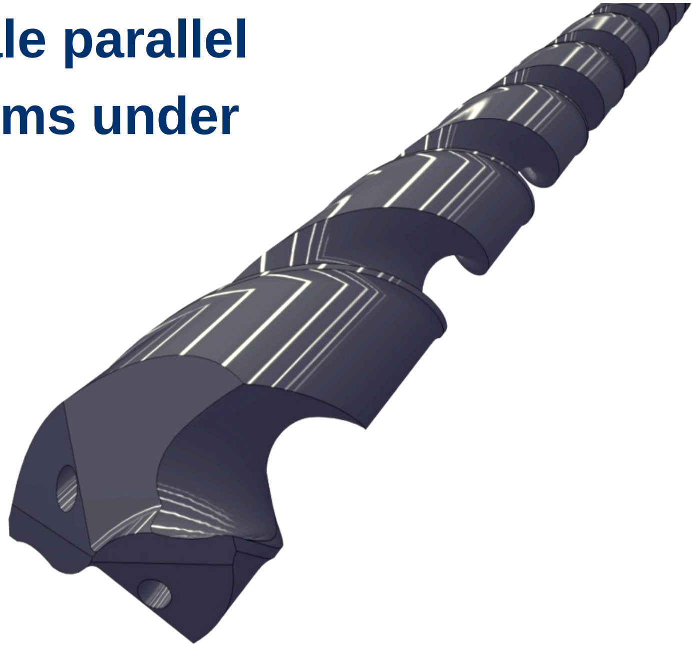
technische universität dortmund

Efficient numerical methods for the large-scale parallel solution of thermomechanical contact problems under consideration of mesh separation



August, 16. 2013

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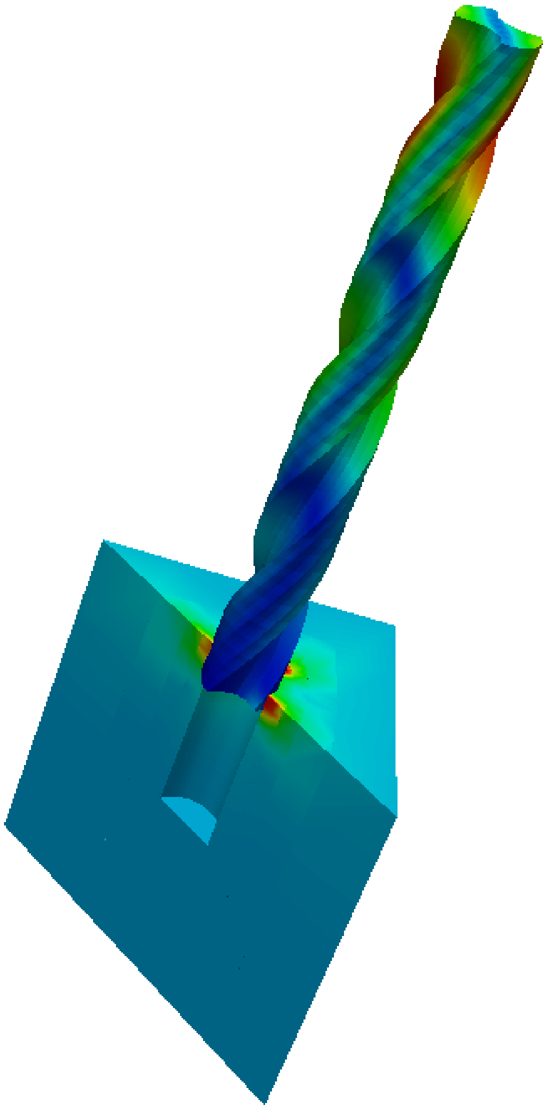
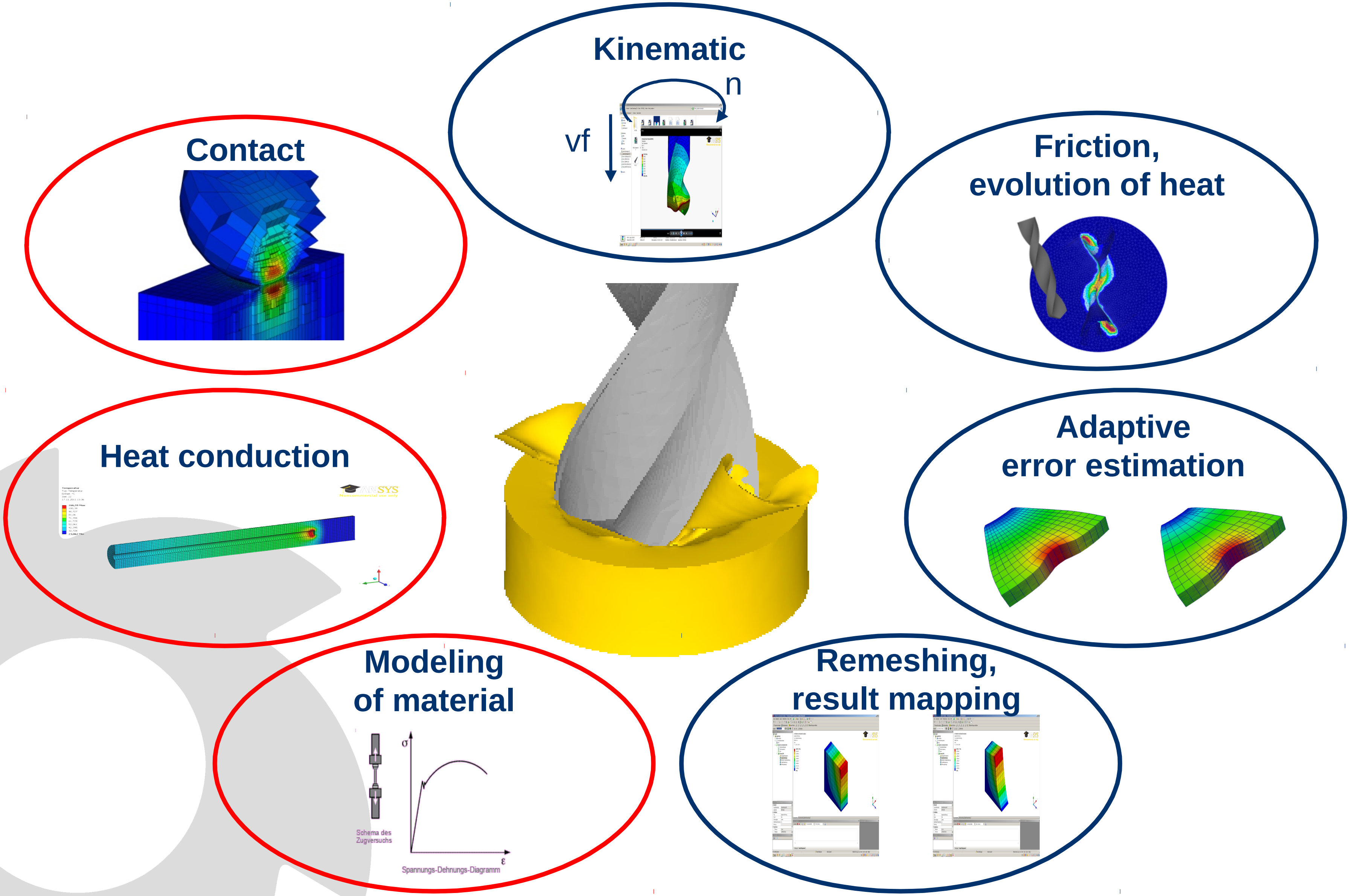
Content

- Motivation
- Modeling of elastoplastic material behavior
  - ➢ Some classical and variational formulations
  - ➢ Including contact problem
- A semismooth Newton method for solving contact and plasticity
- Large-scale parallel solution (Prof. Wolfgang Bangerth and Prof. Timo Heister)
- Coupling with temperature
- Mesh separation by using DG-Elements
- Outlook



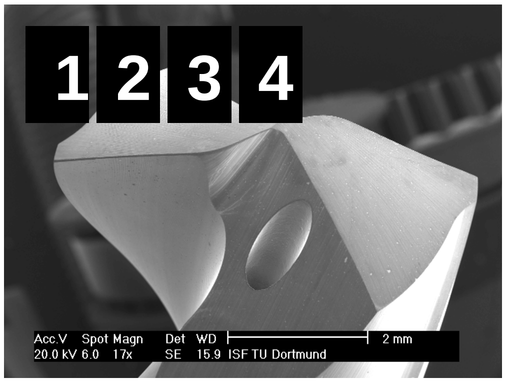
Motivation



Kinematic
n
vf
Contact
Friction,
evolution of heat
Heat conduction
Adaptive
error estimation
Modeling
of material
σ
ε
Schema des
Zugversuchs
Spannungs-Dehnungs-Diagramm
Remeshing,
result mapping

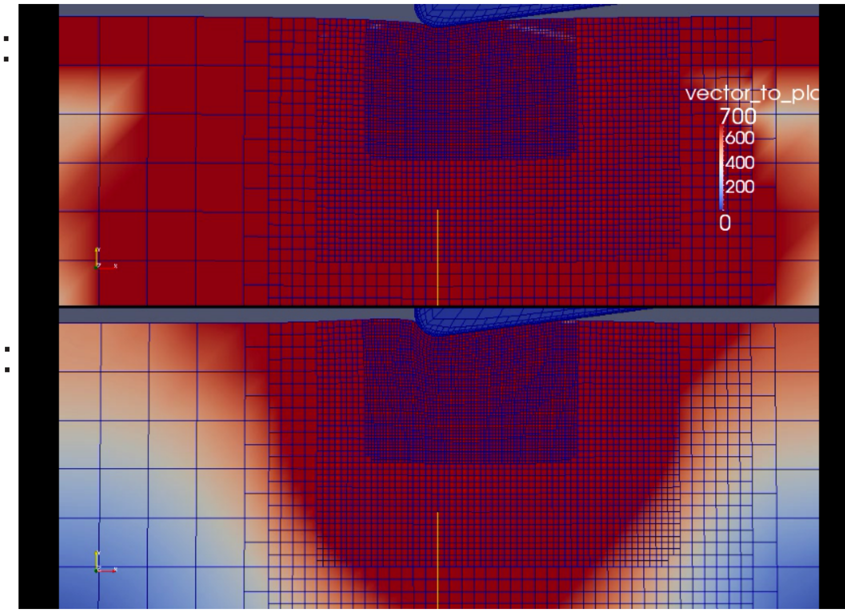
Motivation

Drilling process:



Pure elastic:

Elasto-plastic:



- von. Mises stress intensity:

Classical formulation of the elastic problem

$$-div(\sigma) \geq f \quad , \quad \text{in } \Omega$$ Equilibrium condition

$$u(x,y) = 0 \quad , \quad \text{on } \partial\Omega$$ Boundary condition

$$\sigma = E\nabla u \quad , \quad \text{in } \Omega$$ Hooke's law

Anti-plane shear problem

$$\sigma = \begin{bmatrix} \sigma_{1,1} & \sigma_{1,2} & \sigma_{1,3} \\ \sigma_{1,2} & \sigma_{2,2} & \sigma_{2,3} \\ \sigma_{1,3} & \sigma_{2,3} & \sigma_{3,3} \end{bmatrix} = E \begin{bmatrix} 0 & 0 & \frac{\partial u_3}{\partial x_1} \\ 0 & 0 & \frac{\partial u_3}{\partial x_2} \\ \frac{\partial u_3}{\partial x_1} & \frac{\partial u_3}{\partial x_2} & 0 \end{bmatrix} = E\nabla u$$

Classical formulation of the elastic problem

$$\begin{aligned} -div(\sigma) &= f &&, \quad \text{in } \Omega \\ u(x,y) &= 0 &&, \quad \text{on } \partial\Omega \\ \sigma &= E\nabla u &&, \quad \text{in } \Omega \end{aligned}$$

Equilibrium condition
Boundary condition
Hooke's law

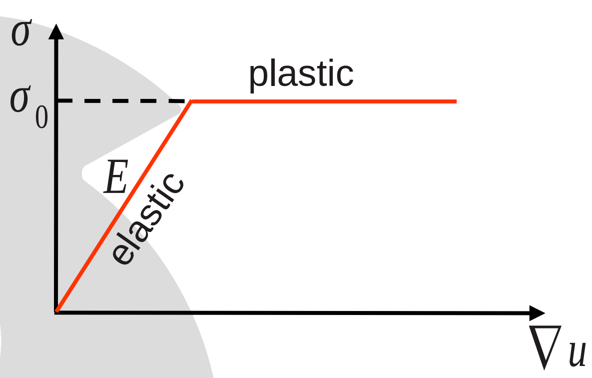
Anti-plane shear problem

$$\begin{aligned} u(x,y) &= u_3(x,y) \\ \sigma &= (\sigma_1,\sigma_2) \\ &= E\left(\frac{\partial u}{\partial x_1},\frac{\partial u}{\partial x_2}\right) \end{aligned}$$

Classical formulation of perfect elastoplasticity

$$
\begin{aligned}
\nabla u &= E^{-1}\sigma + \lambda &&, \text{ in } \Omega && \text{Elasto-plastic formulation}\\
\lambda \cdot (\tau - \sigma) &\leq 0 \quad \forall F(\tau, \ldots) \leq 0 &&, \text{ in } \Omega &&\\
-div(\sigma) &= f &&, \text{ in } \Omega && \text{Equilibrium condition}\\
u(x,y) &= 0 &&, \text{ on } \partial\Omega && \text{Boundary condition}\\
\sigma^{trial} &= E \nabla u &&, \text{ in } \Omega && \text{Hooke's law}
\end{aligned}
$$

Stress-strain diagram:



Some possible yield functions:

$\boxed{F(\tau) = |\tau| - \sigma_0}$ Perfect plastic

$F(\tau, \varepsilon_p) = |\tau| - (\sigma_0 + \gamma_{iso}\varepsilon_p)$ Isotropic hardening

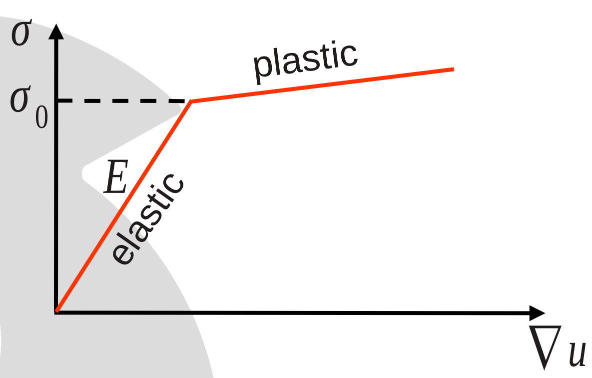
$F(\tau, \varepsilon_p, \dot{\varepsilon}_p, T) = |\tau| - \sigma_y$ Johnson Cook

$$\sigma_y = (A - B\varepsilon_p{}^n)(1 + C\ln(\dot{\varepsilon}_p))(1 - (T - T^R)/(T^m - T^R))$$

Classical formulation of elastoplasticity with linear isotropic hardening

$$
\begin{aligned}
\nabla u &= E^{-1}\sigma + \lambda &&, \text{ in } \Omega && \text{Elasto-plastic formulation}\\
\lambda\cdot(\tau-\sigma) &\le 0 \quad \forall F(\tau,\ldots)\le 0 &&, \text{ in } \Omega &&\\
-div(\sigma) &= f &&, \text{ in } \Omega && \text{Equilibrium condition}\\
u(x,y) &= 0 &&, \text{ on } \partial\Omega && \text{Boundary condition}\\
\sigma^{trial} &= E\nabla u &&, \text{ in } \Omega && \text{Hooke's law}
\end{aligned}
$$

Stress-strain diagram:



Some possible yield functions:

$F(\tau)=|\tau|-\sigma_0$ Perfect plastic

$F(\tau,\varepsilon_p)=|\tau|-(\sigma_0+\gamma_{iso}\varepsilon_p)$ Isotropic hardening

$F(\tau,\varepsilon_p,\dot{\varepsilon}_p,T)=|\tau|-\sigma_y$ Johnson Cook

$$\sigma_y=(A-B\varepsilon_p{}^n)(1+C\ln(\dot{\varepsilon}_p))(1-(T-T^R)/(T^m-T^R))$$

Classical formulation of elastoplasticity with Johnson Cook nonlinear hardening

$$\begin{aligned}
\nabla u &= E^{-1}\sigma + \lambda &&, \text{ in } \Omega \\
\lambda\cdot(\tau - \sigma) &\le 0 \quad \forall F(\tau,\dots)\le 0 &&, \text{ in } \Omega \\
-div(\sigma) &= f &&, \text{ in } \Omega \\
u(x,y) &= 0 &&, \text{ on } \partial\Omega \\
\sigma^{trial} &= E\nabla u &&, \text{ in } \Omega
\end{aligned}$$

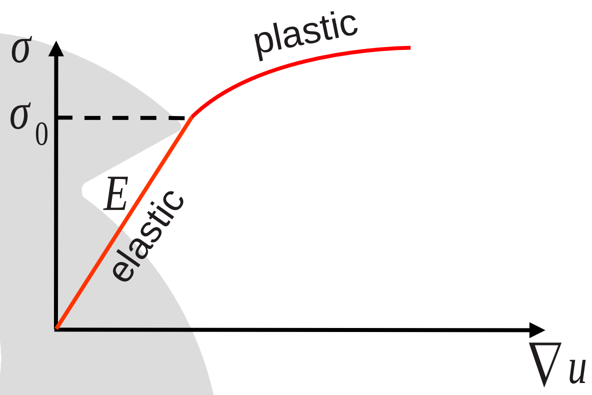
Elasto-plastic formulation

Equilibrium condition

Boundary condition

Hooke's law

Stress-strain diagram:



Some possible yield functions:

$F(\tau) = |\tau| - \sigma_0$ Perfect plastic

$F(\tau, \varepsilon_p) = |\tau| - (\sigma_0 + \gamma_{iso}\varepsilon_p)$ Isotropic hardening

$F(\tau, \varepsilon_p, \dot{\varepsilon}_p, T) = |\tau| - \sigma_y$ Johnson Cook

$$\sigma_y = (A - B\varepsilon_p{}^n)(1 + C\ln(\dot{\varepsilon}_p))(1 - (T - T_R)/(T_M - T_R)^m)$$

Classical formulation of elastoplasticity with contact

$$
\begin{array}{rcll}
\nabla u & = & E^{-1}\sigma + \lambda & , \text{ in } \Omega \\
\lambda \cdot (\tau - \sigma) & \leq & 0 \quad \forall F(\tau, \dots) \leq 0 & , \text{ in } \Omega \\
-div(\sigma) & = & f & , \text{ in } \Omega \\
u(x,y) & = & 0 & , \text{ on } \partial\Omega \\
(\Delta u + f)(u - g) & = & 0 & , \text{ in } \Omega \\
u(x,y) & \geq & g(x,y) & , \text{ in } \Omega \\
\sigma^{trial} & = & E \nabla u & , \text{ in } \Omega
\end{array}
$$

Elasto-plastic formulation

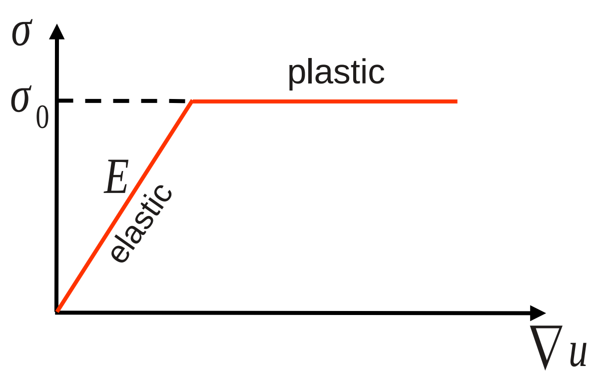
Equilibrium condition

Boundary condition

Contact-conditions

Hooke's law

Stress-strain diagram:



(Dual) Variational formulation of perfect elastoplasticity with contact

Find a pair $(\sigma, u) \in \Pi W_0^{div} \times V^+$

$$\left(E^{-1}\sigma, \tau - \sigma\right) + \left(u, div(\tau) - div(\sigma)\right) \geq 0 \qquad \forall \tau \in \Pi W_0^{div}$$

$$-\left(div(\sigma), \phi - u\right) \geq \left(f, \phi - u\right) \qquad \forall \phi \in V^+$$

$$W_f^{div} := \left\{ \tau \in L^2(\Omega)^2 \,|\, div(\tau) \in L^2(\Omega),\ div(\tau) + f \geq 0 \text{ in } \Omega \right\}$$

$$\Pi W_f^{div} := \left\{ \tau \in W_f^{div} \,|\, |\tau| \leq \sigma_0 \right\}$$

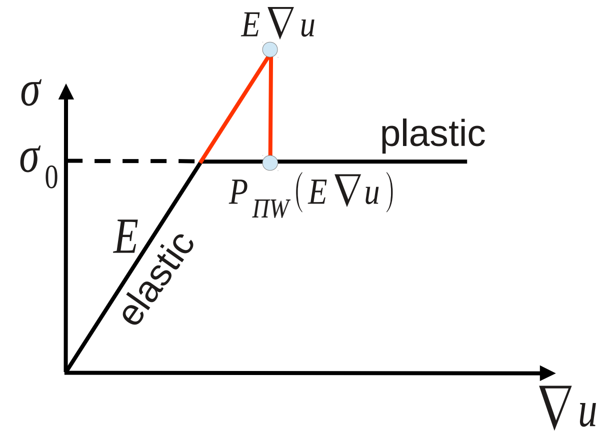
$$V^+ := \left\{ v \in H_0^1(\Omega) : v \geq g \ \text{ a.e. in } \Omega \right\}$$

(Primal) Variational formulation of perfect elastoplasticity with contact

Applying a projection theorem yields:

$$\sigma = P_{\Pi W}(E\nabla u) = \begin{cases} \tau, & |\tau| \leq \sigma^0 \\ \sigma^0 \dfrac{\tau}{|\tau|}, & |\tau| > \sigma^0 \end{cases}$$

Stress-strain diagram:



Find $u \in V^+$

$$\left(P_{\Pi W}(E\nabla u), \varepsilon(\phi) - \varepsilon(u)\right) \geq (f, \phi) \ \forall \phi \in V^+$$

Primal-dual active set method

(1) Initialize A_1 and F_1, such that $S = A_1 \cup F_1$ and $A_1 \cap F_1 = \{\}$

(2) Assemble newton matrix $A^k = a'\left(u^{k-1}; \phi_i, \phi_j\right)$ and right-hang-side $f(u^{k-1})$.

(3) Find primal-dual pair $(\bar{u}^k, \lambda^k)$

$$\begin{aligned} A^k \bar{u}^k + B\lambda^k &= f(u^k), \\ \bar{u}^k_{n,p} &= g_p \quad \forall\, p \in A_k, \\ \lambda^k_p &= 0 \quad \forall\, p \in F_k. \end{aligned}$$

(4) Line search: Find $\alpha \in (0,1]$ with $|f(u^k)| < |f(u^{k-1})|$ for
$u^k = \alpha u^{k-1} + (1-\alpha)\bar{u}^k$

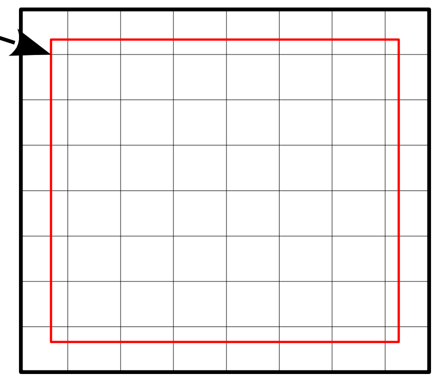
(5) Define new active and inactive sets by

$$\begin{aligned} A_{k+1} &:= \left\{ p \in S : \lambda^k_p + c\left(u^k_{n,p} - g_p\right) > 0 \right\}, \\ F_{k+1} &:= \left\{ p \in S : \lambda^k_p + c\left(u^k_{n,p} - g_p\right) \leq 0 \right\}. \end{aligned}$$

(6) If $A_{k+1} = A_k$, $F_{k+1} = F_k$ and $\boxed{|f(u^k)| < \delta}$ then stop,
else set $k = k+1$ and go to step (2).

all vertices inside the red rectangle

Mesh



Primal-dual active set method

(1) Initialize A_1 and F_1, such that $S=A_1 \cup F_1$ and $A_1 \cap F_1 = \{\}$

(2) Assemble newton matrix $A^k = a'(u^{k-1};\phi_i,\phi_j)$ and right-hang-side $f(u^{k-1})$.

(3) Find primal-dual pair $(\bar{u}^k, \lambda^k)$

$$\begin{aligned} A^k \bar{u}^k + B\lambda^k &= f(u^k), \\ \bar{u}^k_{n,p} &= g_p \quad \forall p \in A_k, \\ \lambda^k_p &= 0 \quad \forall p \in F_k. \end{aligned}$$

Condensation of lambda by biorthogonal ansatz-functions

$$\int \phi_i \varphi_j \, dx = \delta_{i,j} \int \varphi_j \, dx$$

results in a smaller system.

(4) Line search: Find $\alpha \in (0,1]$ with $|f(u^k)| < |f(u^{k-1})|$ for $u^k = \alpha u^{k-1} + (1-\alpha)\bar{u}^k$

(5) Define new active and inactive sets by

$$A_{k+1} := \{ p \in S : \lambda^k_p + c(u^k_{n,p} - g_p) > 0 \},$$

$$F_{k+1} := \{ p \in S : \lambda^k_p + c(u^k_{n,p} - g_p) \leq 0 \}.$$

(6) If $A_{k+1} = A_k$, $F_{k+1} = F_k$ and $\boxed{|f(u^k)| < \delta}$ then stop, else set $k = k+1$ and go to step (2).

M. Hintermueller, K. Ito, K. Kunisch: The primal-dual active set strategy as a semismooth Newton method, 2003.

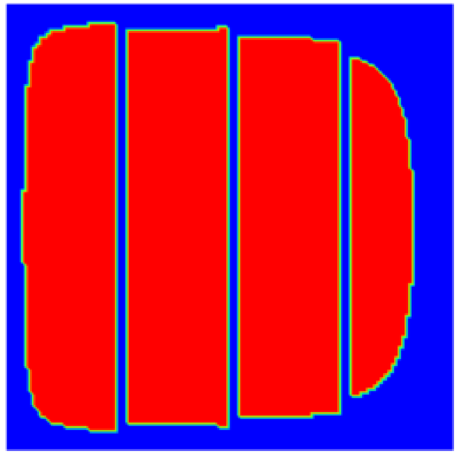
Brunssen, Schmid, Schäfer, Wohlmuth: A fast and robust iterative solver for nonlinear contact problems using a primal-dual active set strategy and algebraic multigrid, Int. J. Numer. Meth. Engng, 2007, 69, pp. 524-543

Frohne, Heister, Bangerth: Efficient numerical methods for large-scale, parallel solution of elastoplastic contact problems, submitted 2013.

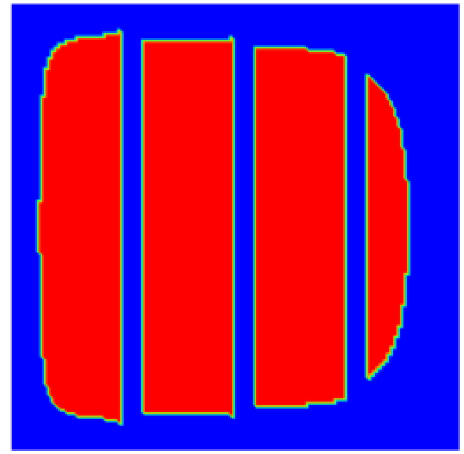
Example for linear elasticity (see step-41)

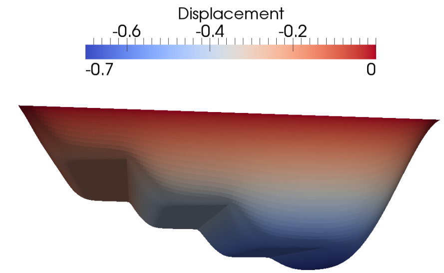
Step 0

Step 3

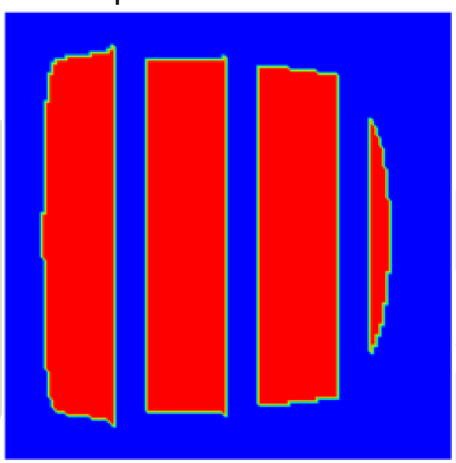


Step 6

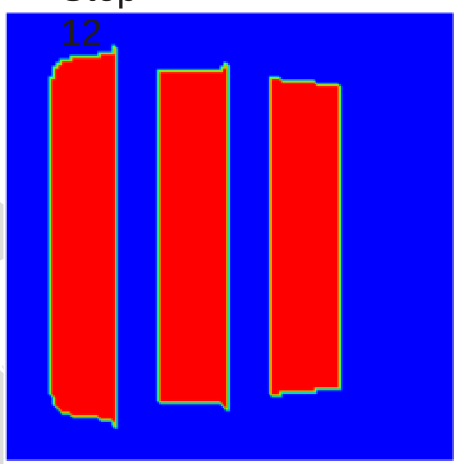




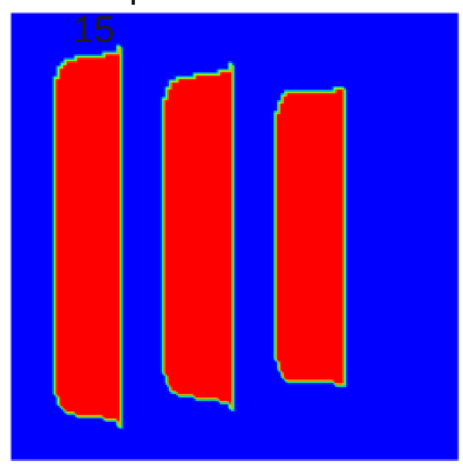
Step 9



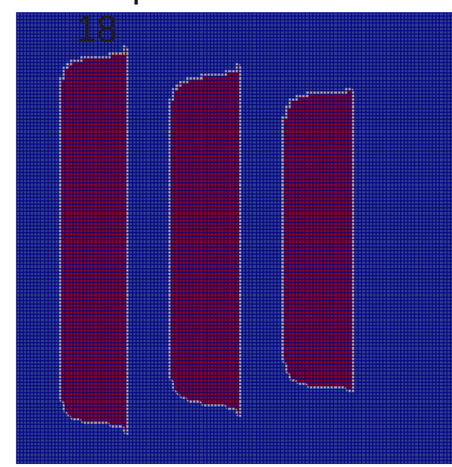
Step 12



Step 15



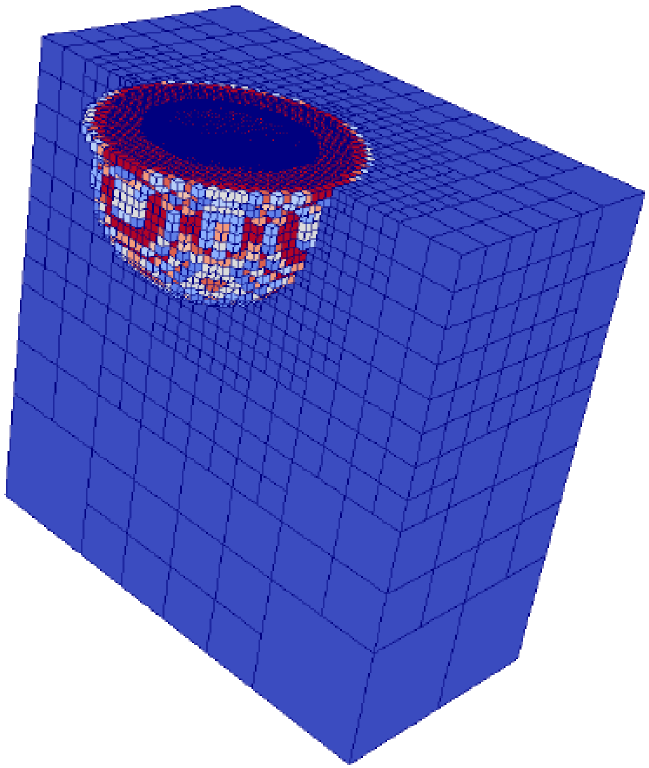
Step 18



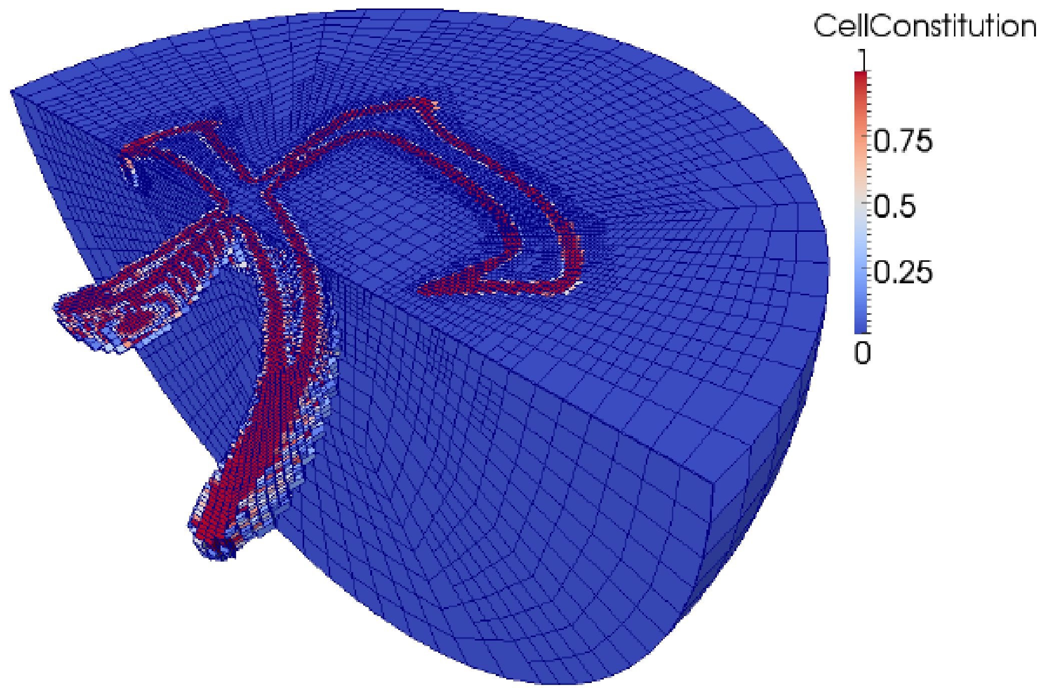
Contact-area red colored

Two examples for the large-scale solution of elastoplasticity with contact (see step-42)

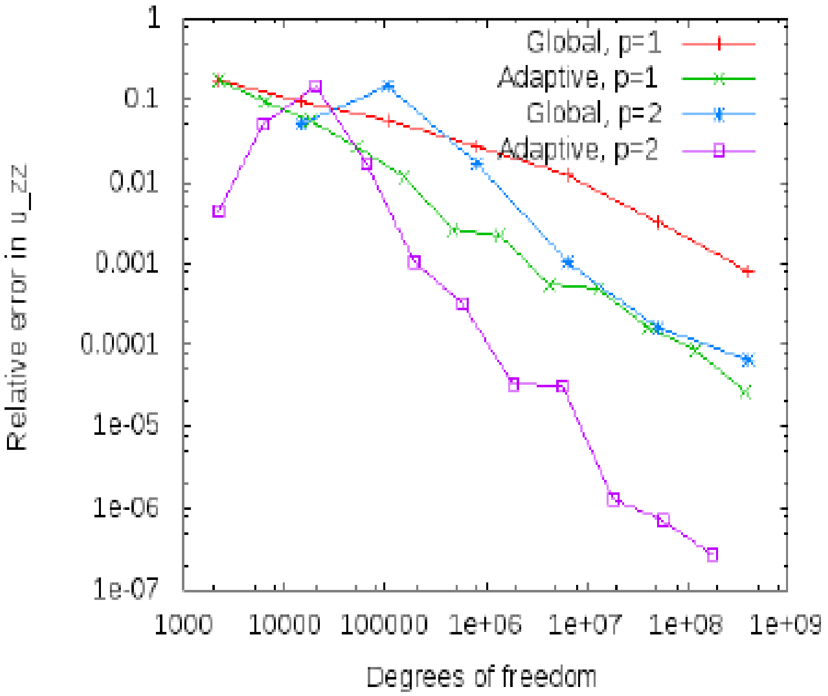
Ball

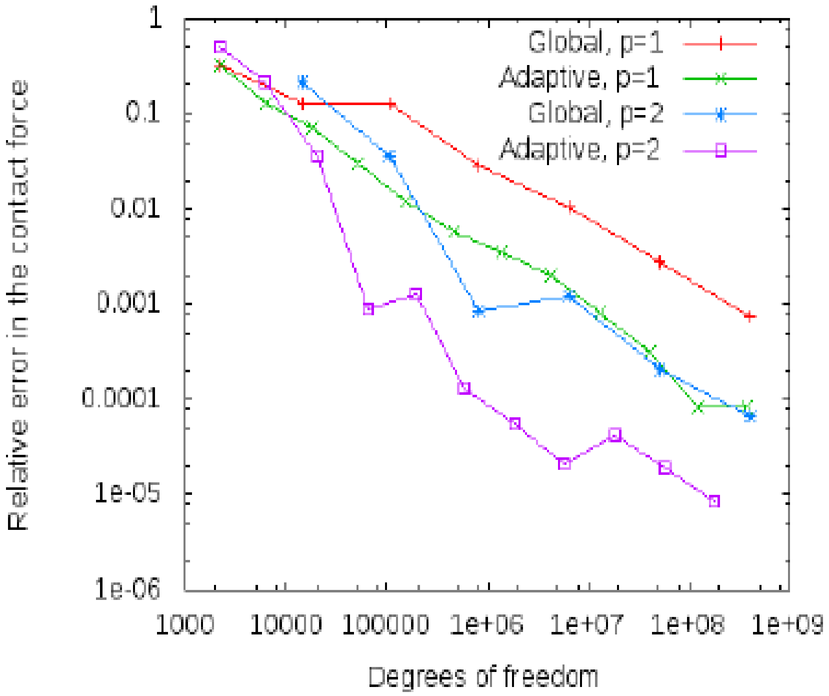


Chinese Symbol for force

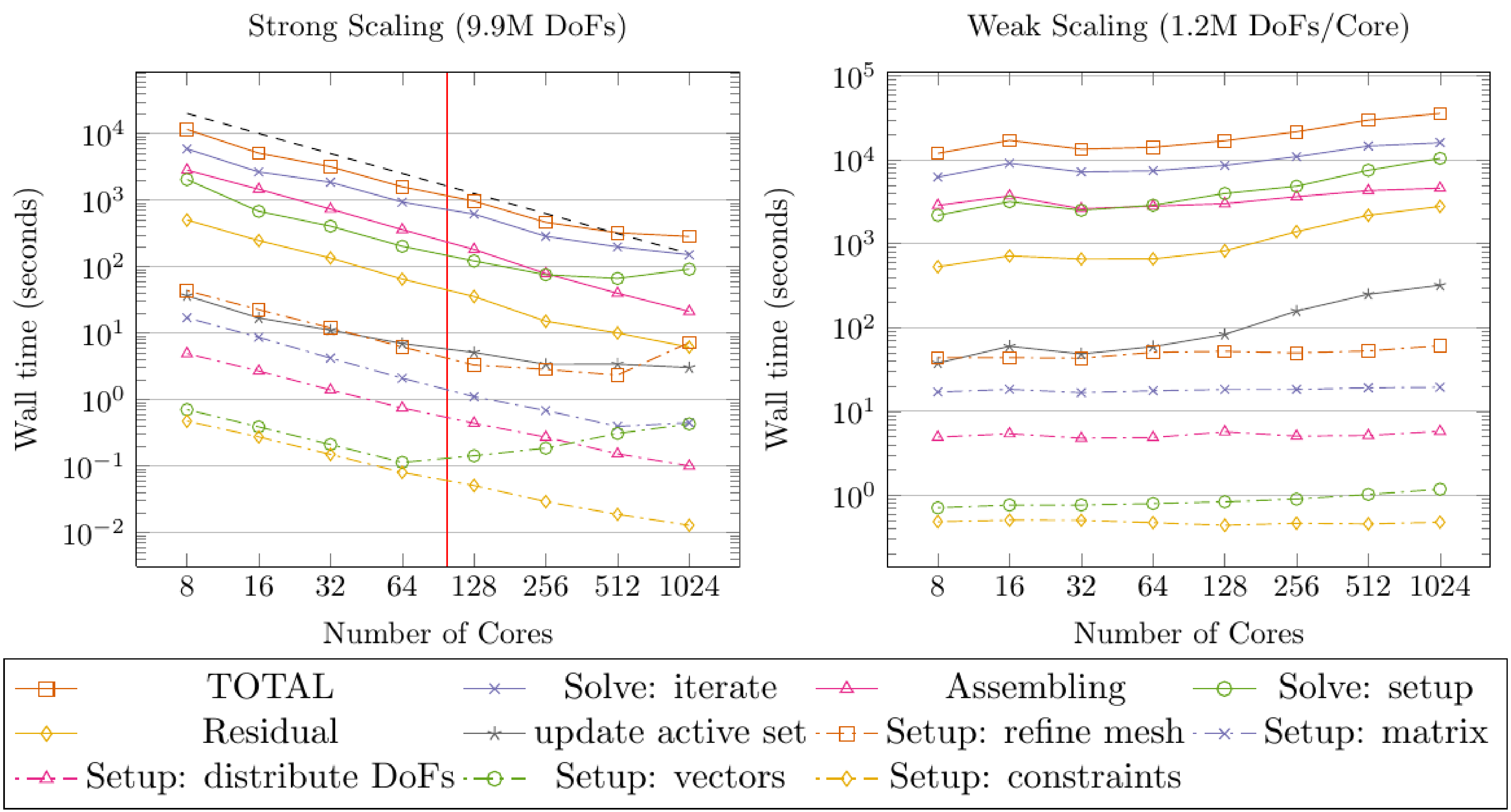


Convergence for the left contact situation with the ball





Strong and weak scaling of our algorithms



Classical formulation of thermomechanical contact problem (with Gough-Joule effect)

$\nabla u = E^{-1}\sigma + \lambda$	,	in Ω	Elasto-plastic formulation
$\lambda \cdot (\tau - \sigma) \leq 0 \quad \forall F(\tau) \leq 0$	,	in Ω	
$-div(\sigma) + dim\, K\, \alpha \nabla T = f$	,	in Ω	Equilibrium condition
$\boxed{c\,\dot{T} + dim\, K\, \alpha\, T_R - \mathrm{div}(\kappa \nabla T) = r}$	,	in Ω	Heat equation
$u(x,y) = 0, \; T = 0$	,	on $\partial\Omega$	Boundary condition
$(\Delta u + f)(u - g) = 0$	,	in Ω	Contact-conditions
$u(x,y) \geq g(x,y)$	,	in Ω	
$\sigma^{trial} = E \nabla u$	,	in Ω	Hooke‘s law

c Specific heat capacity

α Thermal expansion

κ Thermal conductivity

K Bulk modulus

Linearization to apply a Newton method for plasticity

Find $(u^i, T^i) \in V^+$

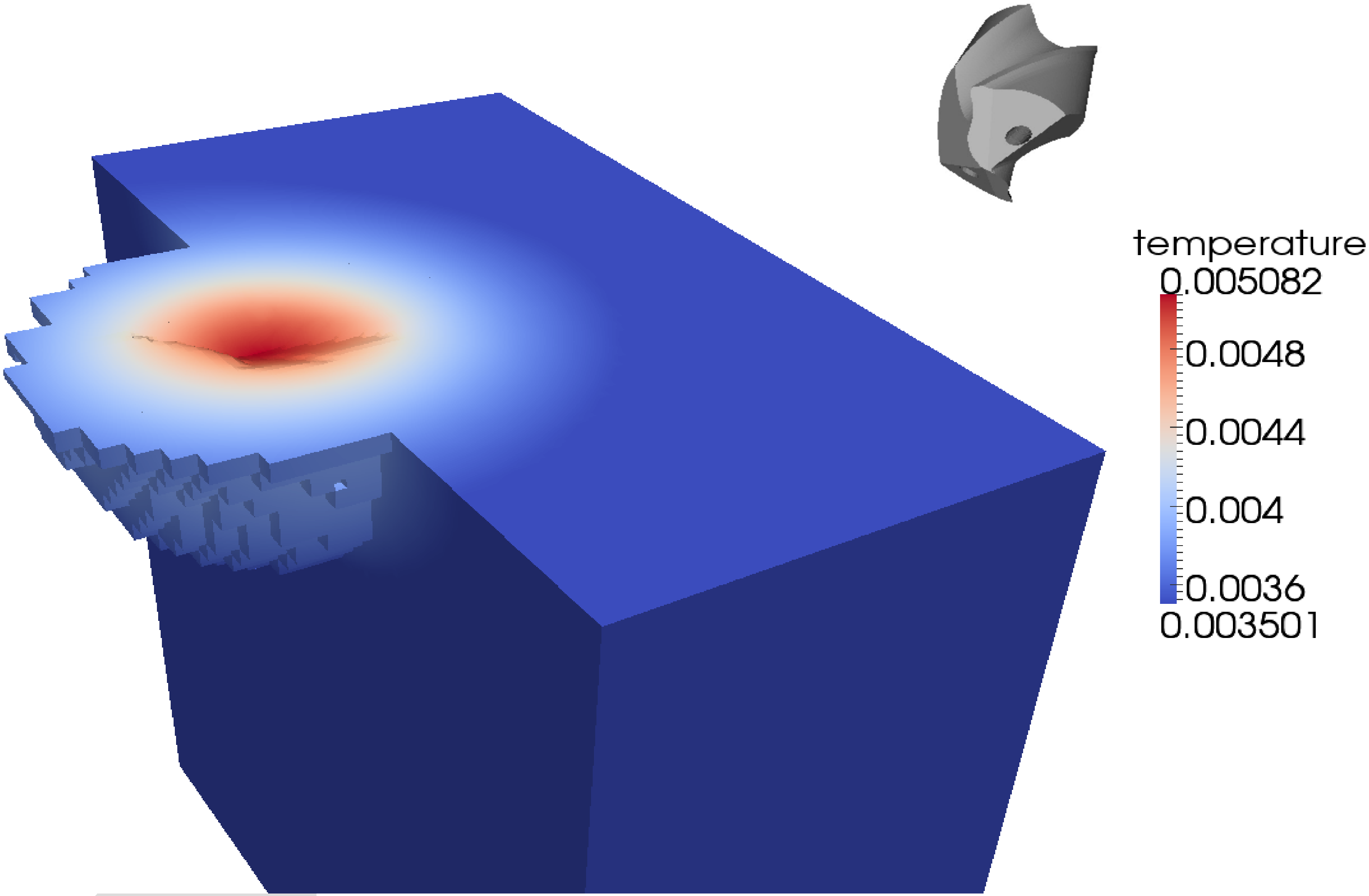
$$\left(P'_{\Pi W}\left(E\nabla u^{i-1}\right)\nabla u^i, \nabla\phi\right) + dim\,K\,\alpha\left(\nabla T^i, \phi\right) \geq \left(f, \phi\right) \;\; \forall \phi \in V^+$$

$$dim\,K\,T_R\,\alpha\left(\mathrm{div}\,u^i, \chi\right) + \kappa\left(\nabla T^i, \nabla\chi\right) = \left(r, \chi\right) \;\; \forall \chi \in H_0^1(\Omega)$$

Alternatively (for very short processes) one can skip the heat equation and the coupling terms and evolute the temperature as another internal variable (adiabatic):

$$\rho_0 c \dot{T} = \beta \sigma_y \dot{\varepsilon}_p, \quad \beta \text{ Taylor-Quinney constant}$$

Solution of a coupled system with Gough-Joule effect

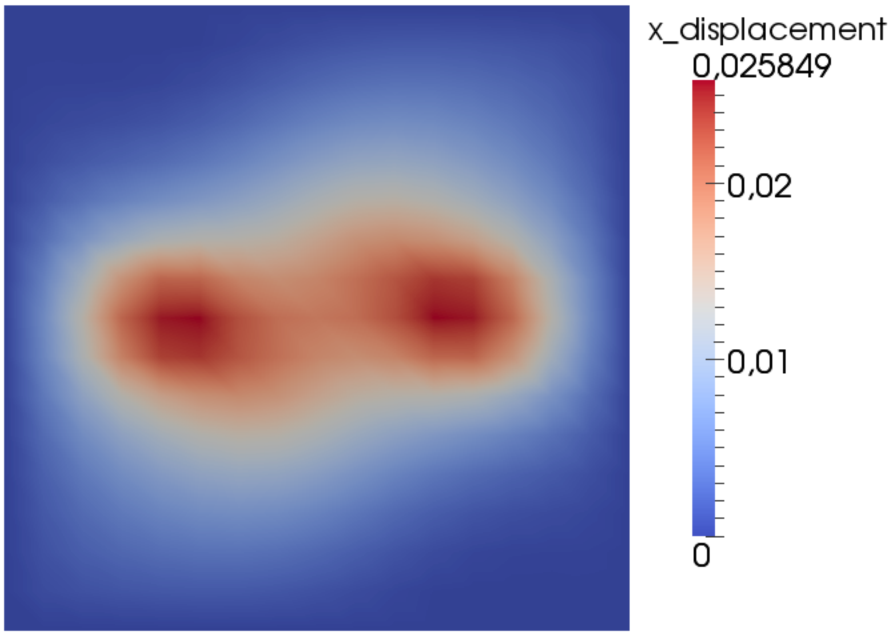


Example of linear elasticity (step-8)

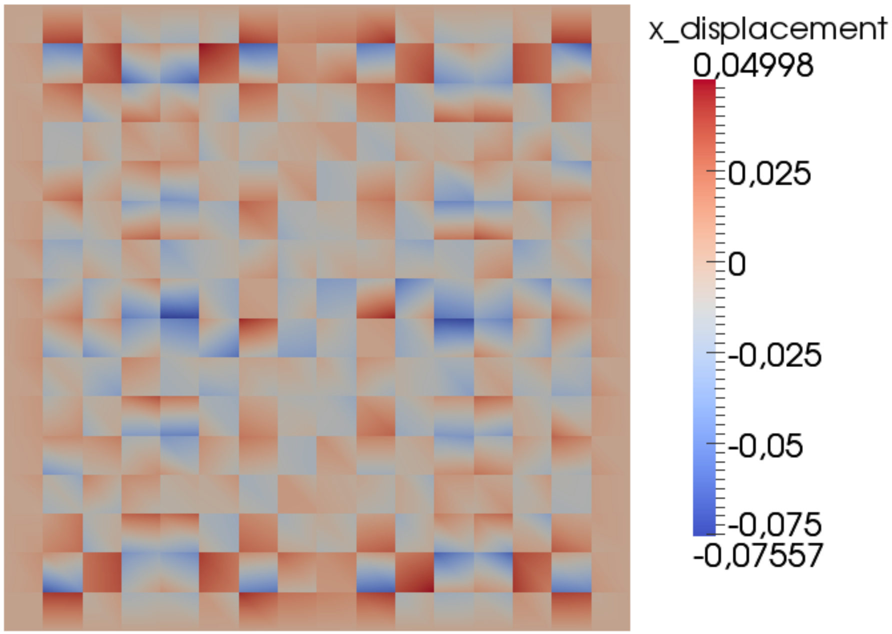
$$
\begin{aligned}
-\operatorname{div}\sigma(u) &= f, && in\ \Omega \\
u &= 0, && \text{auf } \partial\Omega
\end{aligned}
$$

$$f(x) = \begin{pmatrix}1\\0\end{pmatrix}, x \in \mathbb{B}_{0.2}(0.5,0) \cup \mathbb{B}_{0.2}(-0.5,0)$$

CG elements



DG elements



Nitsches method

Weak formulation including:

- Penalty terms for the Dirichlet boundary
- Penalty terms for the interia boundaries

$$a(\mathrm{u},\varphi) = \int_{T} \sigma(u) : \varepsilon(\varphi) dx - \int_{\partial T_{int}} (\langle \sigma(u) \cdot n \rangle \cdot \varphi) + \sigma(\varphi) \cdot n \cdot \frac{[u]}{2} ds + \mu \int_{\partial T_{int}} \frac{\gamma_\mu}{h} \cdot [u] \cdot \varphi$$

$$+\lambda \int_{\partial T_{int}} \frac{\gamma_\lambda}{h} \cdot [u \cdot n] \cdot \varphi \cdot n \, ds - \int_{\partial T_D} \sigma(u) \cdot n \cdot \varphi + \sigma(\varphi) \cdot n \cdot u \, ds + \mu \int_{\partial T_D} \frac{\gamma_\mu}{h} \cdot u \cdot \varphi \, ds$$

$$+\lambda \int_{\partial T_D} \frac{\gamma_\lambda}{h} u \cdot n \, \varphi \cdot n \, ds$$

μ, λ Lamé constants

$\gamma_\mu, \gamma_\lambda$ Penalty parameters

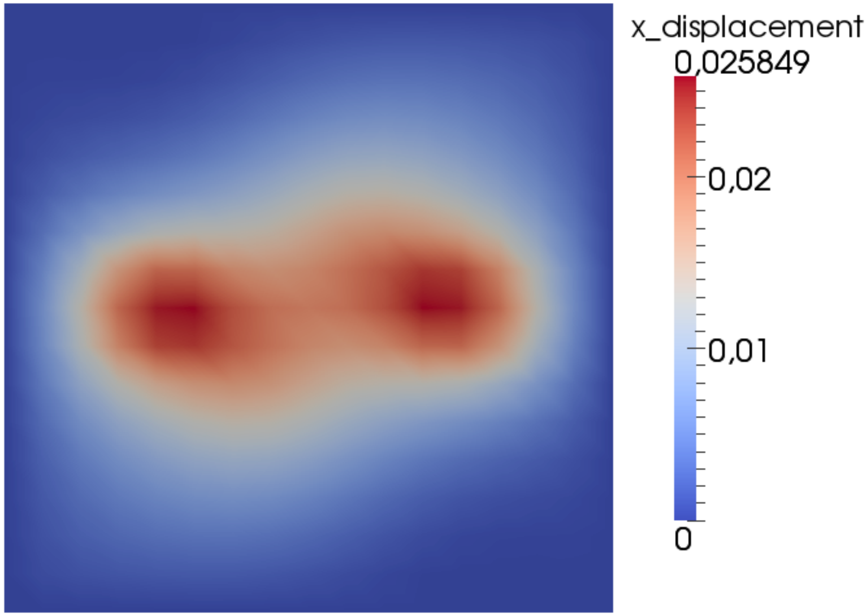
Hansbo / Larson - Discontinuous Galerkin Methods for Incompressible and Nearly Incompressible Elasticity by Nitsche's Method (2002)

Example of linear elasticity (step-8)

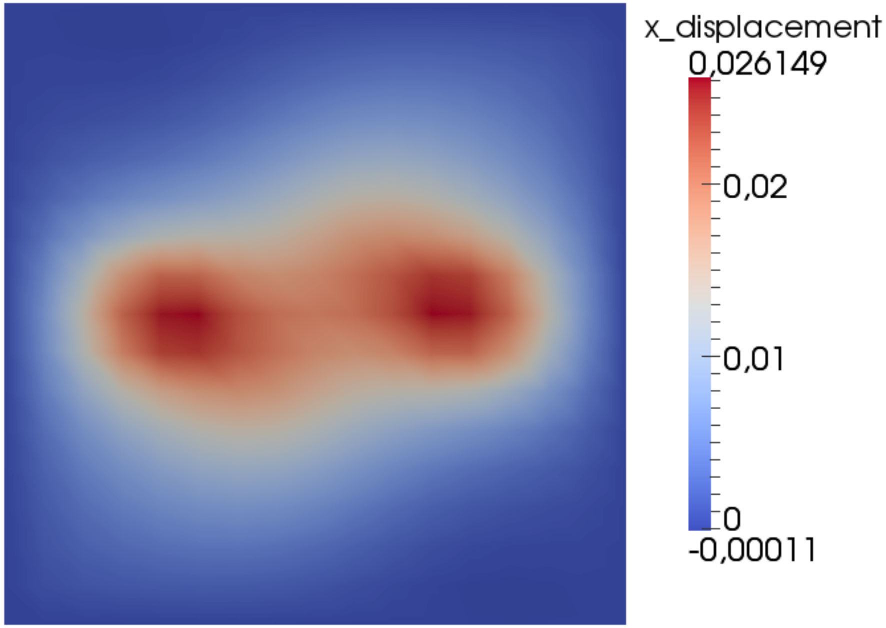
$$-\operatorname{div}\sigma(u) = f, \qquad in\ \Omega$$
$$\mathrm{u} = 0, \qquad \text{auf}\ \partial\Omega$$

$$f(x) = \begin{pmatrix}1\\0\end{pmatrix}, x \in \mathbb{B}_{0.2}(0.5,0) \cup \mathbb{B}_{0.2}(-0.5,0)$$

CG

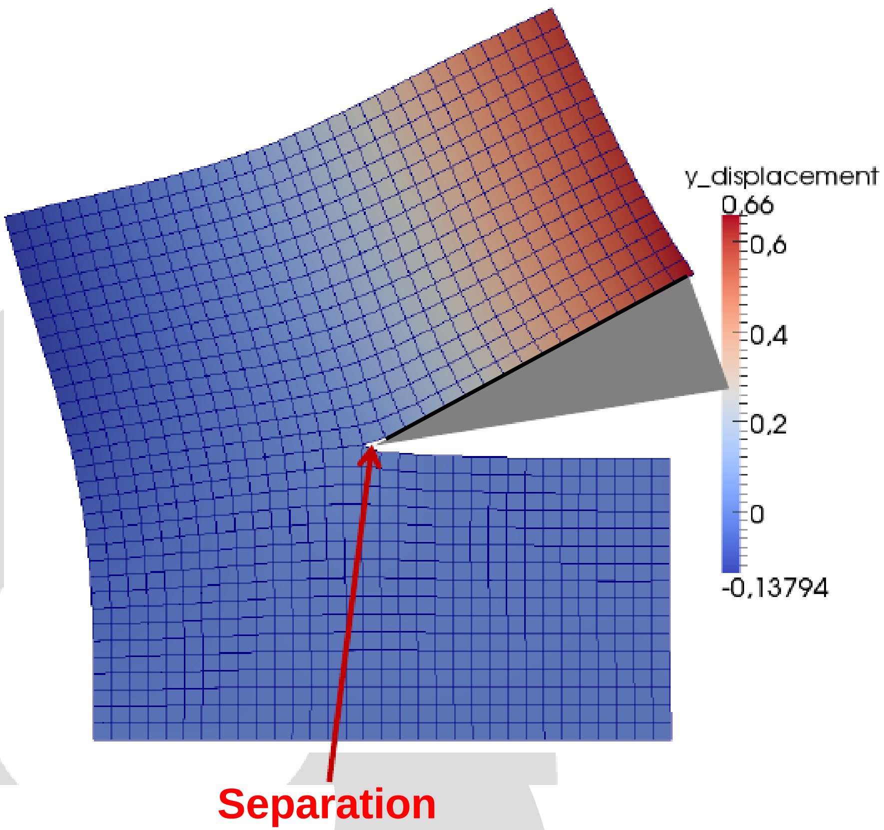


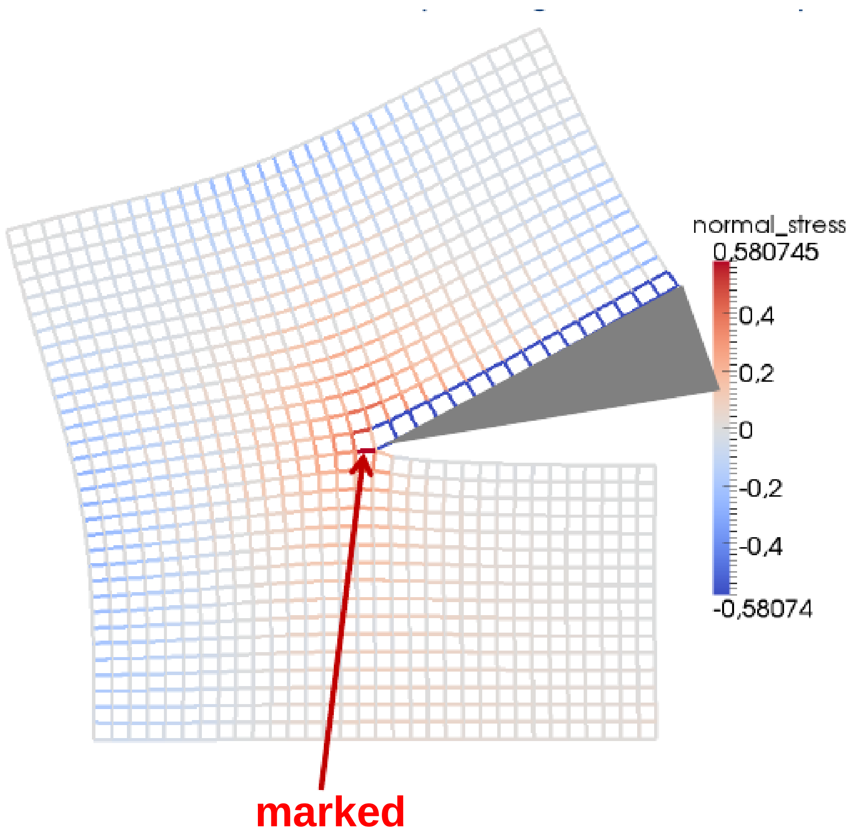
DG



Example for mesh separation for linear elasticity

We need reasonable criteria for separation





Advantage and disadvantage of DG

Advantages:
- One do not have to take care about hanging nodes
- It avoids (volumetric) looking effects
- Easy way to split the mesh along an edge

Disadvantages:
- A larger number of unknowns compared to CG elements
- How to formulate the penalty terms and how to choose the penalty parameters

→ Only local use of DG elements. But this doesn't work in parallel yet.

Hansbo – A discontinuous finite element methods for elasto-plasticity, 2008

Liu, Wheeler, Yotov – On the spatial formulation of discontinuous Galerkin methods for finite elastoplasticity, 2013

Conclusion

What is done:

- Building a parallel framework for solving a coupled thermo-elastoplastic contact problem
- First steps to use the meshworker class for a DG method in linear elasticity

What has to be done:

- Finishing implementing more fancy constitutive laws (Johnson Cook)
- Developing a DG method for thermo-elastoplastic contact problem and mesh separation
- Including friction and heat development by frictional contact
- Including the existing programm in a quasi-static problem (Backward-Euler)
- Remeshing and mapping of internal variables

We would like to have:

- Possibility to mix CG and DG elements in one mesh in a parallel the framework
- Using the meshworker class especially for the DG elements with the penalty terms also in the parallel framework

Thank you!
Questions?

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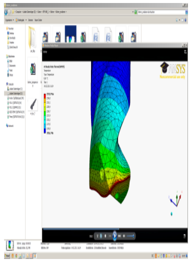
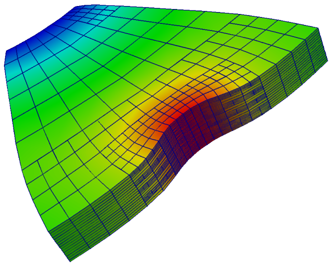
Einleitung

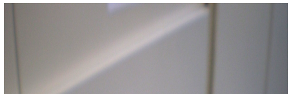


Wendeltiefbohren

Große industrielle Bedeutung – Zylinderkurbelgehäuse

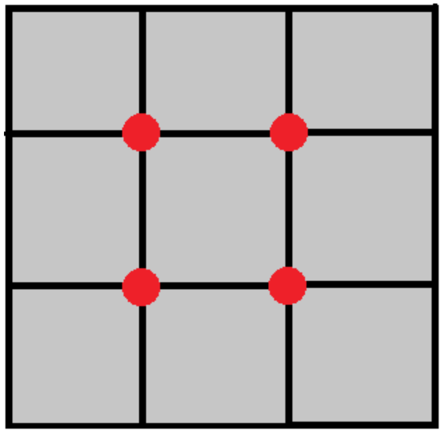
- Stand der Technik – Vollstrahlschmierung
- Herausforderungen beim Einsatz der Minimalmengenschmierung
- Gewendelte Spannuten begünstigen den Spanabtranstort
- Erhöhte mechanische und thermische Belastung

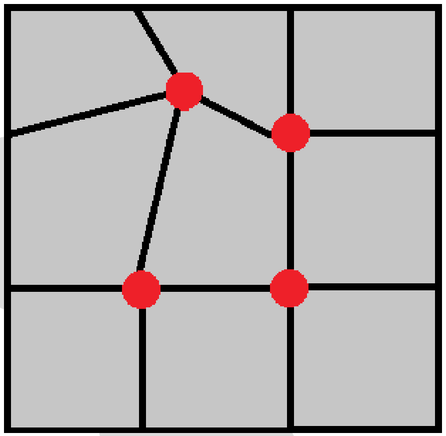




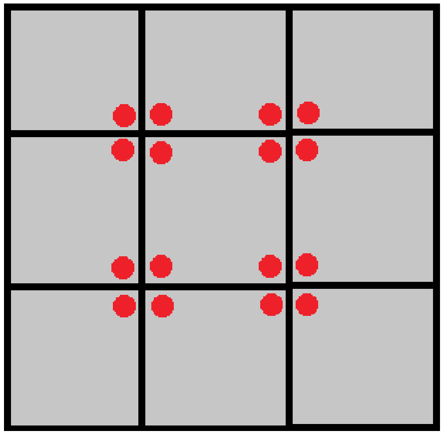
Stetige / Unstetige Elemente

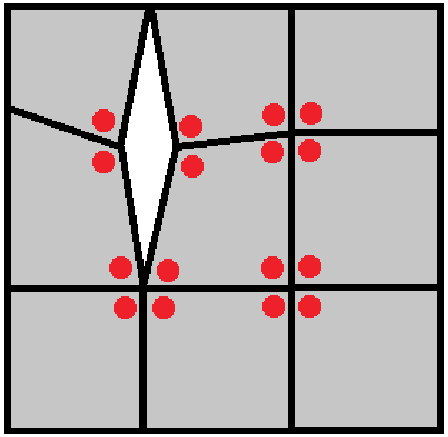
Stetige Ansatzfunktionen (CG)





Unstetige Ansatzfunktionen (DG)





Mehr Freiheitsgrade
Größeres Gleichungssystem