

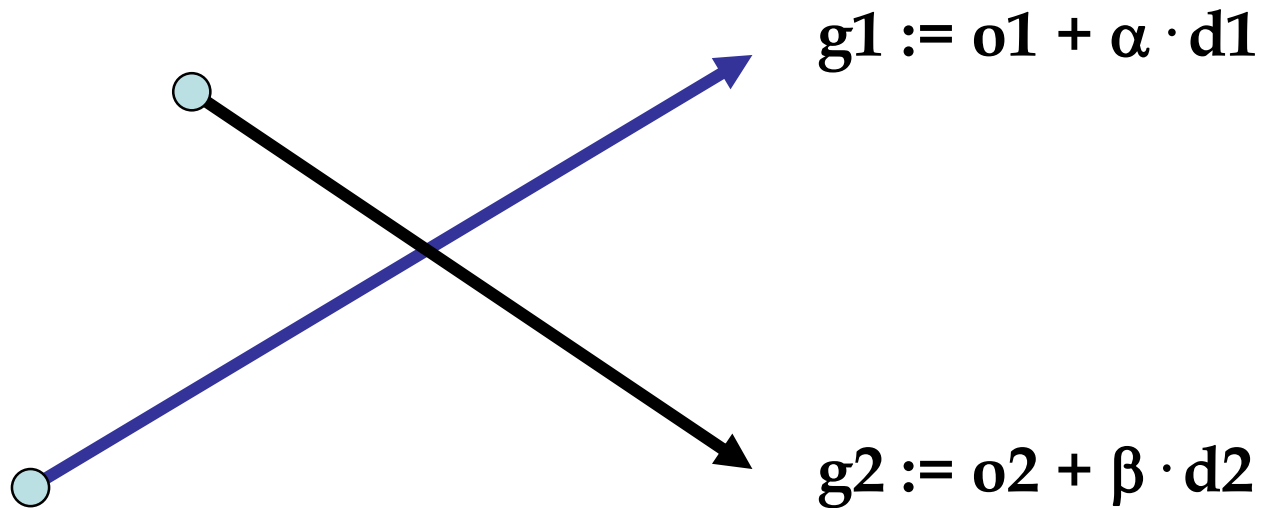
Industrial Applications of Computational Mechanics Extended Civil Engineering Problems

**Prof. Dr.-Ing. Casimir Katz
SOFiSTiK AG**

Beyond Structural Analysis

- **Multiphysics**
 - » **Heat Conduction, Radiation**
 - » **Potential Flow (Laplace)**
 - » **Fluid mechanics (Navier Stokes)**
 - » **Wind engineering**
 - » **Fire and Blast**
 - » **Combustion**

Mathematical Excursion



Intersection of two lines in 3D

- $g_1 = g_2$

$$x_1 + \alpha \cdot dx_1 - x_2 + \beta \cdot dx_2 = 0$$

$$y_1 + \alpha \cdot dy_1 - y_2 + \beta \cdot dy_2 = 0$$

$$z_1 + \alpha \cdot dz_1 - z_2 + \beta \cdot dz_2 = 0$$

- 3 equations for 2 unknowns α, β
- You need some case constructs to select the optimal solution strategy !

Alternate approach

- Distance (g1 - g2) = Minimum

$$(x_1 + \alpha \cdot dx_1 - x_2 - \beta \cdot dx_2)^2 +$$

$$(y_1 + \alpha \cdot dy_1 - y_2 - \beta \cdot dy_2)^2 +$$

$$(z_1 + \alpha \cdot dz_1 - z_2 - \beta \cdot dz_2)^2 = A^2$$

- 2 equations for 2 unknowns α, β

$$\partial A / \partial \alpha = 0$$

$$\partial A / \partial \beta = 0$$

Minimum Approach

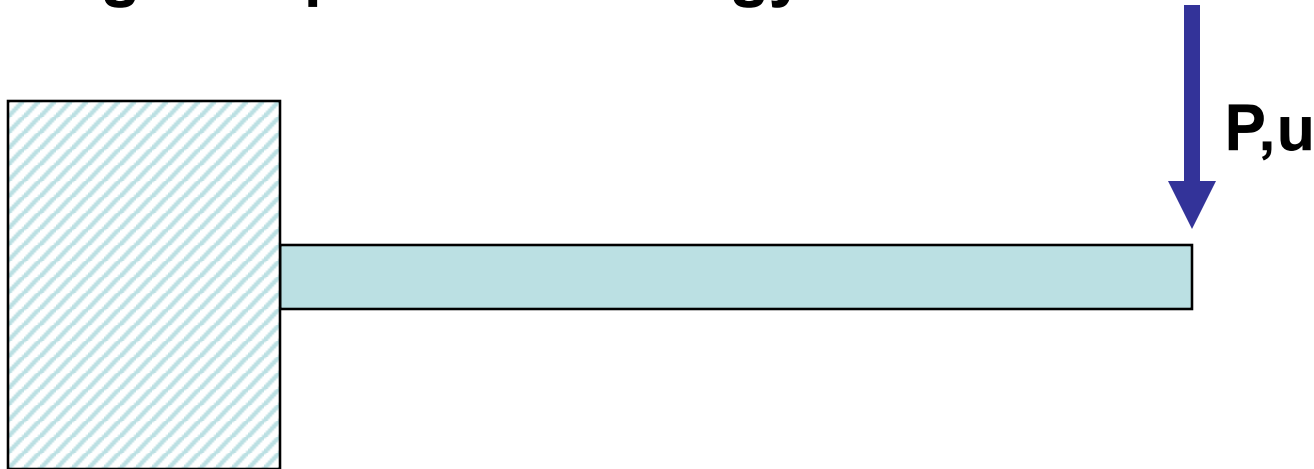
$$\begin{bmatrix} dx_1^2 + dy_1^2 + dz_1^2 & dx_1 dx_2 + dy_1 dy_2 + dz_1 dz_2 \\ \text{sym} & dx_2^2 + dy_2^2 + dz_2^2 \end{bmatrix} \cdot \begin{bmatrix} \alpha \\ \beta \end{bmatrix} =$$

$$\begin{bmatrix} (x_1 - x_2) dx_1 + (y_1 - y_2) dy_1 + (z_1 - z_2) dz_1 \\ (x_1 - x_2) dx_2 + (y_1 - y_2) dy_2 + (z_1 - z_2) dz_2 \end{bmatrix}$$

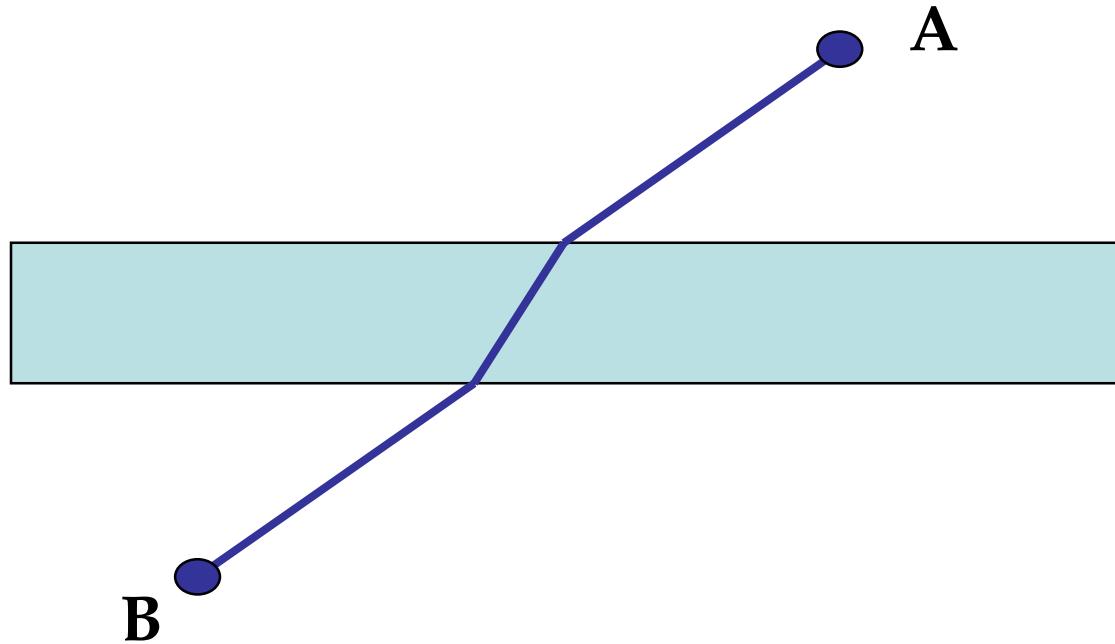
- **16 lines of code instead of 200**
- **Only two conditions to check**
 - » **Determinant becomes zero if and only if lines are parallel**
 - » **Resulting distance gives skewed lines problem for free**

Minimum of Energy

- Each mechanical system will deform in such a way that the total energy will become a minimum.
- Positive deformation Energy $\frac{1}{2} \cdot u^T \cdot K \cdot u$
- Negative potential Energy $P \cdot u$



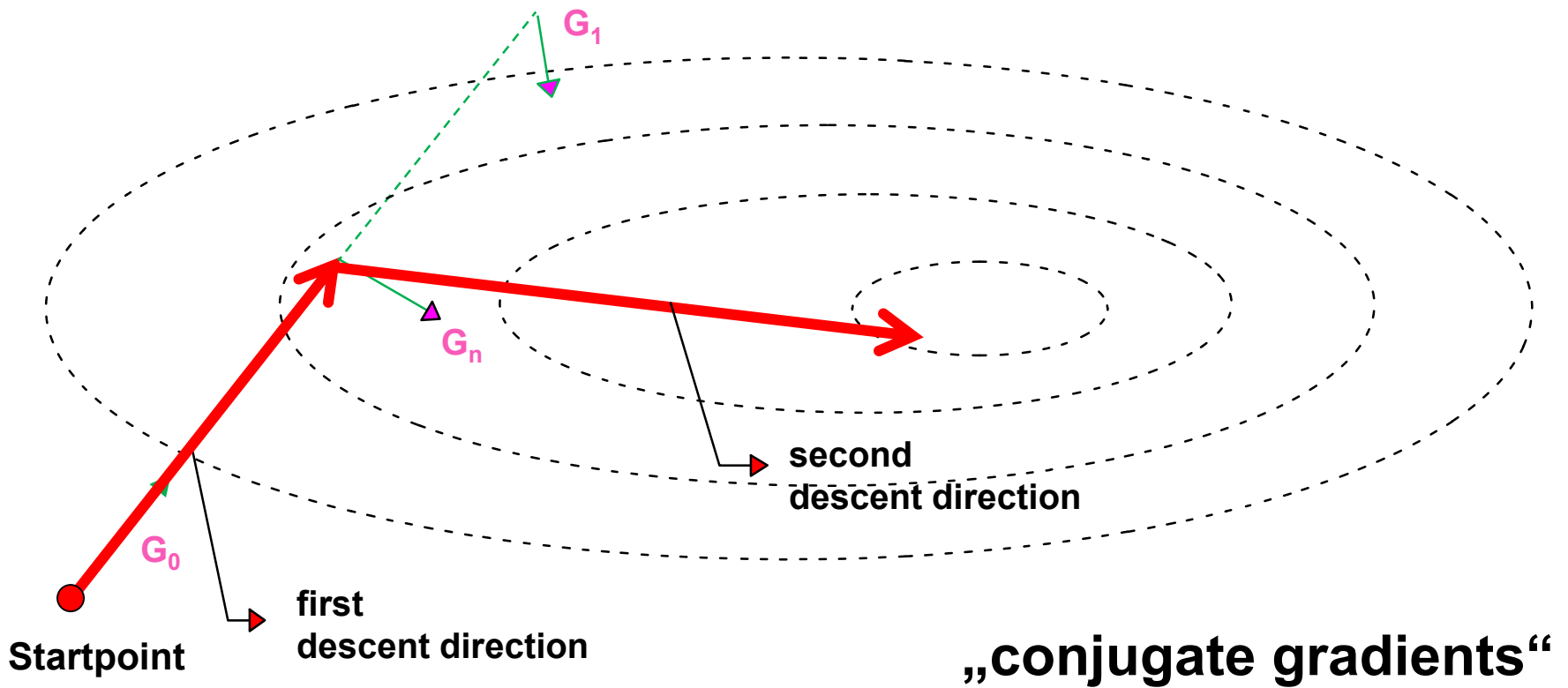
Refraction of light (QED)



What is the fastest (most probable) way for the light from A to B if the speed in the blue body is slower ?

Optimization and Line-Search

$$\min \Pi \Leftrightarrow \frac{\partial \Pi}{\partial x} = 0$$



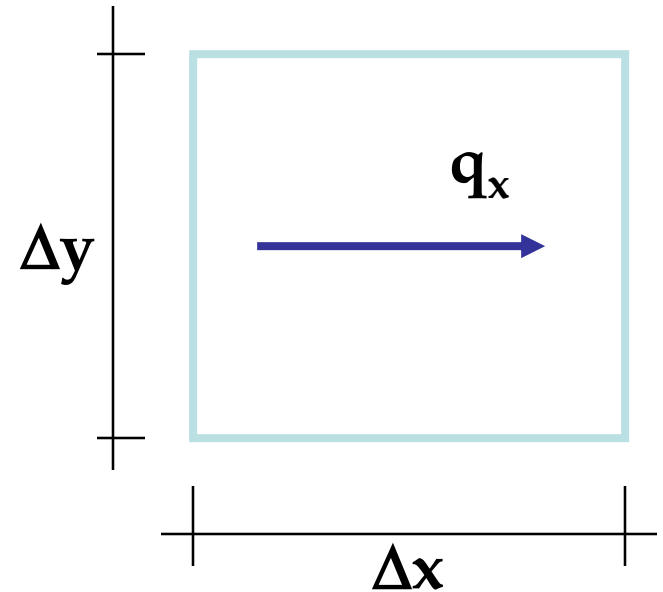
Heat Conduction 2D

Requested:
Temperature field $T(x,y)$

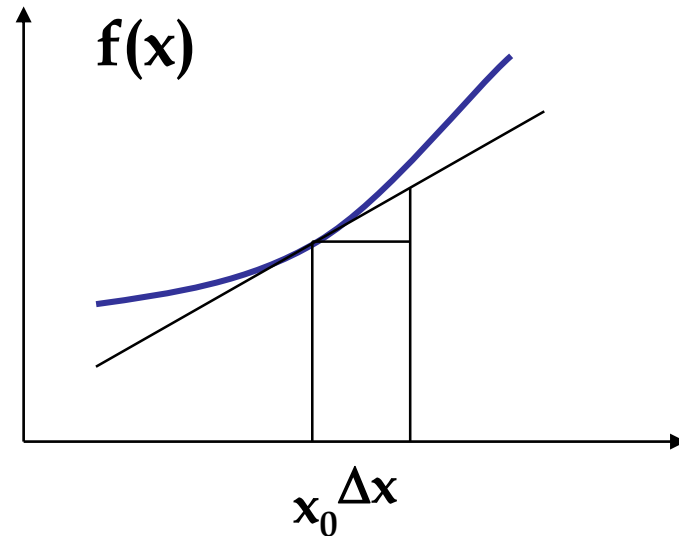
Heat conductivity k

$$q_x = k \cdot \frac{\Delta T}{\Delta x} \Rightarrow q_x = k \cdot \frac{\partial T}{\partial x}$$

$$q_y = k \cdot \frac{\Delta T}{\Delta y} \Rightarrow q_y = k \cdot \frac{\partial T}{\partial y}$$



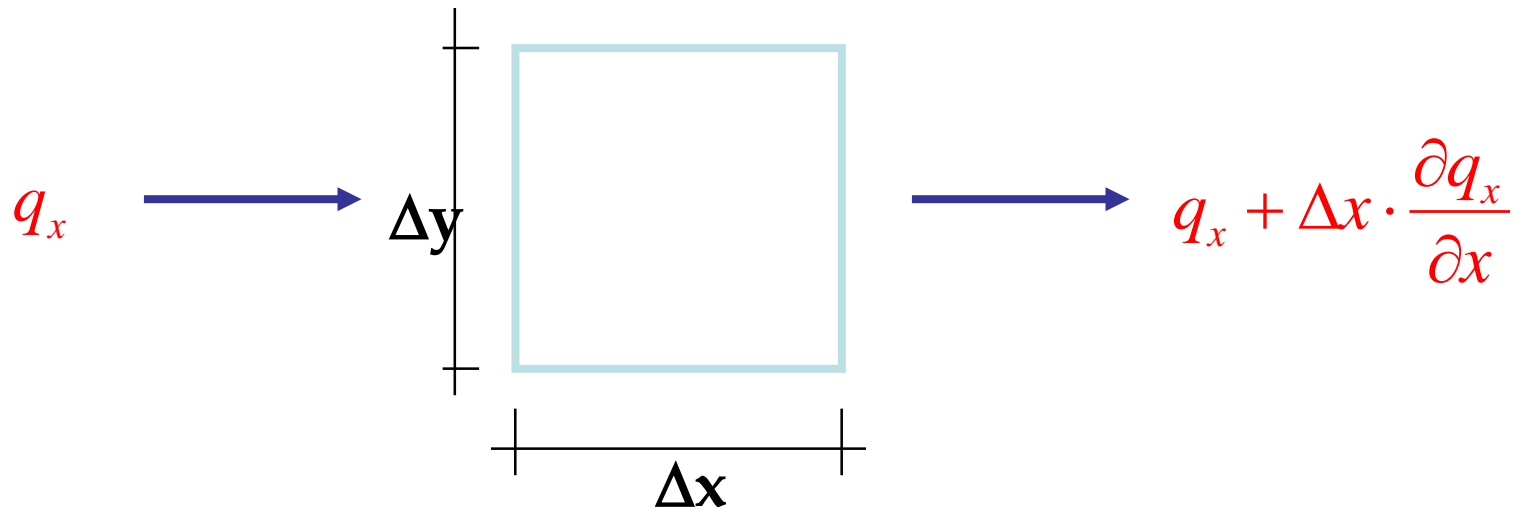
Taylor Series



$$f(x + \Delta x) = f(x_0) + \Delta x \cdot \frac{df(x_0)}{dx} + \frac{\Delta x^2}{2!} \cdot \frac{d^2 f(x_0)}{dx^2} + \dots$$

(for $\Delta x \rightarrow 0$ all contributions of higher order will vanish!)

Heat quantity conservation



$$\Delta y \cdot \left(q_x + \Delta x \cdot \frac{\partial q_x}{\partial x} - q_x \right) + \Delta x \cdot \left(q_y + \Delta y \cdot \frac{\partial q_y}{\partial y} - q_y \right) = 0$$

Laplace Equation

$$\Delta y \cdot \left(q_x + \Delta x \cdot \frac{\partial q_x}{\partial x} - q_x \right) + \Delta x \cdot \left(q_y + \Delta y \cdot \frac{\partial q_y}{\partial y} - q_y \right) = 0$$

$$q_x = k \cdot \frac{\partial T}{\partial x} \quad q_y = k \cdot \frac{\partial T}{\partial y}$$

$$\Rightarrow \frac{\partial}{\partial x} \left(k \cdot \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \cdot \frac{\partial T}{\partial y} \right) = 0$$

$$\Rightarrow k \cdot \Delta T = 0$$

The complete picture

$$\operatorname{div}(k \cdot \operatorname{grad} T) + S \frac{\partial T}{\partial t} - q = 0$$

- **Where**
 - » **T is potential value (e.g. Temperature)**
 - » **k is conductivity**
 - » **S is the storage coefficient**
 - » **q is a source term within the domain**
- **And the basic boundary conditions**
 - » **$T = T_1$ on Γ_1**
 - » **$\mathbf{u}^t \cdot \mathbf{n} = \mathbf{q}_2 + \alpha (T - T_2)$ on Γ_2**

Fields and Gradients

- A scalar value U which is defined in every point of space with a distinct value (eg. Temperature) is called a scalar field.
- A value u which is defined in every point of space as a vector (e.g. flow velocities) is called a vector field.
- A partial derivative of a scalar field U defines a vector field:

$$u = \text{grad } U = \begin{bmatrix} \frac{\partial U}{\partial x} \\ \frac{\partial U}{\partial y} \\ \frac{\partial U}{\partial z} \end{bmatrix}$$

Divergence

- Differentiating a vector field we have the divergence and the curl or rotation given by:

$$\operatorname{div} u = \nabla U = \left[\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \right]$$

$$\operatorname{rot} u = \begin{bmatrix} \frac{\partial u_z}{\partial y} - \frac{\partial u_y}{\partial z} \\ \frac{\partial u_x}{\partial z} - \frac{\partial u_z}{\partial x} \\ \frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y} \end{bmatrix}$$

Potential Fields

- A conservative field or potential field is a vector field, where the integral along a curve $\int_C \mathbf{u} \cdot d\mathbf{r}$ depends only on the start point A and the end point B, but not on the integration path.
- A conservative field is free of vortices, i.e. the closed integral with $A=B$ is zero.
- If sources or sinks are present in the system however the closed integral will be equal to the sum of sources (vortices).
- A conservative field has its largest and smallest value at the boundary (Maximum principle).

Uniqueness of Solutions

- **There are many cases where a quantity is only as a derivative within the equations. Then its value is only defined by the selection of a reference value in any arbitrary point.**
 - » e.g. displacements for rigid body movements
 - » e.g. pressure for a flow problem
- **As the fundamental solution (Greens function) of a 2D problem is the logarithm function, while in 3D it is the $1/r$ function, there is an important difference.**

In 3D we may easily select a zero potential at infinity, for 2D we have to select this point within a finite distance. This makes 2D solutions in many cases less unique than 3D solutions.

Analytical Solutions of the Laplace-Equation

- All functions of a complex Variable will solve the Laplace equation with their real and their imaginary part (conformal mapping).

$$F(z) = g(z) + i * h(z)$$

e.g.

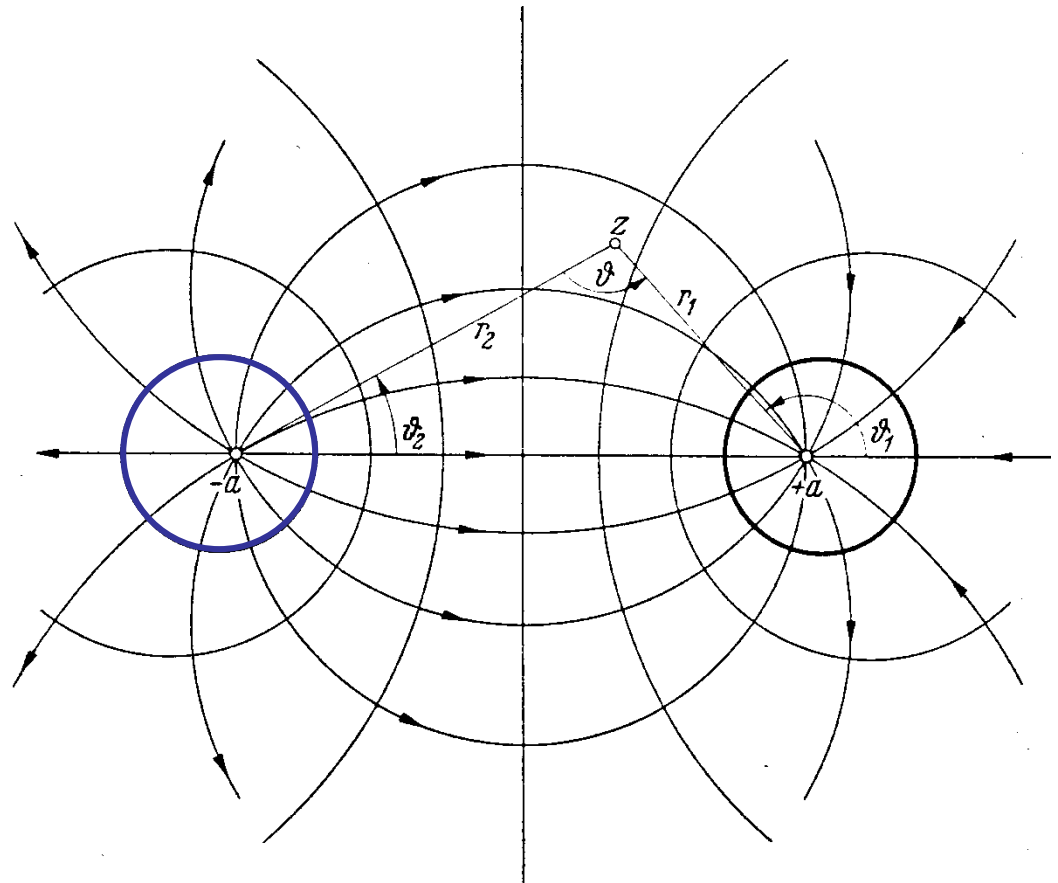
$$\text{Ln}(z) = \ln(\sqrt{x^2+y^2}) + i * \text{atan}(y/x)$$

- In 3D the fundamental solution is $1/r$ but there are no equivalent techniques available

Two Point Flow

- Combination of functions will yield more solutions:

$$\frac{1}{2\pi} \ln \left(\frac{z+a}{z-a} \right)$$



Laplace Solutions

- **Principal Problem: Boundary Conditions**
Beside some special cases it is impossible to find a solution fulfilling the boundary conditions.
- **General Solution Possibility:**
Use a limited but large set of fundamental solutions and try to full fill the boundary conditions point wise or with a weighted approach approximately.
Example: Integral equations

Alternate Formulations

- **Variational Approach**
Integral over the domain Ω and the boundary Γ

$$\iint k \cdot \left(\frac{\partial T}{\partial x} \right)^2 + k \cdot \left(\frac{\partial T}{\partial y} \right)^2 d\Omega - \int q \cdot T d\Gamma = \textit{Minimum}$$

- **Method of weighted Residuals**

$$\iint W \cdot (L(u) - L(u)) d\Omega - \int w \cdot (R(u) - R(u)) d\Gamma = \textit{Min}$$

The complete picture

$$\begin{aligned} & \frac{1}{2} \int_{\Omega} k_{ij} \frac{\partial T}{\partial x_i} \frac{\partial T}{\partial x_j} d\Omega + \int_{\Omega} T \left(S \frac{\partial T}{\partial t} - q \right) d\Omega \\ & + \int_{\Gamma_1} (T - T_1) k_{ij} \frac{\partial T}{\partial x_j} d\Gamma_1 - \int_{\Gamma_2} T \cdot \left(q - \frac{1}{2} \alpha T \right) d\Gamma_2 \end{aligned}$$

■ Remarks

- » The function T is selected best to fulfil the Dirichlet boundary condition $T=T_1$ on Γ_1 in advance
- » On all boundaries without an explicit integral we will obtain the natural boundary condition $u^t \cdot n = 0$
- » The transient term is only correct if we assume the time derivative to be constant

Numerical variational analysis

- Instead of the unknown function we use a series of known functions with variable parameters and integrate the functional (analytically or even numerically)

$$y = \sum_{i=1}^n a_i \cdot N_i(x)$$

$$\Pi = \Pi(a_1, a_2, \dots, a_n)$$

Numerical variational analysis

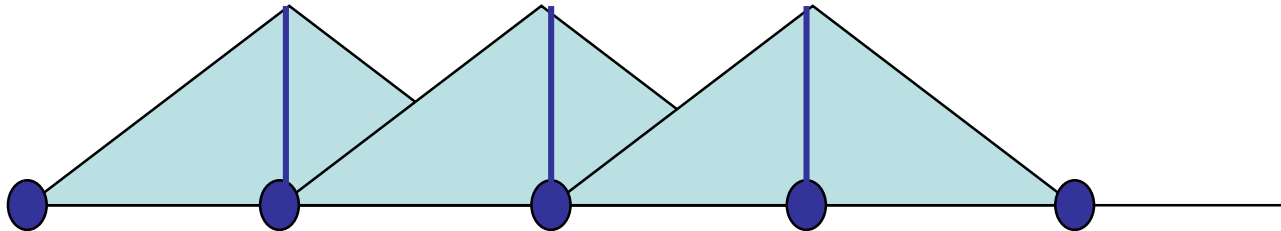
- Then we calculate the derivatives and get an equation system

$$J = J(a_1, a_2, \dots, a_n)$$

$$\frac{dJ}{da_i} = \text{equation}(a_1, a_2, \dots, a_n)$$

Base of Finite Elements

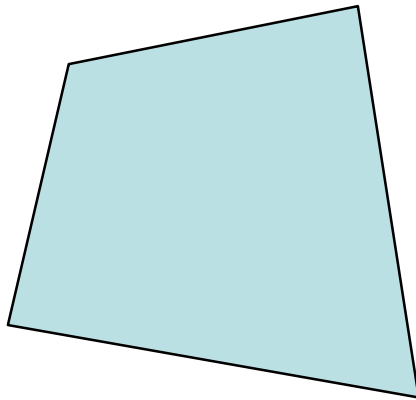
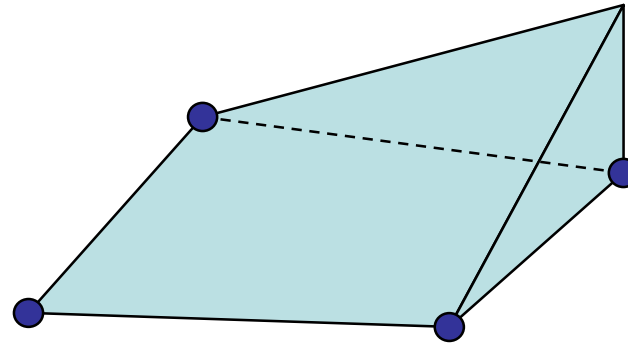
- **Select special simple trial functions with only a local influence !**
- **Example along an edge**



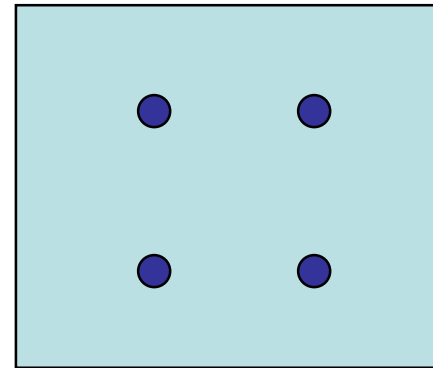
- **Local triangular (linear) functions**
Sum of functions is 1.0 everywhere

Discretisation of an area

- **Triangles**
- **Quadrilaterals**



Real Geometry



**Unit square
with 4 Gauss-Points**

Element matrices

- **Linear Functions**
=> constant derivatives
- **Although the selected functions do not fulfil the DE, the solution may be obtained by the variational principle and numerical integration**
- **Each „node“ is one unknown and we might have millions of them**
- **„Elements“ have only local influence**
- **Large equation systems have sparse matrices allowing for fast solution.**

Discretisation in Time

- **Assumption:**

$$\frac{\partial T}{\partial t} = \frac{T_i - T_{i-1}}{\Delta t}$$

- **Establishing the Equations for time $t_{i-1} + \Theta \Delta t$**

$$\left(\Theta \cdot A + \frac{1}{\Delta t} C \right) T_i = \left((\Theta - 1) \cdot A + \frac{1}{\Delta t} C \right) T_{i-1} - Q$$

$$A = \int_{\Omega} k_{ij} \frac{\partial N}{\partial x_i} \frac{\partial N}{\partial x_j} d\Omega ; C = \int_{\Omega} S (N^T N) d\Omega$$

Stability of Method

- The parameter Θ of the Crank-Nicholson Method may be selected between 0.5 and 2.0 to obtain stable Methods. The default is **0.7**
- The time step has to be selected to allow the physical effects to be traced properly. An adaptive selection may be needed for many cases.
- For small time steps the matrix **C** will become dominant. For a certain critical value of Δt the sum of $a_{ij} + c_{ij}/\Delta t$ will change the sign. If this happens the discrete maximum principle is violated and we will get perceptable oscillations in our solution.
Remedy: use lumped (diagonal) matrices for **C**

Heat Flow Material constants

- **T = Temperature [° K]**
- **u = Vector of heat fluxes [W/m²]**
- **q = Power of sources or sinks [W/m³]**
- **S = $\rho \cdot c_p$ = Storage coefficient in [Wsec/K·m³]**

where

ρ = specific weight of the material [kg/m³]

c_p = specific thermal capacity [Wsec/K·kg]

Heat Flow

Boundary Conditions

- Prescribed temperature

$$T = T_0 [^\circ \text{C}]$$

- Prescribed flux

$$q = q_0 [\text{W/m}^2]$$

- Prescribed resistance to environment temperature

$$q = \alpha (T - T_0)$$

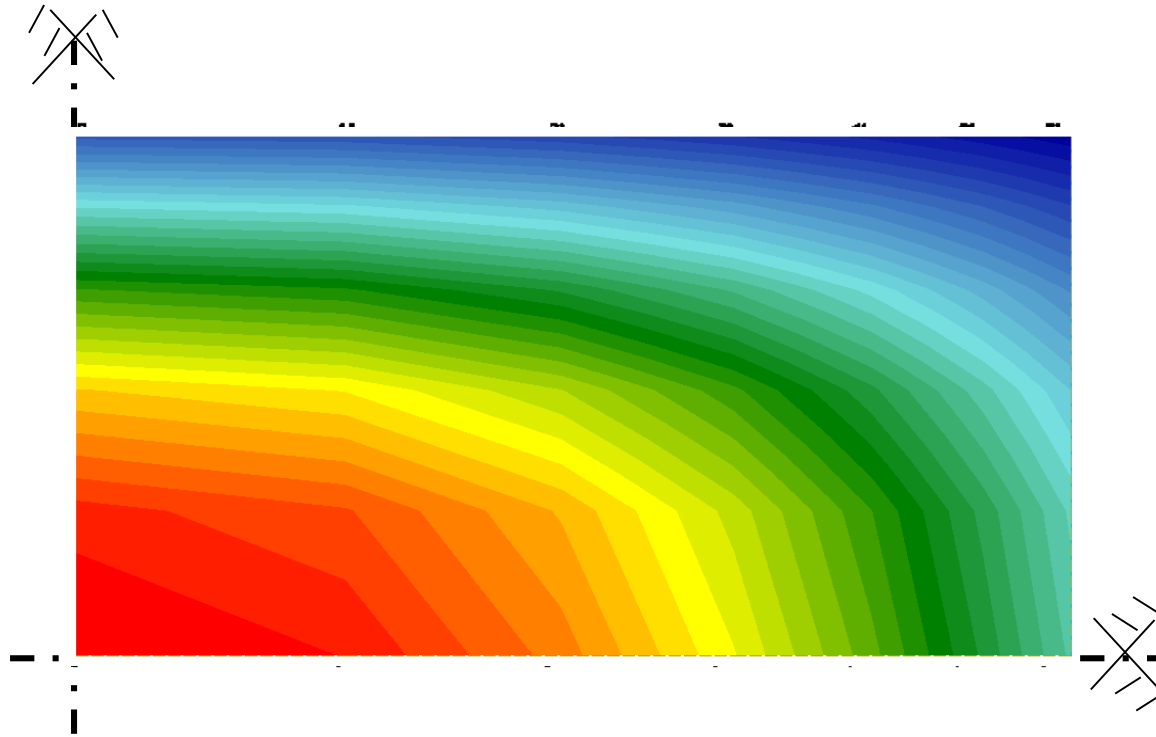
- Radiation

$$q = \varepsilon k (T^4 - T_0^4)$$

ε = Emission grade

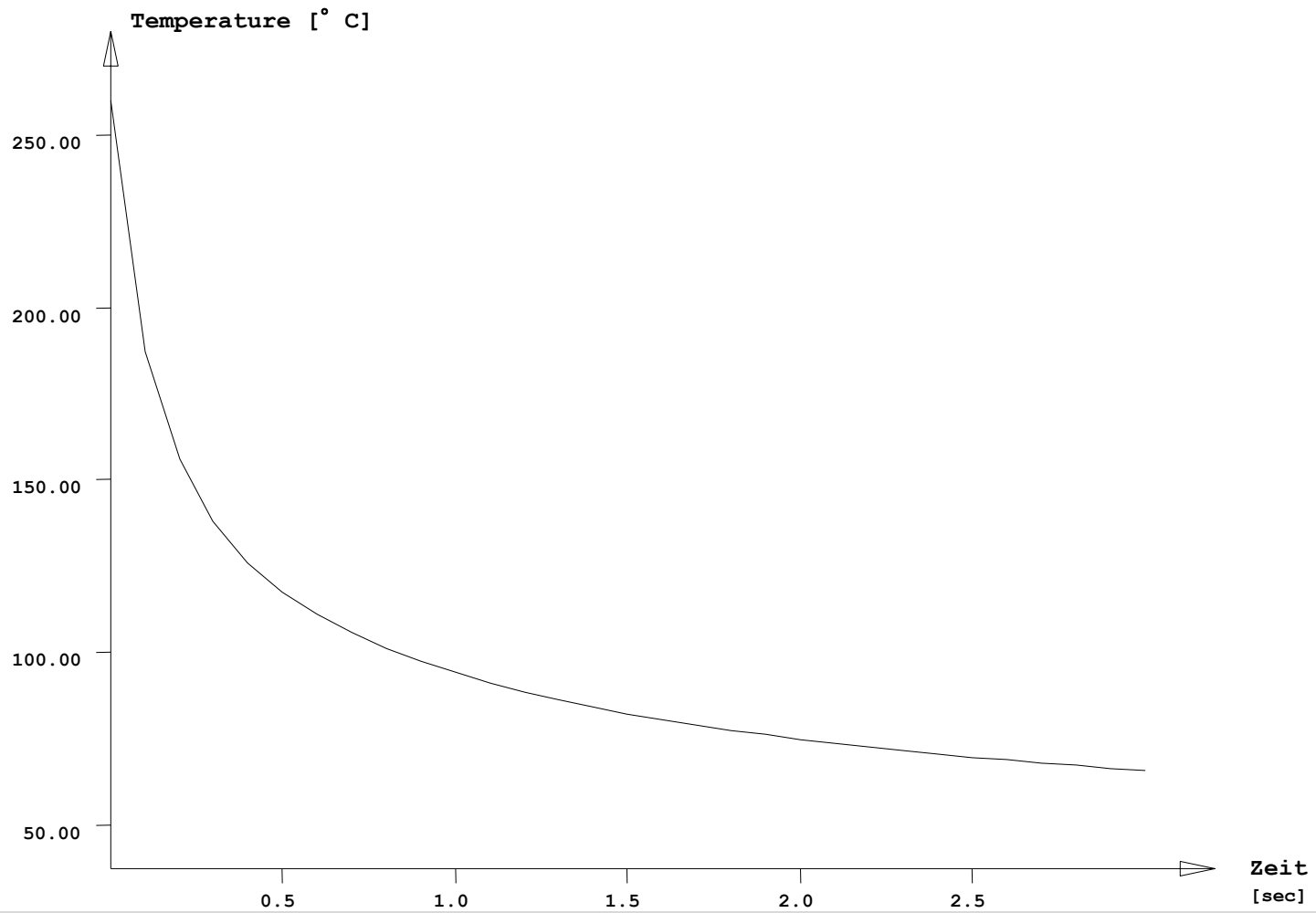
k = Boltzmann constant

Example

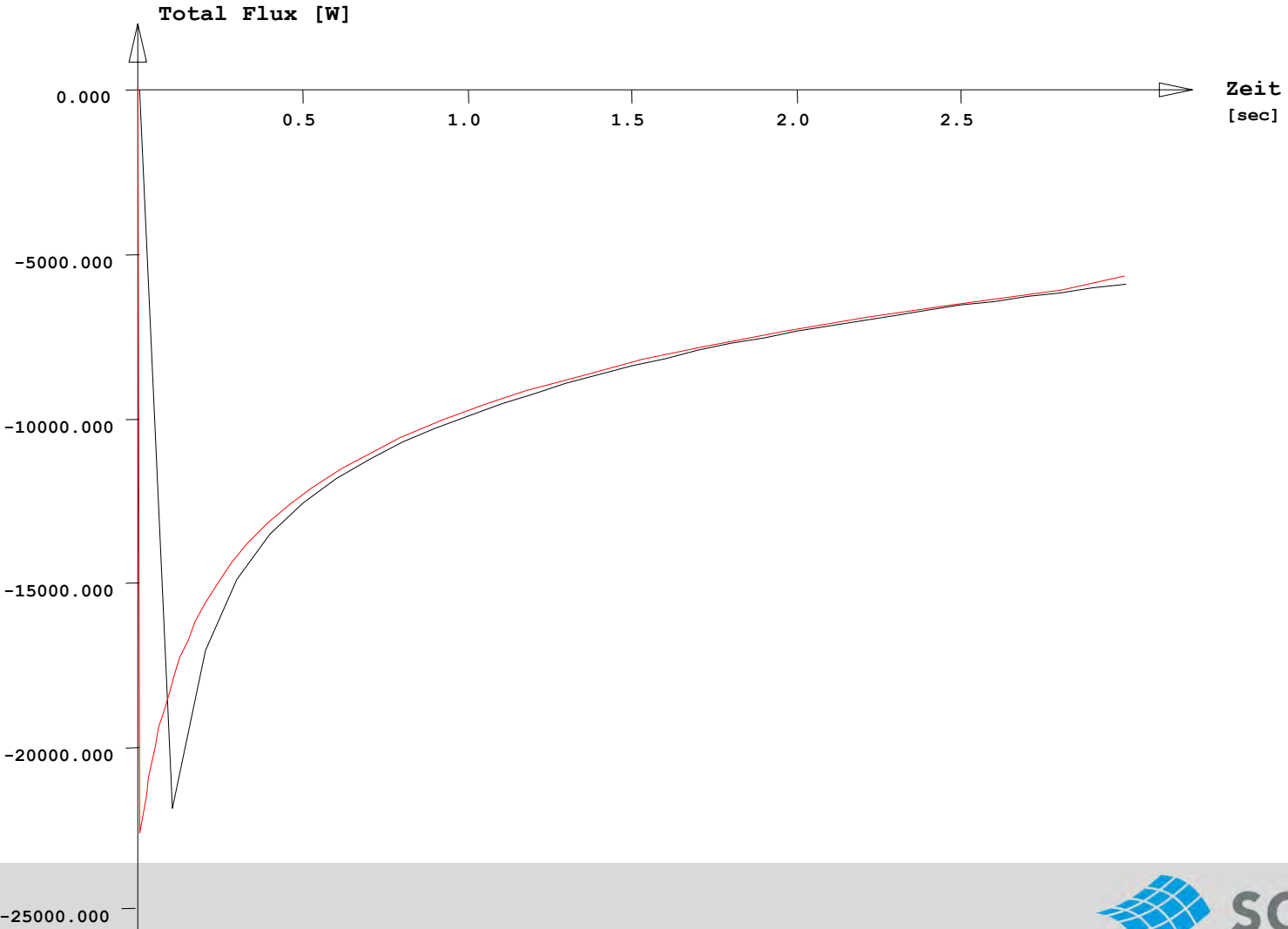


- A hot block with 260 degrees is thrown in a isothermal oil with 37 degrees.
- A sudden heat flow is created at the surface, propagating into the internal area, reducing within time.

Temperature



Heat Flux



Hydration of Concrete

- **During the hydration of concrete heat is produced. The production of heat is dependant on the heat.**
- **The thermal heating and cooling creates stresses**
- **The tensile strength is developing with the time**
- **The sensibility of the required reinforcement is highly dependant on the parameters of that process.**
- **First problem is to find basic rules behind that process**
- **Second problem is to convert those rules to software**
- **And the last problem is to get the real material data**

Basics

- **Base for all properties, strength, elasticity modulus and heat production is the hydration grade α , defined as the ratio of the heat already produced to the maximum heat possible at the end of time:**

$$\alpha = \frac{Q(\tau_w)}{Q(\infty)}$$

The heat production per time is then given by the derivative of that function

Effective Age of Concrete

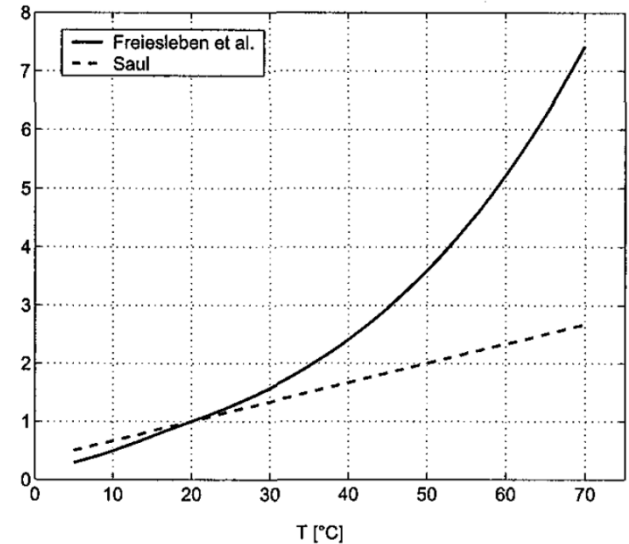
- Empirical (Saul etc.)

$$\tau_w = \int \left[\frac{T + T_{ref}}{20 + T_{ref}} \right]^S dt$$

- Theoretical (Freiesleben etc.)

$$\tau_w = \int \exp \left(\frac{A}{R} \left(\frac{1}{293} - \frac{1}{273 + T} \right) \right) dt$$

$$R = 8.3143 [J / mol K] ; A = 33500 + 1470 \cdot \max(0, 20 - T)$$



Hydration Relations

- **Jonasson**

$$\alpha = \exp \left[b \cdot \ln \left(1 + \frac{\tau_w}{\tau_k} \right)^a \right]$$

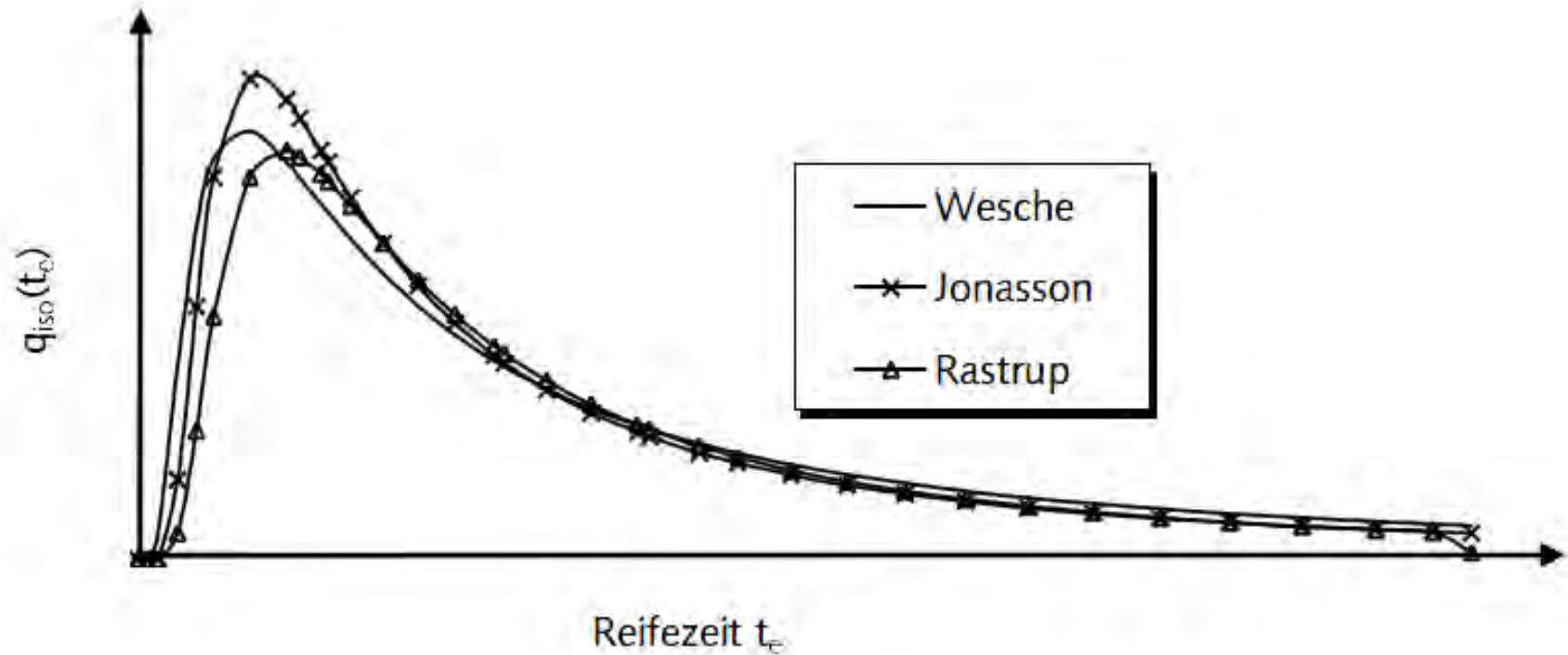
- **Shrinkage Core**

$$\alpha = \frac{a \cdot (\tau_w - \tau_k)}{1 + a \cdot (\tau_w - \tau_k)}$$

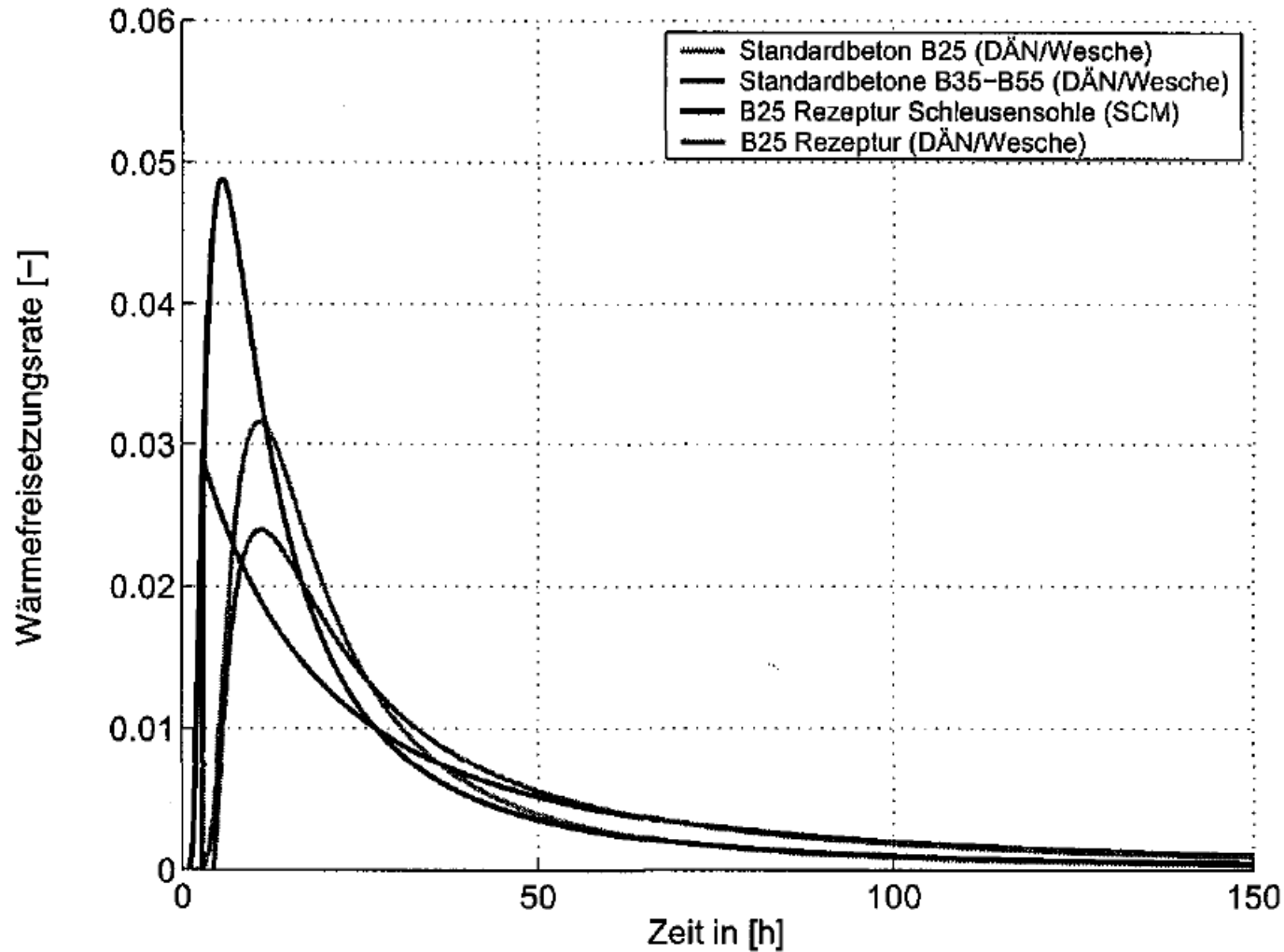
- **Wesche**

$$\alpha = \exp \left[- \left(\frac{\tau_w}{\tau_k} \right)^b \right]$$

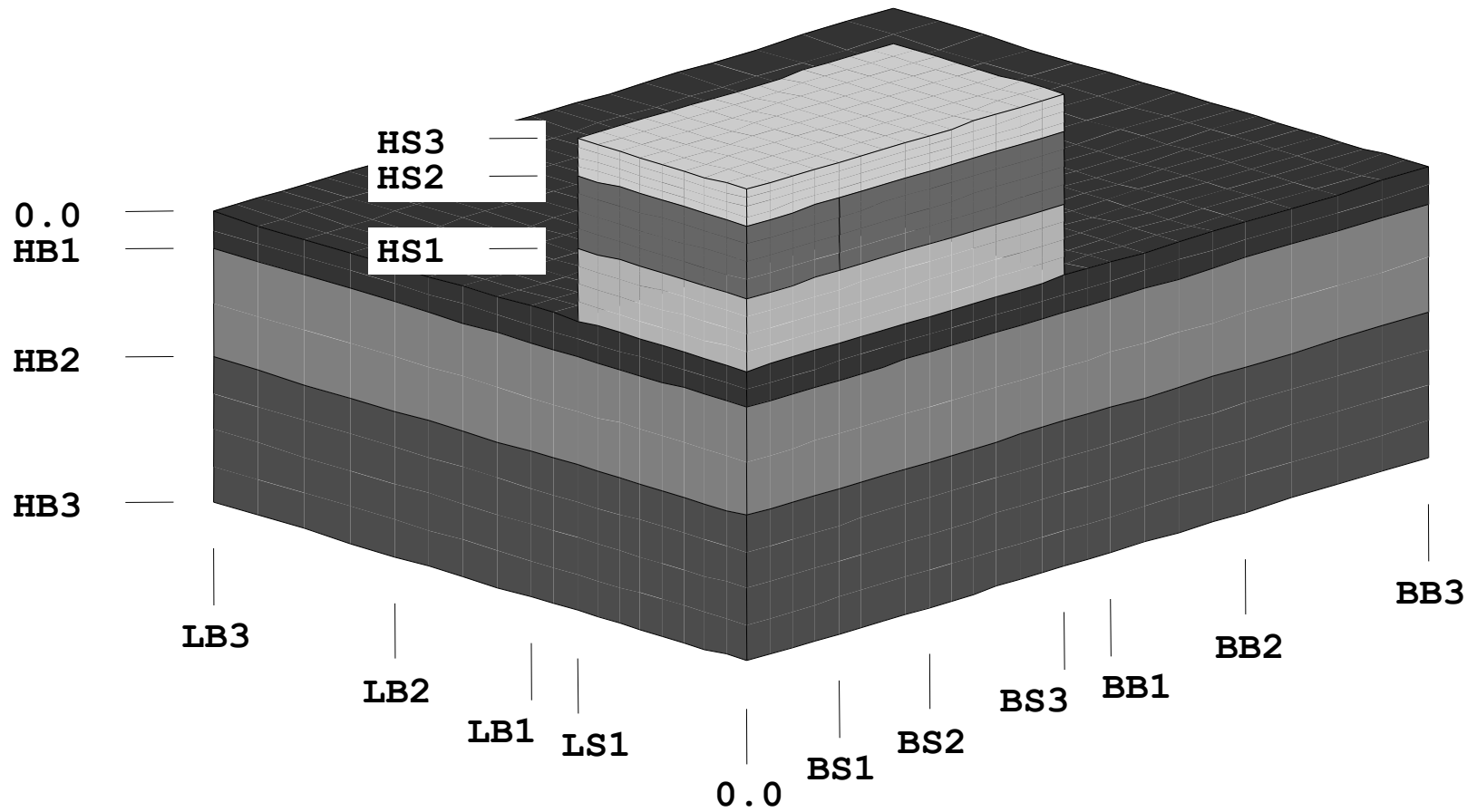
Hydration Relations



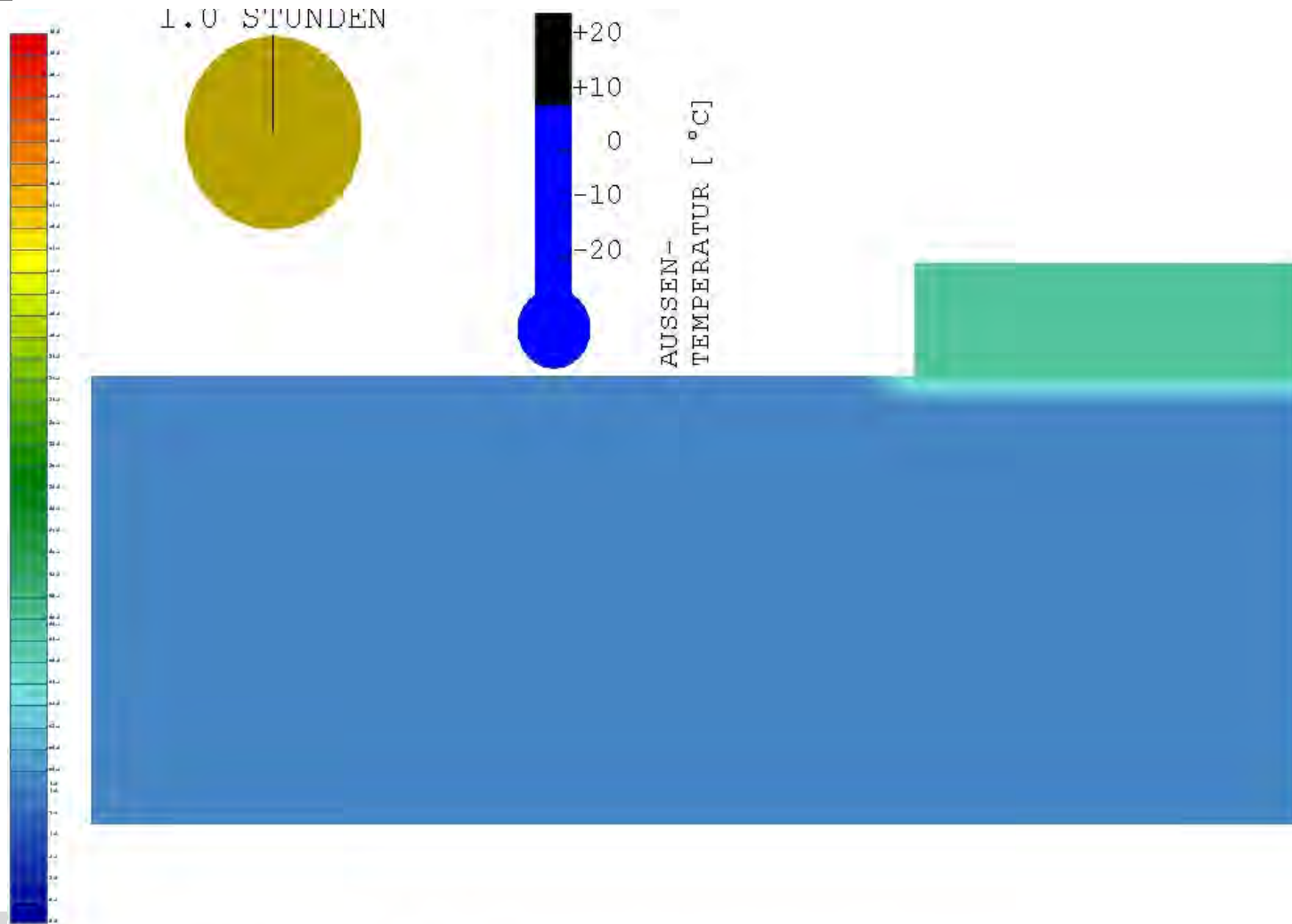
Hydration Relations



Example Hydration



Temperatures of Hydration



Example: Fire Design

- **Materials, especially steel loses its strength when exposed to fire.**
- **So steel will be covered/combined with concrete to protect it.**
- **To design a column we need the heat distribution within the section after 90 min (Fire class R90)**
- **From that we may calculate the hot ultimate bearing capacity**

Parameters for Analysis

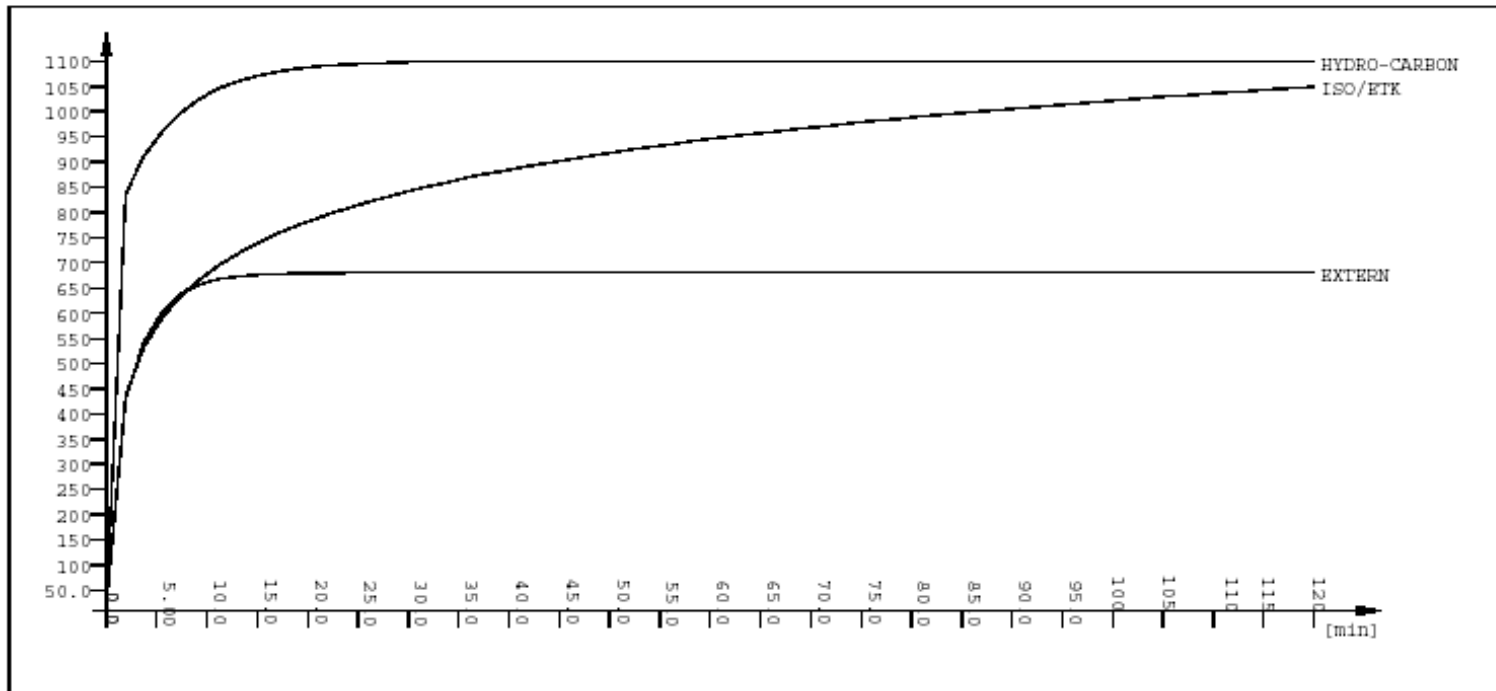
- **Transient analysis**
- **Standard fire design temperature curve**
 $T=T(t)$
- **Radiation boundary conditions are dominant**
- **Temperature dependant conductivity**
- **Temperature dependant capacity including evaporation of pore water in concrete at 100 degree**

Temperature Curves

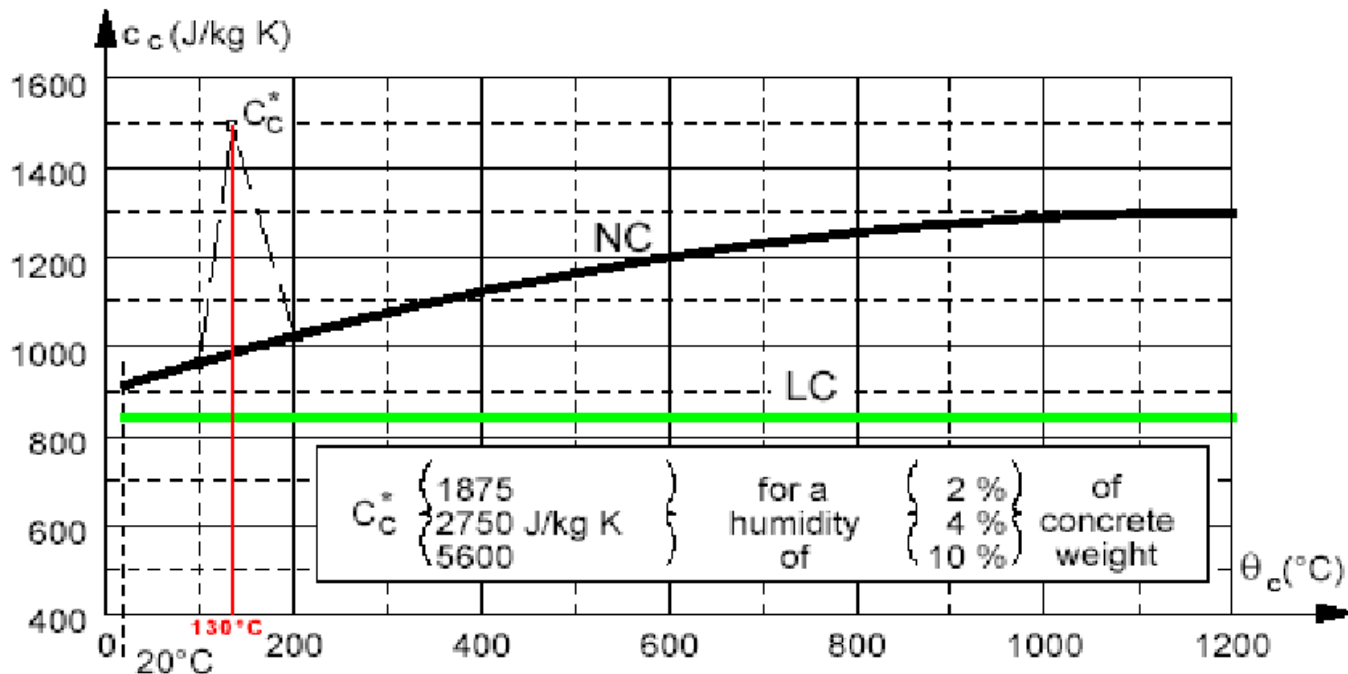
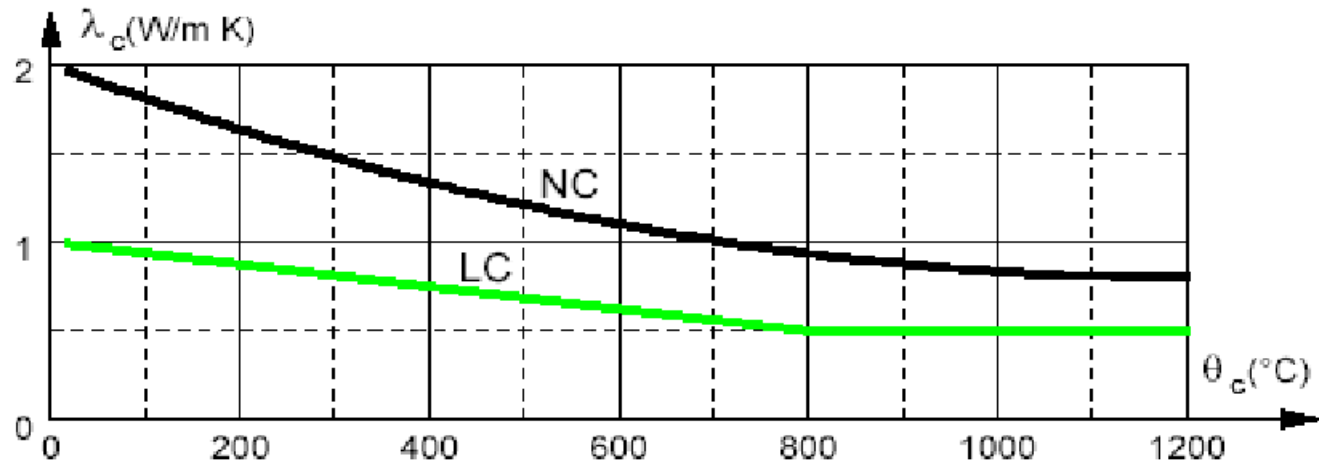
$$T = 20 + 345 \log_{10}(8t + 1) \quad (53)$$

$$T = 20 + 660 \cdot (1 - 0.687 \cdot e^{-0.32t} - 0.313 \cdot e^{-3.8t}) \quad (54)$$

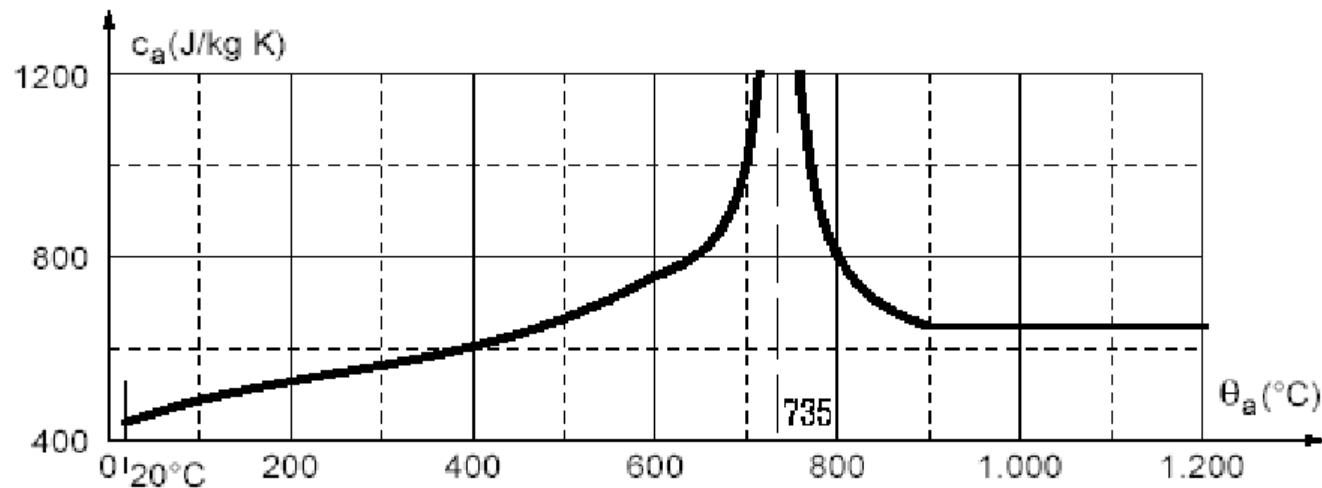
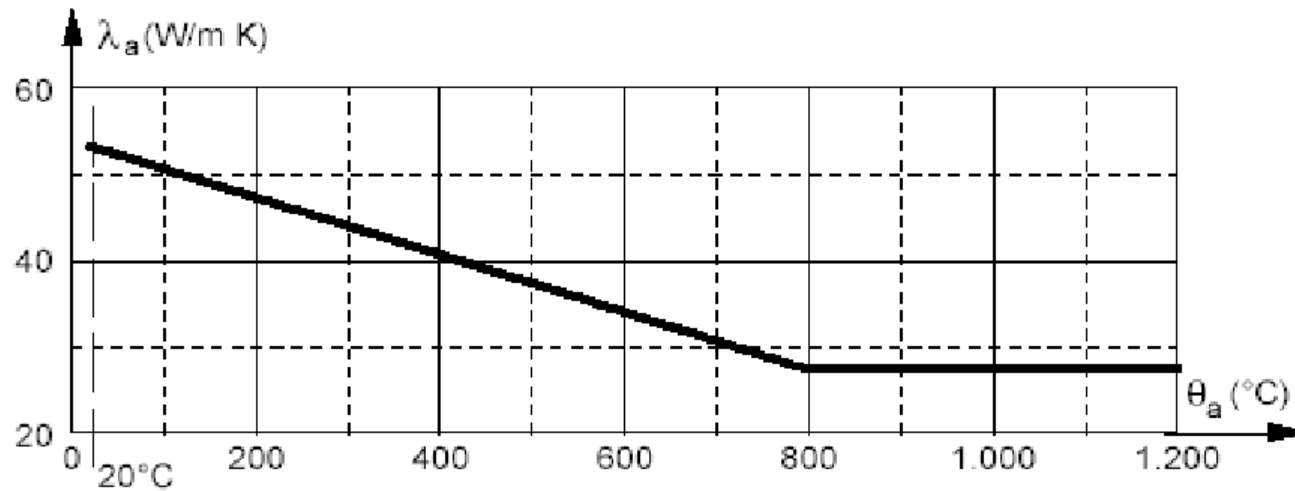
$$T = 20 + 1080 \cdot (1 - 0.325 \cdot e^{-0.167t} - 0.675 \cdot e^{-2.5t}) \quad (55)$$

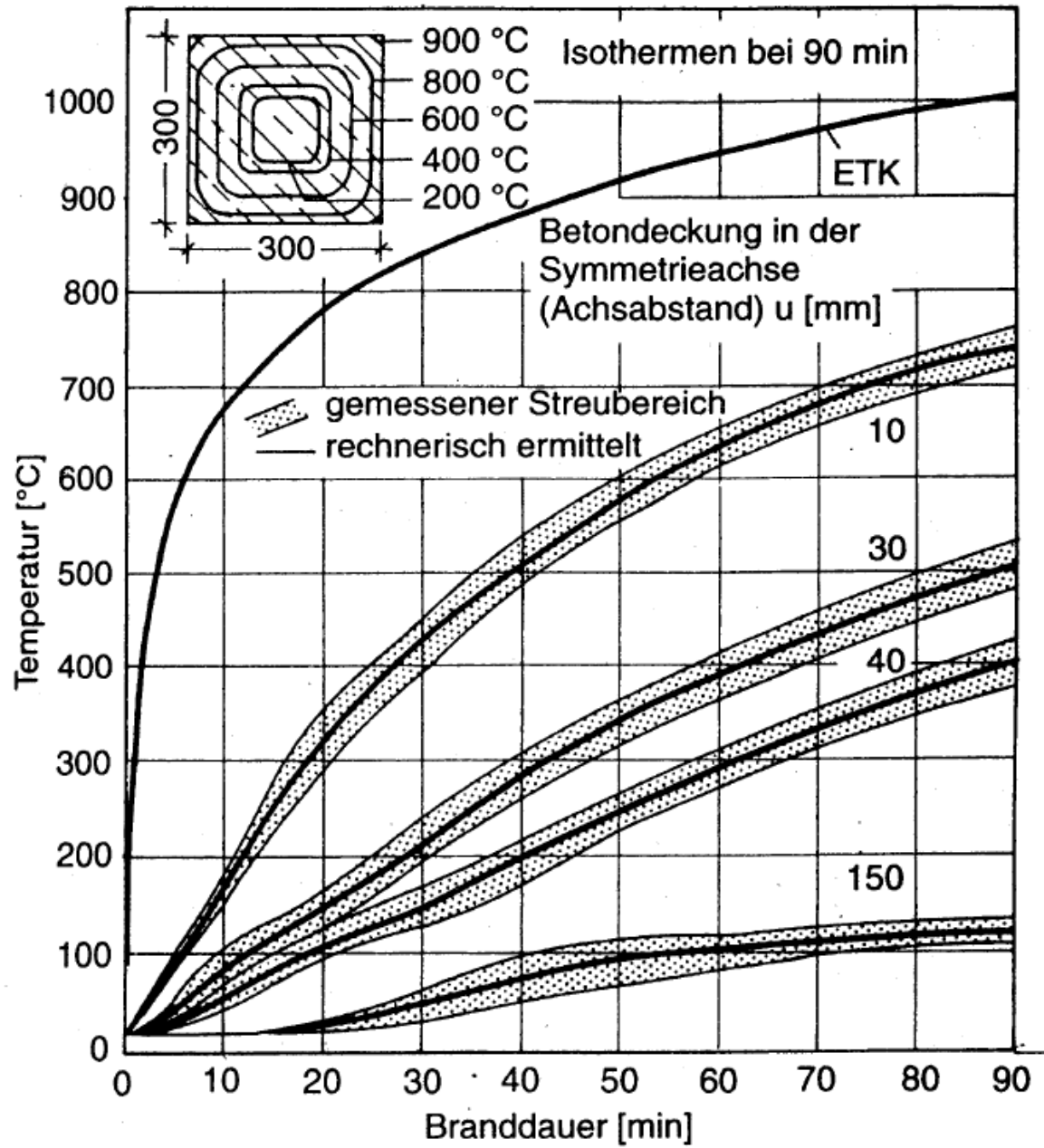


Concrete

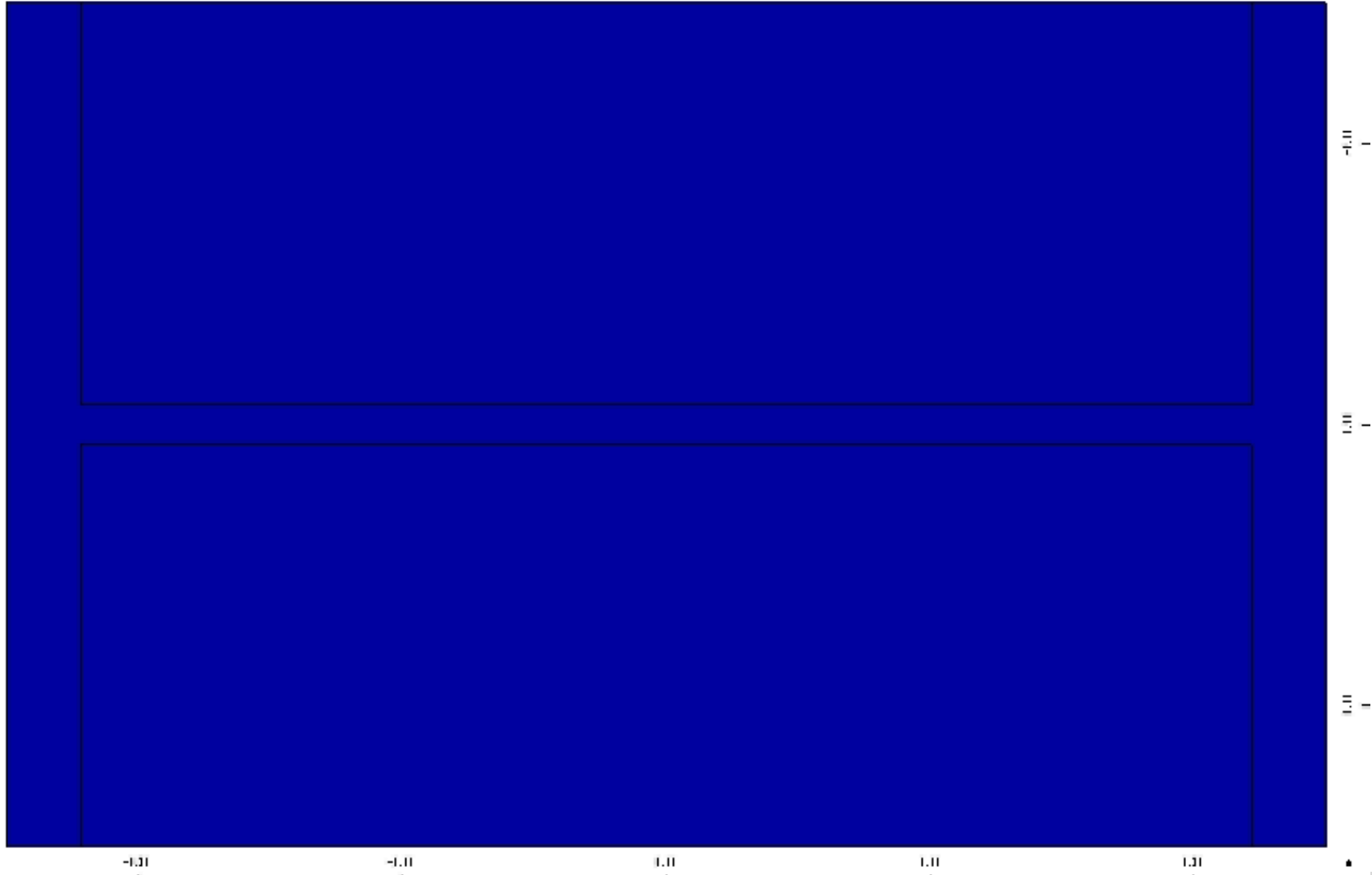


Steel





FE for composite Column



Temperatur in Knoten, Lastfall 1 Zeitpunkt 1.00 sec, von 01.1 bis 1001. Stufen 100.0 grad



Kontur

Example: Heat Storage System

Der Boden als Wärmespeicher

+80°C



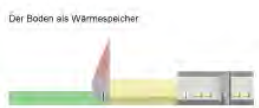
+30°C

+20°C

0°C

-20°C

SOFiSTiK - Temperaturanimation über 1 Jahr



Further fields of application

- **Groundwater seepage**
- **Moisture transport**
- **Electric Fields**
- **Magnetic fields**
- **Shear stress in bars**
- **Lubrication problems**