christian Hesch (*Chair of Computational Mechanics, University of Siegen*), Maik Dittmann (*Chair of Computational Mechanics, University of Siegen*), Stefan Schuß (*Chair of Computational Mechanics, University of Siegen*), Simon Eugster (*Institute of Nonlinear Mechanics, University of Stuttgart*), Marco Favino (*Institute of Computational Science, Università della Svizzera italiana*), Rolf Krause (*Institute of Computational Science, Università della Svizzera italiana*)

10:10–10:30

In the present contribution, we introduce a new Galerkin based formulation for transient continuum problems, governed by partial differential equations in space and time, see [1] for details. Therefore, we aim at a direct finite element discretization of the space-time, suitable for massive parallel analysis of the arising large-scale problem. To be specific, a Bubnov-Galerkin approach with continuous finite elements in the whole space-time is used, i.e. we apply the same shape functions for the solution as well as for the test functional space.
We will present in detail the application to mechanical systems, using a direct discretisation of Hamilton's principle of varying action in the Hamiltonian framework. This approach has already been addressed in the fundamental papers of Emmy Noether within a continuous setting. This allows us to formulate the system in a variationally consistent way in the discrete space, hence we can demonstrate all necessary conservation properties of the different systems under consideration.
For two-dimensional problems in space, existing solvers for three-dimensional problems can be applied directly to solve the arising, massive large-scale problem. Eventually, we will demonstrate the applicability of the proposed formulations to a wide range of problems.

[1] C. Hesch, S. Schuß, M. Dittmann, S.R. Eugster, M. Favino and R. Krause. Variational space-time elements for large-scale systems. Comput. Methods Appl. Mech. Engrg., 326:541-572, (2017).

S22.05 | Scientific computing

Date 22.03.2018
Room 0534

DNS / LES simulation of aeroacoustics based on the Cumulant Lattice Boltzmann Method

Konstantin Kutscher (*Inst. for Computational Modeling in Civil Engineering, TU Braunschweig*), Martin Schönherr (*Inst. for Computational Modeling in Civil Engineering, TU Braunschweig*), Martin Geier (*Inst. for Computational Modeling in Civil Engineering, TU Braunschweig*), Andrea Pasquali (*FluiDyna GmbH*), Manfred Krafczyk (*Civil Engineering, TU Braunschweig*)

14:00–14:20

Flow induced noise can be modeled on different levels. The most prominent models typically use a decoupled approach based on aeroacoustic analogies [1]. With the advent of more efficient numerical methods and massively parallel hardware, direct solutions of the weakly compressible flow equations including acoustic time scales come into reach even for moderately turbulent flows. In this contribution we report on three-dimensional transient DNS / LES simulations of flow induced acoustic spectra using a new numerical approach [2] for two application fields: A generic flute at Re $\approx 5 \cdot 10^4$ and a wing profile at Re $\approx 10^6$. While the first test case is computed

on a GPGPU, the second setup required a massively parallel computation with 4000 cores on an Intel-Cluster to handle the setup with more than $5 \cdot 10^{10}$ degrees of freedom. Both simulations have been successfully validated with experimental data.

[1] Williams, J. E. F.; Hawkings, D. L. (1969). "Sound Generation by Turbulence and Surfaces in Arbitrary Motion". Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences. 264 (1151): 321. doi:10.1098/rsta.1969.0031.

[2] Geier, M., Schönherr, M., Pasquali, A., Krafczyk, M., The cumulant lattice Boltzmann equation in three dimensions: Theory and validation, In Computers & Mathematics with Applications, Volume 70, Issue 4, 2015, pp. 507-547, ISSN 0898-1221, https://doi.org/10.1016/j.camwa.2015.05.001.

Thermodynamically consistent finite volumes and pressure robust finite elements for electroosmotic flow

Jürgen Fuhrmann (*Numerical Mathematics and Scientific Computing, Weierstraß-Institut*), Alexander Linke (*Weierstraß-Institut*), Christian Merdon (*Weierstraß-Institut*) 14:20–14:40

Electroosmotic flows occur in many interesting applications, including pore scale processes in fuel cell membranes and sensing with nanopores. We present a new approach for the numerical solution of coupled fluid flow and ion transport in a self-consistent electric field. Ingredients of the method are
- Pressure-robust, pointwise divergence free finite element discretization of the Stokes equations describing the barycentric velocity of the ionic mixture
- Thermodynamically consistent, maximum principle observing finite volume method for ion transport including competition for finite available volume
- Coupling approach between fluid flow and mass transport together with a fixed point iteration to solve the combined system.
The talk introduces the discretization approach and provides results of numerical simulations confirming the validity of the approach. A number of open problems and challengig directions will be described.

Domain decomposition applied to the thermal model of selective beam melting processes

Dominic Soldner (*Maschinenbau, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Paul Steinmann (*Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*), Julia Mergheim (*Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)*) 14:40–15:00

The utilization of additive manufacturing enables the realization of rather complex part geometries. In the context of powder bed based selective beam melting processes, parts are built in a layer-by-layer fashion by locally fusing powdered material using either a laser or electron beam. The simulation of powder bed based additive manufacturing processes for both, polymers as well as metals, is usually a computationally expensive task. This is especially due to the different involved time and length scales, highly non-linear material behaviour and dynamic growth of the simulation domain. Hence, several numerical methods are ought to be combined in order to reduce the associated computational cost.
Therefore we employ adaptivity in the spatial and temporal domain. This allows to have locally refined regions that are currently exposed to the beam, while coarsening the discretization in

areas that are currently not exposed to the beam. In addition the path of the heat input is integrated in time, which renders a line heat input model. Furthermore, domain decomposition (multi-time-stepping) is applied to account for the different requirements regarding the temporal discretization of different parts of the considered domain. This renders a time integration scheme with distinct time step sizes for different parts of the domain.

Multi-level preconditioning and eigenvector approximation for axisymmetric Maxwell eigenproblems

Marija Kranjcevic (*Computer Science Department, ETH Zurich*), Peter Arbenz (*Computer Science Department, ETH Zurich*), Andreas Adelmann (*Paul Scherrer Institut (PSI)*) 15:00–15:20

Radio frequency (RF) cavities are elements in which an oscillating electric field is used to accelerate charged particles. We compute the resonant modes in vacuated axisymmetric RF cavities by solving time-harmonic Maxwell's equations with perfectly electrically conducting boundary conditions. The finite element method leads to a sequence of decoupled real symmetric generalized eigenvalue problems (GEVPs). In practice, only a few of these GEVPs need to be solved and, for each eigenproblem, only the eigenpairs corresponding to the few smallest non-zero eigenvalues have to be found.
We solve these GEVPs using the symmetric Jacobi–Davidson (JDSYM) algorithm, focusing in particular on the parallelization and the use of the multi-level Maxwell preconditioner from Trilinos.
Furthermore, we compute eigenvector approximations by sampling the solutions on a much coarser mesh. If only one eigenpair needs to be found, we use the computed approximation as the initial vector in the JDSYM algorithm. In case more eigenpairs need to be found, we compare three different ways of using the computed approximations: using their average as the initial vector in the JDSYM algorithm, initializing the search space to all computed approximations, or running the block version of the JDSYM algorithm, with the block size set to the number of computed approximations and these approximations as the initial guesses.
We show the scaling and the timings for the use of eigenvector approximations on the problem of computing a few of the lowest resonant modes of a real-world cavity.

Numerical Shape Optimization to Decrease Failure Probability of Ceramic Structures

Camilla Hahn (*Fakultät 4, Bergische Universität Wuppertal*), Matthias Bolten (*Bergische Universität Wuppertal*), Hanno Gottschalk (*Bergische Universität Wuppertal*) 15:20–15:40

Ceramic is a material frequently used in industry because of its favorable properties. Common approaches in shape optimization for ceramic structures aim to minimize the tensile stress acting on the component, as it is the main driver for failure. In contrast to this, we follow a more natural approach by minimizing the component's probability of failure under a given tensile load. Since the fundamental work of Weibull, the probabilistic description of the strength of ceramics is standard and has been widely applied. Here, for the first time, the resulting failure probabilities are used as objective functions in PDE constrained shape optimization. To minimize the probability of failure, we choose a gradient based method combined with a first discretize then optimize approach. For discretization finite elements are used. Using the Lagrangian formalism, the shape gradient via the adjoint equation is calculated at low computational cost. The implementation is verified by comparison of it with a finite difference method applied to a minimal 2d example. Furthermore, we construct shape flows towards an optimal / improved shape in the case of a simple beam and a bended joint.

Gradient-based optimisation of TU Berlin Stator with constraint imposition using a differentiated CAD kernel

Mladen Banovic (*Institut für Mathematik, Universität Paderborn*), Salvatore Auriemma (*Open Cascade*), Orest Mykhaskiv (*Queen Mary, University of London*), Kshitij Kulshreshtha (*Universität Paderborn*), Andrea Walther (*Universität Paderborn*), Jens-Dominik Müller (*Queen Mary, University of London*) 15:40–16:00

To perform aerodynamic shape optimisation of a CAD-based model using the gradient-based methods, one requires the calculation of geometrical derivatives w.r.t. design parameters of the CAD model. Within a CAD system this information is usually not available and obtained using inaccurate finite differences. To have exact geometrical derivatives, algorithmic differentiation (AD) is applied to the open-source CAD kernel Open Cascade Technology (OCCT), in forward and reverse mode, using the AD software tool ADOL-C (Automatic Differentiation by Overloading in C++). The performance of differentiated OCCT is improved by developing a new feature in ADOL-C, named activity analysis, that can dramatically reduce the temporal complexity of the derivative computation. The differentiated OCCT kernel is coupled with a discrete adjoint CFD solver and applied to the gradient-based optimisation of the TU Berlin TurboLab Stator to minimise the total pressure loss. The stator's geometry is parametrised in differentiated OCCT, which allows to handle several manufacturing constraints during the optimisation loop. One constraint specifies that the blade has to accommodate four cylinders used to fix the blade to its casing. To find the best position of cylinders at each iteration, we have developed an automatic process that is driven by differentiated OCCT. Starting from a guess position, it calculates possible intersections between the cylinders and the blade, and then uses the gradient information to locate the position of minimal intersection. If some intersections still exist, we increase the thickness of the blade in the corresponding intersection areas until the cylinders are completely inside the blade.

S22.06 | Scientific computing

Date 22.03.2018
Room 0534

Interactive High-Performance-Computing with Common Lisp

Nicolas Neuß (*Mathematik, FAU Erlangen-Nürnberg*) 17:30–17:50

Although Common Lisp is a programming language with a long tradition, it is not a mainstream language. Nevertheless it combines four important language features in a way which cannot easily be achieved by other approaches:

1. Interactivity: Common Lisp is normally used in interaction with the user and/or the programmer.
2. Reflection: A Common Lisp program can use the same introspective features as the user/programmer.
3. Performance: Common Lisp allows compilation at runtime of highly efficient low-level code which can compete with the speed of code written in C.
4. Abstraction: Common Lisp has a uniform syntax which allows for syntax transformation that are formulated in Common Lisp itself. Especially, it does not need a separate language for meta-programming.

We show how these features play together when solving several PDE problems interactively and in parallel with the Finite Element library FEMLISP (see [1]) which is written in Common Lisp. Additionally, we will compare the performance of FEMLISP with the performance of some other Finite Element frameworks.

[1] http://www.femlisp.org

Task-Based Approaches for Molecular Dynamics Simulations

Fabio Alexander Gratl (*Department of Informatics, Technical University of Munich*), Nikola Tchipev (*Department of Informatics, Technical University of Munich*), Steffen Seckler (*Department of Informatics, Technical University of Munich*), Hans-Joachim Bungartz (*Department of Informatics, Technical University of Munich*), Philipp Neumann (*Department of Informatics, Universität Hamburg*) 17:50–18:10

Molecular dynamics simulations are tools of increasing importance in many different disciplines such as life sciences, thermodynamics, and chemical engineering. They are applied to investigate for example nucleation or cavitation processes in nanofluids with the advantage of providing clearly definable scenarios and reproducible results.
Computing the interaction forces in a molecular system poses an N-body problem whose computational complexity through direct methods lies in $O(N^2)$, where N is the number of particles in the system. Parallel implementations of established algorithms for short-range considerations such as *Linked-Cells* as well as for long-range corrections such as the *Fast-Multipole-Method*, which reduce the complexity to $O(N)$, typically require several synchronization steps during the computation of a single time-step. These steps are necessary to avoid race conditions or reflect dependencies in the simulation. The barriers always induce a certain overhead since all threads need to wait for the slowest to reach a certain state. Task-based parallelization approaches offer a way of removing these global barriers and replacing them with local task-dependencies.
This talk looks at task-based shared-memory parallelization approaches for force calculations in *ls1-mardyn*, a highly efficient molecular dynamics simulation code which currently holds the record for the largest simulation consisting of more than 10^{13} molecules. We demonstrate how the *QuickSched* library was used to re-structure existing implementations into task-patterns and how it provided an efficient load-balancing of the tasks. First results show nearly linear scaling up to 64 threads on a single Knights Landing processor, which compares well against a competing MPI parallelization.

A hybrid parallelization strategy for a modular multiresolution compressible flow solver

Nils Hoppe (*Lehrstuhl für Aerodynamik und Strömungsmechanik, Technische Universität München (TUM)*), Felix Späth (*Technische Universität München*), Igor Pasichnyk (*IBM Deutschland GmbH*), Momme Allalen (*Leibniz-Rechenzentrum (LRZ) der Bayerischen Akademie der Wissenschaften*), Stefan Adami (*Technische Universität München*), Nikolaus A. Adams (*Technische Universität München*) 18:10–18:30

We present a parallelization strategy for a modular block-based multiresolution framework for compressible flows. We are solving the Euler Equations using second-order TVD Runge-Kutta time integration with local time-stepping and high-order WENO space discretization. Our framework allows full flexibility at compile time in the choice of the Riemann solver (e.g. Roe average or HLLC), the space discretization (e.g. WENO-5 or WENO-CU6) and the level-set treatment when

dealing with multiple phases (e.g. different mixing- or reinitialization-schemes). The proposed parallelization strategy combines MPI and OpenMP to achieve high efficiency for the block-based data structure, that is optimized for the multiresolution discretization. OpenMP is used for the local computations on individual blocks without communication. More complex, the global domain decomposition of the multiresolution octree is handled with MPI and allows arbitrary cuts in the tree-based data layout. Besides SIMD optimizations, overlapped MPI-communication is employed to maximize parallel efficiency. The overall goal of the parallelization strategy is high efficiency for todays and next-generation (heterogeneous) architectures without loss of flexiblity in numerical model choices. We present latest performance data on various architectures including a KNL cluster and the SuperMUC system at the Leibniz Rechenzentrum.

S23 | Applied operator theory

Organiser Felix Schwenninger (*Dep. of Mathematics, University of Hamburg*)
András Bátkai (*Pädagogische Hochschule Voralrberg*)

S23.01 | Applied operator theory

Date 21.03.2018
Room 1400

Challenges in non-selfadjoint spectral problems

Christiane Tretter (*Mathematisches Institut (MAI), Universität Bern*) 14:00–14:40

In this talk different techniques to address the challenges arising in spectral problems for non-selfadjoint operators will be presented. The methods and results will be illustrated by several applications from mathematical physics.

Eigenvalue inequalities for the Laplacian with mixed boundary conditions

Jonathan Rohleder (*Stockholm University*) 14:40–15:00

Inequalities for the eigenvalues of the Laplacian subject to mixed boundary conditions on polyhedral and more general bounded domains are established. The eigenvalues subject to a Dirichlet boundary condition on a part of the boundary and a Neumann boundary condition on the remainder of the boundary are estimated in terms of either Dirichlet or Neumann eigenvalues. Moreover, an ordering result for the first mixed eigenvalues of polygons depending on the choice of the Dirichlet part of the boundary is presented. Parts of the results are joint work with Vladimir Lotoreichik.

The Inverse scattering problem for the matrix Schrödinger equation

Ricardo Weder (*Institute for Applied Mathematics and Systems, Universidad Nacional Autonoma de Mexico*) 15:00–15:20

The matrix Schrödinger equation is considered on the half line with the general selfadjoint boundary condition at the origin described by two boundary matrices satisfying certain appropriate conditions. It is assumed that the matrix potential is integrable, is selfadjoint, and has a finite first moment. The corresponding scattering data set is constructed, and such scattering data sets are characterized by providing a set of necessary and sufficient conditions assuring the existence and uniqueness of the correspondence between the scattering data set and the input data set containing the potential and boundary matrices. The work presented here provides a generalization of the classical result by Agranovich and Marchenko from the Dirichlet boundary condition to the general selfadjoint boundary condition. The theory presented is illustrated with various explicit examples. This is a joint work with Tuncay Aktosun.

Spectral analysis of the biharmonic operator subject to Neumann boundary conditions on dumbbell domains

Francesco Ferraresso (*Institute of Mathematics, University of Bern*) 15:20–15:40

A dumbbell domain is the union of two bounded domains joined by a thin channel. We will give an account of recent advances in the spectral analysis of the biharmonic operator subject to Neumann boundary conditions on a planar dumbbell domain. The principal aim is to identify the limit of the eigenvalues and of the eigenprojections as the width of the channel goes to zero. We prove spectral convergence results in the spirit of the articles by J.M. Arrieta et al. for the Neumann Laplacian. In particular we prove that the limiting spectrum is strictly bigger than the sequence of eigenvalues obtained by solving the eigenvalue problem for Δ^2 in the two disjoint domains (corresponding to the dumbbell without the connecting channel). In applications to linear elasticity, the fourth order operator under consideration models the deformation of an elastic plate, a part of which shrinks to a lower dimensional manifold. In contrast to what happens with the classical second order case, it turns out that the limiting equation is here distorted by a strange factor depending on a parameter which plays the role of the Poisson coefficient of the represented plate.
These results were obtained in collaboration with J.M. Arrieta and P.D. Lamberti.

Local convergence of spectra and pseudospectra

Sabine Bögli (*Mathematisches Institut, LMU München*) 15:40–16:00

In general, the spectra of realistic problems in physics cannot be determined analytically and one is forced to use numerical approximations, such as numerical computation of differential equations on the whole $\mathbb{R}^d$ truncated to finite domains $\Omega_n \subset \mathbb{R}^d$, or computation of the spectrum of an infinite matrix cut down to finite sections, i.e. to finite dimensions. These approximations, however, are prone to be unreliable. *Spectral pollution* may occur where approximating operators T_n have eigenvalues λ_n that accumulate at a point λ that does not belong to the spectrum of the limiting operator T. In addition, especially for non-selfadjoint operators, not every true eigenvalue of T may be approximated. An approximation is called *spectrally exact* if these two unwanted phenomena do not occur. Stability problems are simpler when passing from spectra to pseudospectra; in particular, they converge (*pseudospectral exactness*) under norm resolvent convergence. However, if the resolvents converge only strongly, *ε-pseudospectral pollution* may occur.
We prove local convergence results for spectra and pseudospectra, i.e. we identify regions in the complex plane where we can prove local spectral exactness (outside the so-called *limiting essential spectrum*) and local ε-pseudospectral exactness (outside the so-called *limiting essential ε-near spectrum*).

S23.02 | Applied operator theory

Date 21.03.2018
Room 1400

Lipschitz metrics for a nonlinear PDE

Katrin Grunert (*Norwegian University of Science and Technology (NTNU)*) 16:30–16:50

Solutions of the Hunter-Saxton equation might enjoy wave breaking in finite time. This means that solutions in general do not exist globally, but only locally in time since their spatial derivative might become unbounded from below pointwise in finite time, while the solution itself remains bounded. In addition, energy concentrates on sets of measure zero when wave breaking occurs. The prolongation of solutions beyond wave breaking is therefore non-unique. We show how the stability of conservative solutions, i.e., solutions where the energy is not manipulated at breaking time, can be analyzed by constructing a Lipschitz metric, which is based on the use of the Wasserstein metric, in the case of the Hunter-Saxton equation. This is joint work with J. A. Carrillo and H. Holden.

Nonautonomous Flow Semigroups

Frank Neubrander (*Mathematics, Louisiana State University*) 16:50–17:30

This talk reviews some recent results, obtained in collaboration with A. Scirratt from Houston Baptist University, on Bernhard Koopman's operator theoretic, global linearization approach to study nonlinear, nonautonomous flows based on the "dynamics of observables" picture.

Positive Operator Semigroups and Sherman's Theorem on Lattice Ordered C^*-Algebras

Jochen Glück (*Institute of Applied Analysis, Universität Ulm*) 17:30–17:50

A classical theorem of Sherman asserts that, if the self-adjoint part of a C^*-algebra $\mathcal{A}$ is a lattice with respect to its canonical order, then $\mathcal{A}$ is commutative. This result has later been generalised in several directions.
We present a new proof of Sherman's theorem which relies on the spectral theory of positive operator semigroups, i.e. on the so-called *Perron-Frobenius theory*. The point of our approach is not to prove a new theorem or to seek for outmost generality, but to highlight a connection between two different areas of operator theory.

Subordination for strongly continuous semigroups of sequentially equicontinuous operators

Karsten Kruse (*Institut für Mathematik, Technische Universität Hamburg-Harburg*), Jan Meichsner (*Institut für Mathematik, Technische Universität Hamburg-Harburg*), Christian Seifert (*Institut für Mathematik, Technische Universität Hamburg-Harburg*) 17:50–18:10

Let $A : \mathcal{D}(A) \to X$ be a generator of a equibounded, locally equicontinuous C_0-semigroup of sequentially continuous linear operators $(T_t)_{t\geq 0}$ in a sequentially complete Hausdorff locally convex space X. Further let $f : (0,\infty) \to (0,\infty)$ be a Bernstein function. We study so-called subordinated semigroups which are associated to $(T_t)_{t\geq 0}$ and f. The generators can be seen as $f(A)$. The results are motivated by [1] and [2] and can later be found in [3].

[1] R. L. Schilling, R. Song and Z. Vondracek. Bernstein Functions: Theory and Application. De Gruyter Studies in Mathematics 2012

[2] S. Federico and M. Rosestolato. C_0-sequentially equicontinuous semigroups and applications to Markov transition semigroups. arxiv preprint `https://arxiv.org/abs/1608.05707`

[3] K. Kruse, J. M. and C. Seifert. Subordination for sequentially equicontinuous C_0-semigroups. in preparation

Intermediate and extrapolated spaces for bi-continuous semigroups

Christian Budde (*Mathematics, Bergische Universität Wuppertal*) 18:10–18:30

In this talk we discuss the construction of the full Sobolev Hölder scale for non-densely defined operators on a Banach space with rays of minimal growth. In particular, we give a construction for extrapolation- and Favard spaces of generators of (bi-continuous) semigroups, or which is essentially the same, Hille-Yosida operators on Saks spaces.

S23.03 | Applied operator theory

Date 22.03.2018
Room 1400

Stabilization of port-Hamiltonian systems by nonlinear dynamic boundary control

Jochen Schmid (*Institute of Mathematics, Julius-Maximillians Universität Würzburg*) 08:30–08:50

In this talk, we will consider an infinite-dimensional linear port-Hamiltonian system coupled to a dynamic nonlinear controller by standard feedback interconnection: $y = u_c$ and $u = d - y_c$, where u, u_c and y, y_c are the input and output of the port-Hamiltonian system and the controller, respectively, and where d is an external disturbance signal affecting the output of the controller before being fed back into the system. We will establish some fundamental properties of the resulting nonlinear closed-loop system with input d and output y, namely (i) its well-posedness, that is, the existence and continuous dependence of (generalized) solutions and outputs for arbitrary initial states and arbitrary locally square-integrable inputs (ii) its stability, that is, the convergence of the solutions to 0 for arbitrary initial states and arbitrary square-integrable inputs. Joint work with H. Zwart.

Boundedness of solutions of Riccati equations

Christian Wyss (*Mathematik, Bergische Universität Wuppertal*) 08:50–09:10

We consider the operator Riccati equation from systems theory

$$A^*X + XA - XBB^*X + C^*C = 0.$$

An operator X is a solution of the Riccati equation if and only if its graph is an invariant subspace of the associated Hamiltonian operator matrix

$$T = \begin{pmatrix} A & -BB^* \\ -C^*C & -A^* \end{pmatrix}.$$

Hence one approach to solve the Riccati equation is to construct invariant graph subspaces of T. This method yields solutions which may be unbounded in general. In this talk we present conditions ensuring that certain solutions are in fact bounded. We will be particularly interested in the case where T is defined in an extrapolation space setting.

Remarks on Crouzeix's conjecture

Felix Schwenninger (*Dep. of Mathematics, University of Hamburg*) 09:10–09:30

In 2007 Crouzeix showed that there exists a constant $C \leq 11.08$ such that for any square matrix A with complex entries and any f holomorphic on the numerical range $W(A)$, it holds that

$$\|f(A)\| \leq C \sup_{z \in W(A)} |f(z)|,$$

where $\|\cdot\|$ denotes the spectral norm and $W(A) = \{\langle x, Ax\rangle \colon \|x\| = 1\}$. Crouzeix's conjecture claims that the optimal constant C equals 2, whereas, as proved by Crouzeix and Palencia in 2017, only $2 \leq C \leq 1 + \sqrt{2}$ is known so far. In this talk, recent progress around the conjecture is reported. This is joint work with T. Ransford (Université Laval).

On operator-norm convergence in time-dependent homogenisation problems

Marcus Waurick (*Mathematics and Statistics, University of Strathclyde*) 09:30–09:50

Considering homogenisation problems in a space-time framework, we will provide both quantitative and qualitative operator-norm convergence results for the solution operators to certain partial differential equations. In the literature, one can find a great deal of research devoted to operator-norm convergence for semi-groups and/or cosine families or devoted to showing operator convergence in the weak operator topology, only. Our results complement the former research by allowing for mixed type problems and improve the latter research by strengthening the convergence statements.

S24 | History of mechanics and history, teaching and popularization of mathematics

Organiser Peter Eberhard (*Institute of Engineering and Computational Mechanics, University of Stuttgart*)
Herbert Mang (*Institute for Mechanics of Materials and Structures, Technische Universität Wien*)

S24.01 | History of mechanics and history, teaching and popularization of mathematics

Date 21.03.2018
Room 0540

Historical Evolution of Thin-walled Structures – Formfinding and Analysis

Ekkehard Ramm (*Bau- und Umweltingenieurwissenschaften, Universität Stuttgart*) 16:30–17:10

The contribution on thin-walled structures like beams, plates and shells addresses two aspects in the historical perspective. For the first one, related to design processes, we concentrate on shell structures where the determined shape plays a decisive role. Since this has been recognized already in early times it is exemplarily referred to some prominent dome type of masonry structures, from the Greek and Roman times up to the Renaissance. With Hooke's Riddle of the Arch a new form-finding paradigm entered the scene, looking at a material oriented optimal shape. Since than it has been applied by several master builders like Wren, Rondelet, Gaudi and later by Otto as well as Isler. It will be mentioned that in recent times experimental and numerical form-finding principles, applied for membranes and shells, have reached an amazingly advanced stage in the design practice. The second aspect of the lecture addresses the mechanics of thin-walled structures which essentially follows the idea which is nowadays denoted as dimensional reduction. We will briefly report on the well-known beam theories, followed by a more detailed reference to equivalent plate and shell theories. Up to the first half of the 20th century the developments were mainly driven by reduction to the essential and the capability of existing analytical solutions schemes. We will also discuss the evolution of formulations and simulations since the advent of modern computers. This will end in some remarks to the recent development of the Isogeometric Analysis.

Gyrolog – Development of a Digital Collection of Gyro Instruments for Historical and Didactical Research

Maria Niklaus (*ISD, Universität Stuttgart*), Jörg Wagner (*ISD, Universität Stuttgart, Sprachenzentrum*) 17:10–17:30

Mechanical instruments form an essential part of cultural heritage. If historically analyzed and suitably explained, they provide insights into technical devices which have a significant influence upon our present civilization. Without any explanation and contextualization, however, these objects will remain stubbornly silent, especially if they are technically complex or highly encapsulated.
The Gyrolog project intends to take gyroscopes out of their black boxes by digital means. These inconspicuous yet indispensable objects of many of today's key technologies (from automatic car navigation to handheld devices) are of prime interest to historians of mechanics as well as to

technical didactics and to technical museums. The project will render the unique gyroscope collection founded by Kurt Magnus at the University of Stuttgart digitally accessible and, moreover, will virtually unite it with smaller collections at other institutions.
Gyrolog aims at a basic digital representation of all gyroscopes found in German collections. At the centerpiece of the project, however, cutting edge imaging and digitalizing technologies will exhibit carefully selected objects literally in depth. By combining advanced animation and optical technologies in doing so, Gyrolog seeks to present a unique technical collection in digital format as well as an elaborated methodical approach for exploring complex small technical artefacts.

200 years of mechanics at the Technical University of Vienna

Herbert Mang (*Institute for Mechanics of Materials and Structures, Technische Universität Wien*) 17:30–17:50

The historical retrospect at 200 years of mechanics at the Technical University of Vienna, which is the topic of this presentation, consists of three sections. The first one refers to the period of time from the foundation of the k.k. Polytechnic Institute in Vienna to the collapse of the Austro-Hungarian monarchy, the second one to the First Republic and World War II, and the third one to the Second Republic. With reference to the work of individual professors, the important role of mechanics as a basic discipline of the engineering sciences with a strong impact on engineering practice is elucidated in a historical context.

A brief history of logarithmic strain measures in nonlinear elasticity

Robert Martin (*University of Duisburg Essen*), Patrizio Neff (*University of Duisburg Essen*), Ingo Münch (*Karlsruhe Institute of Technology - KIT*), Bernhard Eidel (*University of Siegen*) 17:50–18:10

Historically, there have been a number of different motivations for the use of logarithmic strain measures in nonlinear elasticity, dating back to the end of the 19^{th} century. Today, the first practical applications of logarithmic strain are often attributed to P. Ludwik, for example in Truesdell's *Classical Field Theories*. The earliest mention of the logarithmic strain by Ludwik appears in his 1909 monograph *Elemente der technologischen Mechanik* on plastic deformations, where he arrived at the logarithmic strain measure via the integral $\int_{l_0}^{l} \frac{\mathrm{d}l}{l} = \log \frac{l}{l_0}$ over the *instantaneous strain* $\frac{\mathrm{d}l}{l}$ for uniaxial elongations.
A fully three-dimensional logarithmic elastic law, widely considered to be the first of its kind, was introduced by Heinrich Hencky in his 1928 article *Über die Form des Elastizitätsgesetzes bei ideal elastischen Stoffen*.
However, the first known introduction of the logarithmic strain tensor to fully three-dimensional nonlinear elasticity is actually due to the famous geologist George Ferdinand Becker. In his 1893 article *The Finite Elastic Stress-Strain Function*, he proposed a linear relation between the (material) logarithmic strain tensor $\log U$ and the *Biot stress tensor*, using a systematic approach remarkably similar to Hencky's.
Although it was reviewed in *Beiblätter zu Wiedemanns Annalen der Physik* and cited in Lueger's *Lexikon der gesamten Technik*, Becker's work seems to have gone unnoticed in continuum mechanics until its recent rediscovery. The introduction of the logarithmic strain to elasticity theory is therefore currently misattributed in the literature. This error of attribution seems to originate from Hencky himself who, in a 1931 article, refers to a brief section on plastic deformations in *Hütte: Des Ingenieurs Taschenbuch* where Ludwik is cited. The same misattribution to Ludwik is given by Truesdell, who does not mention Becker at all.

Analytical modelling of autofrettage processes – historical approaches and new results

Franz G. Rammerstorfer (*Institute of Lightweight Design ans Structural Biomechanics, TU Wien, Vienna University of Technology*), Stefan Bauer (*TU Wien, Vienna University of Technology*), Jakob Scheidl (*TU Wien, Vienna University of Technology*) 18:10–18:30

There exist a number of classical analytical solutions for the calculation of the residual stresses as produced by autofrettage, for instance, in order to increase the endurable pressure load of hydraulic devices or the lifetime of cyclically loaded metallic structures with stress concentations. These historical analytical solutions are based on assumptions, which are approximate in comparison with reality and limited in the range of applicability. Especially, by considering the solutions at the free end of pressurized tubes or at the surface of structures with stress concentrations by boreholes, it is shown that due to the free surface boundary conditions some peculiar phenomena can be observed. Furthermore, unconventional mechanical responses can appear when the autofrettage pressure approaches or exceeds certain limits.

S24.02 | History of mechanics and history, teaching and popularization of mathematics

Date 21.03.2018
Room 0540

Theory of Science, Mechanica Rationalis and Construction of Machinae Arithmeticae in the 17th Century

Erwin Stein (*Civil Engineering and Geodesy, Leibniz Universität Hannover*) 14:00–14:40

The infinitesimal calculus by Newton and Leibniz and the variational calculus by Jakob Bernoulli as the bases of mathematical analysis as well as the axiomatic theory of solid mechanics, Newton's Mechanica Rationalis, were developed in the early period of the age of enlightenment in the second half of the 17th century, being the cradle of modern mathematics, natural sciences and technical inventions. Descartes created the new mechanistic philosophy with the metaphor Man and Machine, and the universal scholar Leibniz solved the 100-year-problem of the Vis viva, the so-called True measure of the living force, namely the kinetic energy of a mass moving by gravity, and he substantially contributed to the Theory of Science for logical and mathematical modeling of measurable and non-observable objects and processes by scientific and metaphysical theories, with a relative truth for a certain time. Kant criticized Leibniz according to his transcendental philosophy, emphasizing the importance of experience and observations of reality. According to Leibniz' postulate Theoria cum praxi, technical inventions of mechanical calculators were equally important: the first Two-Step Four-Species Decimal Calculator by Schickard, the Two-Species Decimal Calculator by Pascal, the famous Pascaline, and especially the first true Four-Species Decimal Calculator by Leibniz, his Machina Arithmetica, as the basis for mechanical calculators until the 1950s, as well as his description of a Two-Species-Binary-Calculator, the Machina Dyadica with metal spheres rolling down, in connection with the binary calculus, and finally his description of a Cypher machine, the Machina Deciphratoria. In the Leibniz Exhibition of the Leibniz Universität Hannover we established complete mathematical models and Pareto-Optimizations of the Leibniz Machines and constructed fully functional replicas.

Interactive Web Apps for Visualizations in Mathematics and Engineering

Francesca Taddei (*TUM Department of Civil, Geo and Environmental Engineering, Chair of Structural Mechanics, Technical University of Munich*), Benjamin Rüth (*Institut für Informatik, Technical University of Munich*), Christian Karpfinger (*TUM Department of Mathematics, Research Group Algebra, Technical University of Munich*), Gerhard Müller (*TUM Department of Civil, Geo and Environmental Engineering, Chair of Structural Mechanics, Technische Universität München*) 14:40–15:00

The diversification of the media in teaching has a large impact on the quality and the outcome of the courses. In particular, several studies have shown [1,2] the positive effects of interactive visualization in the learning process. Depicting numbers in a graphical form has always been a crucial way to understand and explain the physical phenomena behind. Making the graphics interactive brings the understanding to a higher level, where the users get actively engaged. Moreover, interactive visualizations of data, number, equations etc... help to motivate students with difficulties and strengthen the sharing of knowledge.
At the TUM, the Chair of Structural Mechanics and the Research Group Algebra developed interactive applications in the fields of Technical Mechanics and Algebra. These are used in teaching and also in research. As programming framework, we have chosen an open-source Python-based library, Bokeh [3]. Bokeh is an interactive visualization library that targets modern web browsers for presentation. It has a concise approach to the construction of novel graphics with high-performance interactivity over very large or streaming datasets. The current state of the application can be freely downloaded from the platform Github [4].
Running examples of the application can be found at the website of our institutes [5]. Students can access the applications online at any time, without installation or special requirements, and can actively explore the contents. For example, they can let a spring-mass-damper system enter the resonance by changing the frequency of the excitation; or they can search for local maxima and minima of a function with side conditions with the Lagrange multipliers.
We believe, the interactive process enhances the understanding, even if the user does not interact with a strategy but just uses his intuition. These applications can be also used to explain complex concepts to the general public.

[1] Kuosa, Kirsi, et al. "Interactive Visualization Tools to Improve Learning and Teaching in Online Learning Environments." International Journal of Distance Education Technologies (IJDET) 14.1 (2016): 1-21.

[2] Schweitzer, Dino, and Wayne Brown. "Interactive visualization for the active learning classroom." ACM SIGCSE Bulletin. Vol. 39. No. 1. ACM, 2007.

[3] https://bokeh.pydata.org

[4] https://github.com/ChairOfStructuralMechanicsTUM/Mechanics_Apps

[5] http://www.bm.bgu.tum.de/lehre/interactive-apps/

Motivation von Schüler/-innen für MINT-Fächer erhöhen: Vorstellung eines Projekts, das Schulen und Industrieunternehmen zusammenbringt

Roland Gunesch (*PH Vorarlberg*), Nicolas Robin (*PH St. Gallen*) 15:00–15:20

In diesem Beitrag wird das Projekt „MINT macht Schule – Brücken zwischen Schulen und Industrie bauen“ vorgestellt, welches die Motivation von SuS für MINT-Themen (Mathematik, Informatik, Naturwissenschaften, Technik) erhöhen soll. Dieses Projekt wird von den Pädagogischen Hochschulen Vorarlberg und St.Gallen durchgeführt und finanziell unterstützt durch die EU.
Fachkräftemangel resultiert u. a. aus nicht genügend großen Interesse Jugendlicher für MINT-Schulthemen und -Berufsausbildungen. In diesem Entwicklungsprojekt wird versucht, Interesse und Motivation von Jugendlichen für diese Themen bereits einige Jahre vor dem Schulabschluss zu gewinnen und zu erhalten.
Partnerschaften zwischen Schulen und geographisch benachbarten Industrieunternehmen werden etabliert, die den SuS erlauben, technische und wissenschaftlichen Inhalte selbst zu erleben.
Zur Untersuchung der Wirksamkeit wird das Interesses und der Motivation der SuS für Mathematik und Technik mit einem Fragebogen gemessen. Alle eingesetzten Fragen wurden bereits in der Vergangenheit getestet und auf Validität, Reliabilität und Relevanz geprüft. Quellen sind u. a. PISA-Fragebögen sowie Enjoyment-Value- und Expectancy-Value-Cost-Modelle der aktuellen Literatur (Aiken, 1974; Kosovich et al., 2014). Diese Modelle gehen davon aus, dass SuS mathematischen Themen sowohl positive Werte zuordnen (enjoyment bzw. expectancy und value) als auch negative (cost).

Aiken, L. (1974). Two Scales of Attitude toward Mathematics. Journal for Research in Mathematics Education, Vol. 5, No. 2, 67-71.

OECD (2012) PISA 2012, Internationaler und nationaler Schülerfragebogen

https://www.bifie.at/system/files/dl/pisa12_internationaler_nationaler_schuelerfragebogen.pdf.

Kosovich, J.J., Hulleman, C.S., Barron, K.E., & Getty, S. (2014). A practical measure of student motivation establishing validity evidence for the expectancy-value-cost scale in middle school. Journal of Early Adolescence, Vol 35, Issue 5-6, 790–816.

A revised taxonomy for the competence orientated description of learning outcomes for study programs in engineering sciences

Franziska Mittermeier (*Lehtstuhl für Baumechanik, Technische Universität München*), Rupert Ullmann (*Technische Universität München*), Gerhard Müller (*Lehrstuhl für Baumechanik, Technische Universität München*) 15:20–15:40

The modularisation of study programs due to the Bologna Process leads to a growing number of selection choices and an increasing flexibility in the individual curriculum design. Therefore an appropriate description of the learning outcomes of the individual modules is crucial for ensuring consistent personal curricula and the continuous acquisition of competencies.
At the Technische Universität München, learning outcomes are currently described in continuous texts using Bloom´s taxonomy. Although this taxonomy is commonly accepted, in practise there are problems regarding a clear description of the acquired competences in engineering sciences. Thus, Anderson's and Krathwohl's revision of Bloom´s taxonomy was extended for the explicit application to engineering studies. In the reformulation the stage of qualification is expressed via a breakdown into quantified levels of knowledge (know what), skills (know how), and competencies (know why). Furthermore, a tabular description is introduced instead of a continuous text. This allows for a systematic storage and analysis in a database. Therefore besides an appropriate and clear description of learning outcomes, the new system delivers access to various possibilities: First, the new taxonomy facilitates the detection of conflicts between learning outcomes of different modules using a web-based tool for the analysis of module interfaces. Furthermore, the

level system eases competence orientated examination via adapting questions to the respective qualification level addressed in the module description. Finally, the new system simplifies the recognition of credits, which becomes more important due to the increasing mobility of students.

Christian Otto Mohr und Friedrich Hebbel - Söhne aus Wesselburen in Dithmarschen

Lothar Gaul (*F07 Konstruktions, Produktions und Fahrzeugtechnik, Stuttgart University*) 15:40–16:00

Christian Otto Mohr wurde 1835 im Hause des Kirchspielvogts Mohr in Wesselburen geboren. Der Vogt beschäftigte einen verarmten Maurer Hebbel als Gärtner, der seinen Sohn Friedrich zur Gartenarbeit mitbrachte. Friedrich Hebbel interessierte sich mehr für die Schreibarbeiten des Vogtes, der seine Begabung erkannte und ihn als Sekretär beschäftigte. Durch die Förderung des Vogtes kam Friedrich Hebbel zum Studium nach Heidelberg und wurde zu Deutschlands bekanntestem Dramatiker. In Wien ehelichte er eine Burgschauspielerin und schrieb seine Hauptwerke 'Die Wikinger' und 'Maria Magdalena'. Christian Otto Mohr wurde 1867 mit 32 Jahren von König Karl von Württemberg an die Polytechnische Schule, die spätere TH und Universität Stuttgart als ordentlicher Professor auf die neu eingerichtete Professur für Mechanik, Eisenbahntrassen und Erdbau berufen. Er hat zuvor von 1851 bis 1854 an der Polytechnischen Schule in Hannover studiert und war bis zu seiner Berufung Eisenbahningenieur im Königreich Hannover und bei der Oldenburgischen Staatsbahn. Christian Otto Mohr bezog mit sechzehn Jahren die Polytechnische Schule in Hannover und wurde dort wie August Wöhler aus Soltau ausgebildet, der die Grundlagen für systematische Materialprüfungen und damit für die Festigkeitslehre als neuer ingenieurwissenschaftlicher Disziplin legte. Jeder angehende Ingenieur lernt die Wöhler-Kurve kennen, in der die ertragbare Beanspruchung der Zahl der Lastwechsel zugeordnet wird. Die Mohrschen Kreise zur graphischen Konstruktion der Transformationsgesetze von Spannungen und Verzerrungen bei Drehung des Koordinatensystems kennt jeder Ingenieur. Wesentliche Beiträge zur Elastostatik und Festigkeitslehre leisteten am Polytechnikum in Stuttgart Christian Otto Mohr (1835 - 1918) und Carl Julius von Bach (1847 - 1931). Während Mohrs vorangegangener zehnjähriger Tätigkeit bei den Staatsbahnen zeigte er seine glänzende Befähigung für die Lösung statischer Aufgaben, und die von ihm entworfene und als erste eiserne Fachwerkskonstruktion bei Lüneburg ausgeführte Eisenbahnbrücke sowie sein Werk über 'Durchlaufträger' lenkten die Aufmerksamkeit der Fachwelt auf ihn. In Stuttgart lehrte Mohr die graphostatische Behandlung von Konstruktionsaufgaben und hatte einen begeisterten Kreis von Schülern um sich, zu denen Carl von Bach gehörte, wie auch August Föppel (1854 – 1924), der 1894 Nachfolger Bauschingers in München wurde. In Stuttgart erforschte Mohr einen Weg zur graphischen Ermittlung komplizierter elastischer Biegelinien von Balken, den er in seinem Beitrag zur 'Theorie der Holz- und Eisenconstructionen' in der Zeitschrift des Architekten- und Ingenieurvereins zu Hannover 1868 veröffentlichte. Mohr erkannte somit als Erster die Analogie zwischen der (linearisierten) Differentialgleichung des Balkens und der Differentialgleichung einer Seilkurve und leitete daraus seine graphische Integration der Biegelinie mit dem Seileckverfahren ab. Ab dem Wintersemester 1867/68 las Mohr die Ingenieur-Mechanik in Stuttgart und behandelte darin 'Die Statik der Baukonstruktionen, Elastizität und Festigkeit der Baumechanik, Balkenträger, Gewölbe, Stütz- und Futtermauern, Auflösung praktischer Aufgaben durch Rechnung und graphische Statik'. Mohr führte 1868 etwa gleichzeitig mit Emil Winkler aber unabhängig von ihm die Einflusslinie ein, welche den Einfluss der Belastungsposition auf die Biegeverformung beschreibt und insbesondere bei wandernden Lasten wie der Eisenbahn kritische Zustände erkennen lässt. 1873 wurde Mohr an das Königlich Sächsische Polytechnikum nach Dresden als Professor für Eisenbahnbau, Wasserbau und Graphostatik berufen, wo er nach dem Tode Zeuners dessen Vorlesungen über Mechanik und Festigkeitslehre fortsetzte. In der Nachfolge des Experten für Lokomotivgetriebe publizierte Mohr wichtige Beiträge zur graphischen Kinematik. Mohr kam als

international anerkannter Ingenieurwissenschaftler von Stuttgart nach Dresden und lehrte hier 27 Jahre. Nach dreiunddreißigjähriger Lehrtätigkeit (6 Jahre in Stuttgart, 27 Jahre in Dresden) setzte sich Mohr zur Ruhe, um als Forscher zu leben. Alljährlich veröffentlichte er Beiträge in Fachzeitschriften, die hohe Anerkennung fanden. Klarheit und Kürze, Einfachheit und Übersichtlichkeit waren die Merkmale seiner Arbeiten. Christian Otto Mohr verdient in besonderer Weise ein ehrendes Andenken als großer Lehrer und Forscher in Stuttgart und Dresden. Er ist als Mitbegründer der seinerzeit neuen Disziplin der graphischen Statik einer jener Ingenieure (wie zuvor Karl Culmann, 1821 - 1881), die im 19. Jahrhundert dem Ingenieurwesen eine wissenschaftliche Grundlage gegeben haben.

List of authors, chairs and organisers

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