SAND2020-1987PE

Polyhedral finite elements and multiscale error estimation of material models

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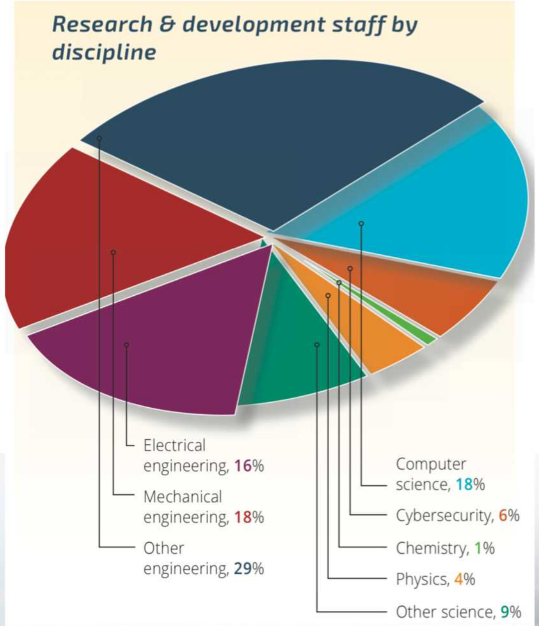
My background

1. Ph.D. Texas A&M Univ., Aerospace Engineering, 1995
2. General Motors, Powertrain Division, 1996 – 2004
    - FEA, thermal-structural analysis of engines
    - “production environment (rapid design to analysis)
    - fatigue (low and high cycle)
    - Group Leader of head and block group, 2002 – 2004
3. Sandia National Laboratories, 2004 – present
    - support of product-development engineering
    - impact/penetration
    - geologic storage of CO_2
    - pervasive fracture modeling
    - polyhedral finite elements
    - meshfree discretizations (rapid design to analysis)
    - multiscale modeling, error estimation
    - metal additive manufacturing
    - department manager, 2018 – present

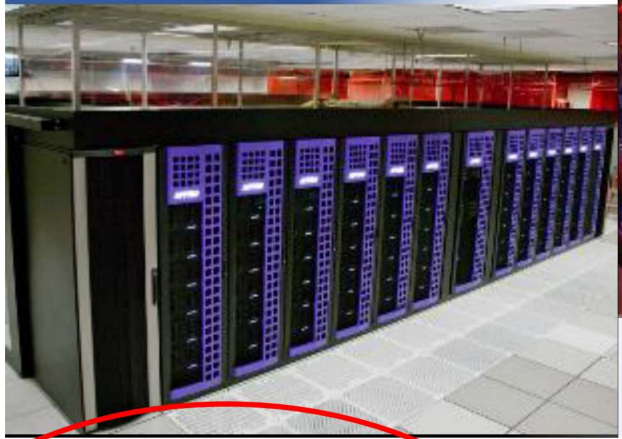
Sandia National Laboratories

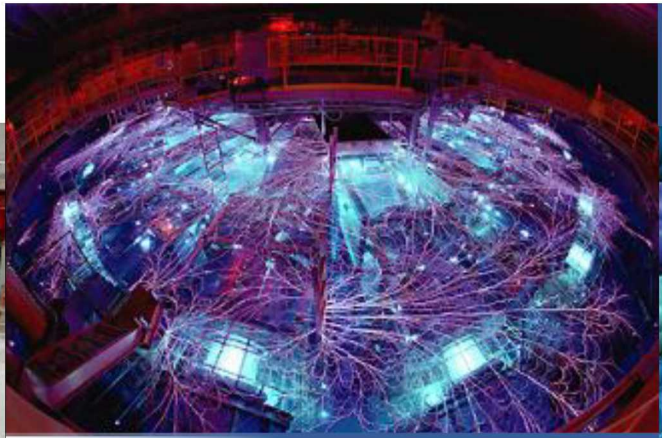
- Established in 1945 as Los Alamos Z division
- Sandia Laboratories established in 1949
- Government owned, contractor operated, for DOE’s National Nuclear Security Administration (NNSA)
- Responsible for design of non-nuclear components for nuclear weapons
- Sandia teams with the two ”physics” laboratories: LANL, LLNL
- First managed by AT&T Bell Labs, 1949-1993
- FFRDC, Federally Funded R&D Center (may perform work for industry)
- $3.8 billion budget
- 14,000 employees: 2600 B.S, 4600 M.S., 2100 Ph.D.
- 950 students; 250 post-docs



Research Foundations (Lab directed R&D)

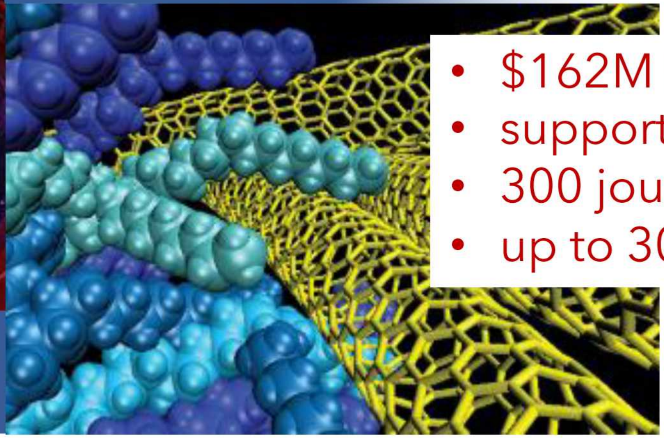
Computing & Information Sciences





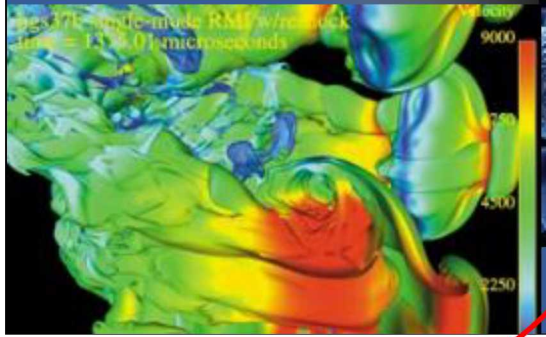
Radiation Effects & High Energy Density Science

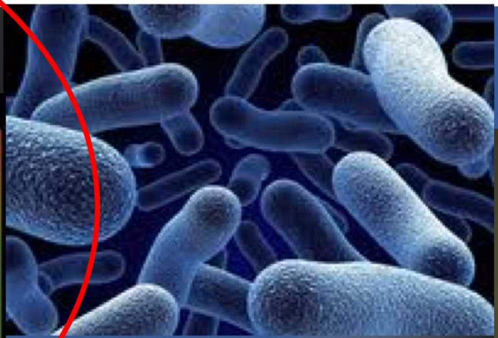
Materials Sciences



- $162M in FY19
- supported 130 post docs
- 300 journal pubs
- up to 30% univ. collab.

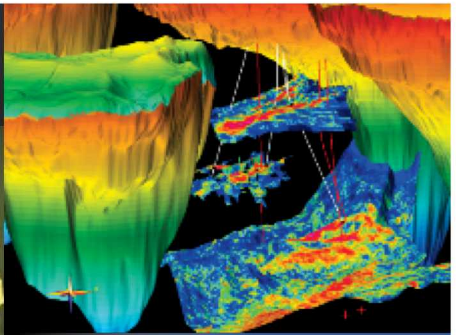
Engineering Sciences





Bioscience

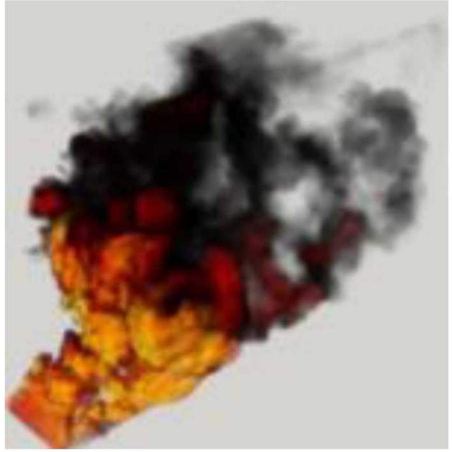
Nanodevices & Microsystems

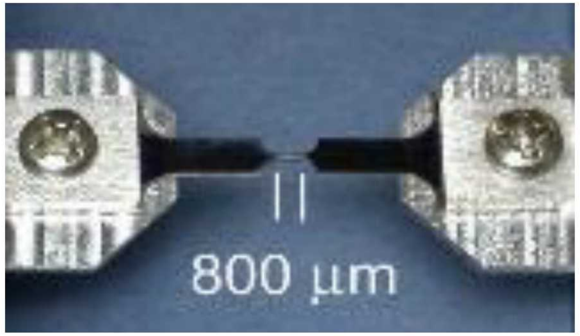


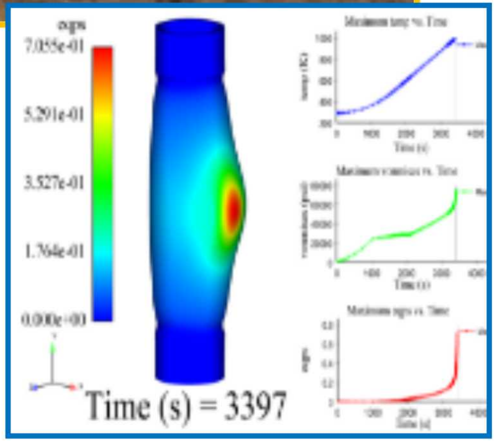
Geoscience

Engineering Sciences Center

- Mission: provide validated, science-based engineering expertise and solutions across the life cycle of products to inform engineering decisions.
- Integrate theory, computational simulation and experimental discovery/validation across length and time scales to develop the technical basis for complex systems.
- 600 staff members
- Core technical areas:
  - shock physics and energetics
  - solid mechanics
  - structural dynamics
  - thermal and fire sciences
  - aerosciences (hypersonics)
  - fluid mechanics







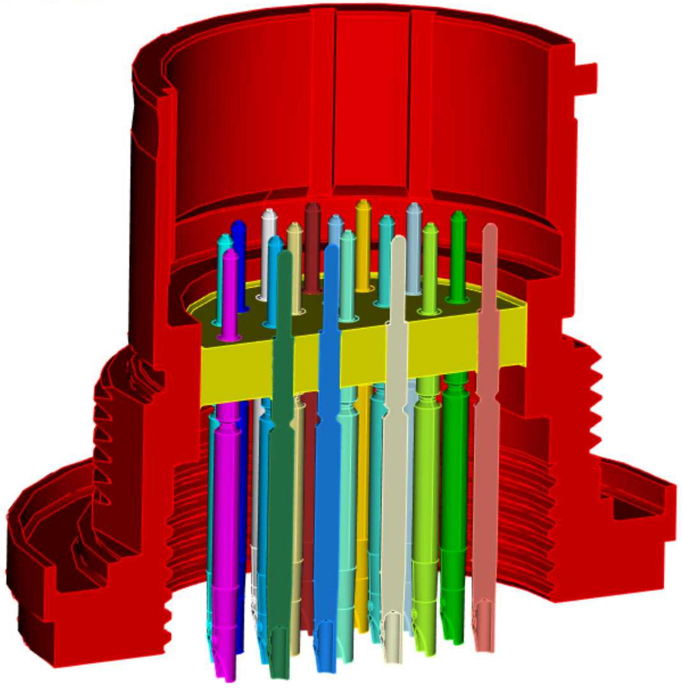
Structural Mechanics and Research Group

- 6 departments:
  - Structural Dynamics (linear)
  - Structural Mechanics (nonlinear)
  - Component Science and Mechanics (engineering mechanics)
  - Computational Material Mechanics (material models)
  - Environments Engineering
  - Computational Shock Physics
- 100 staff members
- Two summer intern institutes:
  - RAMS: Research & Applications of Mechanics of Structures (12 students)
  - NOMAD: Nonlinear Mechanics and Dynamics (18 students)

www.sandia.gov/careers/students_postdocs/

Component Science and Mechanics

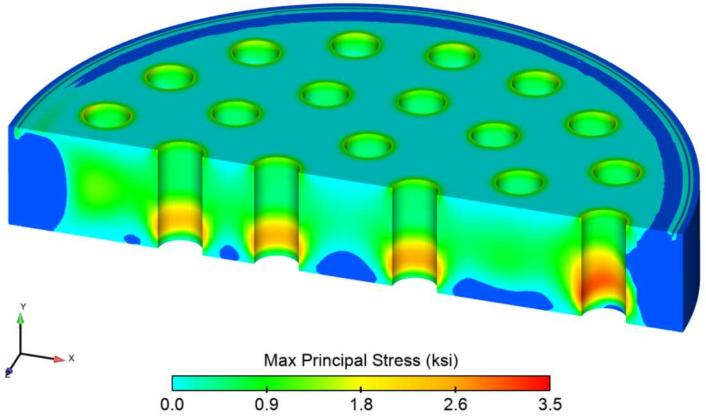
- About 15 staff members: 2/3 M.S., 1/3 Ph.D.
- Tightly integrated with "product realization teams"
- FEA analysis, engineering mechanics



hermitic
connector

Research areas:

- contact mechanics
- fracture mechanics
- advanced stress analysis, error estimation
- parametric reduced-order models (multifidelity)
- object-oriented modeling (e.g. Modelica)
- rapid design to analysis methodologies



Outline

1. Multiscale modeling and model-form error estimation
2. Polyhedral finite element formulation

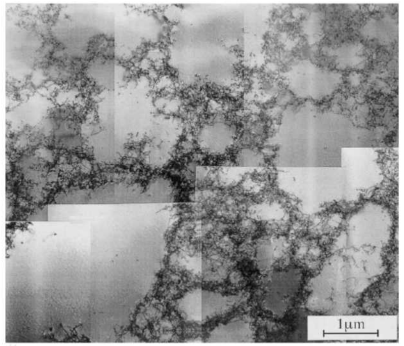
Solid mechanics: multiple scales

dislocation dynamics

Peach-Koehler relation

$$\mathbf{F} = (\mathbf{b} \cdot \sigma) \times \hat{\xi} \quad \sim \quad O(1/r)$$

dislocation cell structure



(Zaiser, M. and P. Hähner, 1999)

crystal plasticity

conservation of linear momentum $\dfrac{\partial \mathbf{P}}{\partial \mathbf{X}} : \mathbf{I} + \rho_o \mathbf{b} = \rho_o \ddot{\mathbf{u}} \quad \text{in} \quad \Omega$

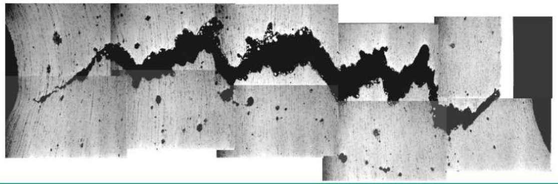
plastic velocity gradient:

$$L^p = \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha P^\alpha$$

$$P^\alpha = m^\alpha \otimes n^\alpha$$

AM 304L microstructure (LENS)

ductile void growth & coalescence



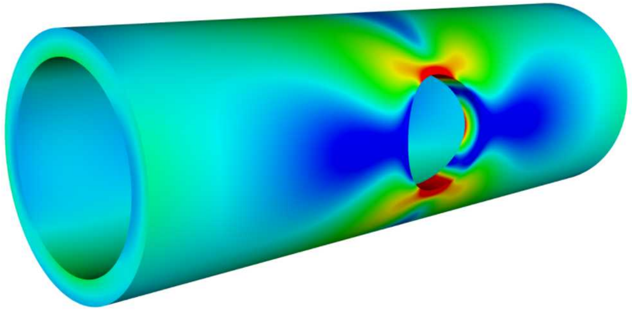
Benzerga, 1999)

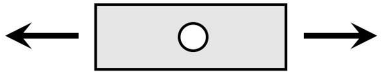
macroscale plasticity

conservation of linear momentum $\dfrac{\partial \mathbf{P}}{\partial \mathbf{X}} : \mathbf{I} + \rho_o \mathbf{b} = \rho_o \ddot{\mathbf{u}} \quad \text{in} \quad \Omega$

yield surface $f(\sigma, \bar{\varepsilon}^p) = \phi(\sigma) - \sigma_y(\bar{\varepsilon}^p) = 0$

$$\phi(\sigma) = \left\{ \frac{1}{2} \left(|\sigma_1 - \sigma_2|^a + |\sigma_1 - \sigma_3|^a + |\sigma_2 - \sigma_3|^a \right) \right\}^{1/a}$$





10^{-6} 10^{-4} 10^{-2}

Length Scale (m), time scale (s)

Multiscale modeling challenges for solid mechanics

1. First principles prediction of strain-hardening behavior in ductile materials
2. Stress-strain behavior is path, rate and T dependent (infinite dimensional).
3. Strain localization, fracture

4. Limits of homogenization theory (lack of scale separation)
5. How to include material variability at macroscale? (homogenization filters fine scale)
6. Concurrent multiscale modeling?
7. error estimation (epistemic uncertainty)

Types of uncertainty (UQ)

Types of aleatory uncertainty

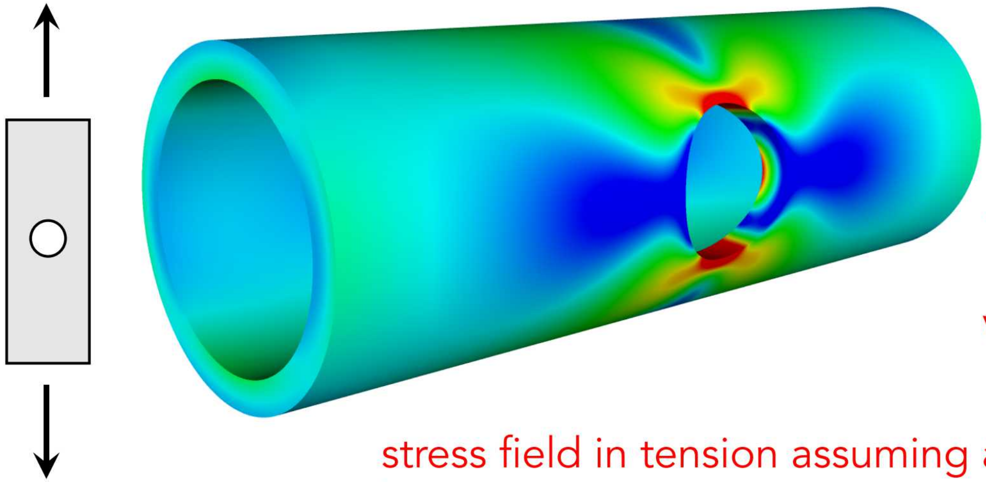
- microstructure (material variability)
- geometric
- loading

Types of errors (epistemic uncertainty)

- model-form error
- homogenization error
  - lack of scale separation
  - surface effects
  - lack of a representative volume element

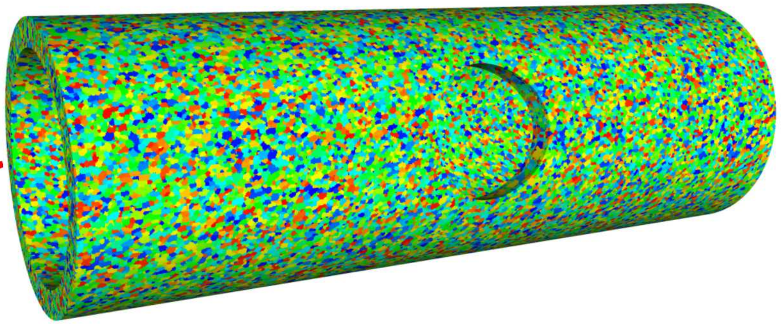
Error estimation as UQ (epistemic)

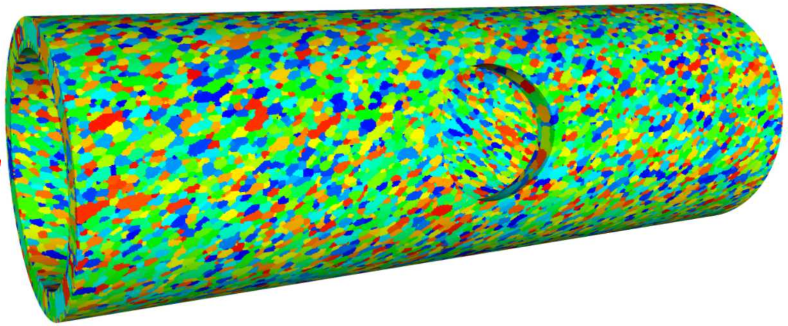
- simple macroscale model
- deterministic (simulate once)
- assess error *a posteriori*

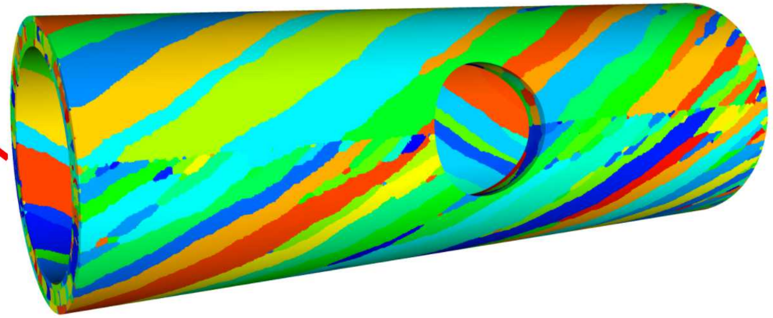


stress field in tension assuming a homogeneous isotropic material

variable microstructure





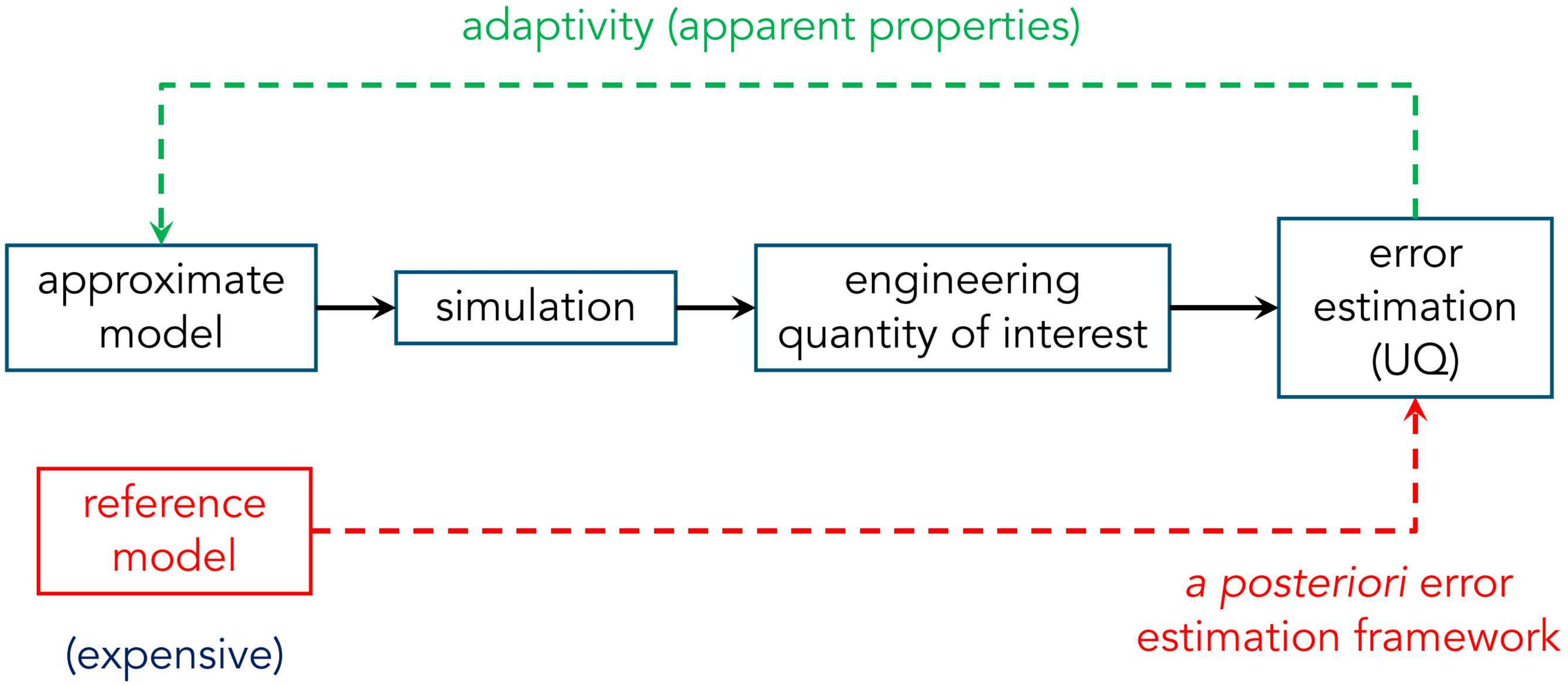


time to failure

stochastic bound

$$t_{\mathrm{f}}(\omega) \longrightarrow t_f \leq \eta(\omega)$$

Error estimation and adaptivity



time to failure

stochastic bound

$$t_{\mathrm{f}}(\omega) \longrightarrow t_f \leq \eta(\omega)$$

Error estimation as UQ

single scale

- Zohdi, T.I., J.T. Oden, and G.J. Rodin, Hierarchical modeling of heterogeneous bodies. Computer Methods in Applied Mechanics and Engineering, 1996, 138:273-298.
- Oden, J.T. and T.I. Zohdi, Analysis and adaptive modeling of highly heterogeneous elastic structures. Computer Methods in Applied Mechanics and Engineering, 1997, 148: 367-391.

multi-scale

- Oden, J.T. and K. Vemaganti, Adaptive hierarchical modeling of heterogeneous structures. Physica D: Nonlinear Phenomena, 1999, 133:404-415.

goal oriented

- Oden, J.T. and K.S. Vemaganti, Estimation of Local Modeling Error and Goal-Oriented Adaptive Modeling of Heterogeneous Materials: I. Error Estimates and Adaptive Algorithms. Journal of Computational Physics, 2000, 164:22-47.
- Oden, J.T. and S. Prudhomme, *Goal-oriented error estimation and adaptivity for the finite element method*. Computers & Mathematics with Applications, 2001, 41:735-756.

nonlinear

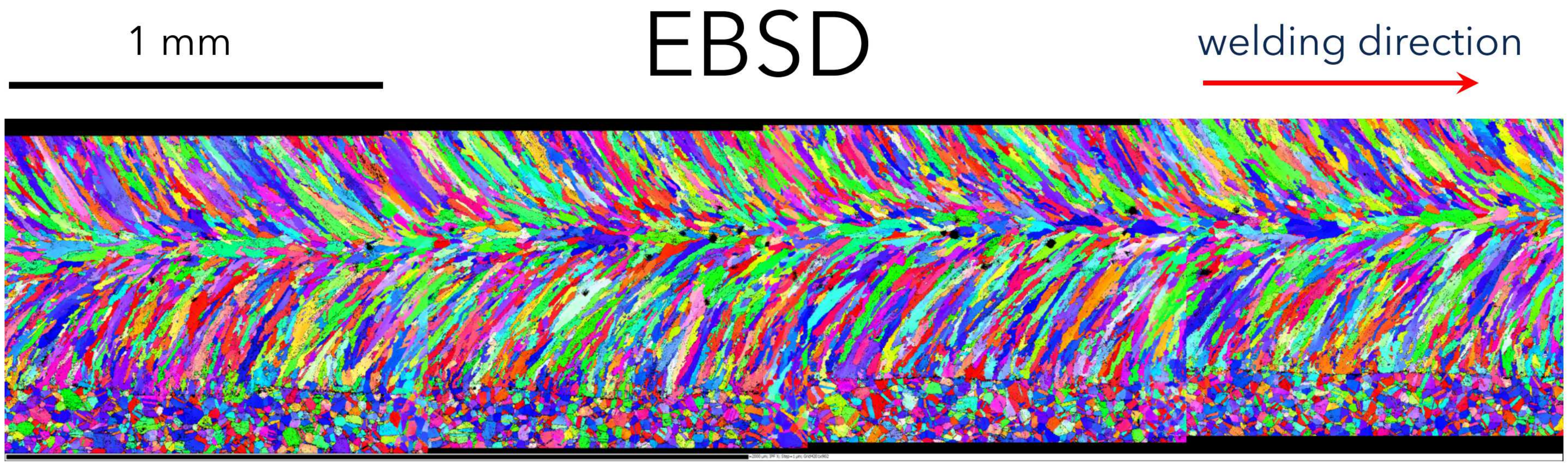
- Oden, J.T., et al., *Modeling error and adaptivity in nonlinear continuum mechanics*. Computer Methods in Applied Mechanics and Engineering, 2001, 190:6663-6684.

UQ

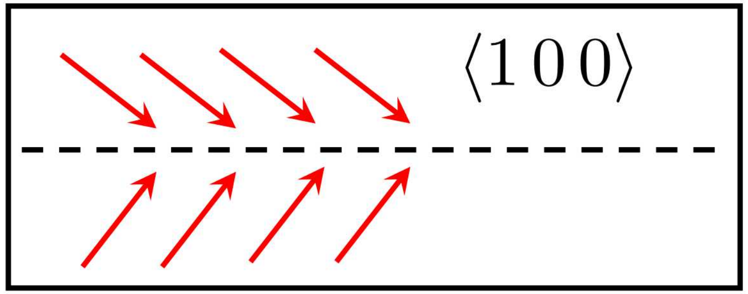
- Romkes, A. and J.T. Oden, Adaptive modeling of wave propagation in heterogeneous elastic solids. Computer Methods in Applied Mechanics and Engineering, 2004, 193:539-559.

- need a “reference model” (or advanced experiments)
- adapt macroscale model to reduce error or uncertainty

Motivation: Laser weld, 304L



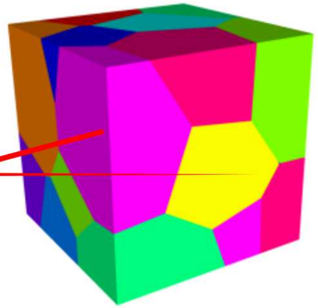
How to homogenize?



Stainless steel 304L single crystal elasticity constants

austenite FCC (cubic symmetry)

$$\left.\begin{aligned} C_{11} &= 204.6 \ \ \mathrm{GPa} \\ C_{12} &= 137.7 \ \ \mathrm{GPa} \\ C_{44} &= 126.2 \ \ \mathrm{GPa} \end{aligned}\right\}$$

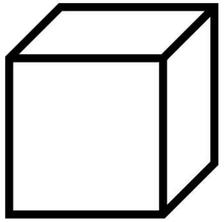


anisotropy ratio $A = \dfrac{2C_{44}}{C_{11} - C_{12}} = 3.8$

(Ledbetter, 1984)

Effect of texture on homogenized elastic properties

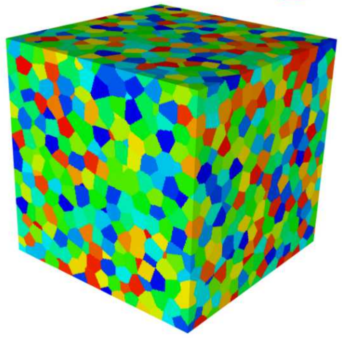
austenite grain (FCC)
304L



cubic symmetry (3 independent)

$$E = 93.8 \text{ GPa}$$
$$\nu = 0.402$$
$$G = 126 \text{ GPa}$$

no texture

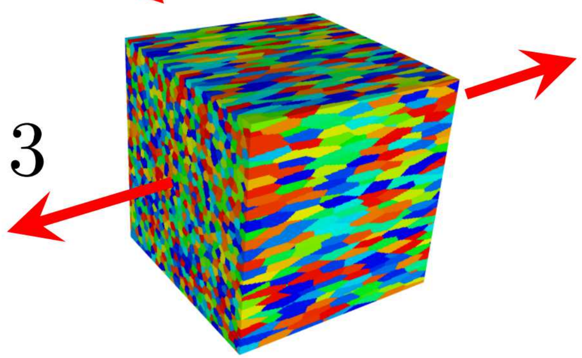


isotropic (2 independent)

$$E = 198 \text{ GPa}$$
$$\nu = 0.294$$
$$G = 76.5 \text{ GPa}$$

$$G = \frac{E}{2(1+\nu)}$$

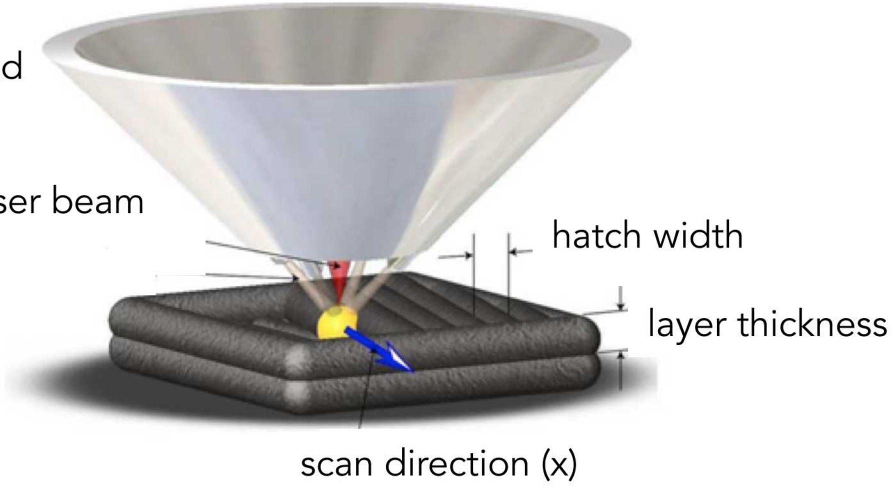
ideal fiber-texture
along [001]

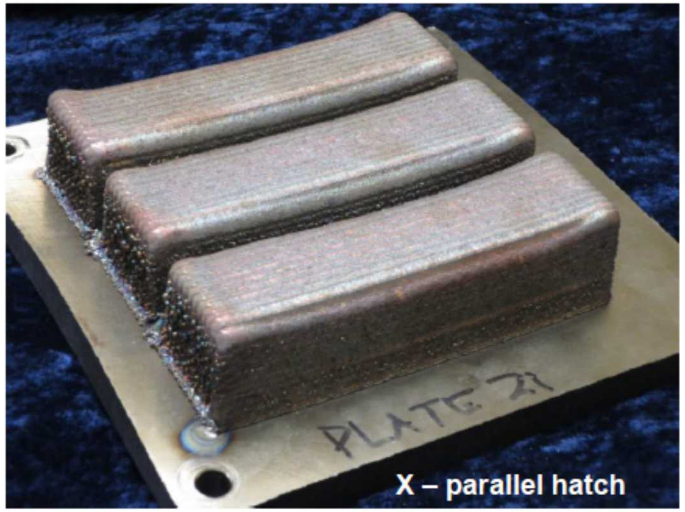


transversely isotropic

$$E_{11} = 143 \text{ GPa}$$
$$E_{22} = 143 \text{ GPa}$$
$$E_{33} = 90.9 \text{ GPa}$$
$$\nu_{12} = 0.114$$
$$\nu_{23} = 0.615$$
$$\nu_{13} = 0.615$$
$$G_{12} = 58 \text{ GPa}$$
$$G_{23} = 126 \text{ GPa}$$
$$G_{13} = 126 \text{ GPa}$$

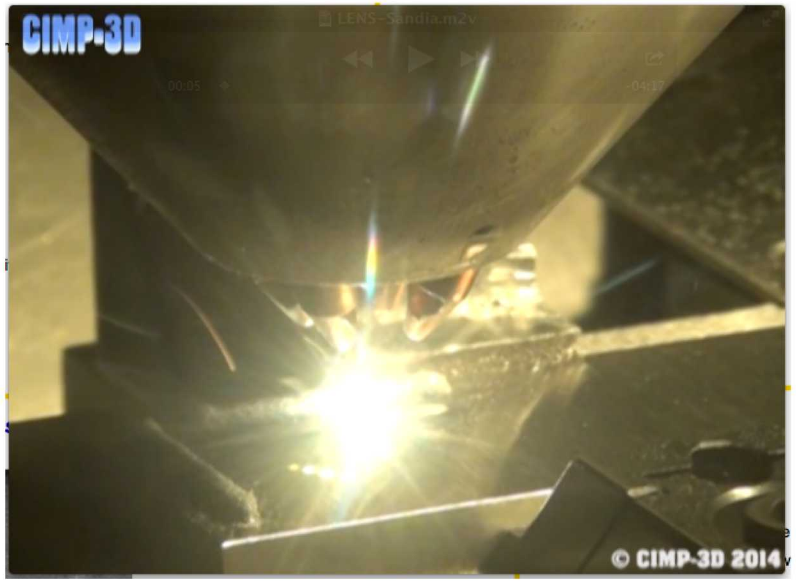
LENS, Laser Engineered Net Shaping



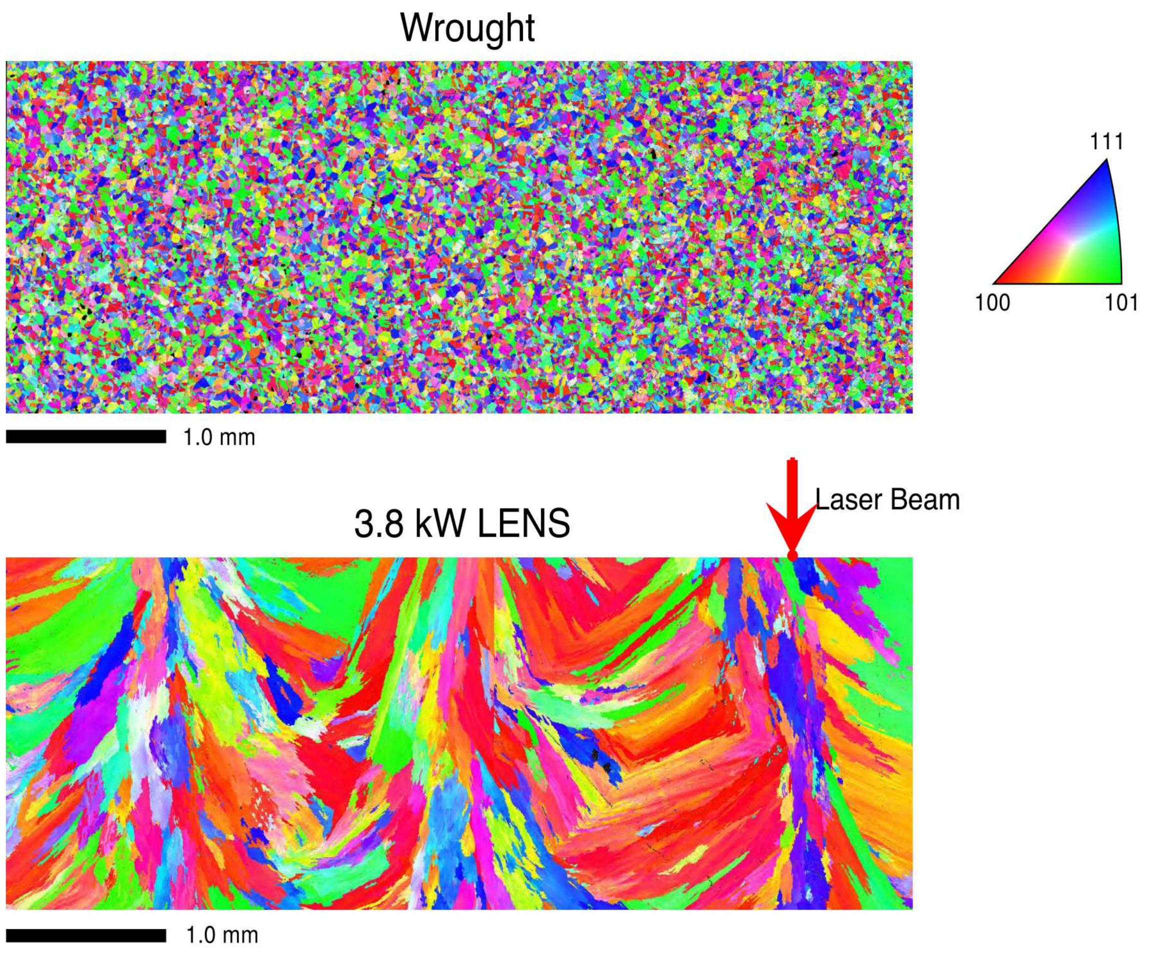


LENS deposition

(T. Palmer, PSU)



Motivation: Microstructure comparison, LENS 304L



- How to homogenize?
- Material or structure?

Error estimation: material-model error

(Zohdi, Oden, Rodin, 1996, CMAME)

$$||\mathbf{u} - \mathbf{u}^0||_E^2 \leq \int_\Omega (\boldsymbol{\varepsilon}^0 - \bar{\boldsymbol{\varepsilon}}) : (\bar{\boldsymbol{\sigma}} - \boldsymbol{\sigma}^0) \, d\Omega$$

displacement field using true material model

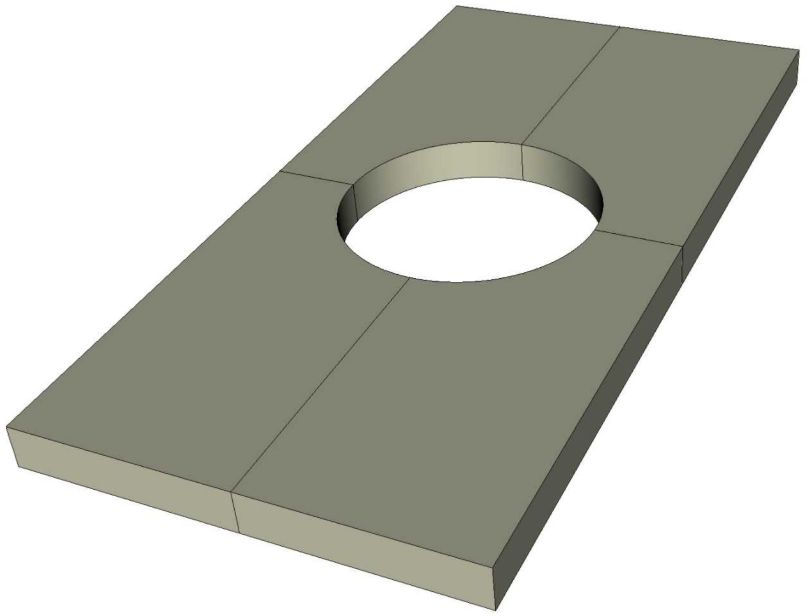
approximate displacement field from simplified or approximate material model

strain field resulting from approx. stress field but true material model

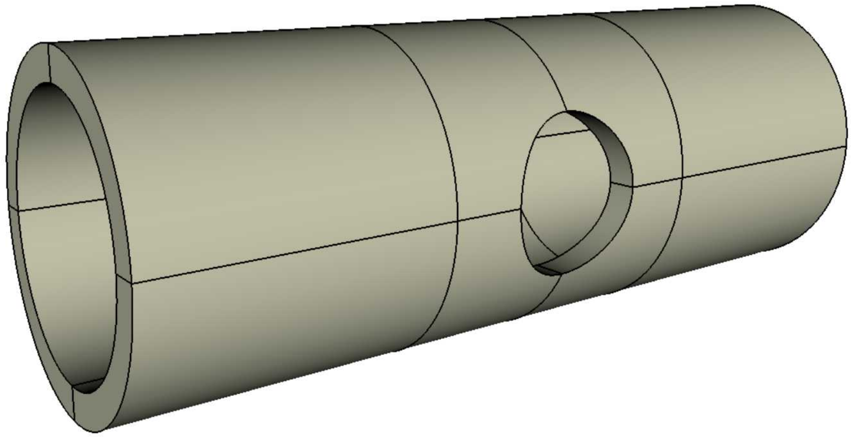
stress field resulting from approx. strain field but true material model

Key point: Can bound error using only known quantities from the approximate simulation. Don't need to run "true" model simulation.

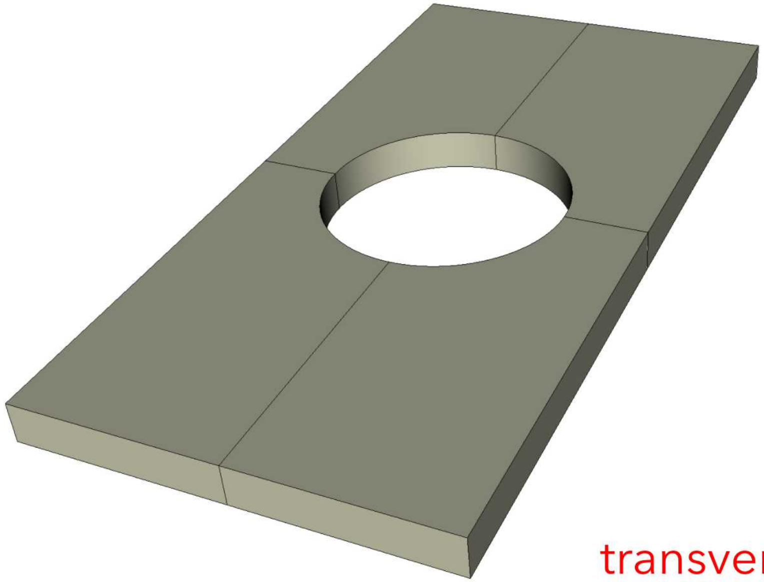
Examples

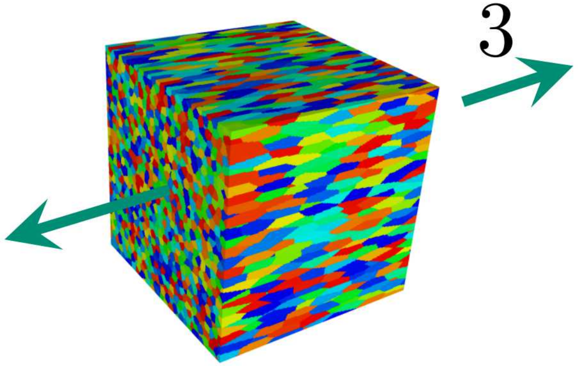


1. anisotropic plate with hole (single scale)
2. tube with side hole: metal additive manufacturing (multiscale)



Example: anisotropic plate with hole





transversely isotropic

$E_{11} = 143$ GPa

$E_{22} = 143$ GPa

$E_{33} = 91.8$ GPa

$\nu_{12} = 0.115$

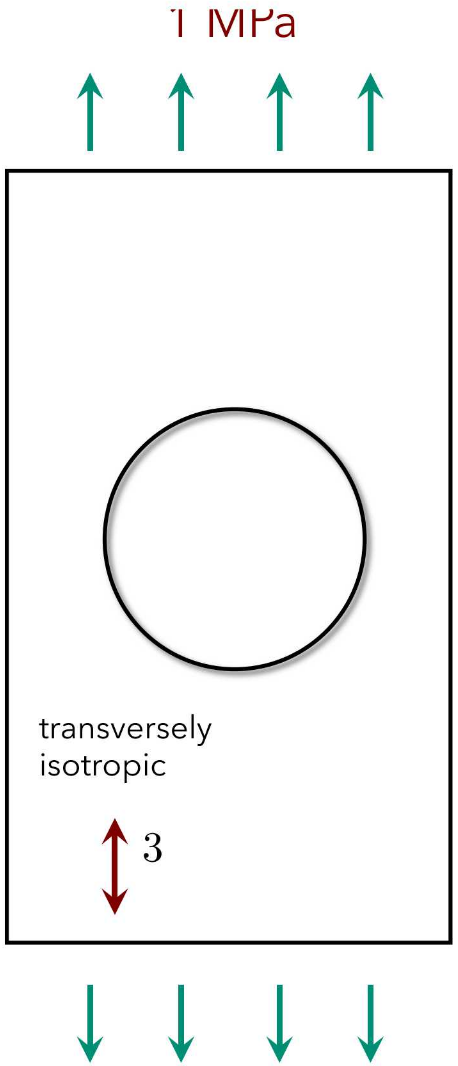
$\nu_{23} = 0.610$

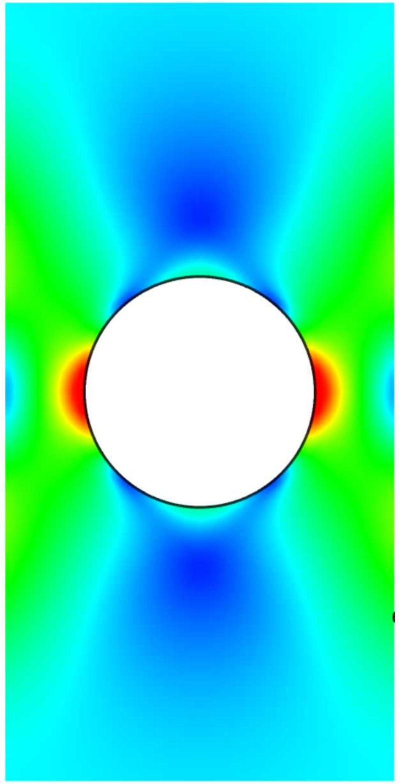
$\nu_{13} = 0.610$

$G_{12} = 64$ GPa

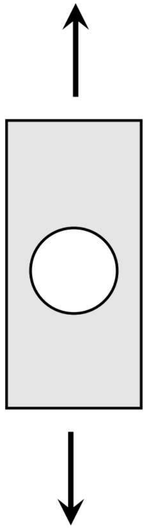
$G_{23} = 126$ GPa

$G_{13} = 126$ GPa

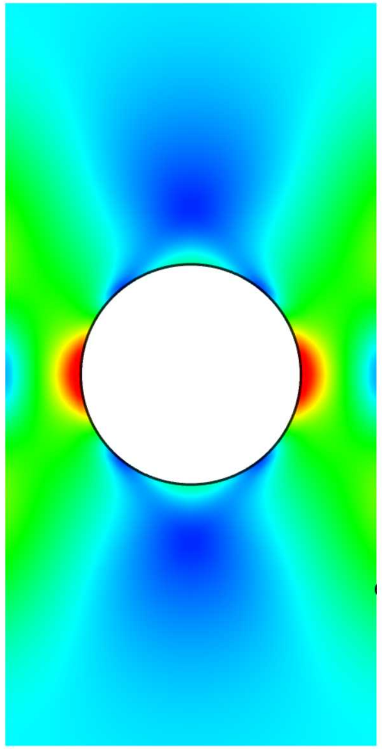




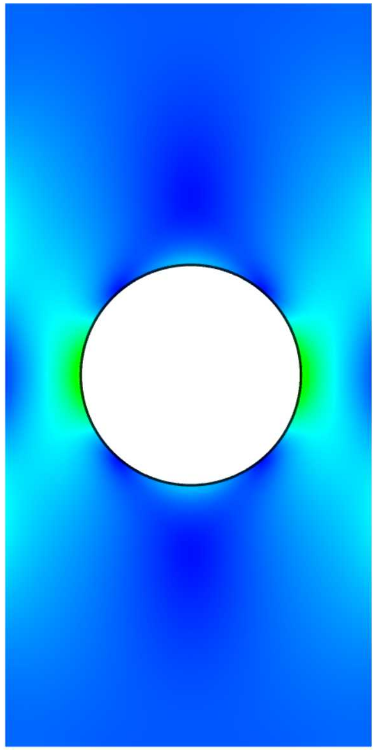
Strain, magnitude



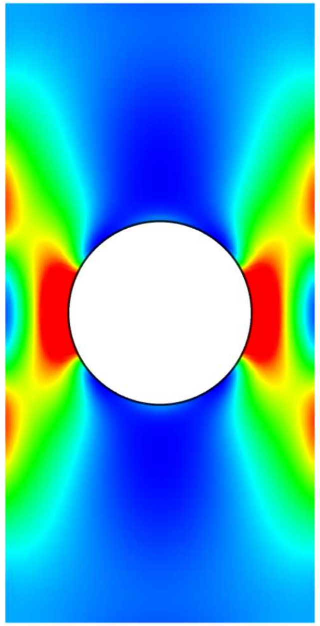
exact



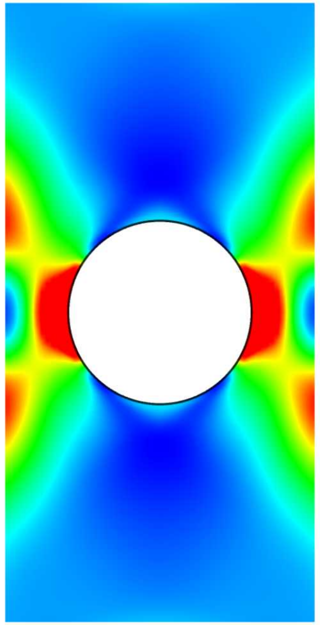
E, $\boldsymbol{\nu}$
homogeneous



estimated
error



9.234×10^{-2}
8.963×10^{-2}



exact error

Model adaptivity

$$\int_\Omega (\mathbf{e}^0 - \bar{\mathbf{e}}) : (\bar{\boldsymbol{\sigma}} - \boldsymbol{\sigma}^0)\, d\Omega \approx \sum_{i=1}^{N} V_e\, \eta_i^2$$

consider fixed

error indicator $\eta_i^2 \approx (\boldsymbol{\epsilon}^0 - \bar{\boldsymbol{\epsilon}}) : (\bar{\boldsymbol{\sigma}} - \boldsymbol{\sigma}^0) = (\mathbb{I} - \mathbb{C}^{-1}\,\mathbb{C}^0\,)\,\boldsymbol{\epsilon}^0 : (\mathbb{C} - \mathbb{C}^0)\,\boldsymbol{\epsilon}^0$

How can we decrease this error, but still use an isotropic material model?

Consider a heterogeneous isotropic material model?

$$\mathbb{C}^0 = \mathbb{C}^{\text{iso}} = a\,\mathbb{J} + b\,\mathbb{K} = 3K\,\mathbb{J} + 2\mu\,\mathbb{K}$$

$\mathbb{J} = \frac{1}{3}\delta_{ij}\delta_{kl}$ hydrostatic operator

$\mathbb{K} = \mathbb{I} - \mathbb{J}$ deviatoric operator

Let bulk modulus *K* and shear modulus μ vary with position.

Model adaptivity

necessary conditions

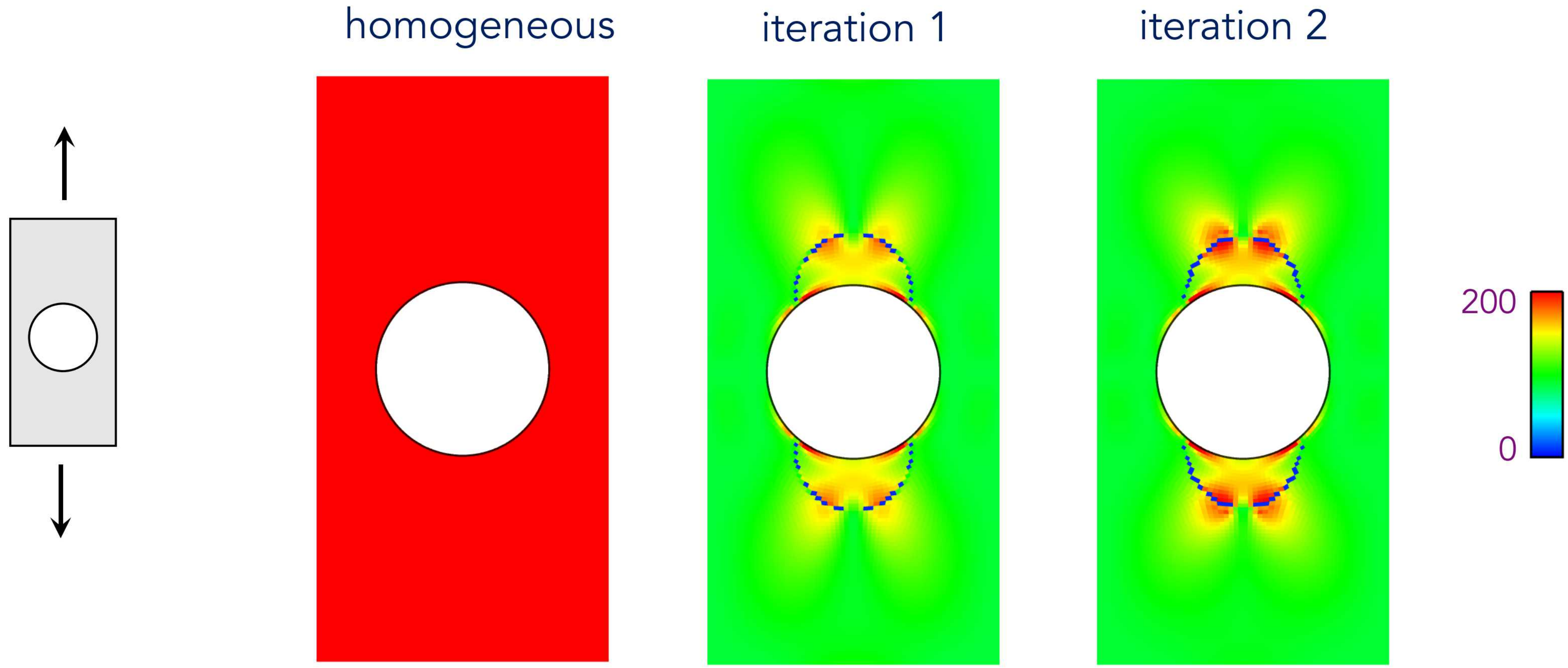
$$\frac{\partial(\eta_i^2)}{\partial a} = 0 \quad \text{and} \quad \frac{\partial(\eta_i^2)}{\partial b} = 0$$

Can derive this 2 by 2 system of equations for the updated bulk and shear moduli.

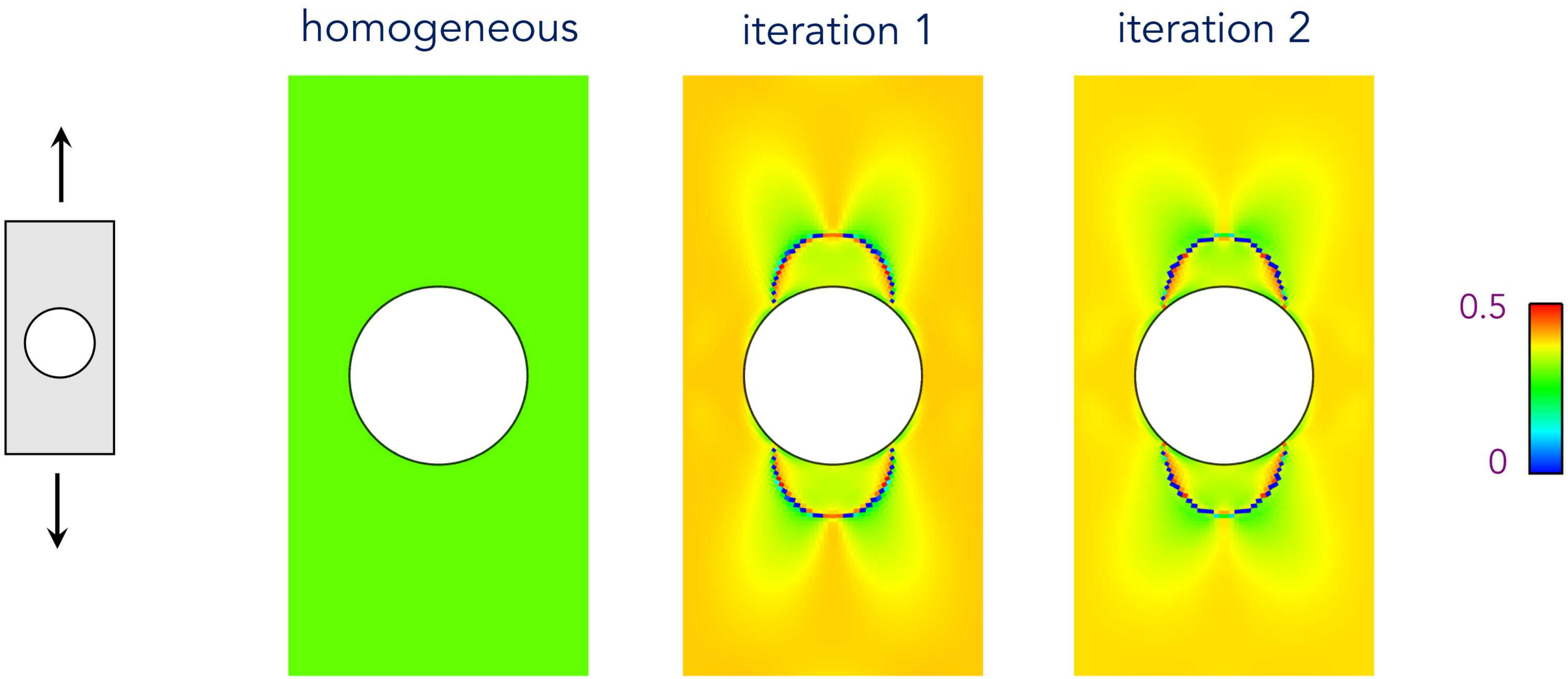
$$\begin{bmatrix} 2(\mathbb{C}^{-1}\,\mathbb{J}\,\boldsymbol{\epsilon}^0) : (\mathbb{J}\,\boldsymbol{\epsilon}^0) & (\mathbb{C}^{-1}\,\mathbb{K}\,\boldsymbol{\epsilon}^0) : (\mathbb{J}\,\boldsymbol{\epsilon}^0) + (\mathbb{C}^{-1}\,\mathbb{J}\,\boldsymbol{\epsilon}^0) : (\mathbb{K}\,\boldsymbol{\epsilon}^0) \\ (\text{sym}) & 2(\mathbb{C}^{-1}\,\mathbb{K}\,\boldsymbol{\epsilon}^0) : (\mathbb{K}\,\boldsymbol{\epsilon}^0) \end{bmatrix} \begin{Bmatrix} 3K_{\text{new}} \\ 2\,\mu_{\text{new}} \end{Bmatrix} =$$

$$\begin{Bmatrix} ||\mathbb{J}\,\boldsymbol{\epsilon}^0||_2^2 + (\mathbb{C}^{-1}\,\mathbb{J}\,\boldsymbol{\epsilon}^0) : (\mathbb{C}\,\boldsymbol{\epsilon}^0) \\ ||\mathbb{K}\,\boldsymbol{\epsilon}^0||_2^2 + (\mathbb{C}^{-1}\,\mathbb{K}\,\boldsymbol{\epsilon}^0) : (\mathbb{C}\,\boldsymbol{\epsilon}^0) \end{Bmatrix}$$

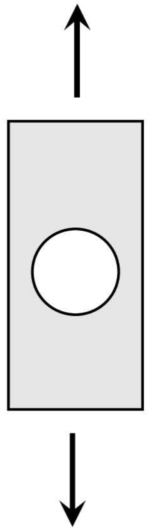
Young's modulus



Poisson's ratio

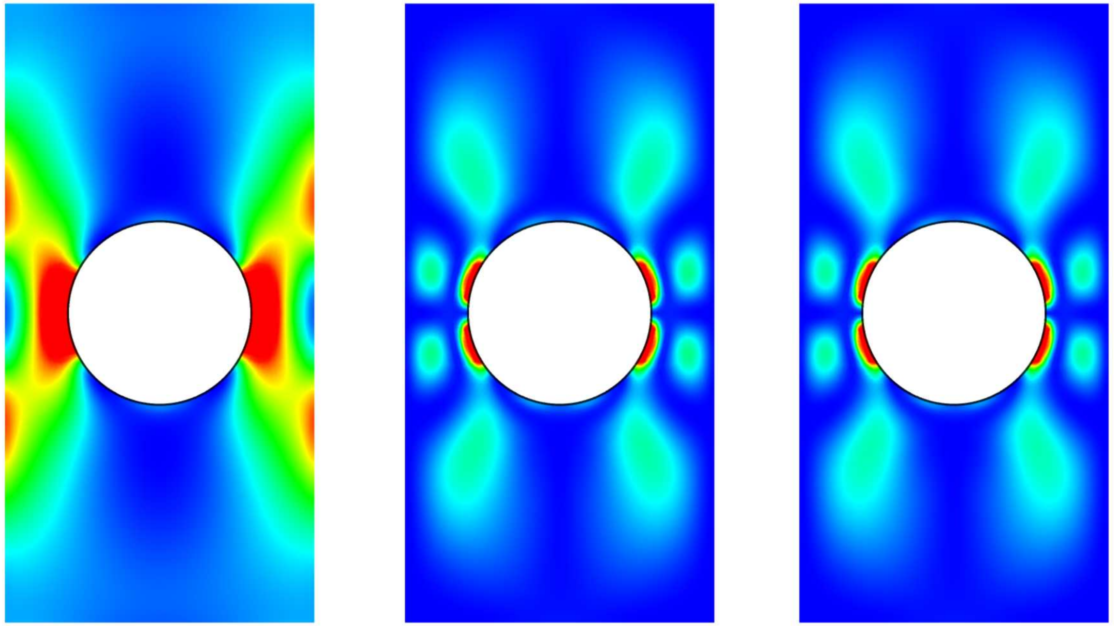


Error bound



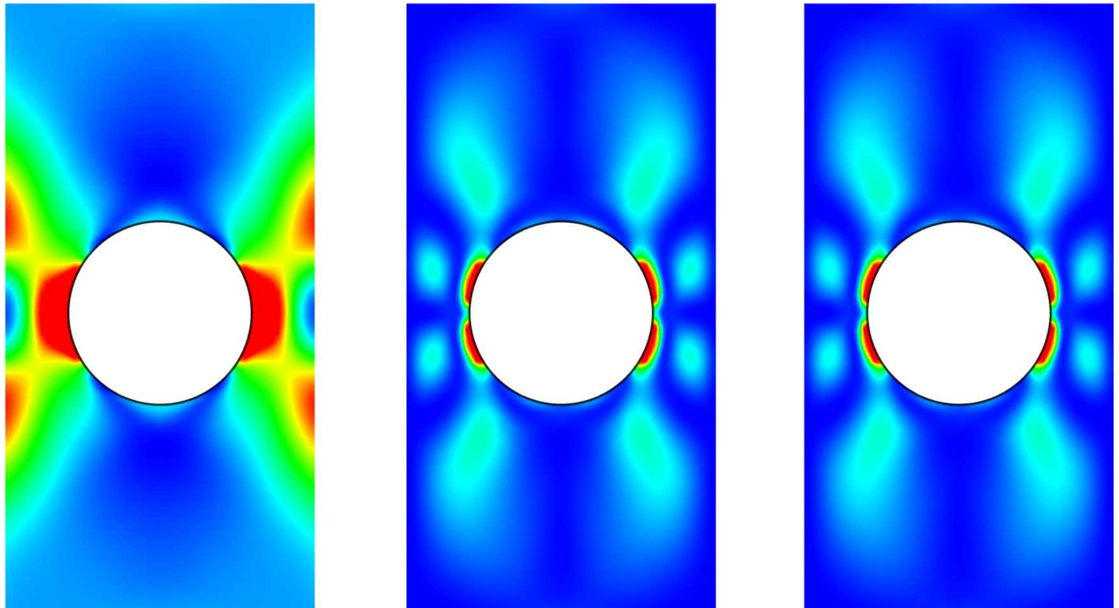
E, ν, homogeneous | iteration 1 | iteration 2

estimated error

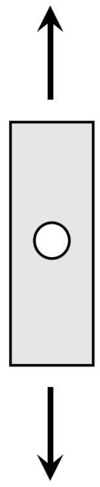


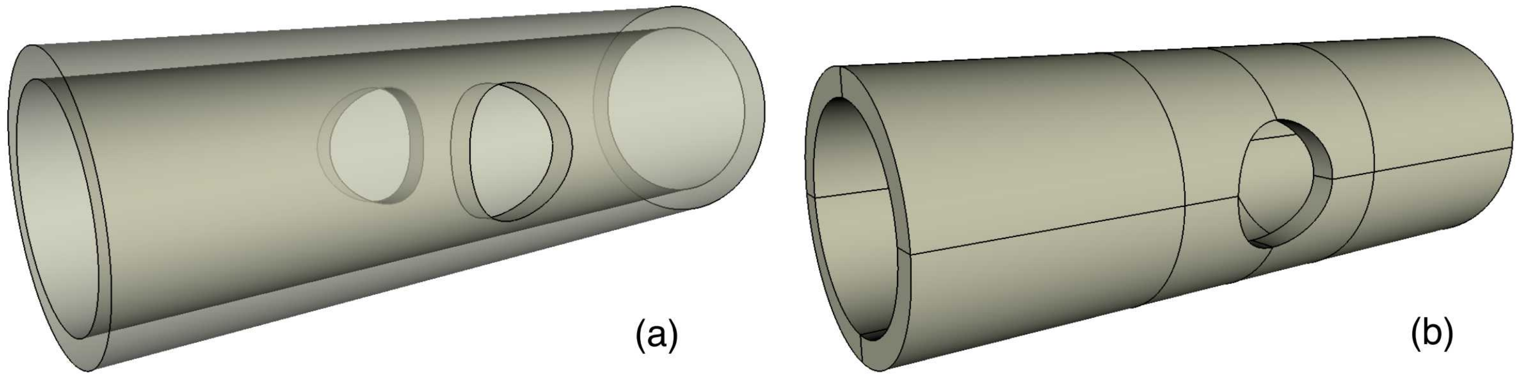
E, ν, homogeneous	iteration 1	iteration 2
9.234×10^{-2}	5.554×10^{-2}	5.482×10^{-2}
8.963×10^{-2}	5.447×10^{-2}	5.378×10^{-2}

exact error



Example (multiscale)





Consider two processing steps

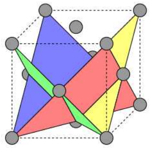
1. AM build for tube (LENS)
2. subtractive machining for side hole

Consider two synthetic microstructures:

1. equiaxed (wrought)
2. additive (LENS using Kinetic Monte Carlo)

FCC crystal plasticity model

plastic velocity gradient: $$L^p = \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha P^\alpha$$



Schmid tensor: $$P^\alpha = m^\alpha \otimes n^\alpha$$

slip system slip rates: $$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left(\frac{\tau^\alpha}{g} \right)^{1/m} \cdot \mathrm{sign}(\tau^\alpha)$$

slip system hardening: $$g = g_o + (g_{so} - g_o) \left[1 - \exp\left(-\frac{G_o}{g_{so} - g_o} \gamma \right) \right]$$

$$\gamma = \sum_{s=1}^{N} |\gamma^s|$$ (sum over slip systems)

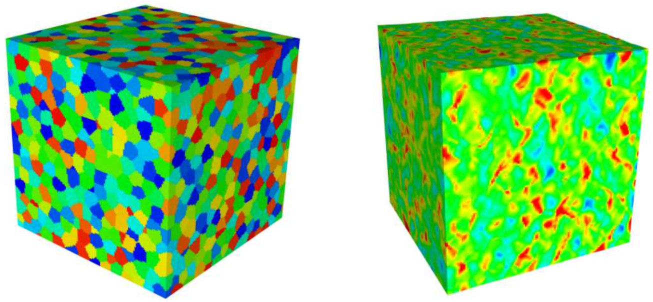
Single crystal elastic constants (austenite)

$$C_{11} = 204.6 \ \text{GPa}$$
$$C_{12} = 137.7 \ \text{GPa}$$
$$C_{44} = 126.2 \ \text{GPa}$$

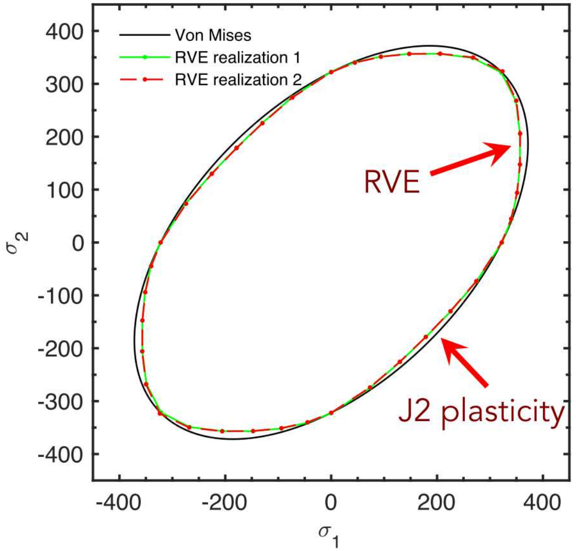
Not considering:

- grain boundary effects (Hall-Petch effect)
- twinning
- dislocation substructures
- latent hardening

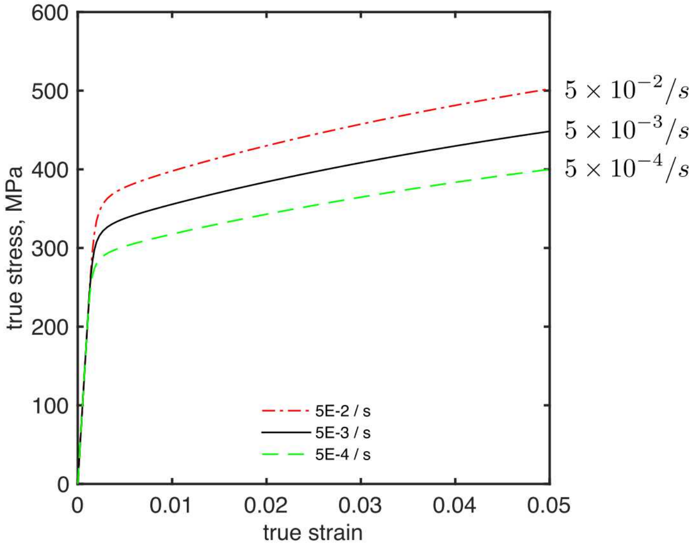
Representative Volume Element (RVE) response



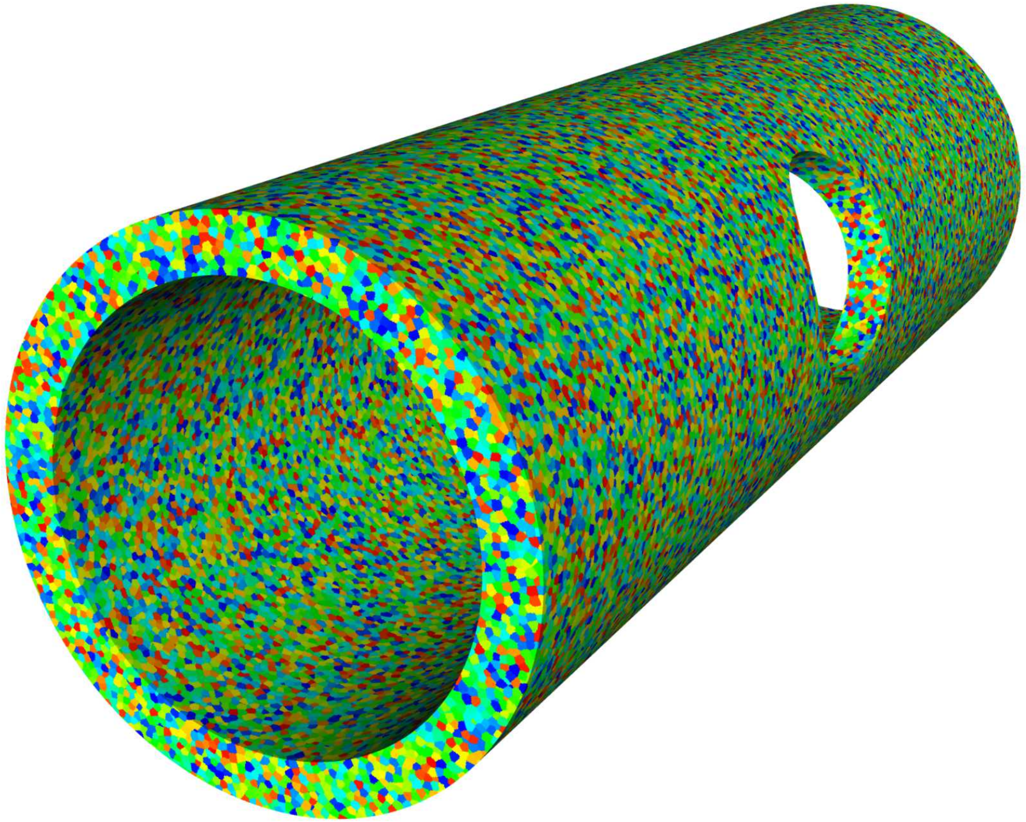
yield surface

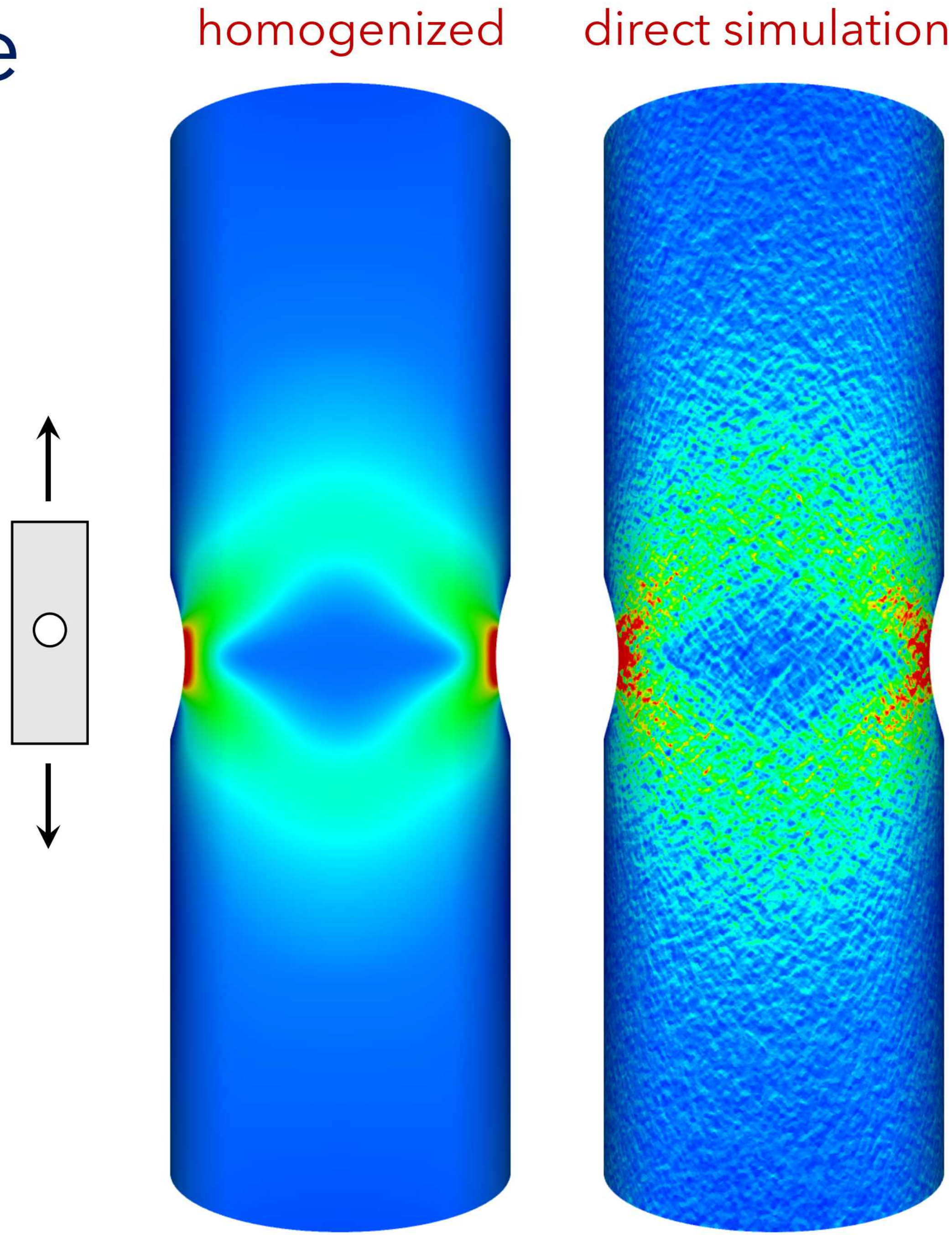


strain-rate dependence



Equiaxed microstructure



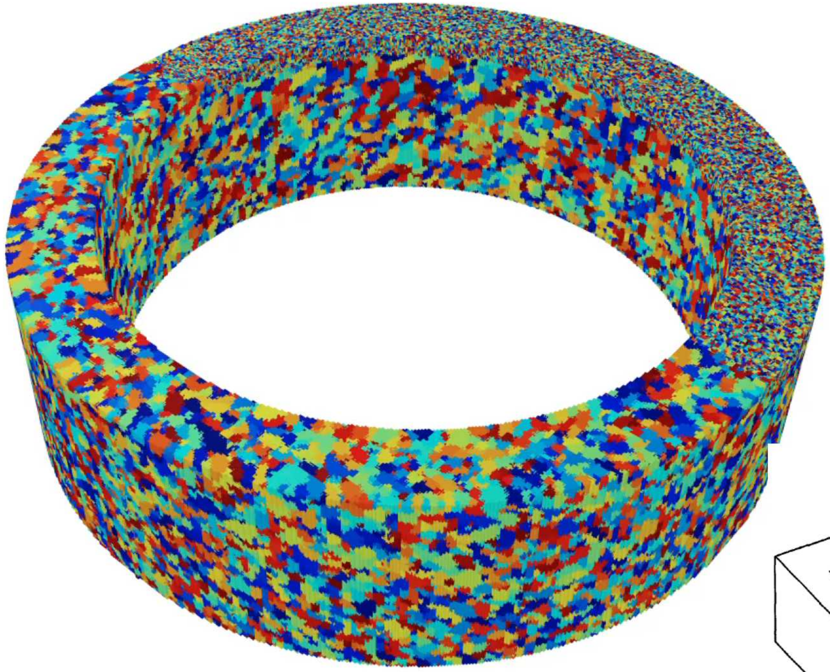


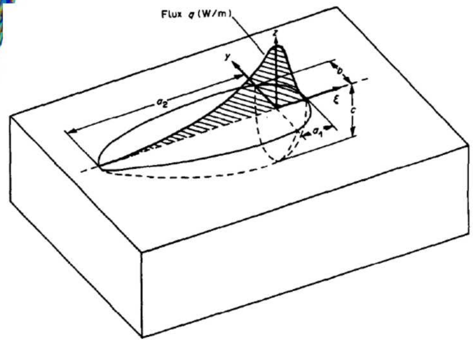
- 358,000 grains
- voxelated with 28M finite elements
- crystal plasticity
- assume no preferred grain orientation (no texture)
- homogenized response is isotropic

Synthetic additive microstructure using Kinetic Monte Carlo (KMC)

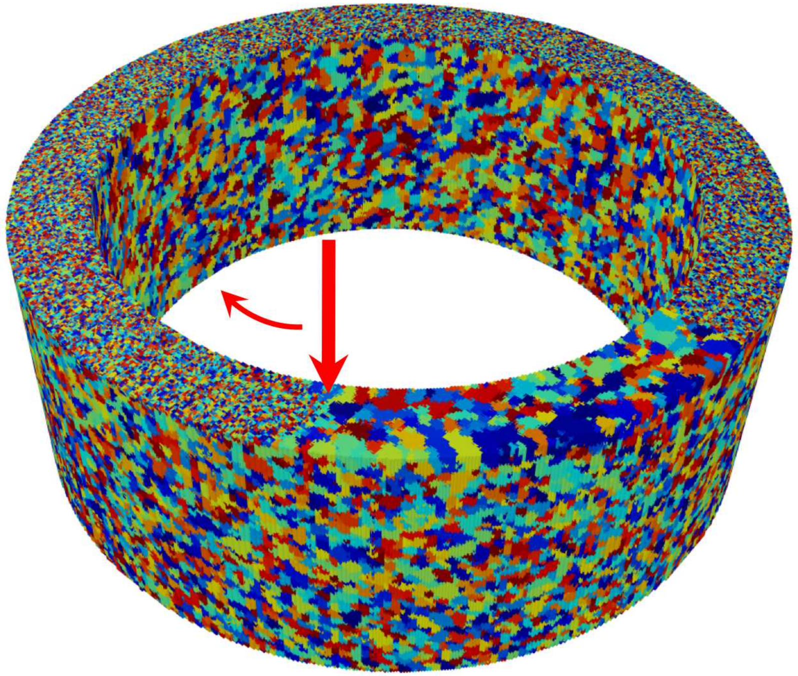
(Theron Rodgers, SNL)

- KMC additive simulation
- single laser pass per layer
- 100 layers
- overlap with previous layer



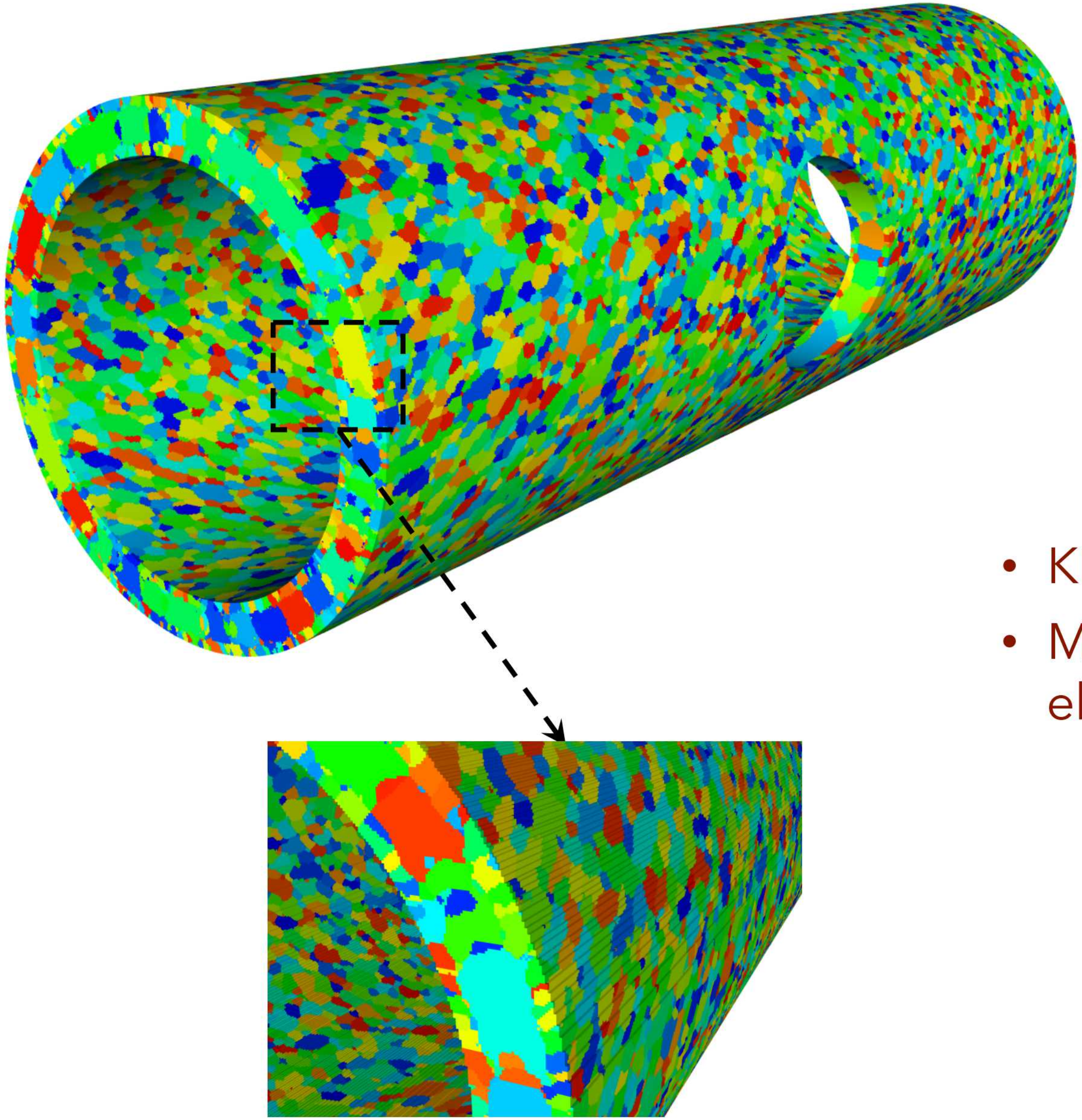


double ellipsoid heat-source model



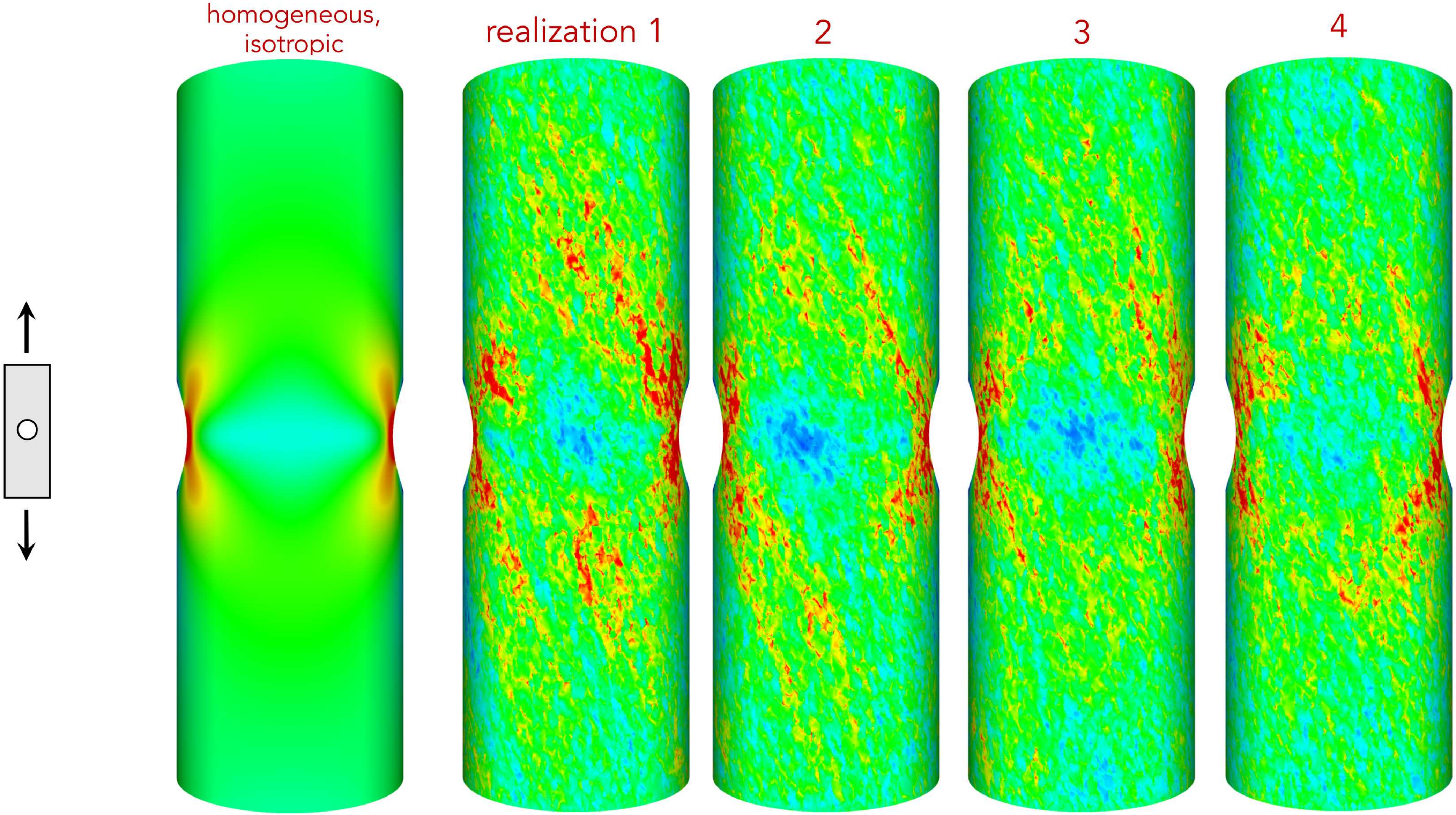
Synthetic additive microstructure using KMC

(Theron Rodgers, Jon Madison, SNL)



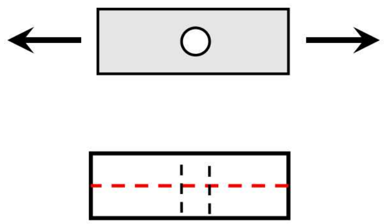
- KMC (SPPARKS) voxelated geometry, 55 million
- Map to a conformal finite-element mesh of 22M elements

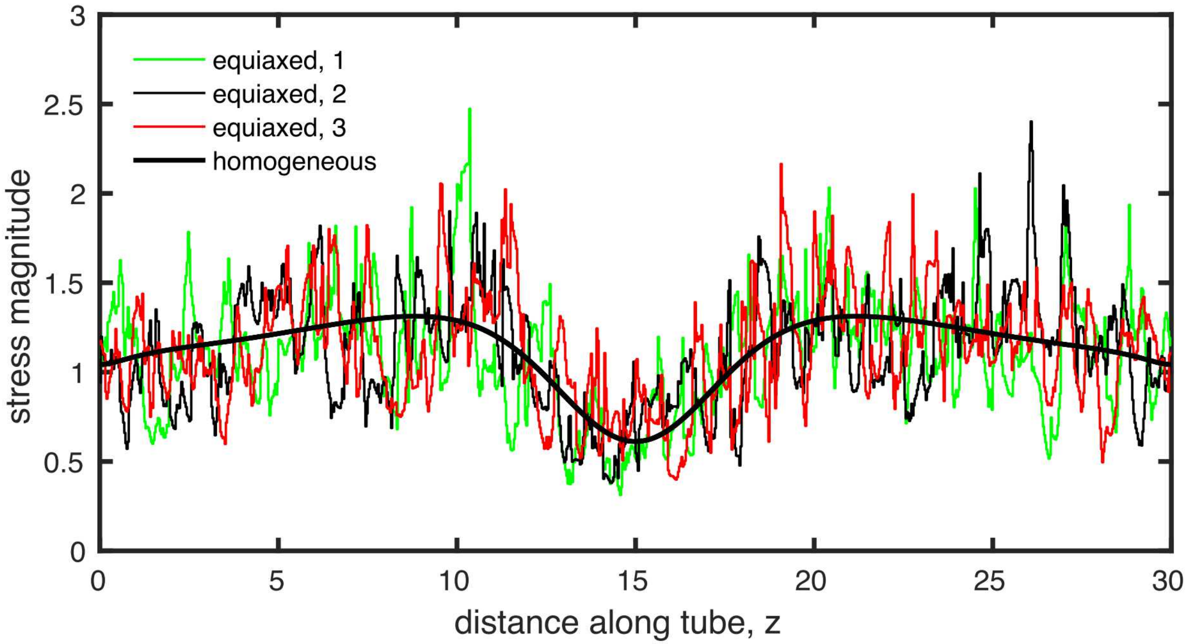
AM stress results (KMC)



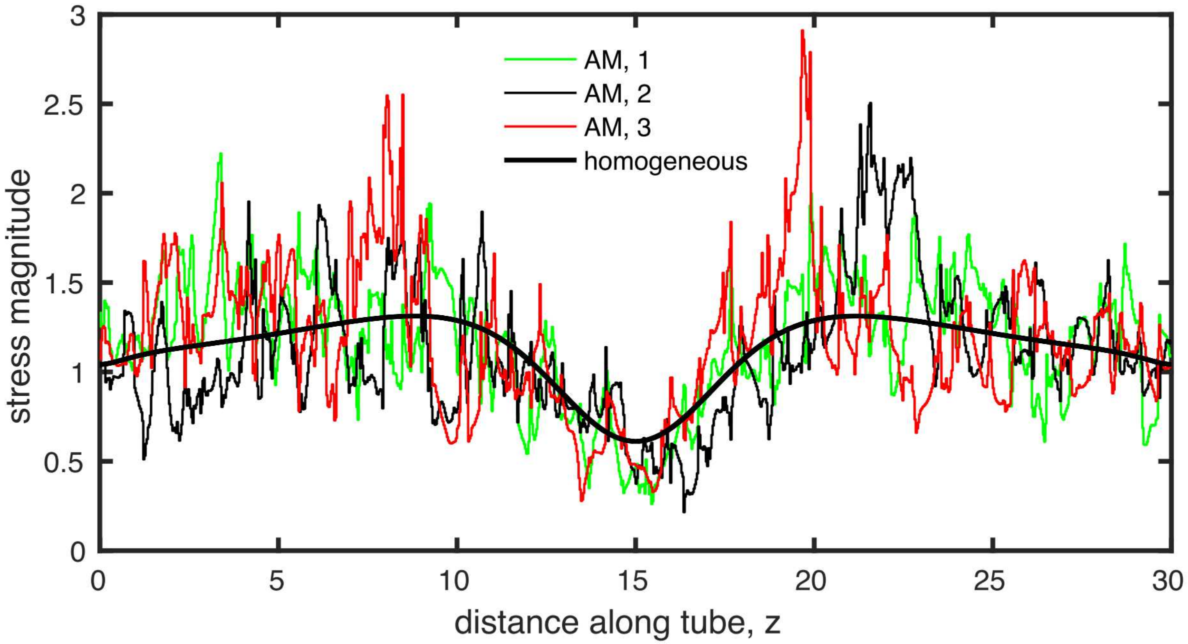
Stress trace

Equiaxed stress result





AM (KMC) stress result



Error estimation: multi-scale

Previous error estimate will perform poorly if applied here.

- similar to Voigt assumption in composites theory (uniform strain)
- need to use a modified error estimate in energy norm.

(Oden, Zohdi, 1997)

$$||\mathbf{w}-\mathbf{u}||_E^2 = 2[J(\mathbf{w}) - J(\mathbf{u}^0)] + \underbrace{||\mathbf{u}-\mathbf{u}^0||_E^2}$$

approximate displacement field from submodeling

displacement field using true material model

potential energy functional

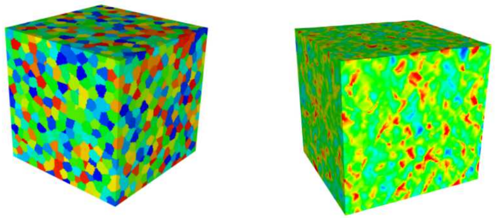
previous estimate

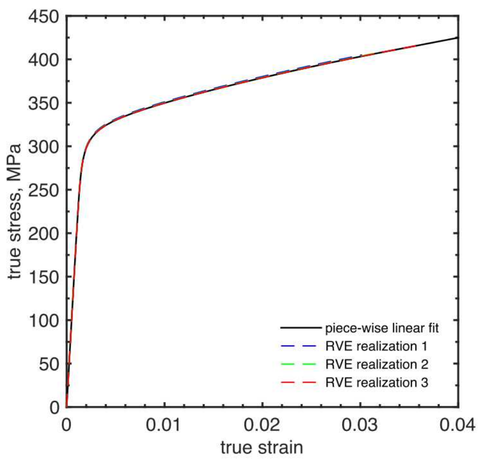
$$||\mathbf{u}-\mathbf{u}^0||_E^2 \leq \sum_{i=1}^{N} V_e\,\eta_i^2$$

How to get approximate microscale displacement field, w?
Use a Dirichlet projection (submodeling)

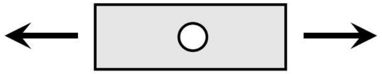
Homogenization-localization duality

Homogenize
(filter fine scale)

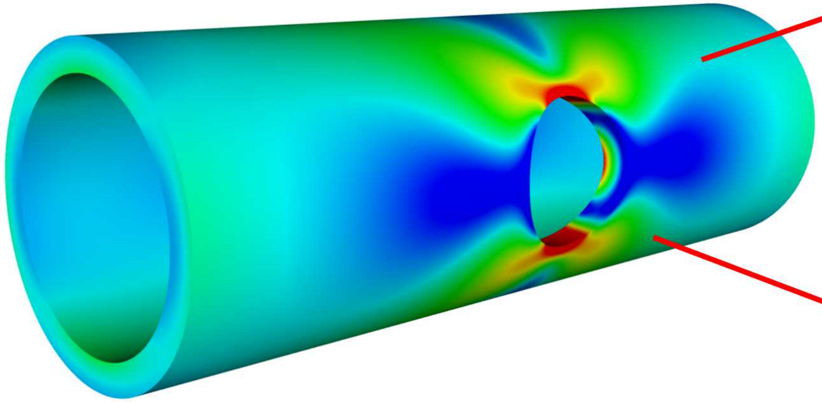




Macroscale simulation



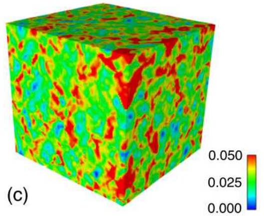
$$\frac{\partial \mathbf{P}}{\partial \mathbf{X}} : \mathbf{I} + \rho_o \mathbf{b} = \rho_o \ddot{\mathbf{u}} \quad \text{in} \quad \Omega$$

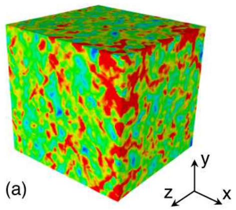


σ_{ij} ε_{ij}

σ_{ij} ε_{ij}

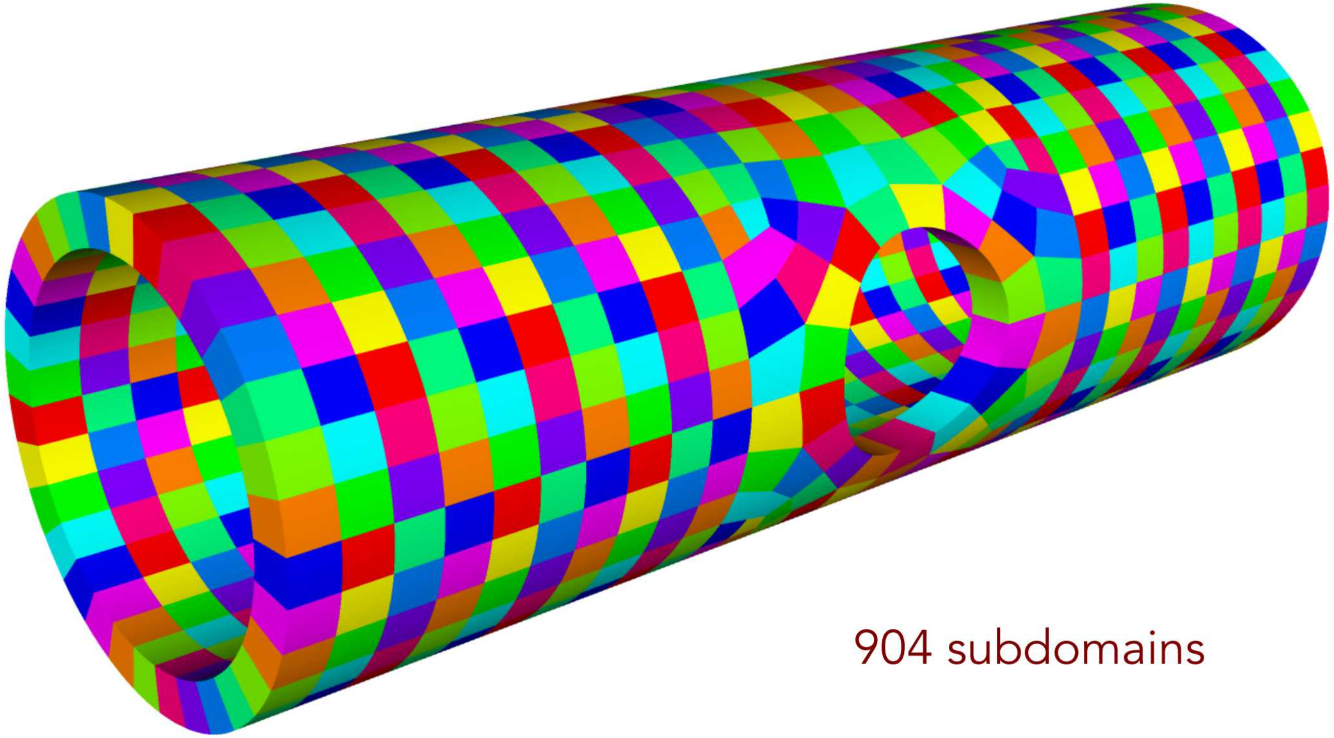
Localization
(recover fine scale)





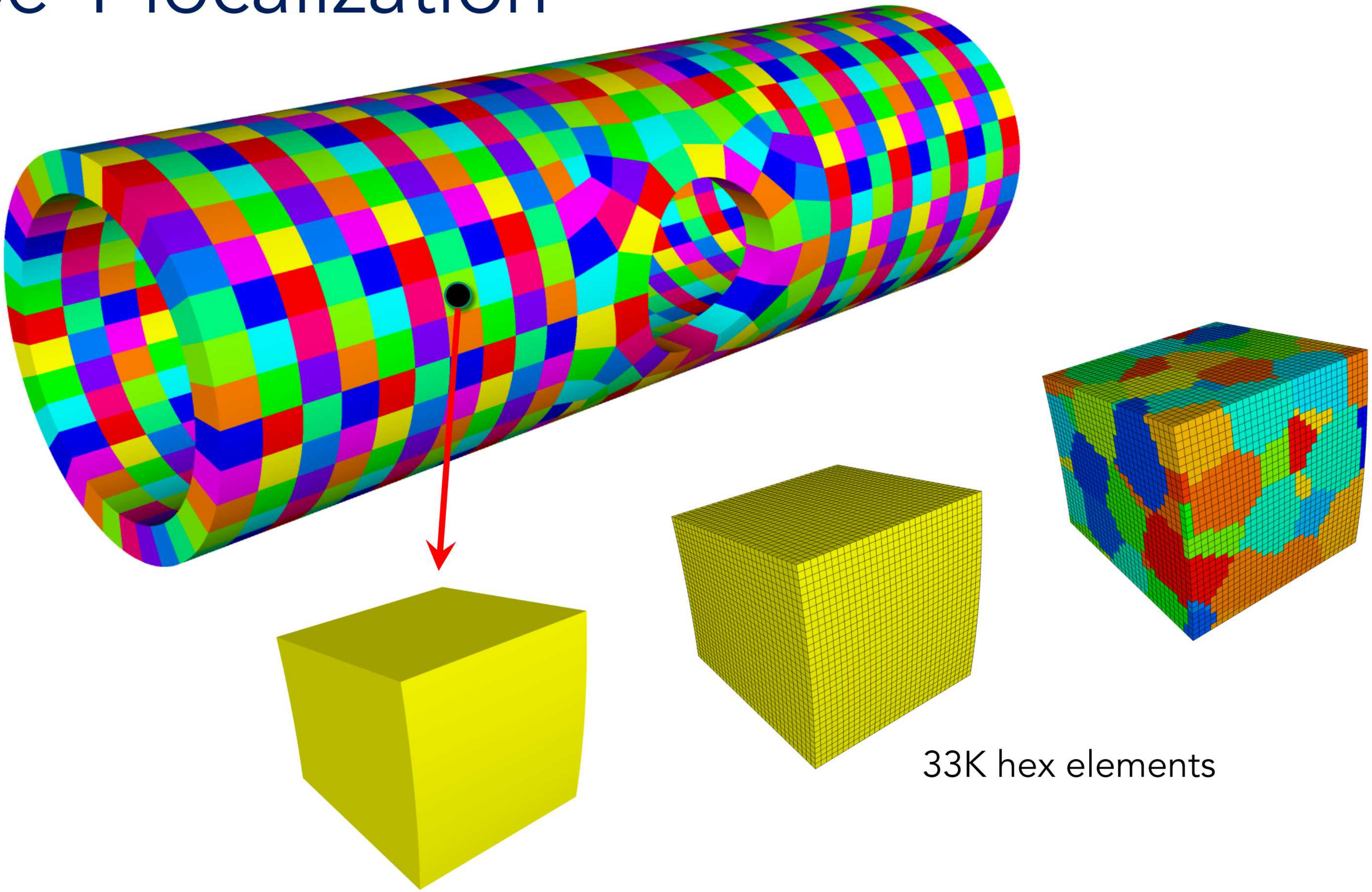
Assumptions:
- scale separation
- RVE well defined
- no surface effects

First, partition structure into non-overlapping subdomains.



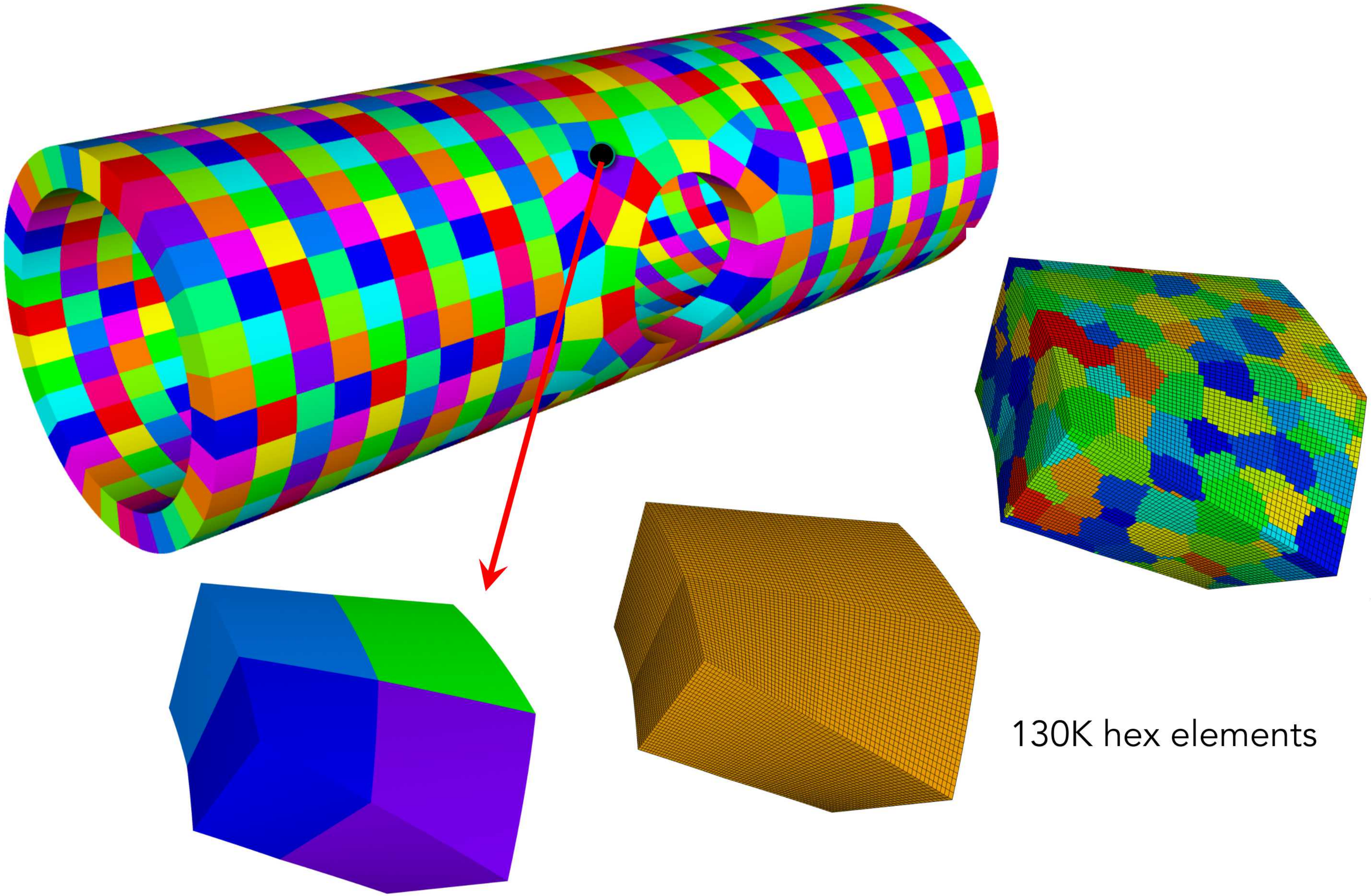
904 subdomains

Type 1 localization



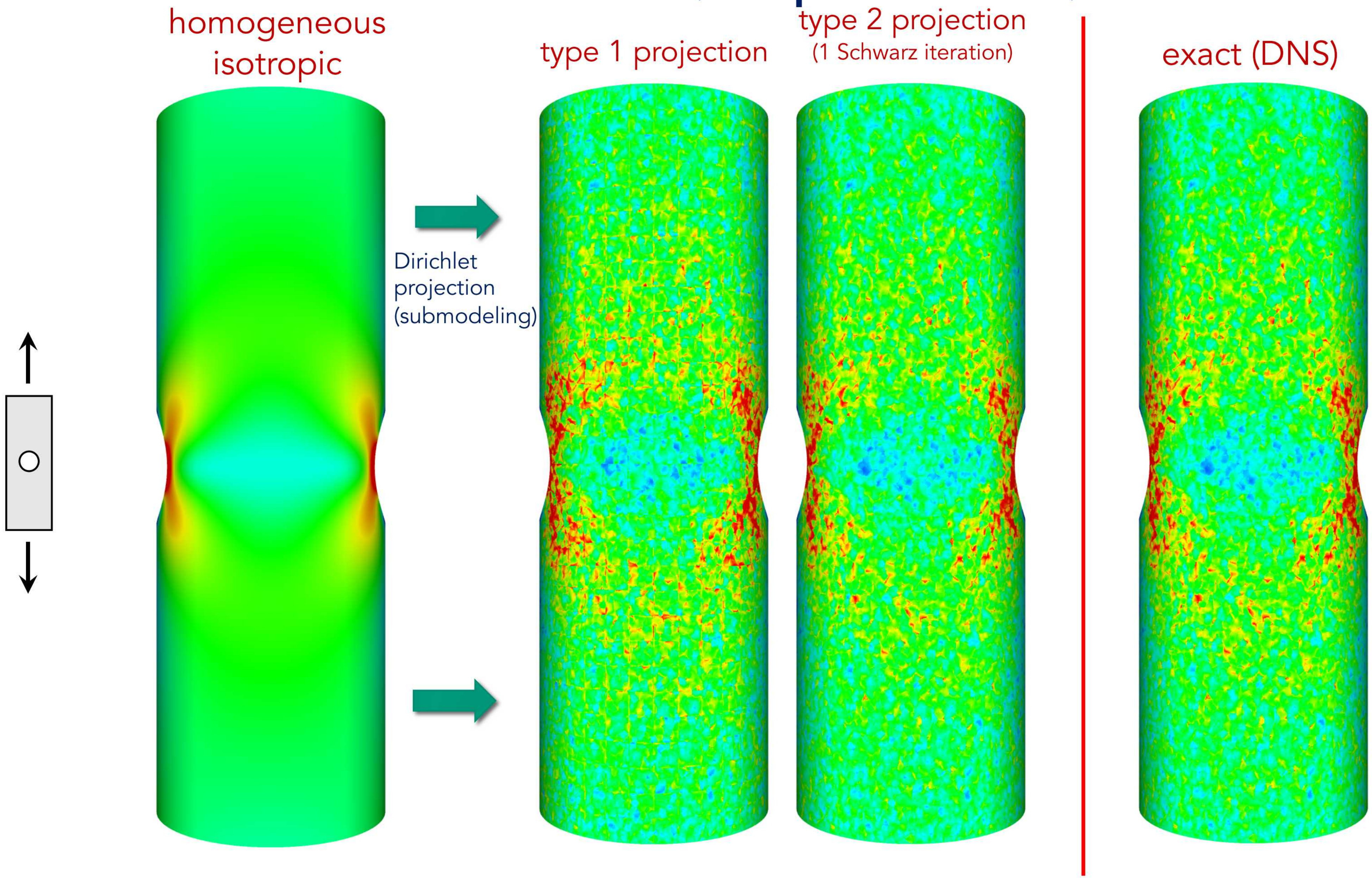
33K hex elements

Type 2 localization (overlapping)

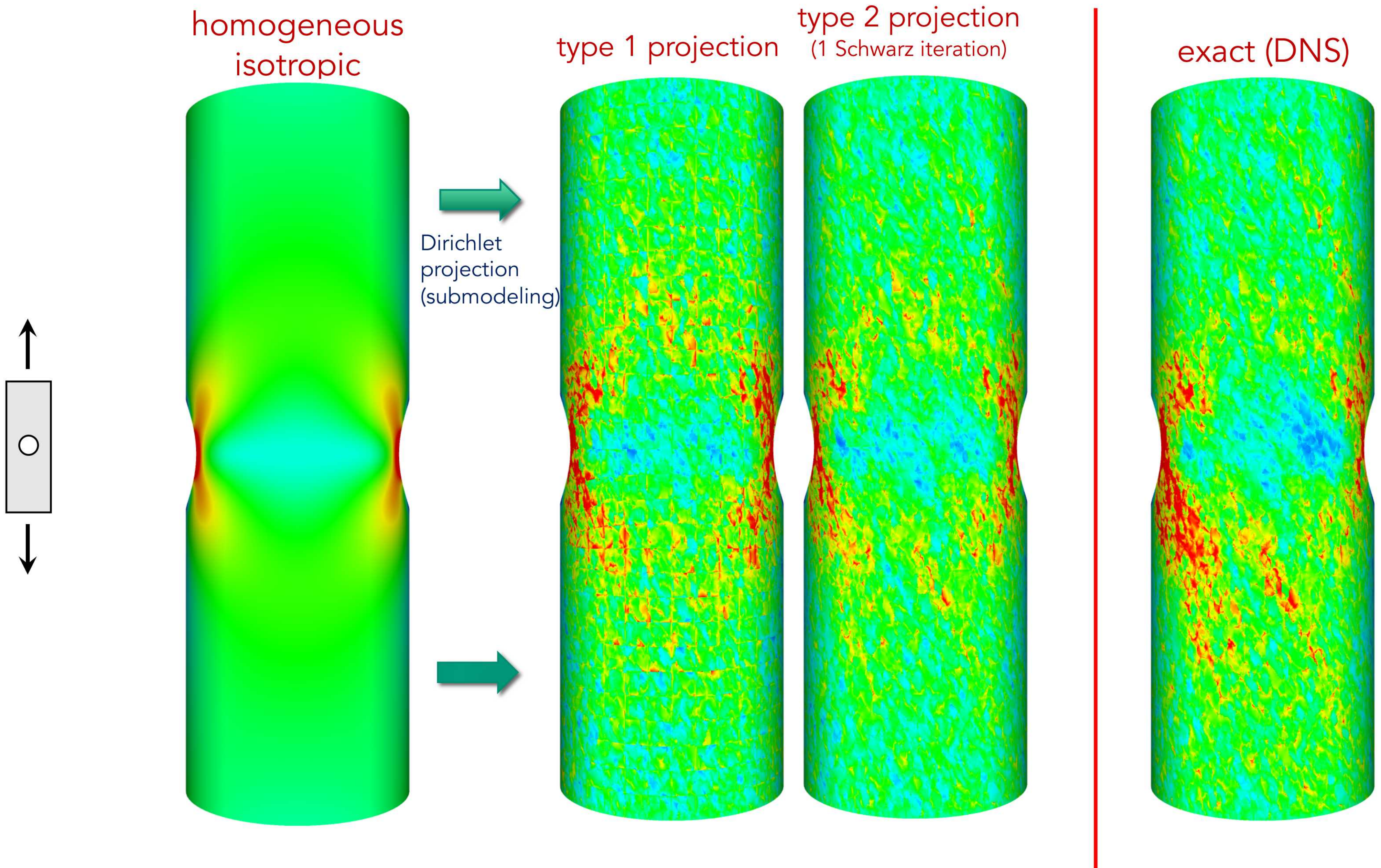


130K hex elements

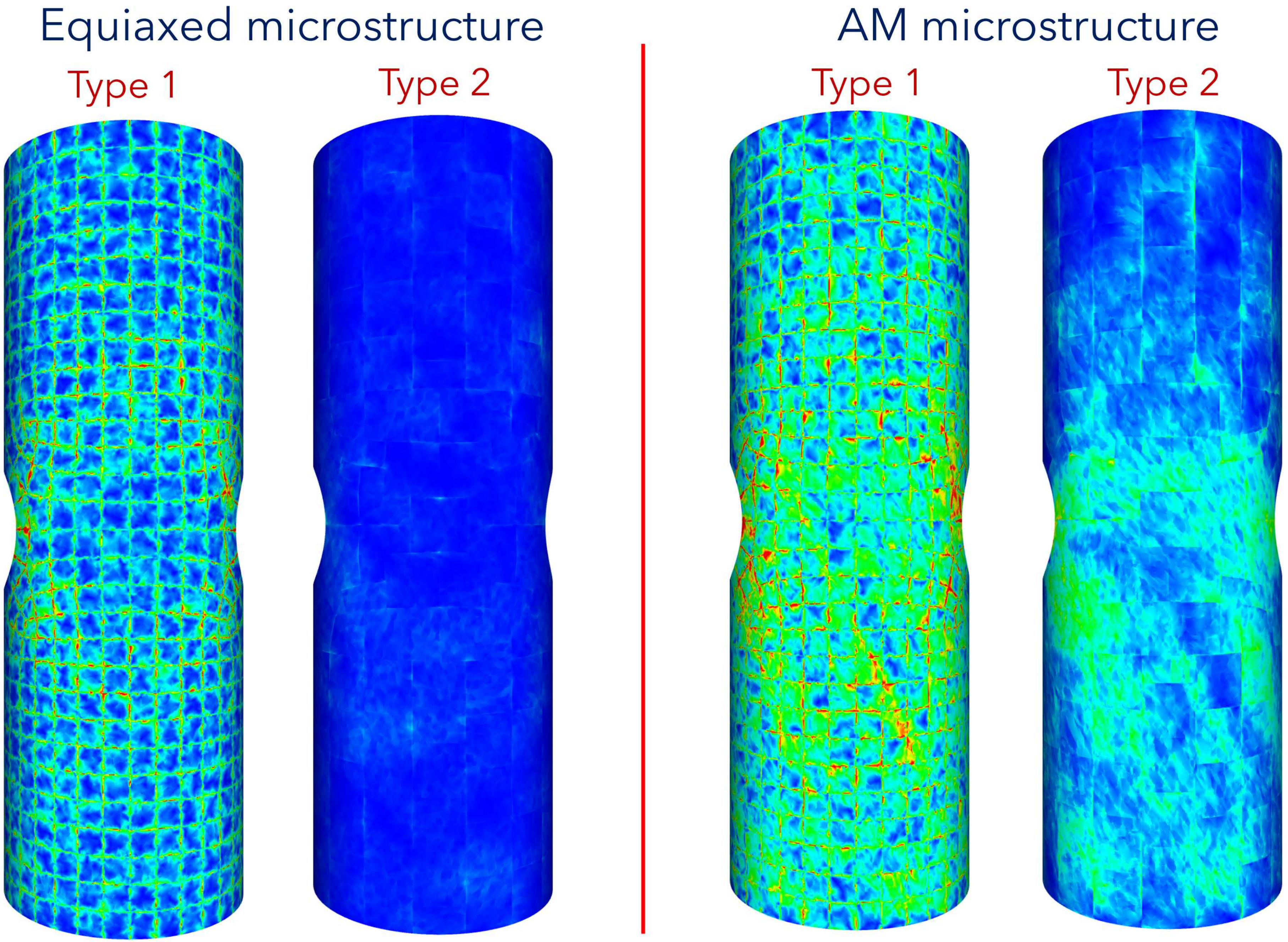
Localization results (equiaxed)



Localization stress results (AM)



Stress error



How to adapt material properties to reduce error?

How can we decrease this error, but still use an isotropic material model?

Consider a heterogeneous isotropic material model?

$$\mathbb{C}^0 = \mathbb{C}^{\text{iso}} = a\,\mathbb{J} + b\,\mathbb{K} = 3K\,\mathbb{J} + 2\mu\,\mathbb{K}$$

$\mathbb{J} = \frac{1}{3}\delta_{ij}\delta_{kl}$ hydrostatic operator

$\mathbb{K} = \mathbb{I} - \mathbb{J}$ deviatoric operator

Let bulk modulus *K* and shear modulus μ vary with position.

Hot to determine? Minimize error mean constitutive response.

$$e_\sigma^2 := ||\langle\boldsymbol{\sigma}\rangle - \mathbb{C}\,\langle\boldsymbol{\epsilon}\rangle||^2$$

$$e_\epsilon^2 := ||\langle\boldsymbol{\epsilon}\rangle - \mathbb{S}\,\langle\boldsymbol{\sigma}\rangle||^2$$

$$e^2 := [\langle\boldsymbol{\sigma}\rangle - \mathbb{C}\,\langle\boldsymbol{\epsilon}\rangle] : [\langle\boldsymbol{\epsilon}\rangle - \mathbb{S}\,\langle\boldsymbol{\sigma}\rangle]$$

$$\frac{\partial\,e^2}{\partial K} = 0$$

$$\frac{\partial\,e^2}{\partial \mu} = 0$$

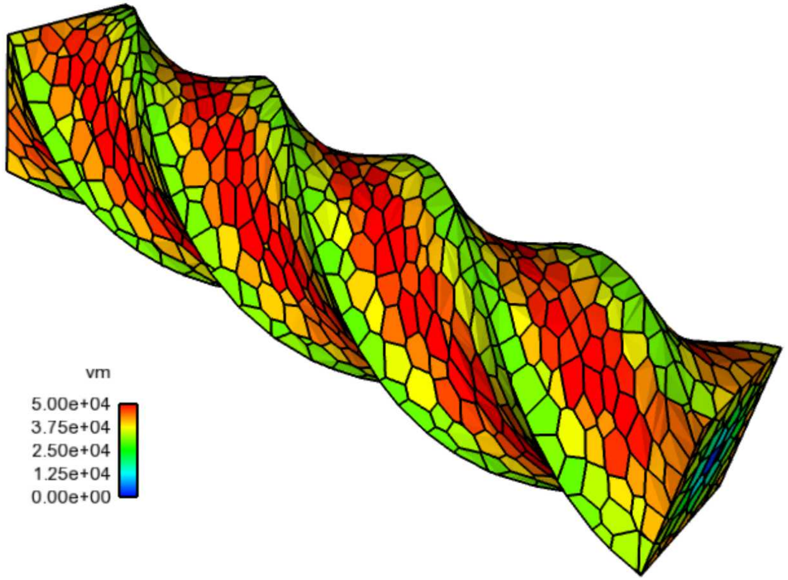
$$3K = \frac{\langle\sigma_{kk}\rangle}{\langle\epsilon_{kk}\rangle}$$

$$2\mu = \frac{\text{dev}\langle\boldsymbol{\sigma}\rangle : \text{dev}\langle\boldsymbol{\epsilon}\rangle}{\text{dev}\langle\boldsymbol{\epsilon}\rangle : \text{dev}\langle\boldsymbol{\epsilon}\rangle}$$

$$2\mu = \frac{\text{dev}\langle\boldsymbol{\sigma}\rangle : \text{dev}\langle\boldsymbol{\sigma}\rangle}{\text{dev}\langle\boldsymbol{\epsilon}\rangle : \text{dev}\langle\boldsymbol{\sigma}\rangle}$$

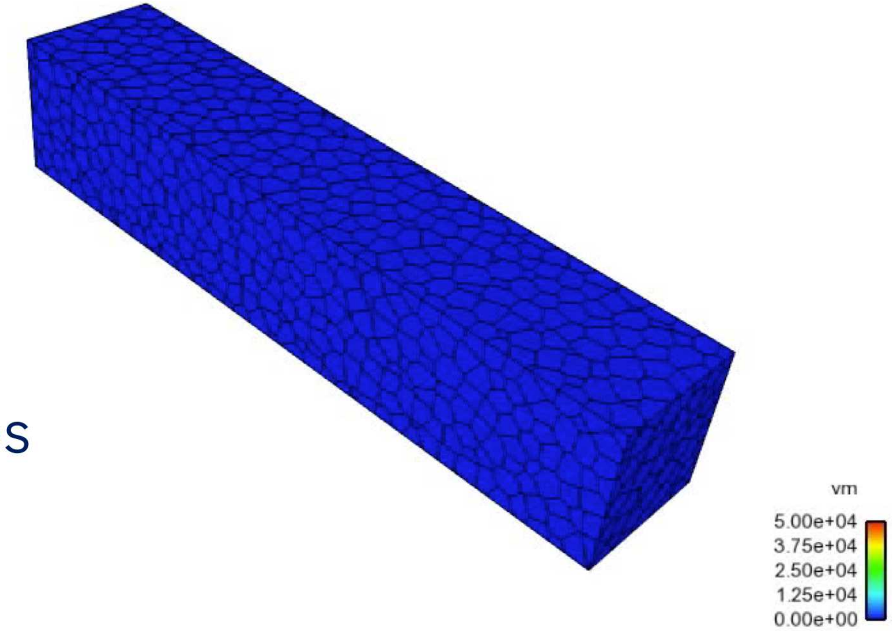
$$2\mu = \frac{\text{dev}\langle\boldsymbol{\sigma}\rangle : \text{dev}\langle\boldsymbol{\sigma}\rangle}{\text{dev}\langle\boldsymbol{\epsilon}\rangle : \text{dev}\langle\boldsymbol{\epsilon}\rangle}$$

Why polyhedra?



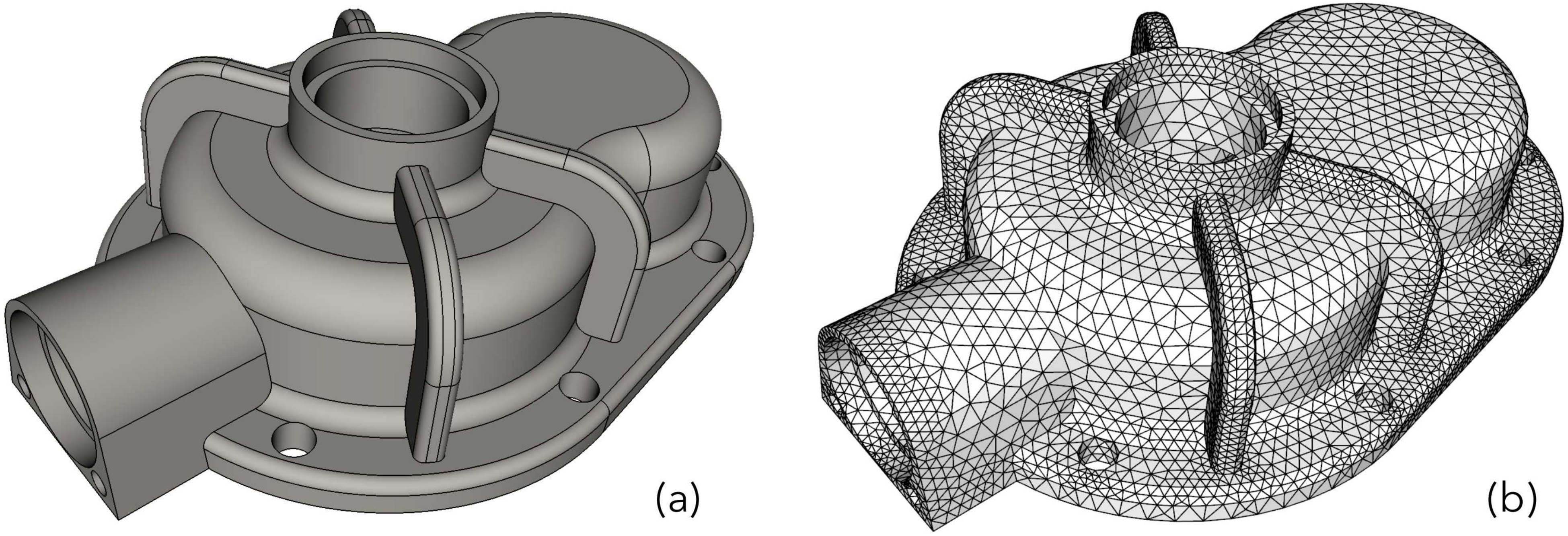
- Increased flexibility in finite element discretizations (tetrahedra and hexahedra are special cases)
- Enables hybrid meshing, e.g. hexahedral-dominant using frame fields
- Enables cut-cell approaches
- Voronoi meshing

How to generate meshes?
Voronoi is challenging on general shapes

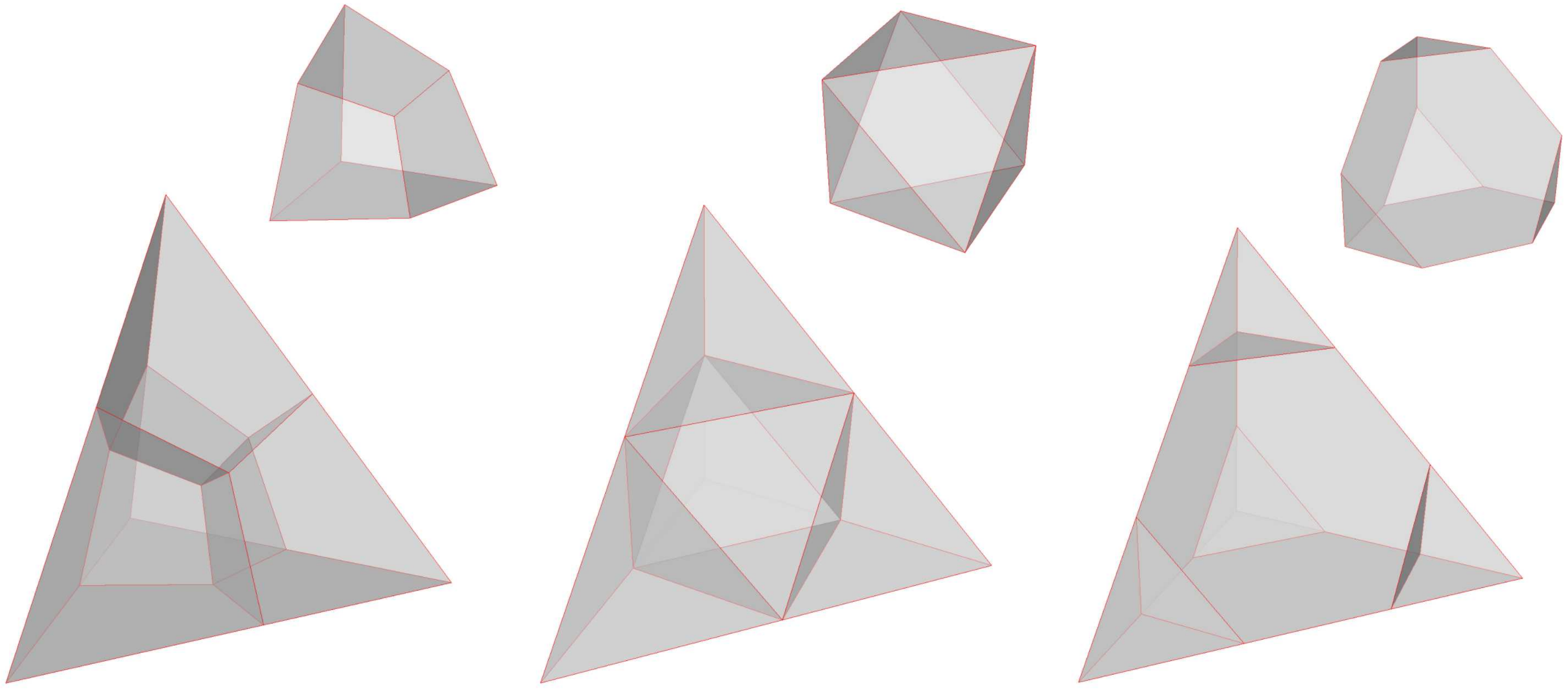


Another approach to forming polyhedral elements

Start with a tetrahedral mesh and then form dual polyhedral cells.

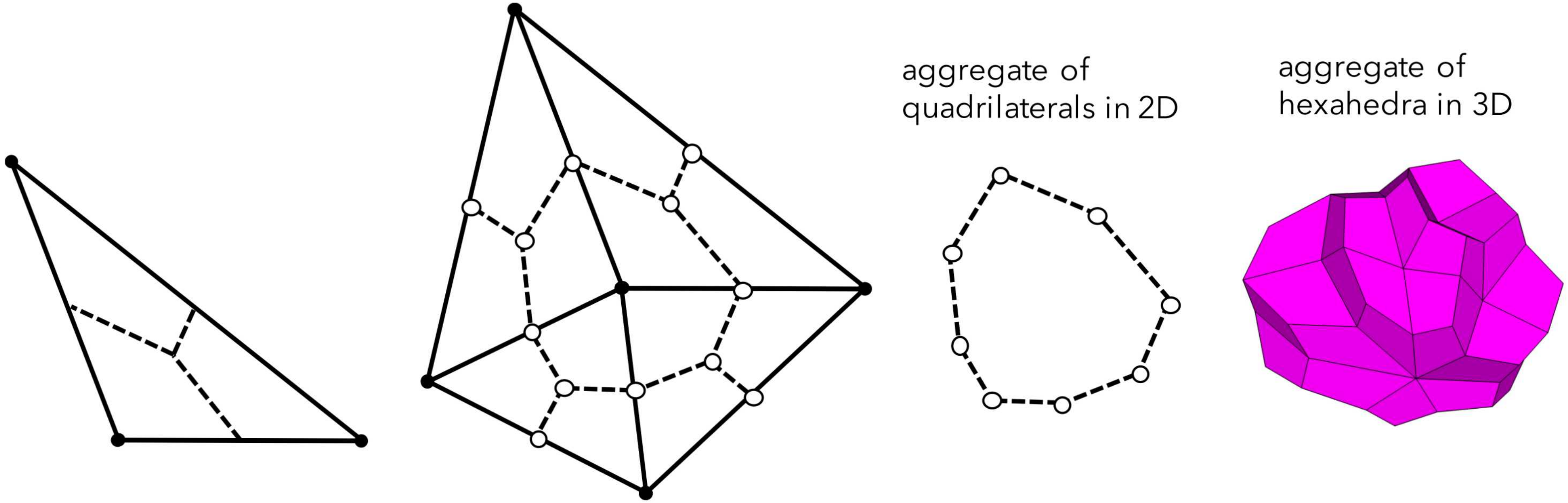


Three types of tetrahedral subdivision



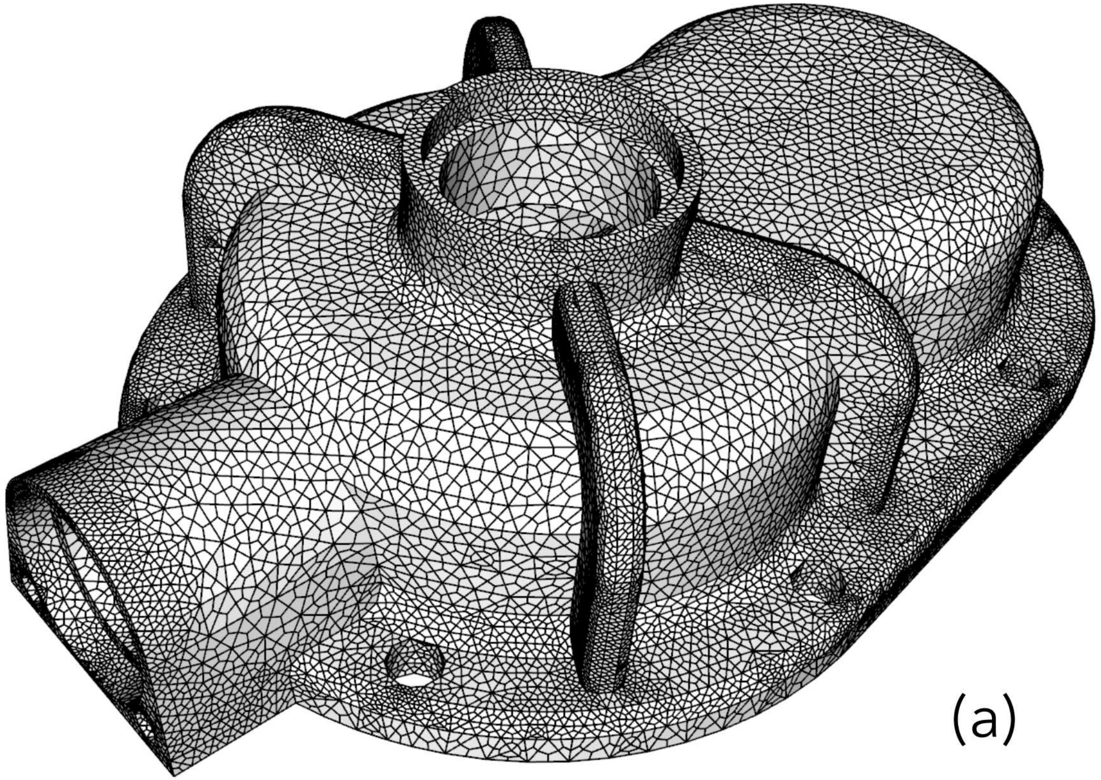
barycentric full truncation partial truncation

Barycentric subdivision and aggregation

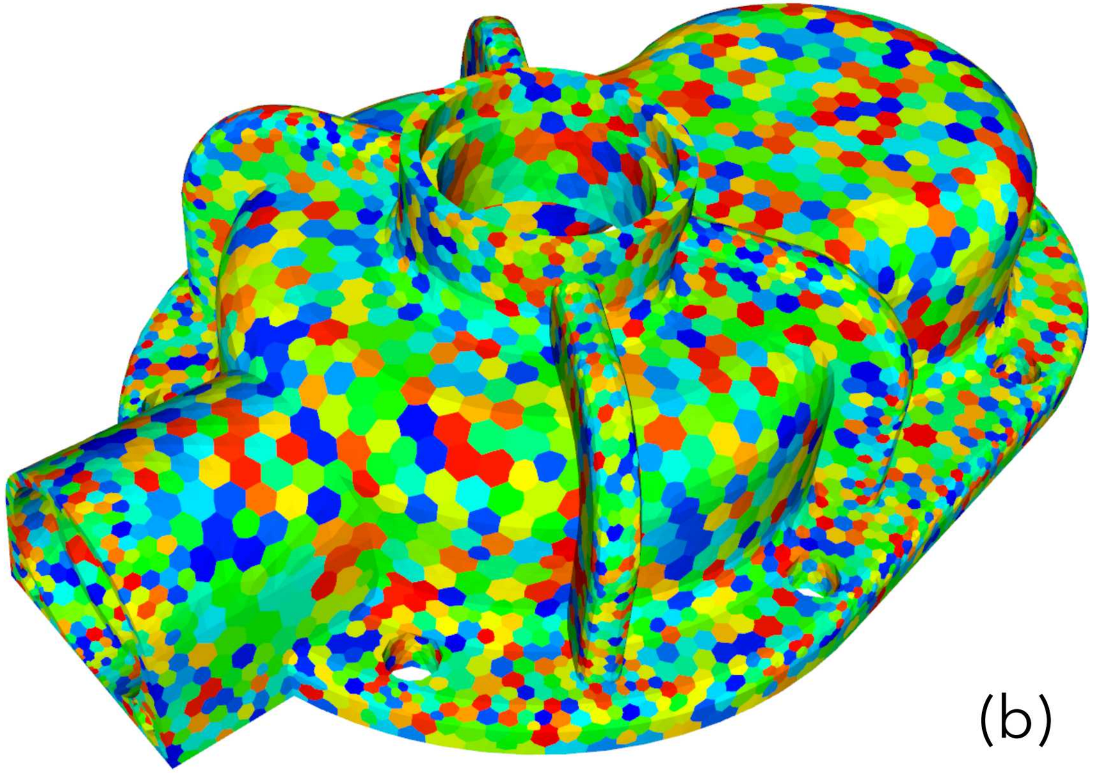


(a) (b) (c) (d)

Barycentric subdivision and aggregation

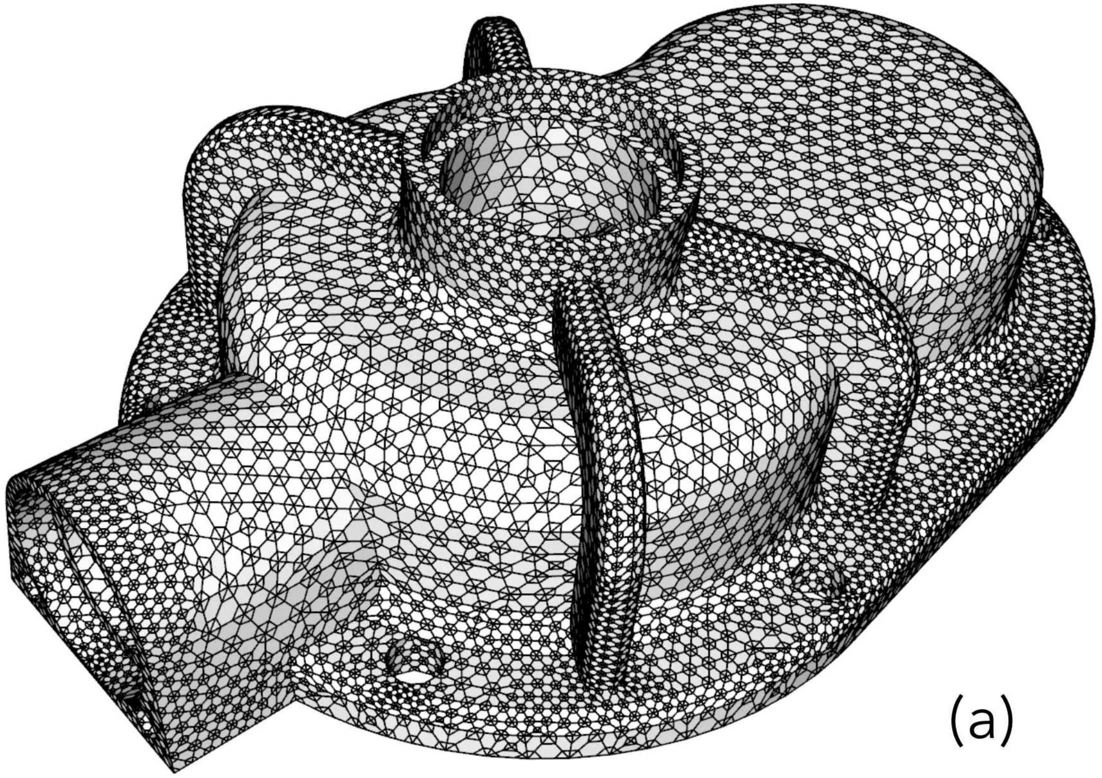


(a)

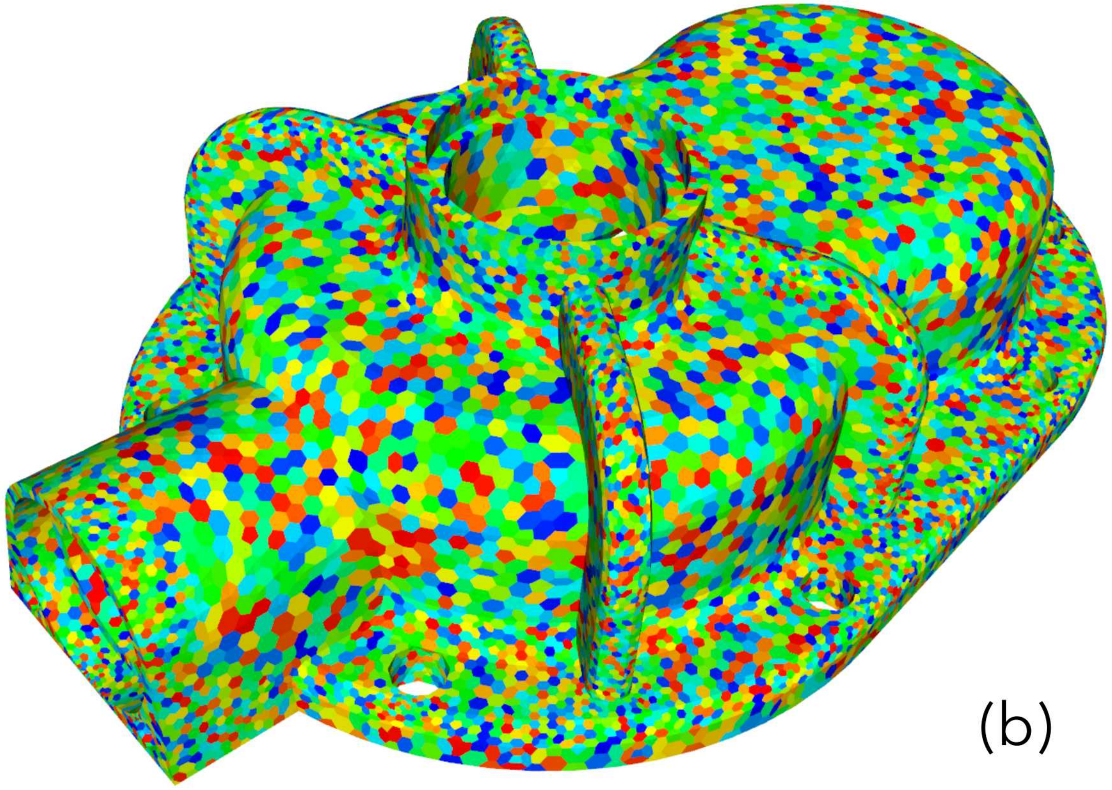


(b)

Partial truncation and aggregation



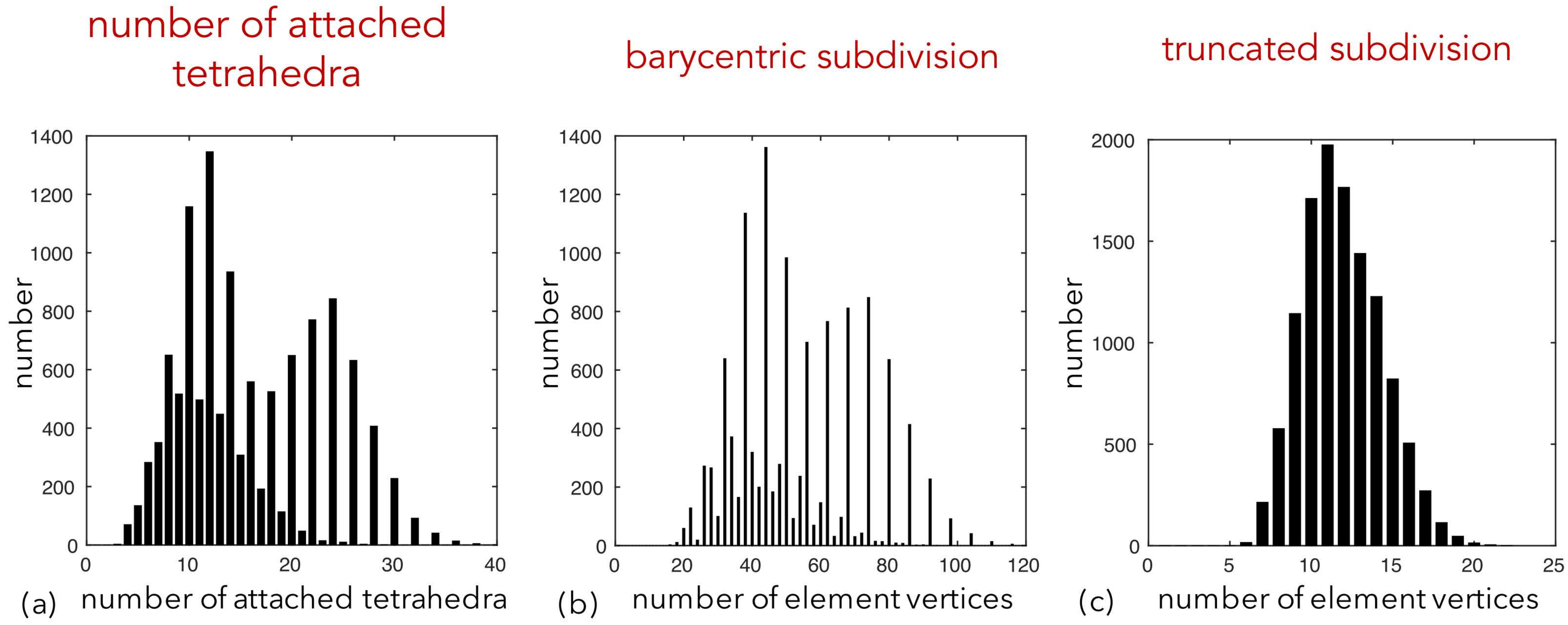
(a)



(b)

Element geometry

number of poly element vertices



Governing equations (total-Lagrangian formulation)

strong form

$$\frac{\partial \boldsymbol{P}}{\partial \boldsymbol{X}} : \boldsymbol{I} = \rho_0 \, \ddot{\mathbf{u}}$$

$$\boldsymbol{u} = \overline{\boldsymbol{u}} \quad \text{on} \quad \Gamma_0^u \quad \text{and} \quad \boldsymbol{P} \cdot \boldsymbol{N} = \boldsymbol{t}_0 \quad \text{on} \quad \Gamma_0^t$$

weak form

find the trial functions $\boldsymbol{u} \in \boldsymbol{H}^1(\Omega_0)$ such that

$$\int_{\Gamma_0^t} \boldsymbol{t}_0 \cdot \boldsymbol{v} \, dS - \int_{\Omega_0} \boldsymbol{P} : (\partial \boldsymbol{v} / \partial \boldsymbol{X}) \, d\boldsymbol{X} = \int_{\Omega_0} \rho_0 \, \ddot{\mathbf{u}} \cdot \boldsymbol{v} \, d\boldsymbol{X}$$

for all test functions $\boldsymbol{v} \in \boldsymbol{H}_0^1(\Omega_0)$

Finite element formulation

- Bubnov-Galerkin formulation (trial and test functions use same space)
- Total-Lagrangian formulation (integrate weak form on original configuration).
- Minimize number of integration points while avoiding artificial stabilization.
- Typically, number of quadrature points ~ number of vertices (first order).
- Mean-dilation (F-bar) formulation for nearly-incompressible materials
- Compatible with standard trilinear hexahedron

- Going to explore the use of two types of shape functions:
  1. harmonic,
  2. maximum entropy (max-ent)

Harmonic shape functions

Harmonic functions minimize the Dirichlet energy given by the following functional:

$$J(\psi) := \frac{1}{2} \int_{\Omega_{\mathrm{e}}} \nabla\psi \cdot \nabla\psi \, d\boldsymbol{X} \qquad \text{with } \psi \in H^1(\Omega_{\mathrm{e}})$$

The minimizer of this functional satisfies the following variational problem:

$$\text{find } \psi \in H^1(\Omega_{\mathrm{e}}) \text{ with } \psi = \overline{\psi} \text{ on } \Gamma_{\mathrm{e}} \text{ such that}$$

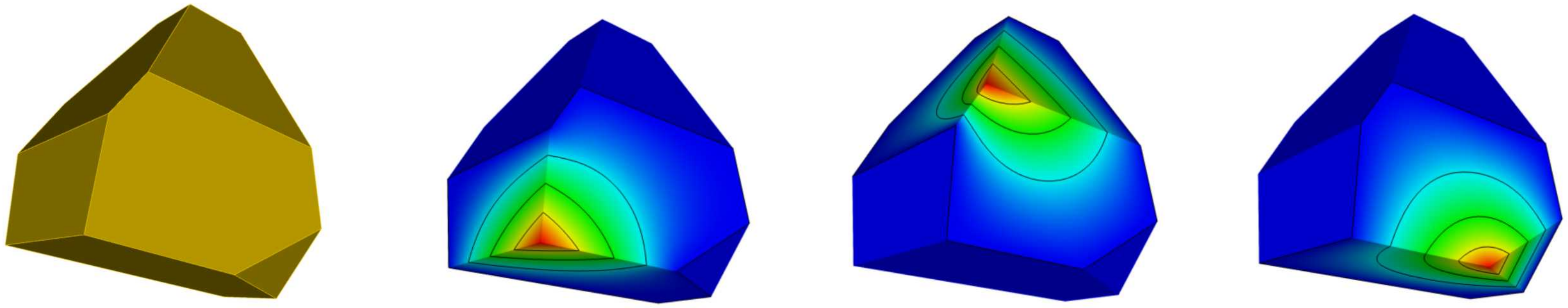
$$\int_{\Omega_{\mathrm{e}}} \nabla\psi \cdot \nabla v \, d\boldsymbol{X} = 0$$

$$\text{for all test functions } v \in H^1_0(\Omega_{\mathrm{e}})$$

The strong form of this variational problem is given by:

$$\nabla^2\psi = 0 \text{ in } \Omega_{\mathrm{e}} \quad \text{with} \quad \psi = \overline{\psi} \text{ on } \Gamma_{\mathrm{e}}$$

Harmonic shape functions



$$\sum_{a=1}^{N_{\mathrm{v}}} \psi_a(\boldsymbol{X}) = 1$$

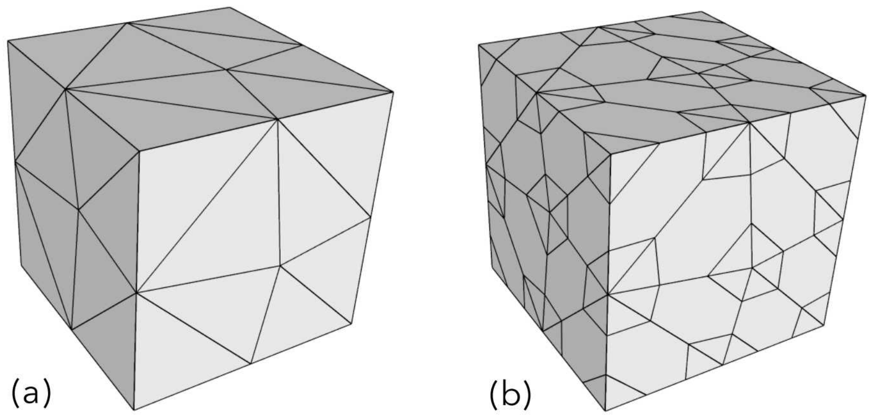
partition of unity

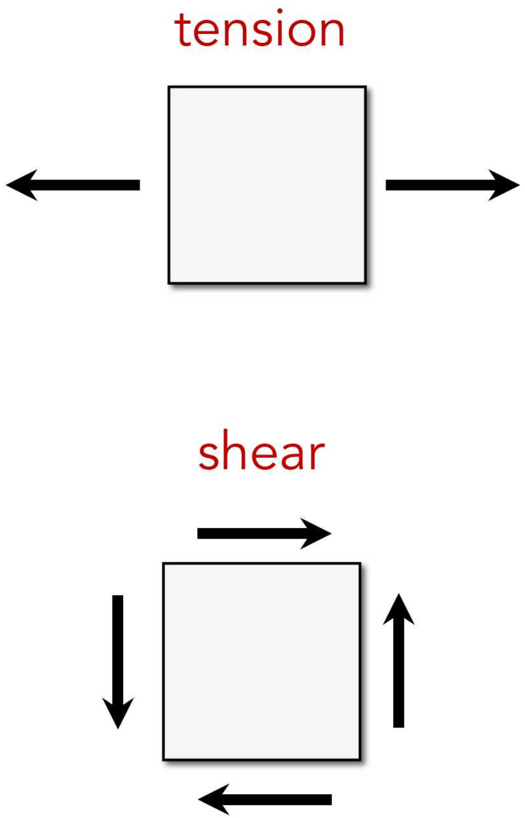
$$\sum_{a=1}^{N_{\mathrm{v}}} \psi_a(\boldsymbol{X})\, \boldsymbol{X}_a = \boldsymbol{X}$$

linear reproducibility

Patch test

- a test for element consistency
- Uniform tractions should result in uniform stress/strain field.

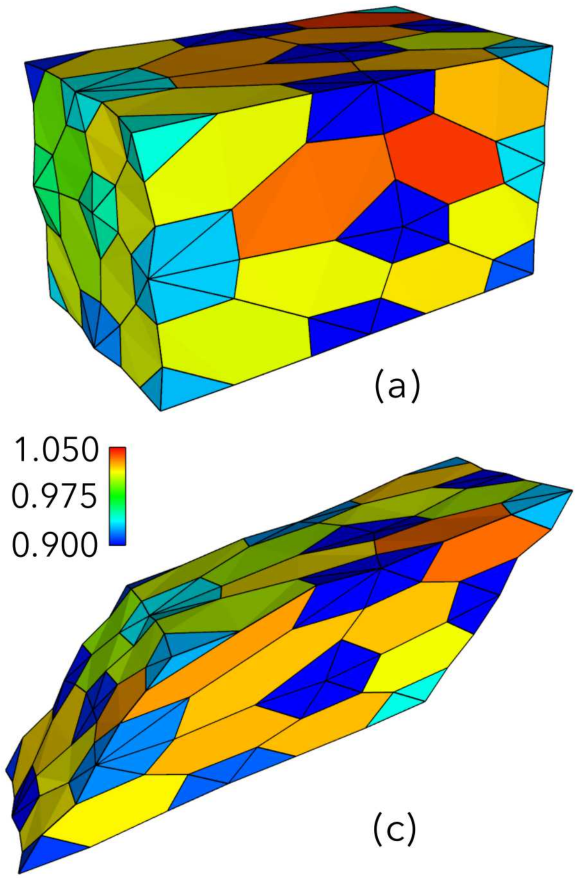




Patch test

tension

shear



- Failed patch test!
- Can be traced to use of low-order integration scheme.
- Due to lack of “integration consistency” or violation of the discrete divergence theorem.

Integration consistency

Divergence theorem states that:

$$\int_{\Omega_{\mathrm{e}}} \nabla\psi_a \, d\boldsymbol{X} = \int_{\Gamma_{\mathrm{e}}} \psi^a \, \boldsymbol{N} \, dS$$

where $\boldsymbol{N}$ is the outward unit normal vector on Γ_{e}

In discrete form:

$$\sum_{k=1}^{N_{\mathrm{Q}}} w_k \nabla\psi_{ak} = \sum_{l=1}^{N_{\mathrm{Q}}^{\Gamma}} w_l^{\Gamma} \, \psi_{al} \, \boldsymbol{N}_l \ , \quad (a = 1, \ldots, N_{\mathrm{v}})$$

where $\psi_{ak} := \psi_a(\boldsymbol{X}_k)$, and $\boldsymbol{X}_k$ is the position of the k-th quadrature point

- For non-polynomial shape functions, this will not be satisfied in general.
- This will results in a lack of consistency (failure of the engineering patch test).

Shape function derivative correction

- "Tweak" the shape function derivatives to satisfy the integration consistency condition.
- Maintain the reproducing properties of the derivatives.
- Minimize the least-squares difference between the new derivatives and the old.
- Only performed once during simulation (pre-processing step).

$$\min_{\boldsymbol{\xi}_k \in \boldsymbol{R}^3} \sum_{k=1}^{N_{\mathrm{Q}}} w_k ||\boldsymbol{\xi}_k - \nabla\psi_{ak}||^2 \qquad \text{subject to the constraints} \qquad \sum_{k=1}^{N_{\mathrm{Q}}} w_k\, \boldsymbol{\xi}_k - \sum_{l=1}^{N_{\mathrm{Q}}^{\Gamma}} w_l^{\Gamma} \psi_{al} \boldsymbol{N}_l = 0$$

This constrained optimization problem can be solved using the method of Lagrange multipliers:

$$\mathcal{L}(\boldsymbol{\xi}_k, \boldsymbol{\lambda}) := \sum_{k=1}^{N_{\mathrm{Q}}} w_k ||\boldsymbol{\xi}_k - \nabla\psi_{ak}||^2 + \boldsymbol{\lambda} \cdot \left(\sum_{k=1}^{N_{\mathrm{Q}}} w_k\, \boldsymbol{\xi}_k - \sum_{l=1}^{N_{\mathrm{Q}}^{\Gamma}} w_l^{\Gamma} \psi_{al} \boldsymbol{N}_l \right)$$

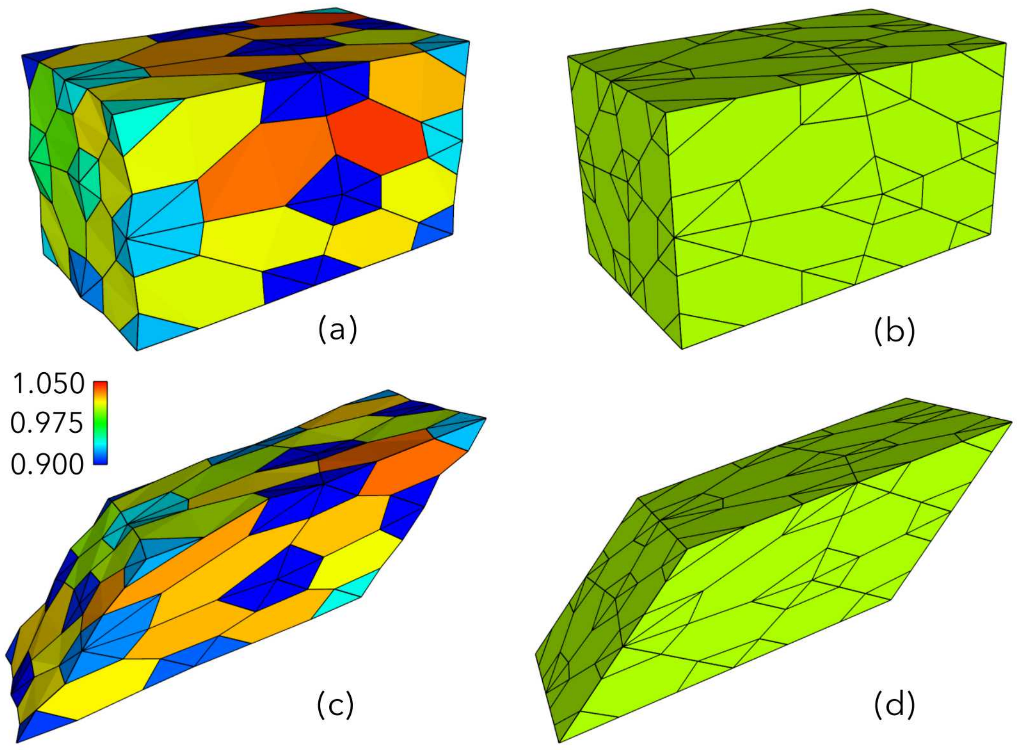
Patch test

failed patch test

successful

tension

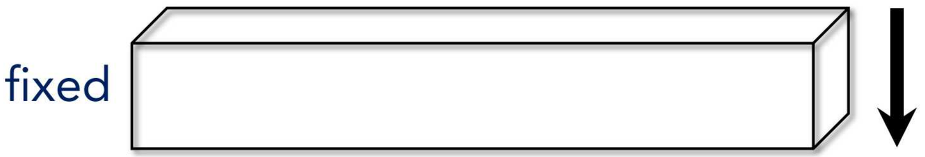
shear

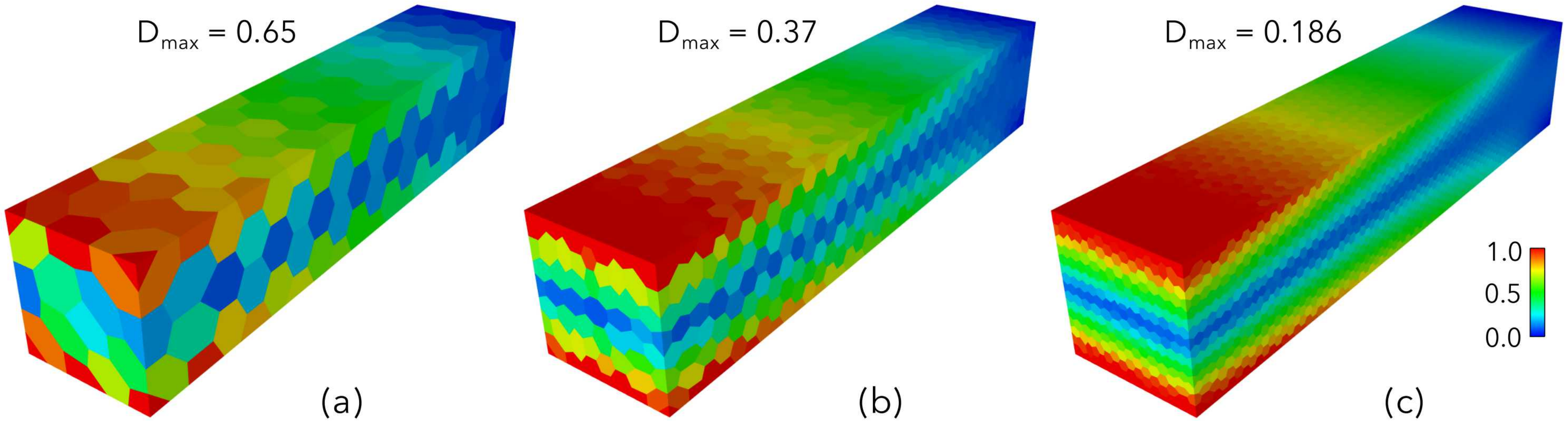


Error in stress with and without correction

applied traction state	without correction	with correction
tension	0.18	$9.6 \cdot 10^{-13}$
shear	0.13	$2.7 \cdot 10^{-12}$

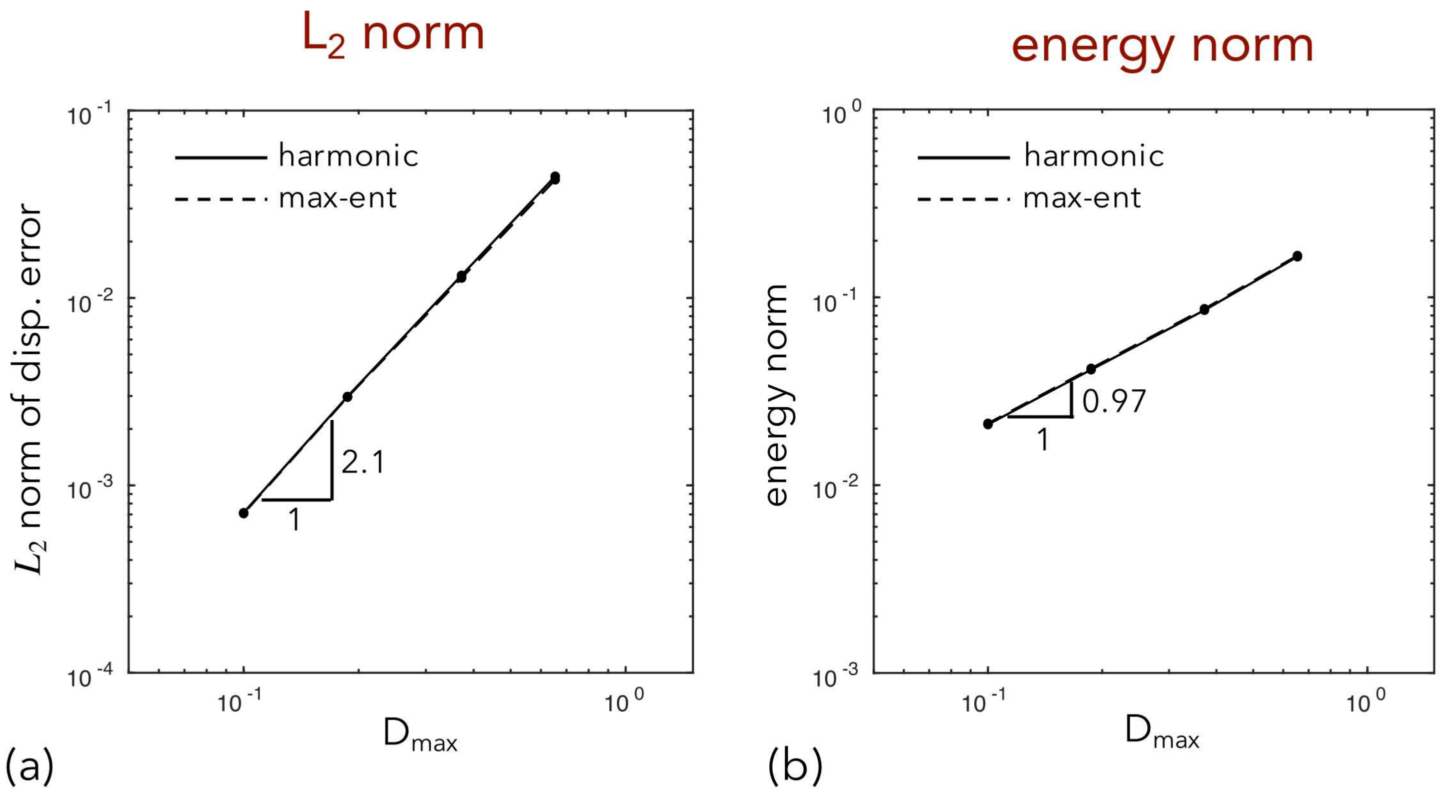
Beam bending with shear load



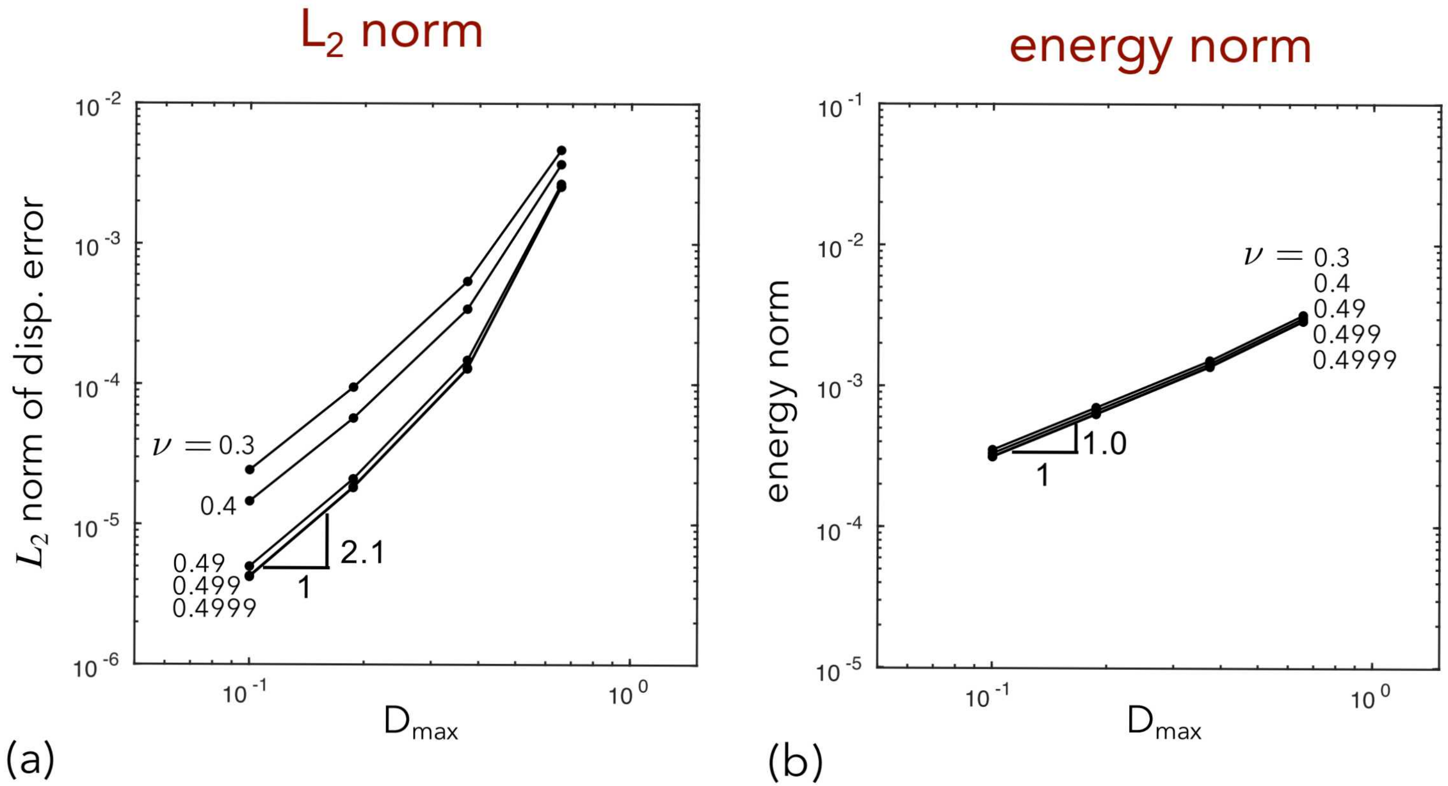


(a) (b) (c)

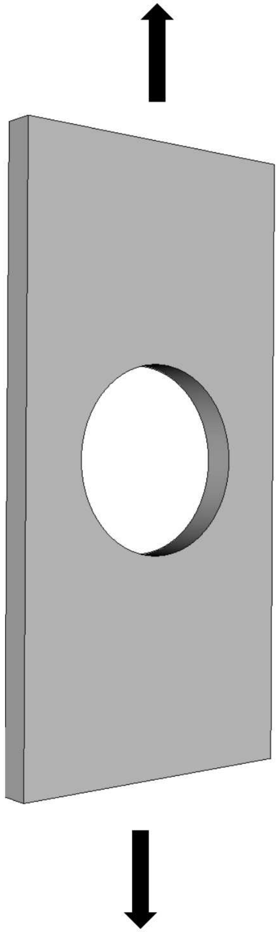
Convergence, harmonic vs. max-ent



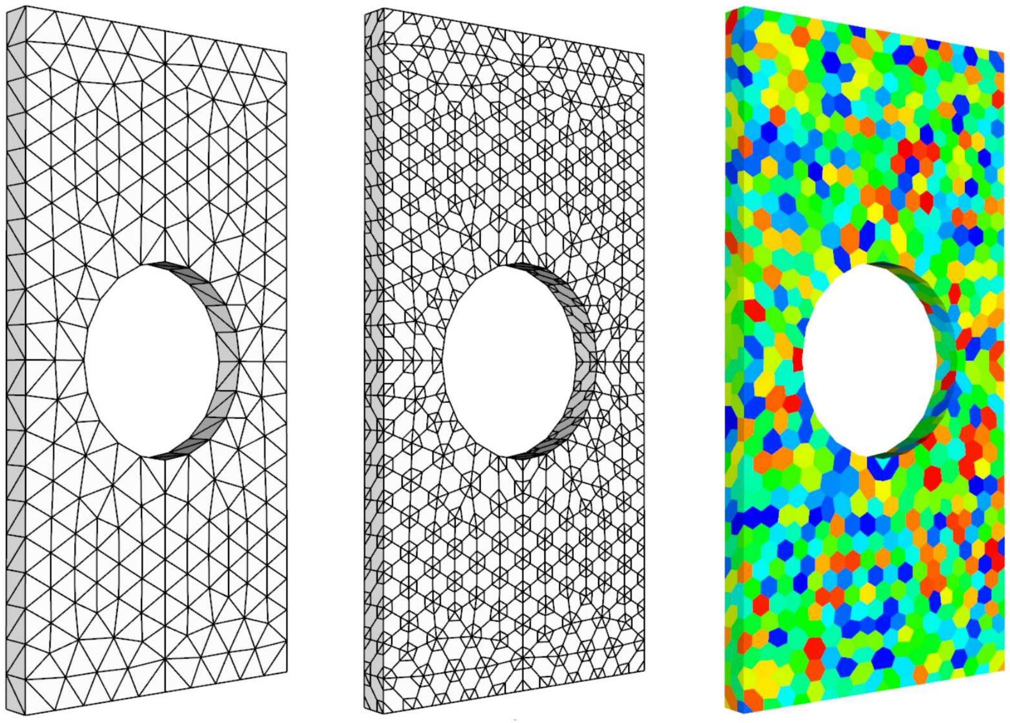
Convergence, harmonic vs. max-ent



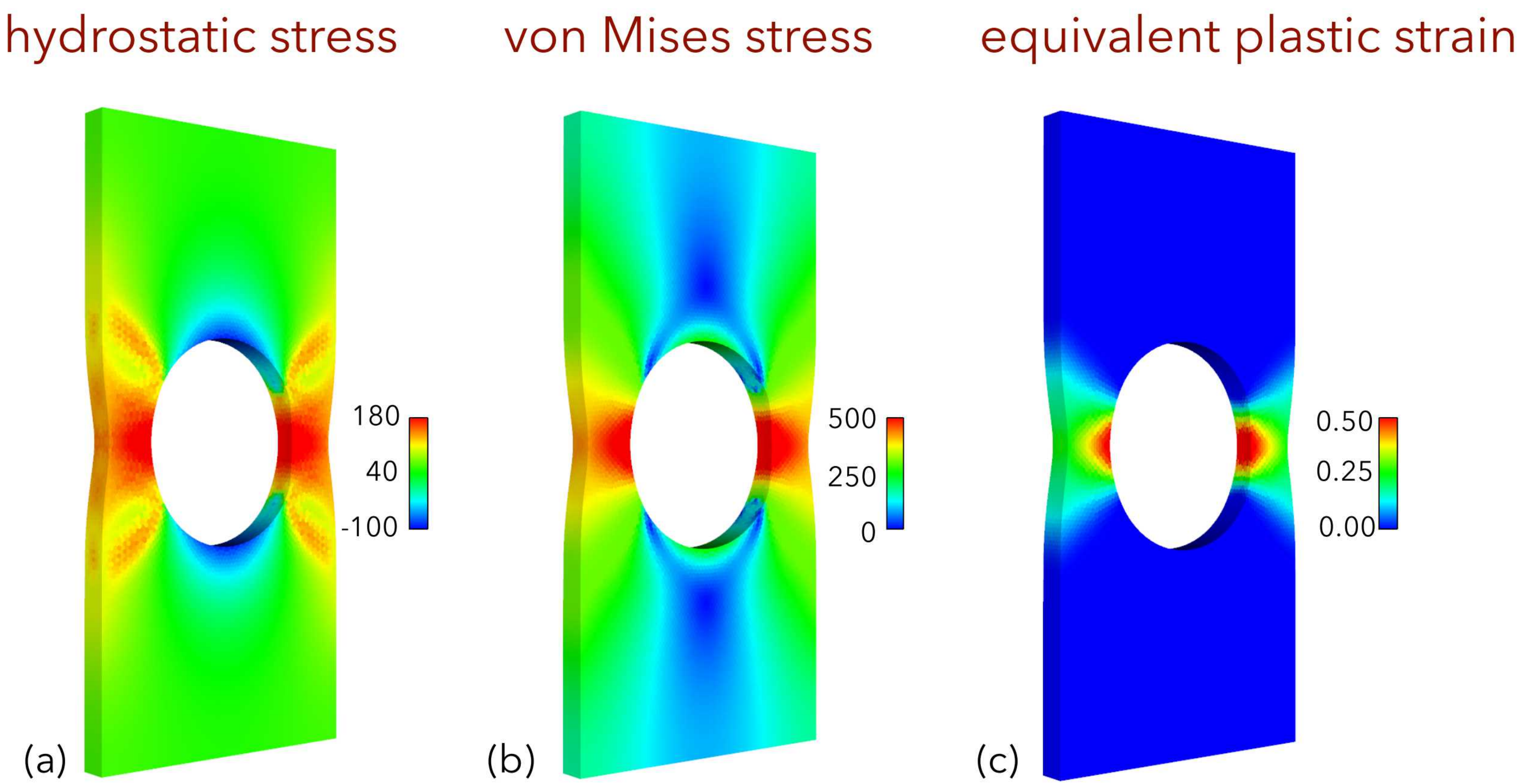
Example: elastic-plastic plate



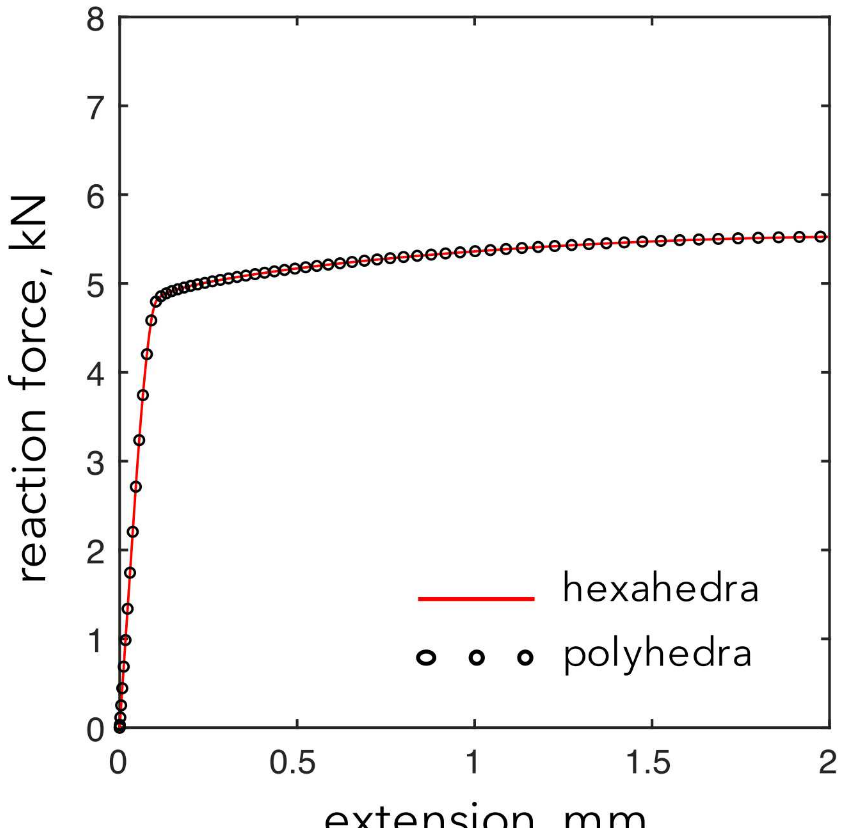
- uniaxial extension
- elastic-plastic constitutive model (J2)



Simulation results



Comparison of reaction forces



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