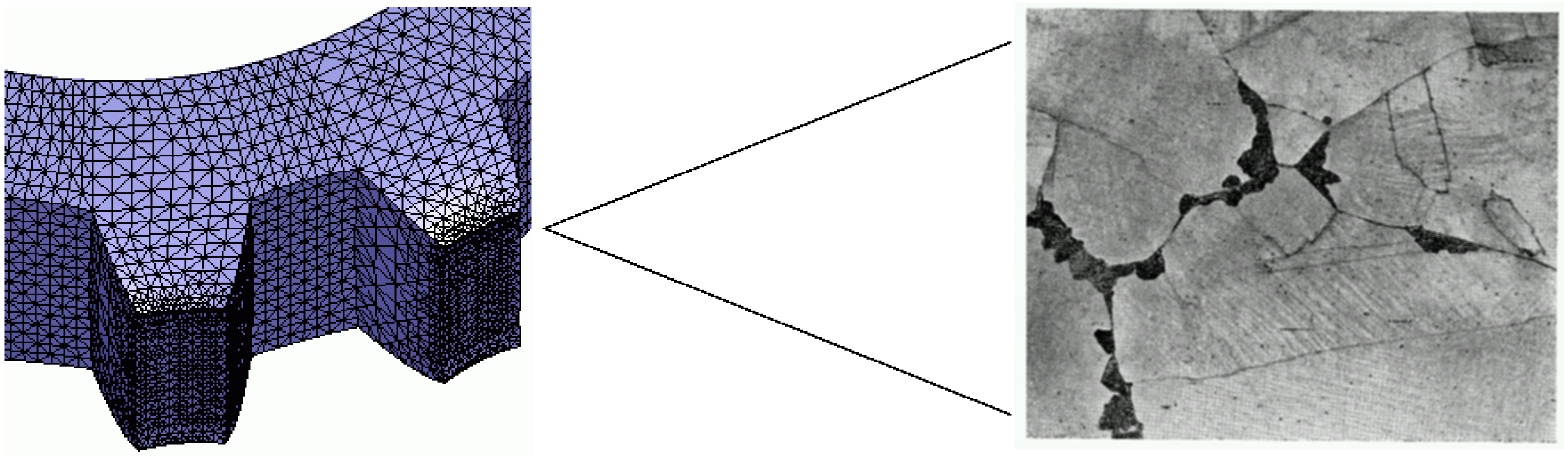


Adaptive Finite Element Methods for Macroscopic and Mesoscopic Models of Steel

Alfred Schmidt

SFB 570

Universität Bremen

Zentrum für Technomathematik

Joint work with M. Böhm, T. Moshagen, B. Suhr, M. Wolff

Work in progress

Background:

Special research program SFB570 "Distortion Engineering"

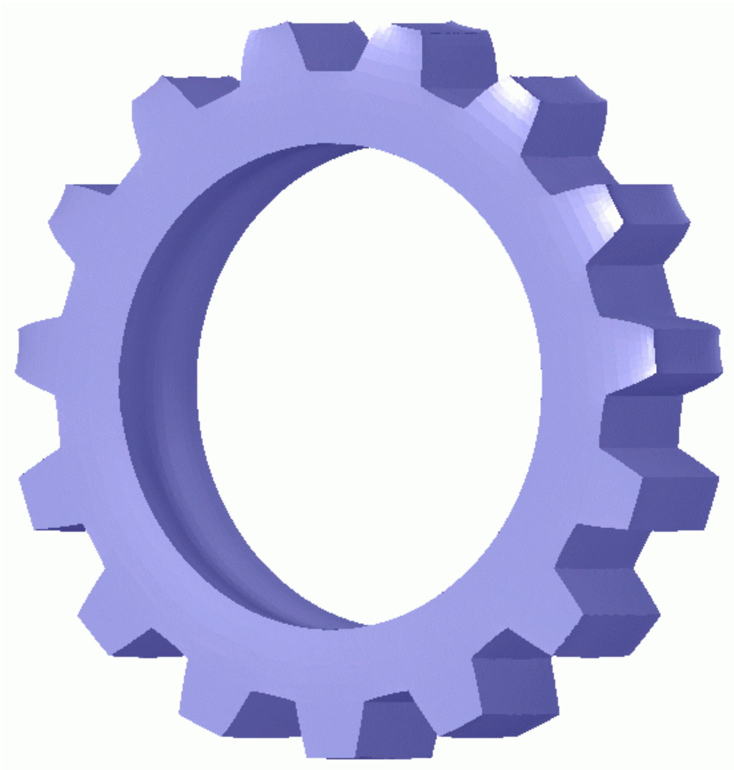
(engineering project, joint with applied math)

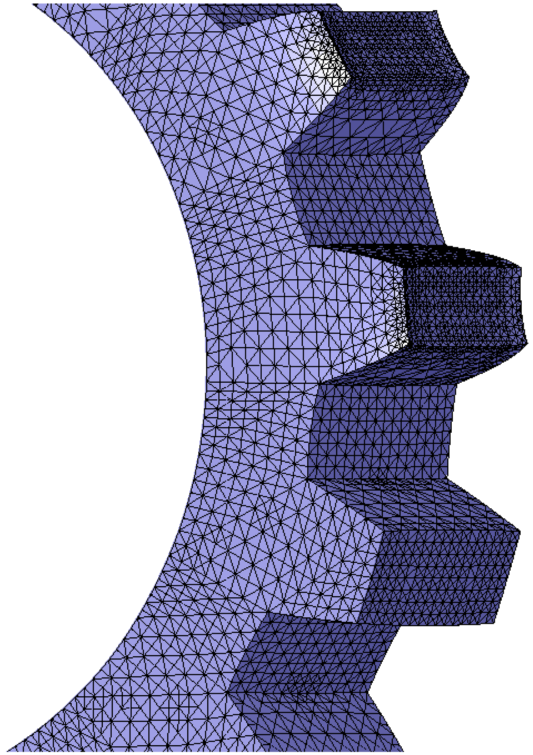
Study (both experimentally and numerically) mechanisms which lead to **distortions** (= unwanted deformations) during production of steel workpieces

Various steps of production: forming, cutting, …, heat treatment

Here:
Solid-solid phase transitions during heat treatment,
cooling of a hot steel workpiece
Phase transitions austenite -> pearlite - bainite - (martensite)

Macroscopic model wanted for simulation of complete workpiece (like a gear, e.g.) in order to study/optimize distortions





Macroscopic variables:

- temperature,
- phase fractions,
- elastic and plastic deformations,
- (concentrations of carbon and other ingredients)

Variables interact !

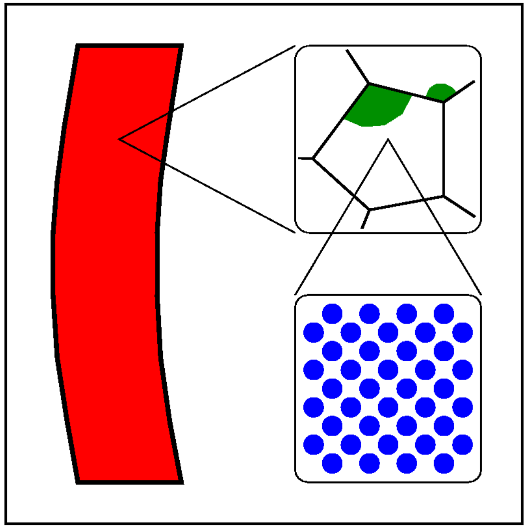
- phase transformations depend on temperature, stress
- density/deformations depend on phase fraction, temperature
- …

Multi-scale phenomenon: various time/space scales

- temperature diffusion: fast, long-range
- chemical diffusion in solids: slow, short-range
- phase transformations: several (many) seconds –
  meanwhile, temperature may change substantially

Phenomena on small scale give effects on large scale !

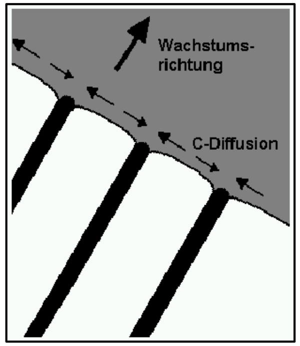
Selection of scale – selection of model:



- Macro: work piece (1 - 100 cm)
  continuum mechanics, no grain structure,
  phase fraction

- Meso 1: multiple grains (10 – 100 μm)
  continuum mechanics, grain structure,
  resolve austenite-pearlite transition, nearly no diffusion of C

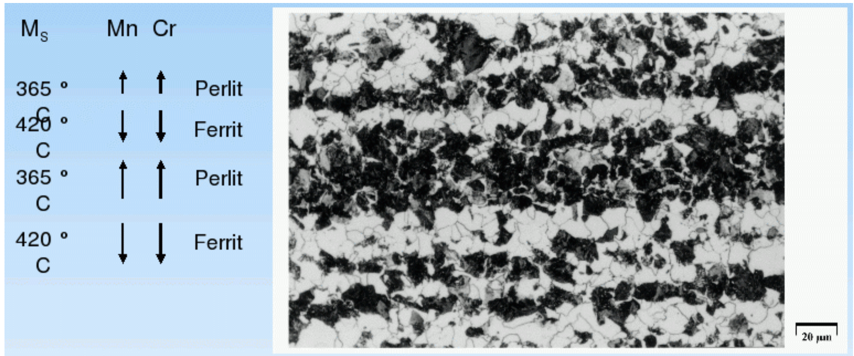
- Meso 2: one or few grains (0.1 – 10 μm)
  continuum mechanics, grain structure,
  resolve structure of pearlite (lamella of ferrite and carbide),
  diffusion of C in transition layer, Fe and C conserved

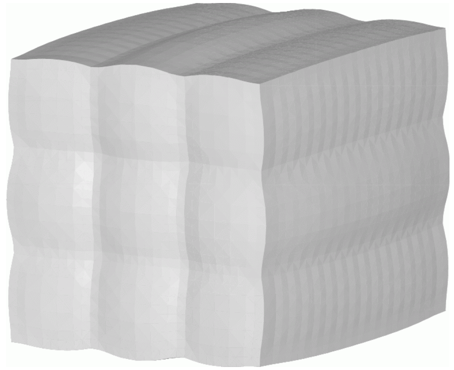


- Micro: scale of atoms / clusters
  plastic deformation by relocation of atoms,
  needs MD/MC simulations

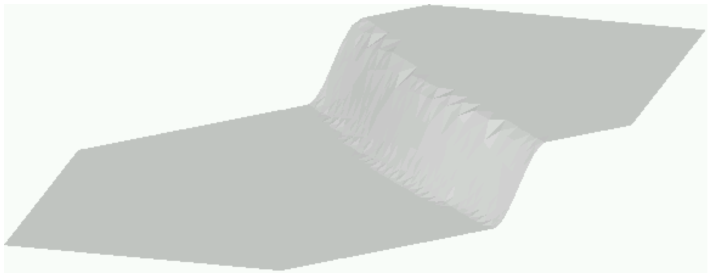
Look here at two special situations:

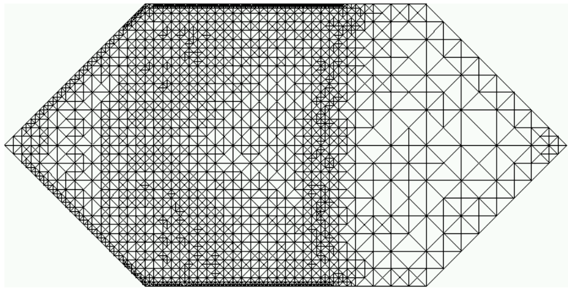
Anisotropic (macroscopic) dilatation behavior of banded material

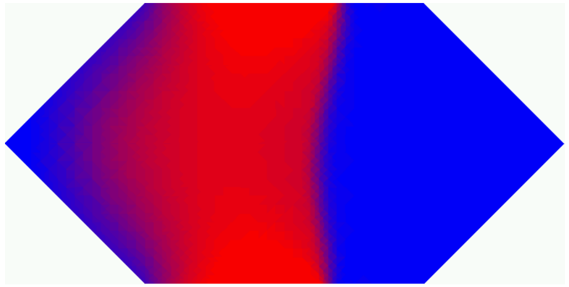




Phase field models for mesoscopic phase transitions





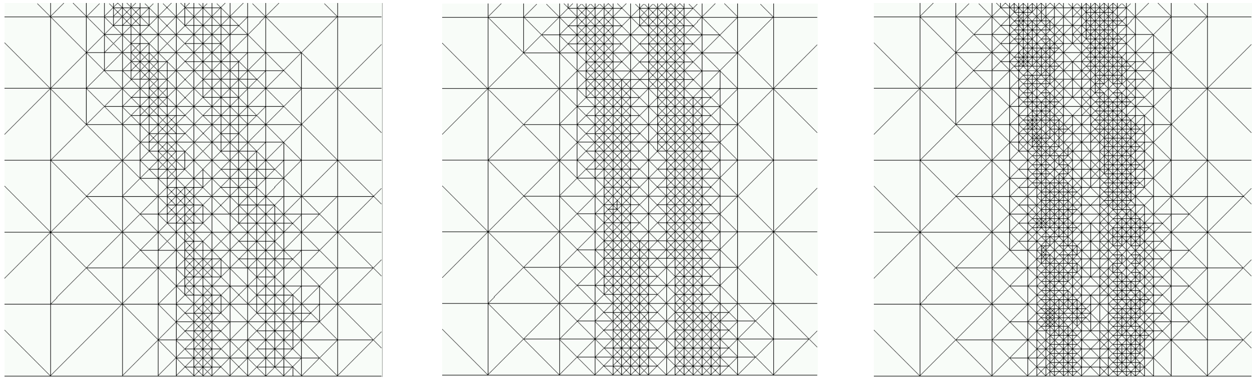


Adaptive Finite Element Methods

Automatic local refinement or coarsening of meshes,
based on numerically computed solution

Generate quasi-optimal meshes for a given error tolerance

Meshes
for different
tolerances:



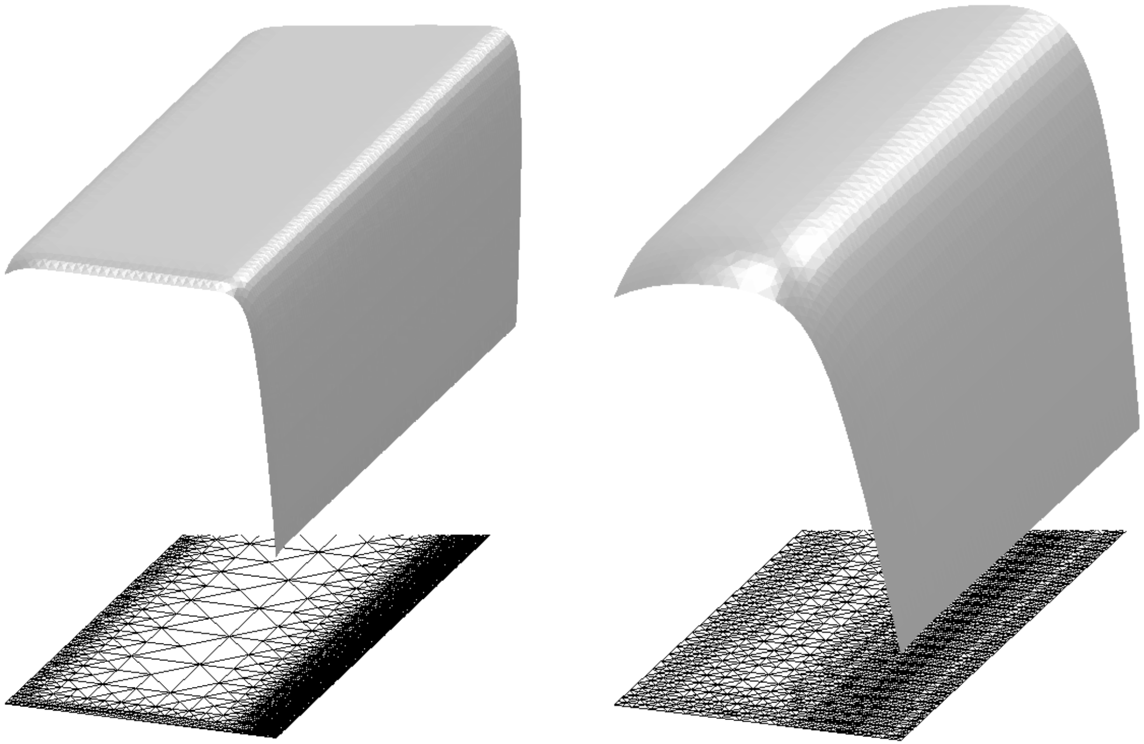
Local error indicators are computed from *numerical* solution and given data of the problem, give error estimate and are used to select mesh elements for refinement/coarsening

Equivalency of the estimate to the error can be mathematically proven (for model problems)

ALBERTA: academic toolbox 1D/2D/3D, open for extensions

Adaptive Finite Element Methods

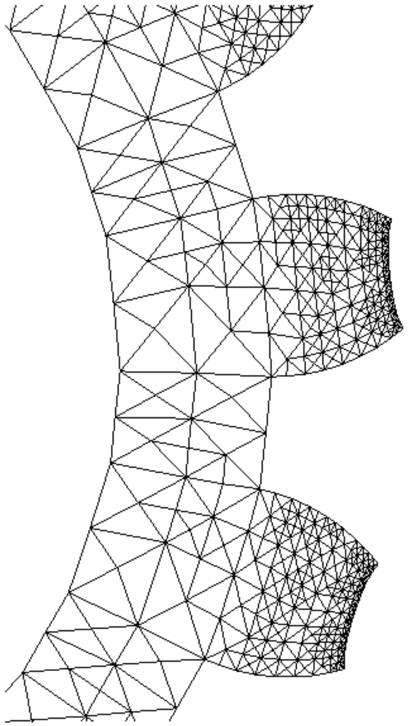
Especially well suited for time dependent situations with time-varying (boundary or interior) layers

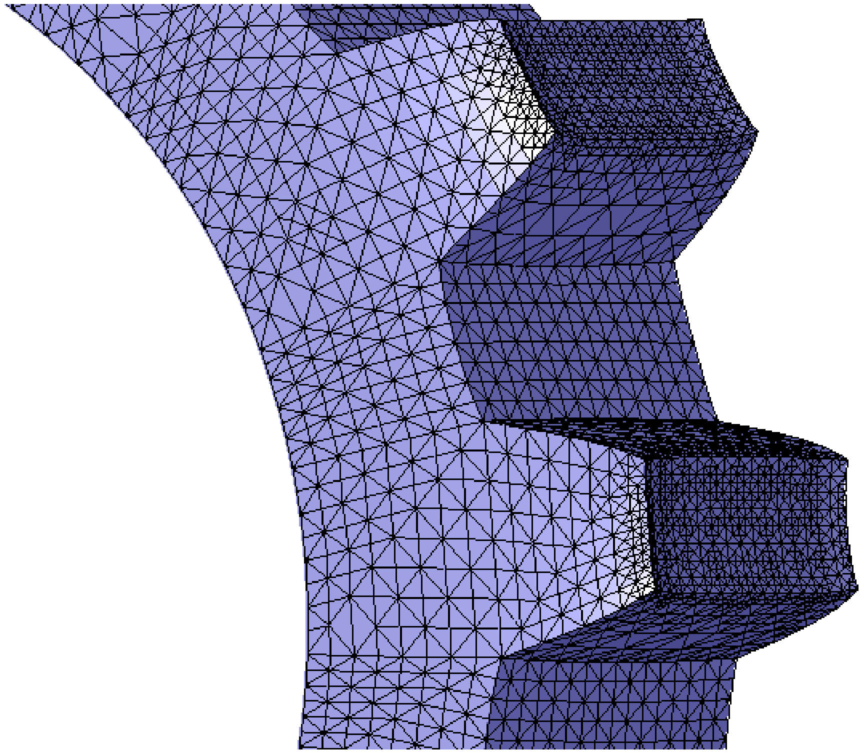


Quenching of a hot steel workpiece (2D): Graphs of temperature and corresponding adaptive meshes at two different times

Adaptive Finite Element Methods

Similar situations occur locally in more complicated geometries

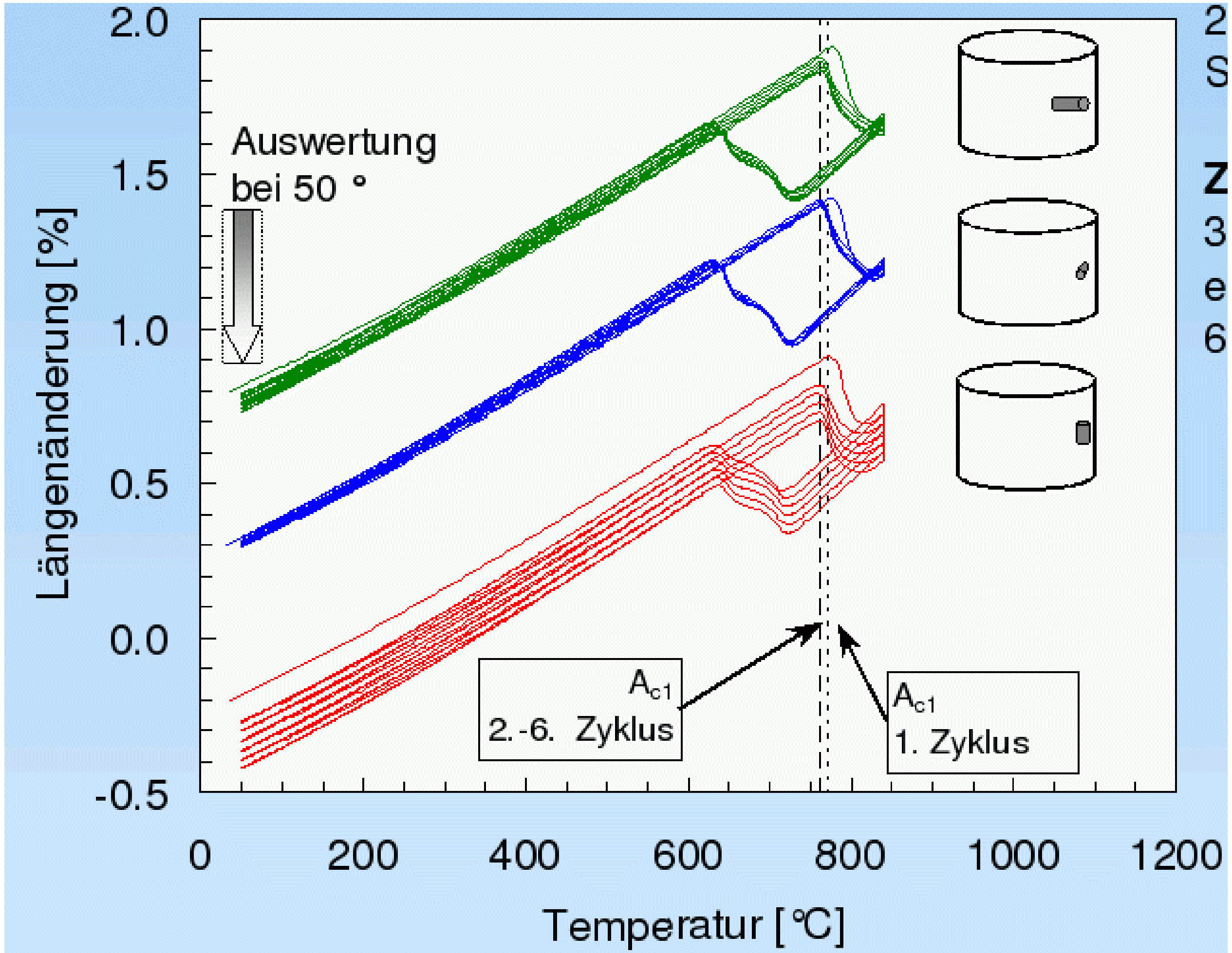




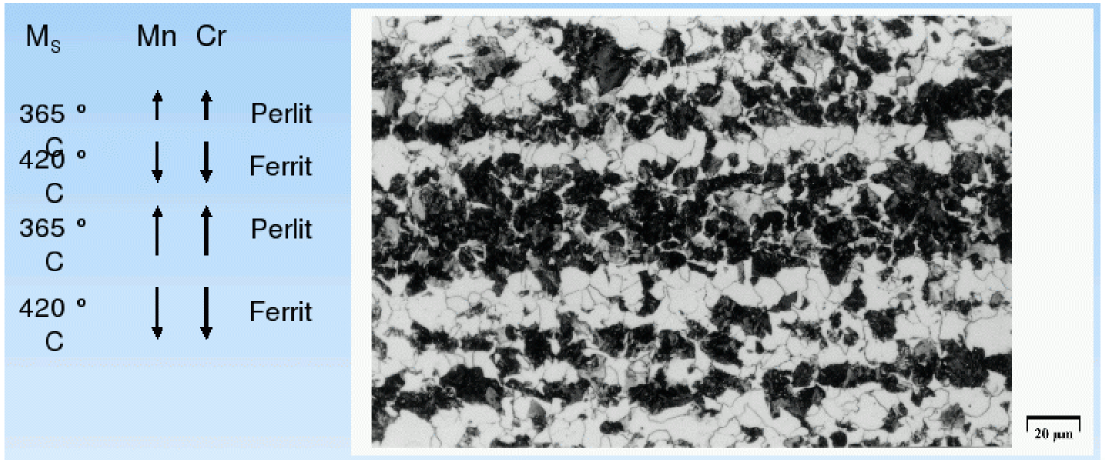
Heat treatment of a (simple) cogwheel in 2D and 3D, with stronger cooling of the cog tips: Adaptive meshes with emphasized deformations.

Anisotropic dilatation behavior of banded material

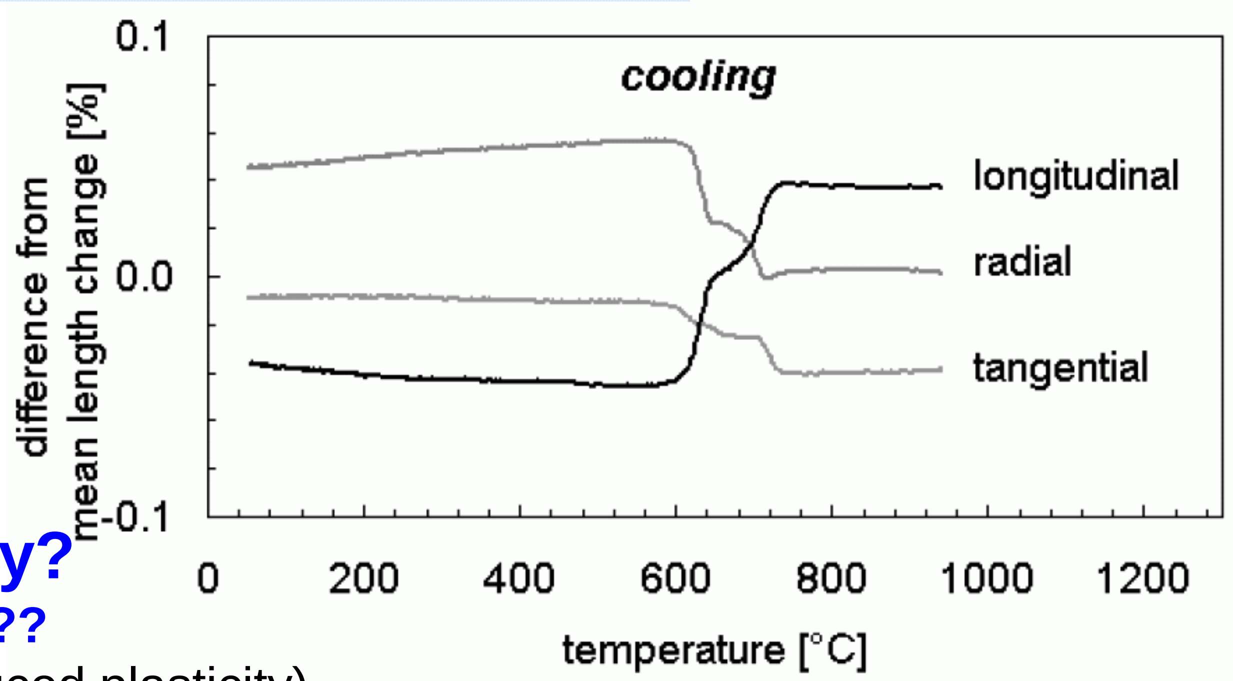
Experimental observation: [Hunkel, Frerichs, Prinz, Surm, Hoffmann, Zoch, 2005]
Samples taken in different direction relative to rolling direction



20MnCr5 with banded chemical inhomogeneities (from segregation and rolling)



Anisotropic length change during each cooling cycle:



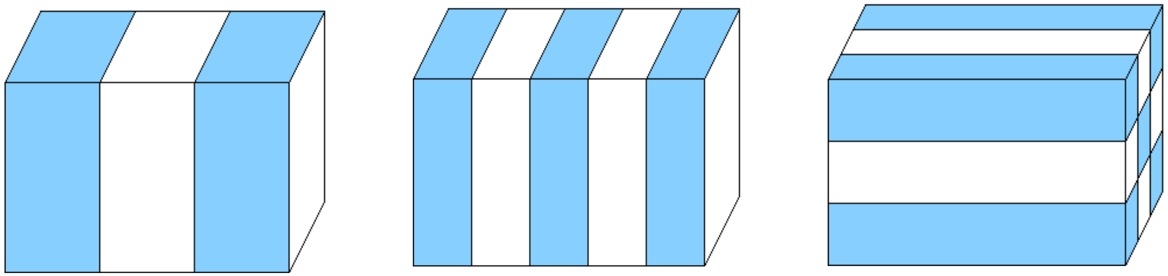
Open question: why?

Is this an effect of TRIP ???

(TRIP = transformation induced plasticity)

Model problem inspired by banded structure:

Don´t look at grain structures, but small sample of layered material:
(planar or checkerboard layer structure)



Different phase change laws in differently colored sub-regions!
(phase change at lower temperatures (later) in blue sub-regions)

Model for thermo-elasticity with phase changes including TRIP

High local stresses near sub-region-boundaries!
Adaptive finite element calculation with (automatic!) fine resolution near well suited

Model for thermo-elasticity with phase changes including TRIP

$$\rho c\dot{T} - div(k\nabla T) = \rho \sum L_i \dot{p}_i$$

$$-div(\sigma) = 0$$

$$\dot{p}_i = f_i(p,T)$$

$$\sigma = \lambda tr(\varepsilon - \varepsilon_{TRIP})I + 2\mu(\varepsilon - \varepsilon_{TRIP}) - (3\lambda + 2\mu)\{\alpha(T - T_0) + (\rho_0 - \rho)/3\rho\}I$$

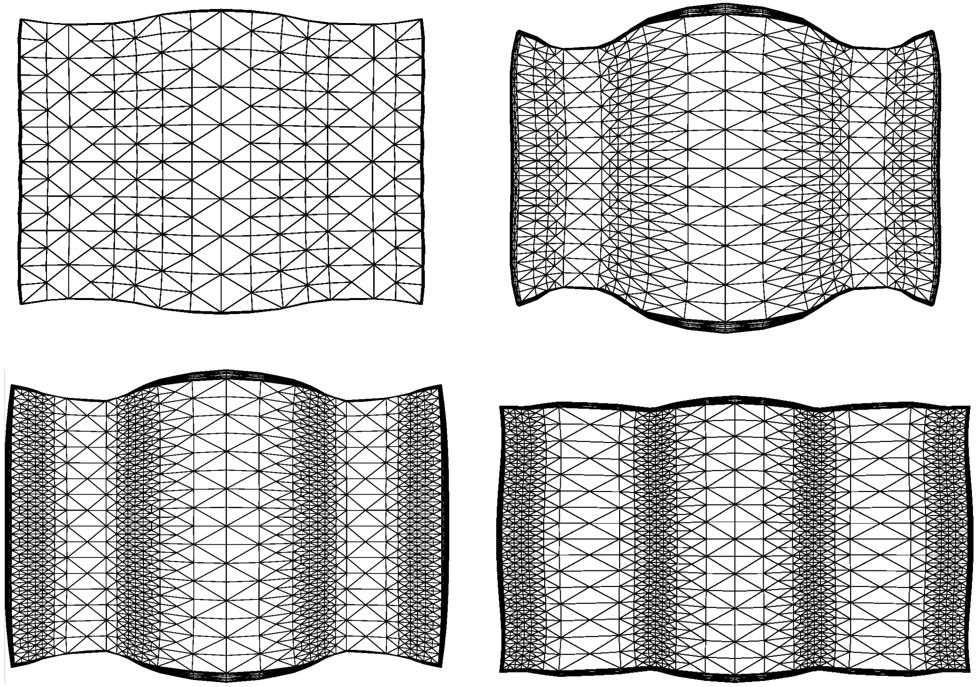
$$\varepsilon = \tfrac{1}{2}(\nabla u + \nabla u^T)$$

$$\dot{\varepsilon}_{TRIP} = \tfrac{3}{2}\kappa\sigma^* \phi'(p)\dot{p} \qquad \varepsilon_{TRIP}(0) = 0$$

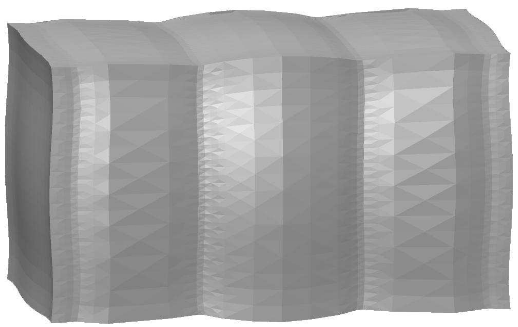
Adaptive finite element calculation: ALBERTA

Not all correct material parameters are used (known) in the moment.
Natural boundary conditions (arguable…)

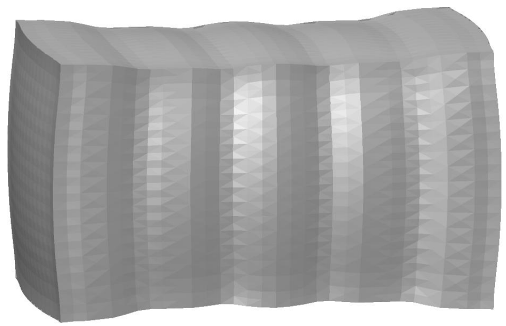
Adaptive finite element calculation: planar layers



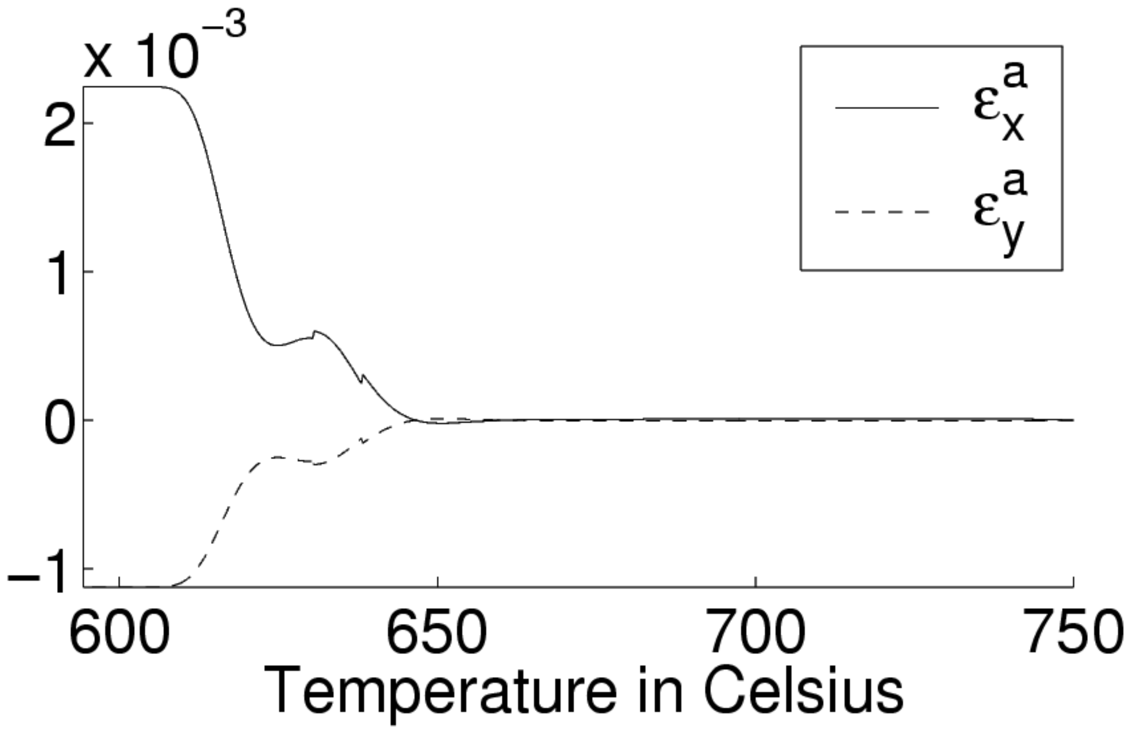
Meshes (3D) and emphasized deformations at different times during the simulation



Final geometry



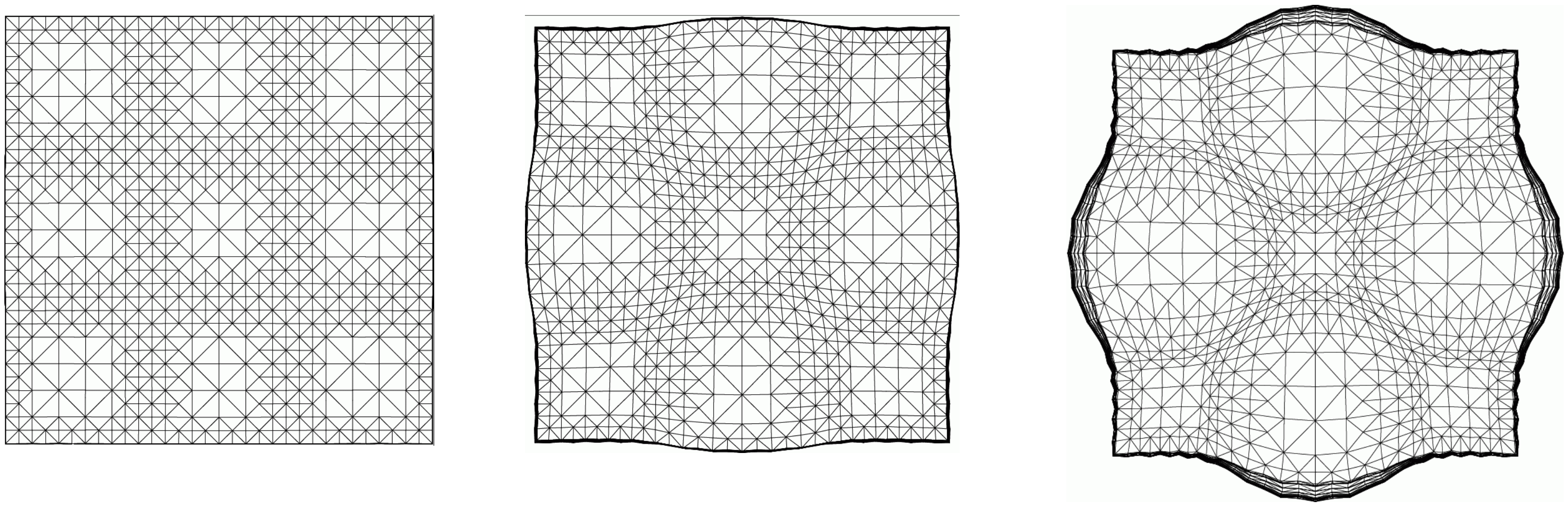
Adaptive finite element calculation: planar layers



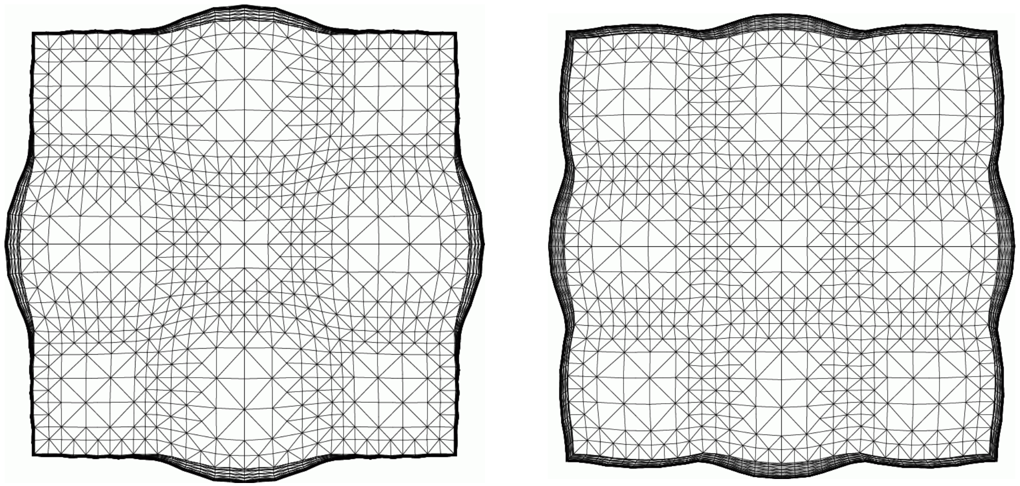
Relative length changes in longitudinal and transversal directions

$$\varepsilon_x^a = \varepsilon_x - (\varepsilon_x + \varepsilon_y + \varepsilon_z)/3 \qquad \varepsilon_y^a = \varepsilon_y - (\varepsilon_x + \varepsilon_y + \varepsilon_z)/3$$

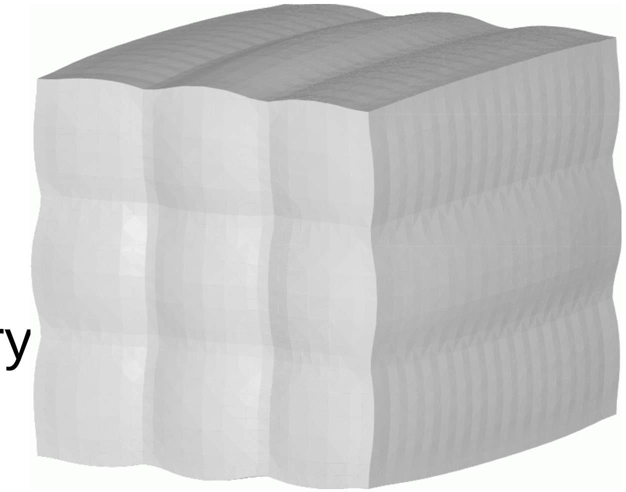
Adaptive finite element calculation: checkerboard layers



Meshes (3D) and emphasized deformations at different times during the simulation

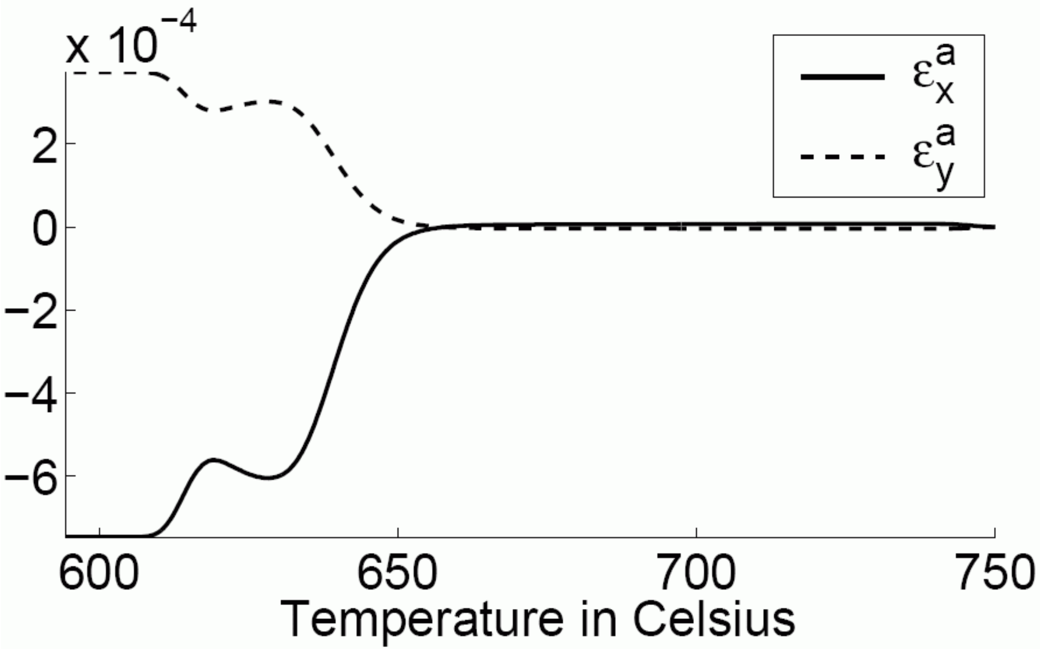


Final geometry



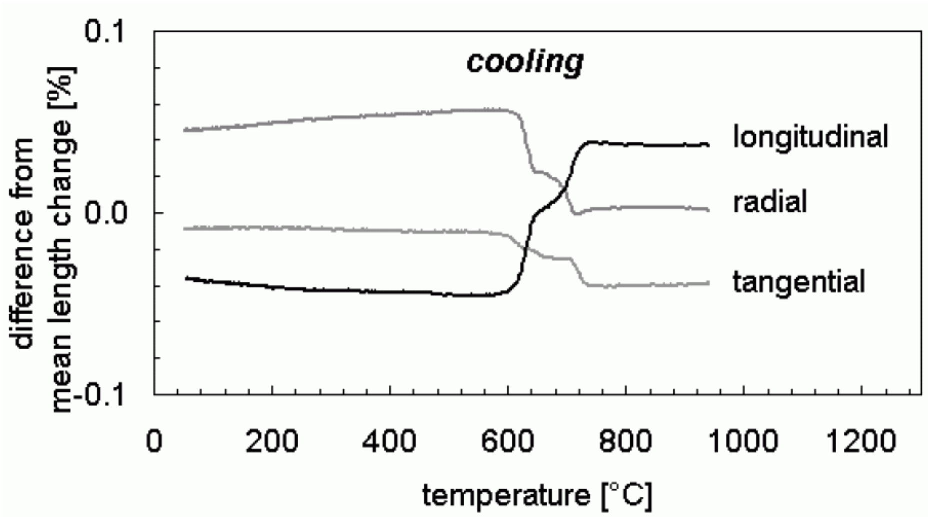
Anisotropic dilatation of banded material

Adaptive finite element calculation: checkerboard layers



Relative length changes in longitudinal and transversal directions

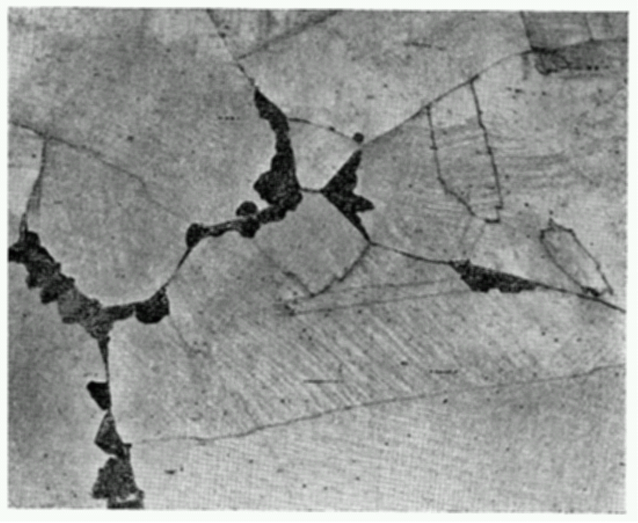
Recall experimental results:



Results are (at least qualitatively) very similar to the experiments

So, **TRIP effect might be the reason for these distortions!**

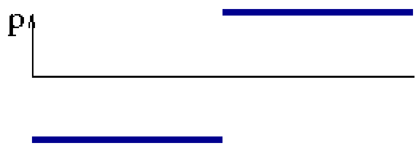
Phase field models for mesoscopic phase transitions



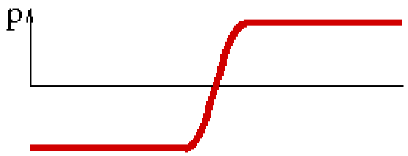
Mesoscopic view on phase transitions:

Sharp interface between
regions of pure phase/constituent
(austenite/pearlite, e.g.)

Motion of interfaces: moving boundary problem
Pure phases described by corresponding characteristic functions



Phase Field Approach:
Introduce a smooth phase variable with a narrow transition region
(width δ) and a corresponding evolution law



Phase field model for stress-dependent mesoscopic phase transitions

Phase Field Model can model geometric effects
(speed of the phase boundary depending on curvature…)

Introduce a (smooth) phase variable
and a corresponding evolution law

$$\delta(\dot{p} - a\Delta p) + \frac{1}{\delta}\Psi'(p) = f$$

instead of the simple ODE law $\dot{p} = f(T, p)$
Underlying principle: double well potential Ψ
with local minima at the values for pure phases.

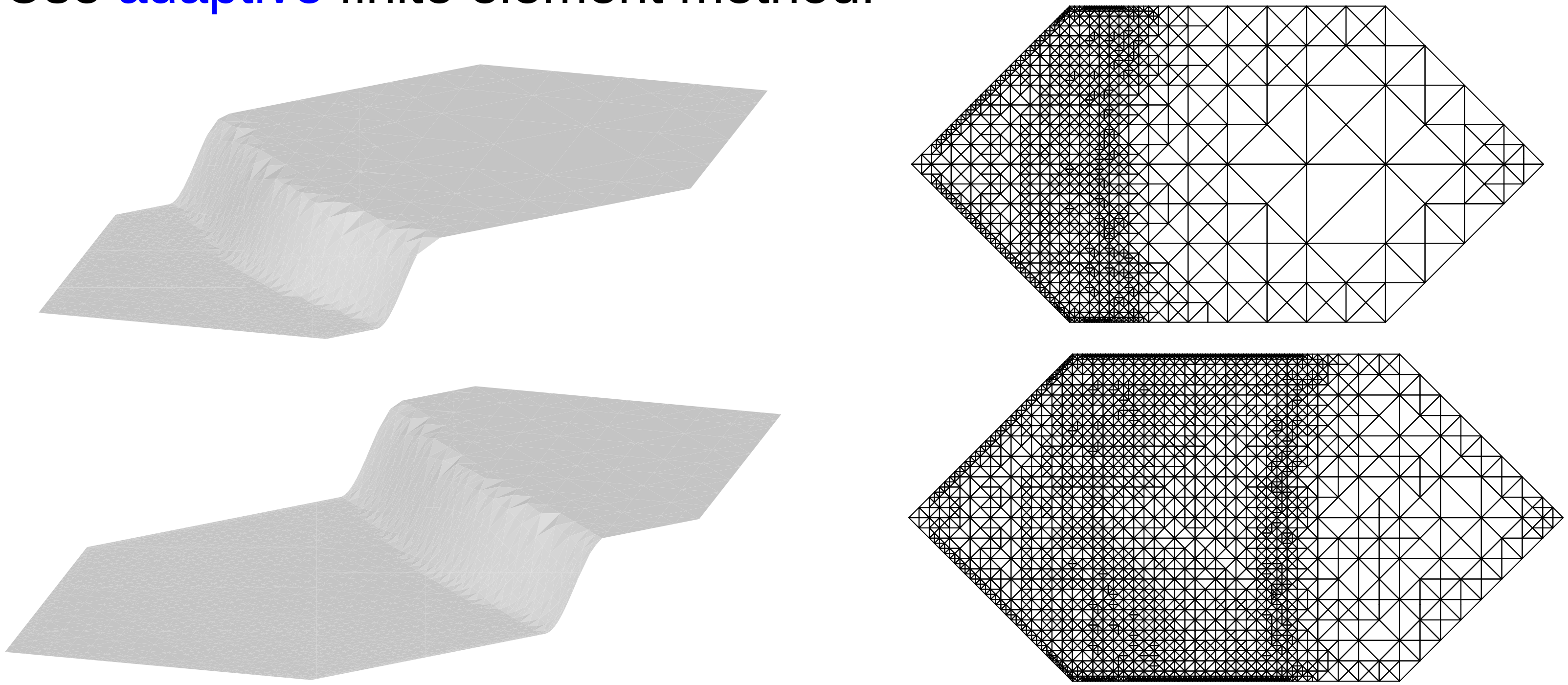
Stress effects modeled via rhs function, e.g.: $f = \gamma T - c \cdot \sigma : \sigma$

Inspired by [Parét 2001, Steinbach et al 2006]

Phase field model for stress-dependent mesoscopic phase transitions

Very simple geometry: one single 2D 6-sided grain

Narrow transition region of width δ needs high resolution!
Use adaptive finite element method!



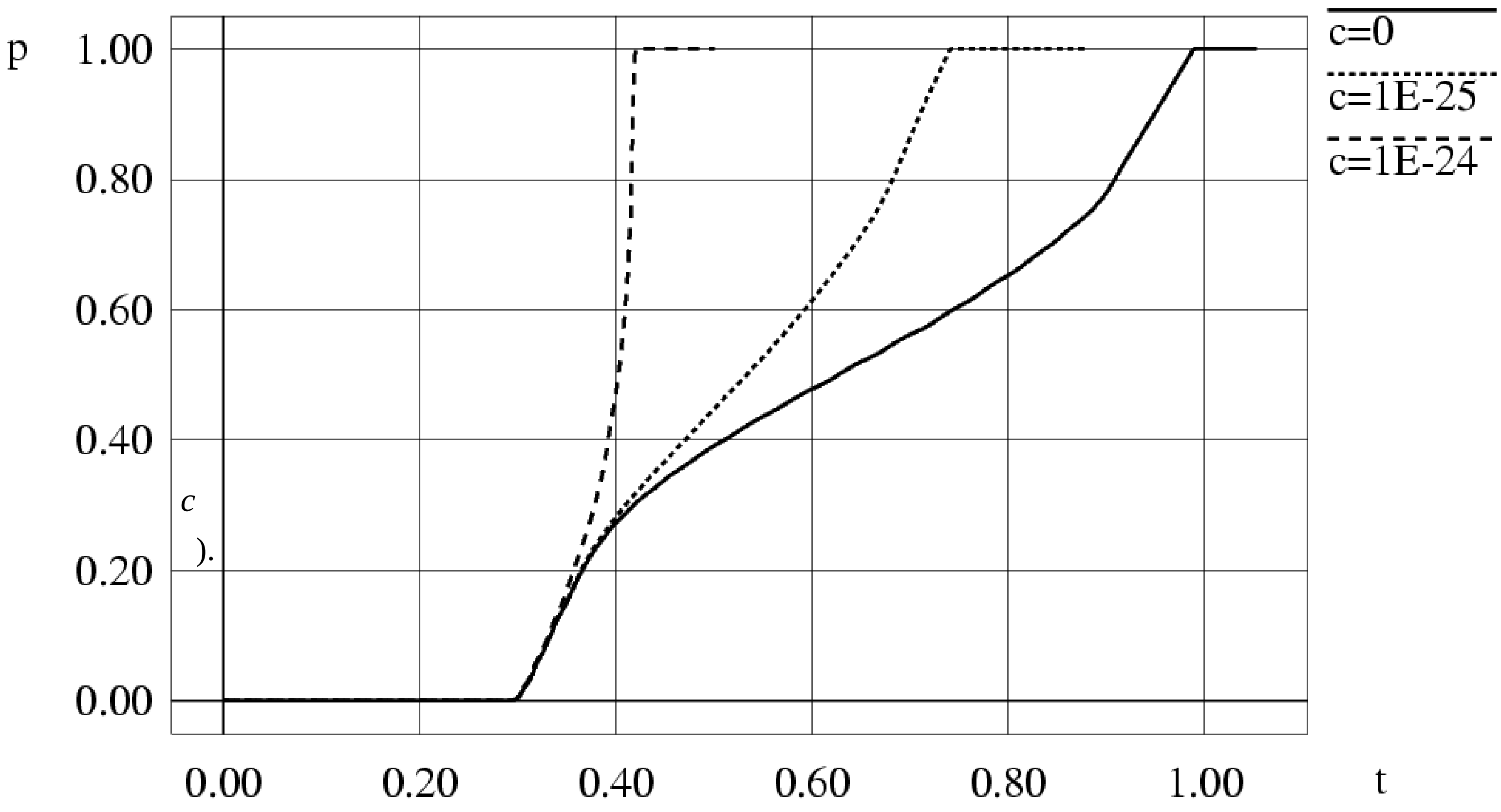
Graphs of phase variable and corresponding meshes at different times

Phase field model for stress-dependent mesoscopic phase transitions

Phase variable, temperature, and modulus of stress tensor

Finite element discretization and adaptive method
based on error indicators presented in joint papers
[Chen, Nochetto, Schmidt 2000], [Kessler, Nochetto, Schmidt 2004]

Phase field model for stress-dependent mesoscopic phase transitions



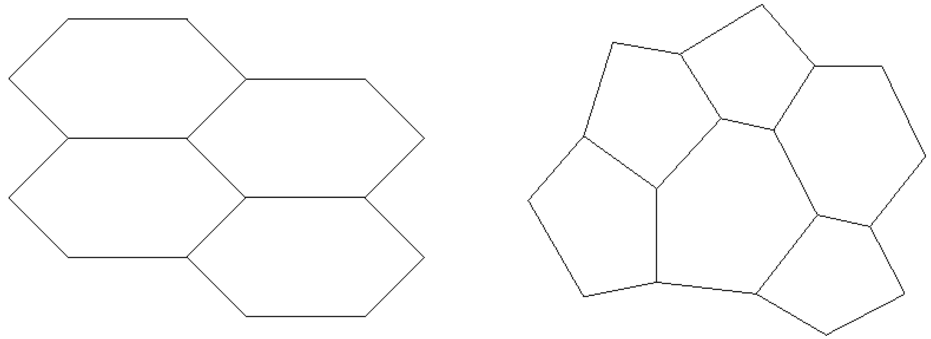
Comparison of volume fractions over time for varying influence of stress (various c)

$$f = \gamma T - c \cdot \sigma : \sigma$$

Phase field model for stress-dependent mesoscopic phase transitions

Work in progress … as shown, just one single grain
Future investigations:

- Multiple, connected grains:
  continuous fields for temperature and deformations,
  separate phase variables on different grains
  with Neumann boundary conditions on grain boundaries

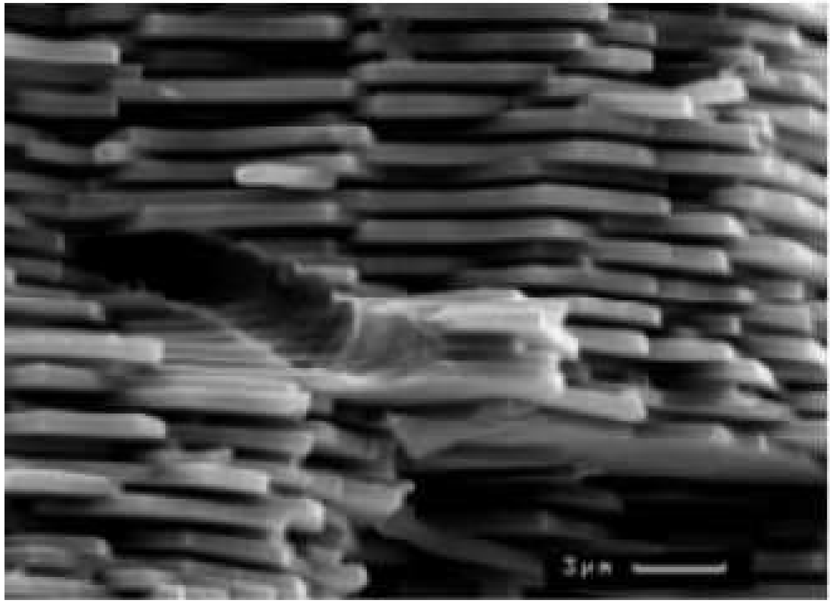


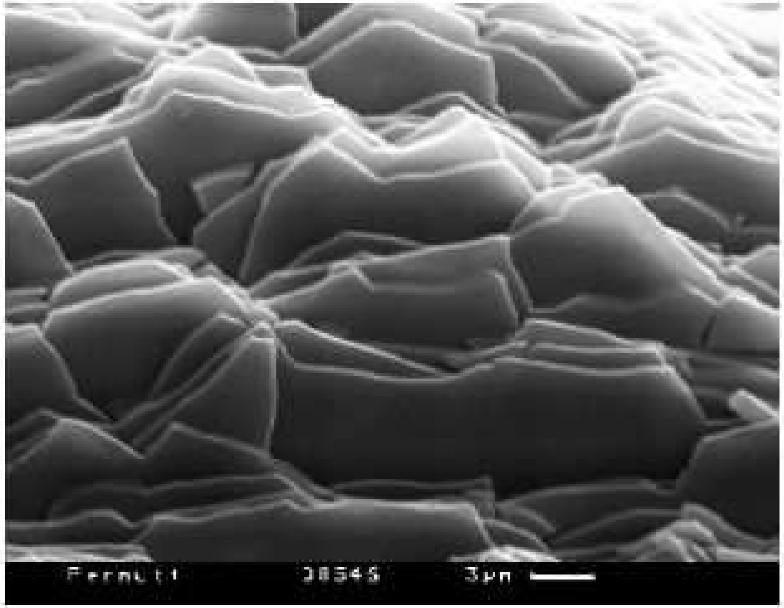
- Apply external stresses:
  Nucleation in various corners ?

- 3D

Nacre

(mother of pearl, material of seashell)

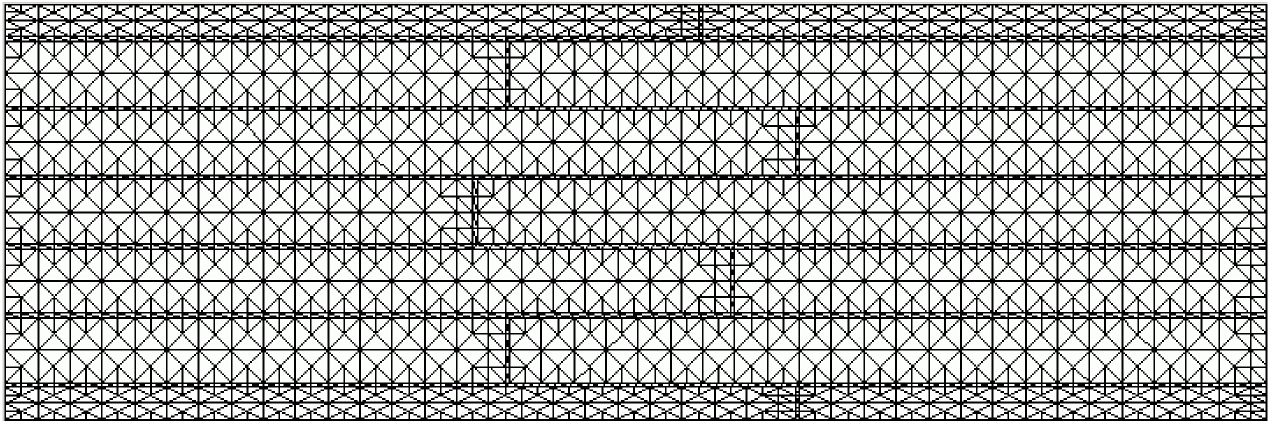




Nacre is a very robust material, built from small aragonite plates (hard and brittle) and biopolymers (softer)
Much higher resistance to fractures than pure aragonite.

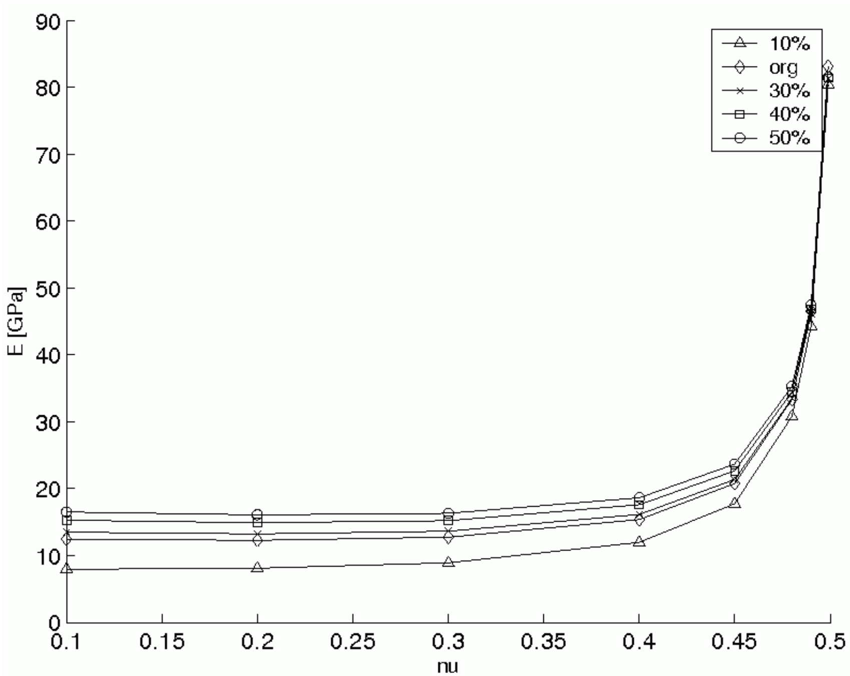
Material properties of biopolymer layer are not well known
(and very hard to determine experimentally)

Parameter identification problem !
Numerical simulations for a small subset (2D)
Here, resolution of thin layers (~mortar) is important !

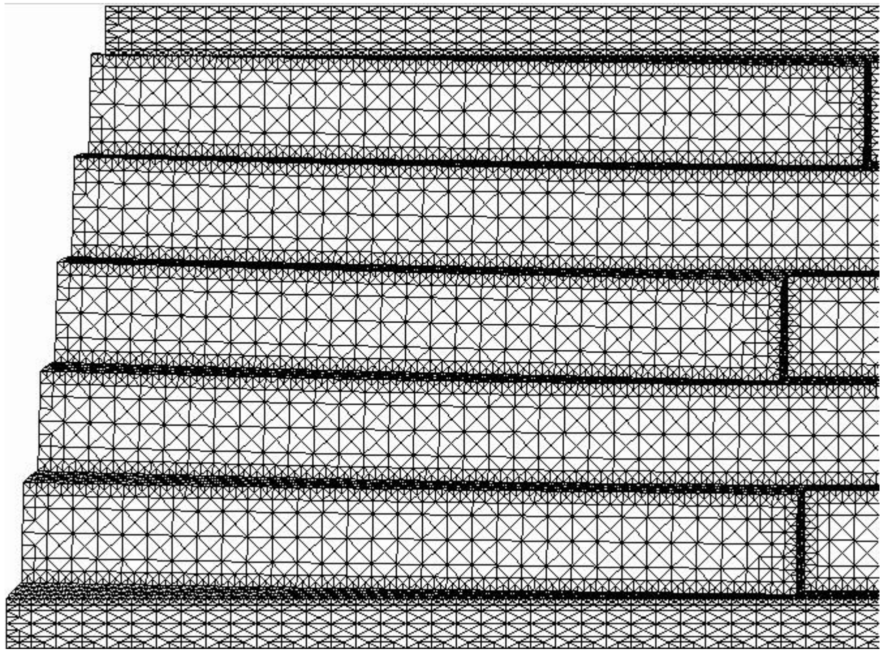


Sample macro triangulation

Some preliminary results:



Dependence of composite E modulus on Poisson number of biopolymers



Simulation of shear deformation

Thank you for your attention !

Acknowledgements

Numerical Simulations: ALBERTA

Graphics: GRAPE

Partly supported by
Deutsche Forschungsgemeinschaft (DFG) via SFB 570 “Distortion Engineering”
and University of Bremen via the Centre for Scientific Computing and Applications (BreSCA)