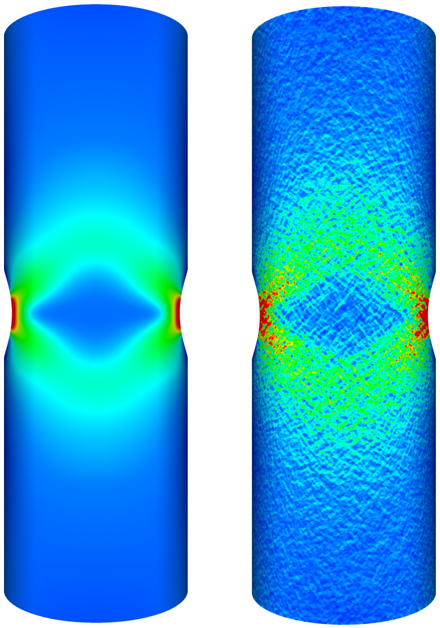
SAND2015-5031C

Direct numerical simulations in solid mechanics for quantifying the effects of microstructure and material-model form error on macroscale quantities of interest



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Albuquerque, NM

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Seattle, WA
June 29 – July 1, 2015

Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Outline

- research questions
- direct numerical simulations in solid mechanics
- example: elastic structure with microstructure
- example: plastic response
- applications to additive manufacturing
- multiscale modeling using geometric multigrid

Research questions (why DNS?)

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- What is “material variability”?
- What is the error in homogenization theory?
- What is the error induced when the assumption of scale-separation no longer holds?
- Can we find evidence of **surface-effects**?
- Can we find evidence of strain-gradient effects or **nonlocality** in the mean-field response?
- How to include known spatial variations in microstructure in our macroscale simulations, e.g. arising from manufacturing processes?
- How does material variability impact engineering quantities of interest?

Direct numerical simulations

- Key postulate: we have a fine scale representation/model that is predictive (e.g. microstructural model, crystal-plasticity model)
- Perform direct numerical simulations (DNS) of macroscopic boundary-value problems with microstructure and compare with the solution from the homogenized PDE.
- Identify any evidence of higher-order effects (gradient or surface effects).
- Can currently model ~ 500,000 grains in a macroscale structure.
- Goal is ~ 100 M grains.

DNS Approach

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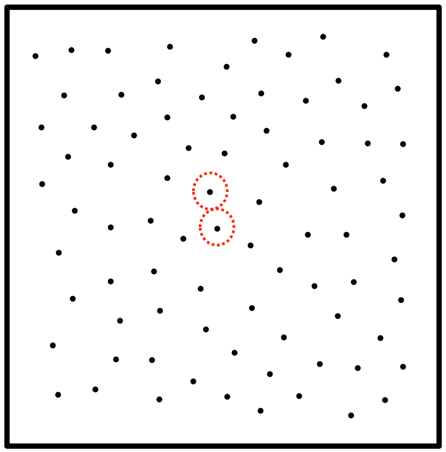
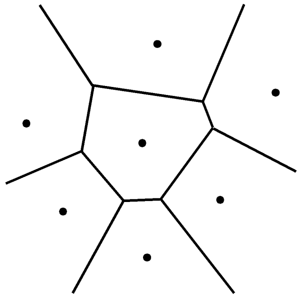
- Use voxelation approach to mesh grains
- Use macroscale hexahedral mesh as "overlay" grid
- Use idealized Voronoi microstructure (for now)
- Use Maximal Poisson Sampling (MPS) to seed Voronoi microstructure (results in equiaxed grain morphology)
- No texture (for now)

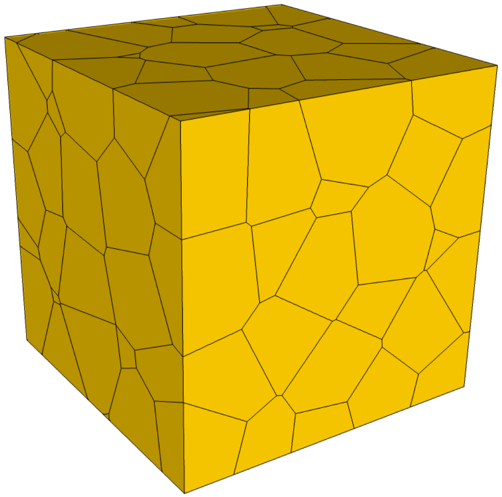
Advantage of voxelation approach

- Easy meshing of microstructure
- Only need implicit representation of microstructure
- Can robustly generate many microstructural realizations
- Robust under large deformation
- Experimental data is typically pixelated anyway

Voronoi Microstructure from MPS Seeding



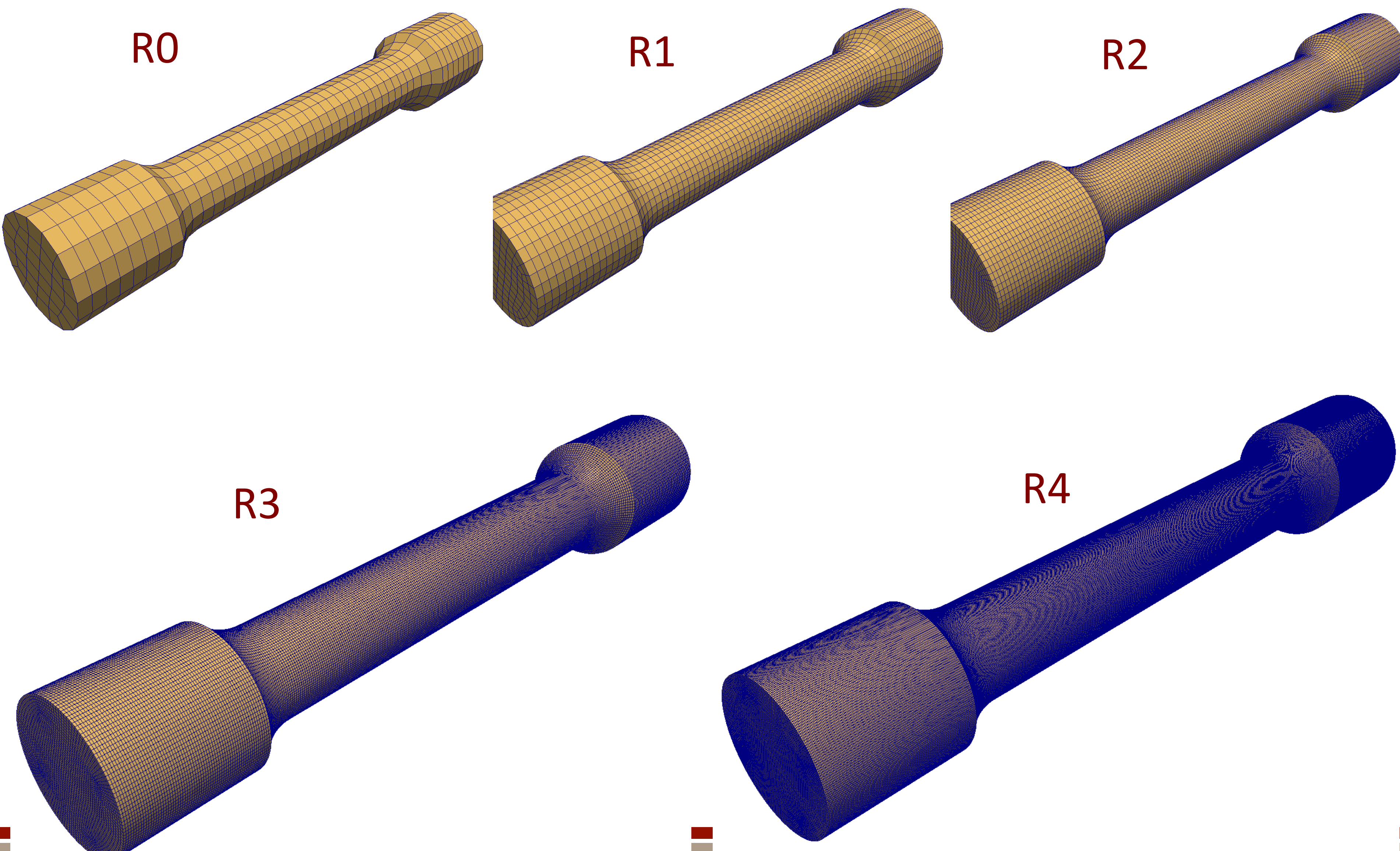




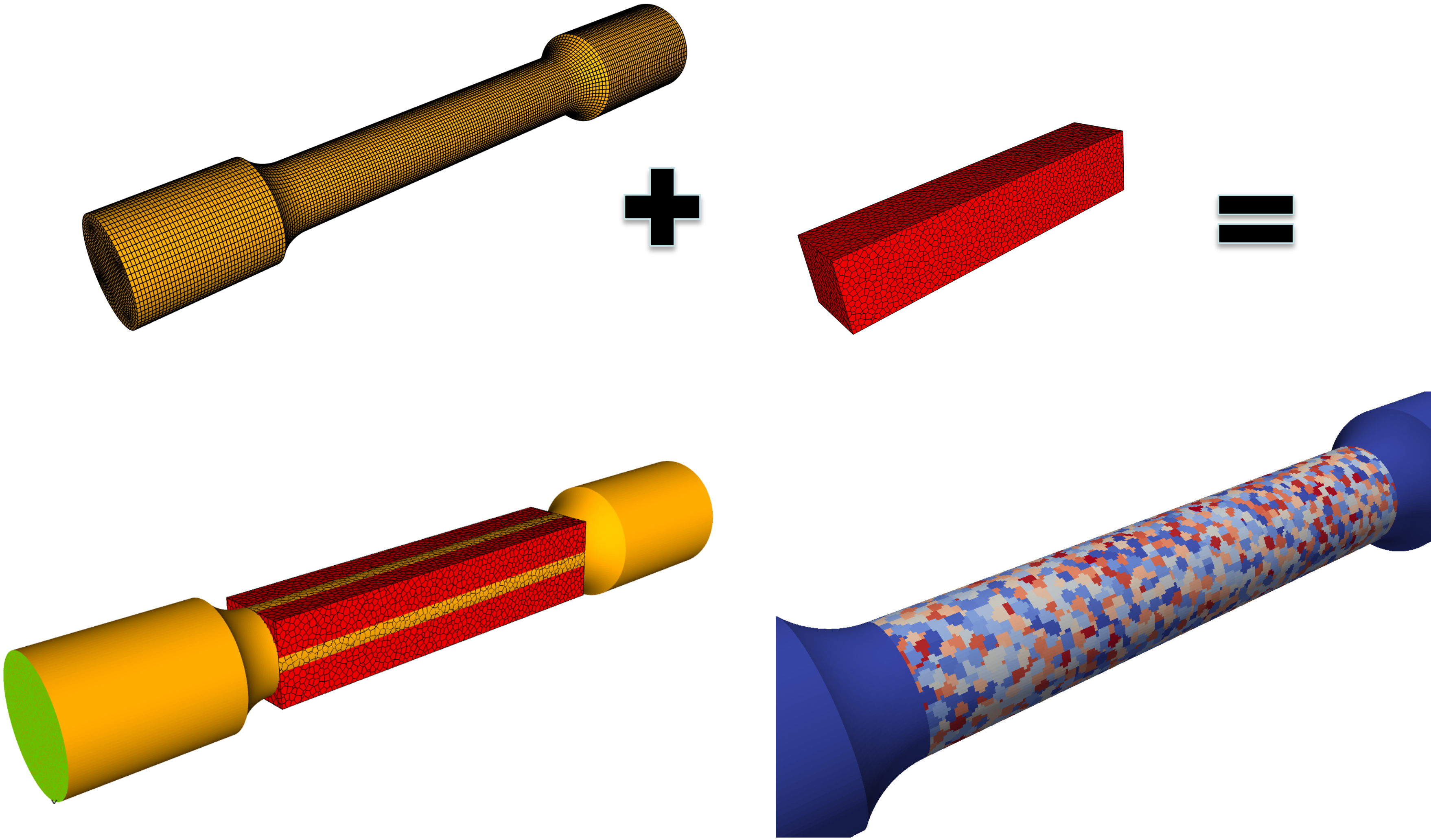
Maximal Poisson Sampling

- constraint on minimum distance
- seed until 'max' packing
- Ebeida/Mitchell Algorithm (1400)

Hierarchy of hexahedral meshes

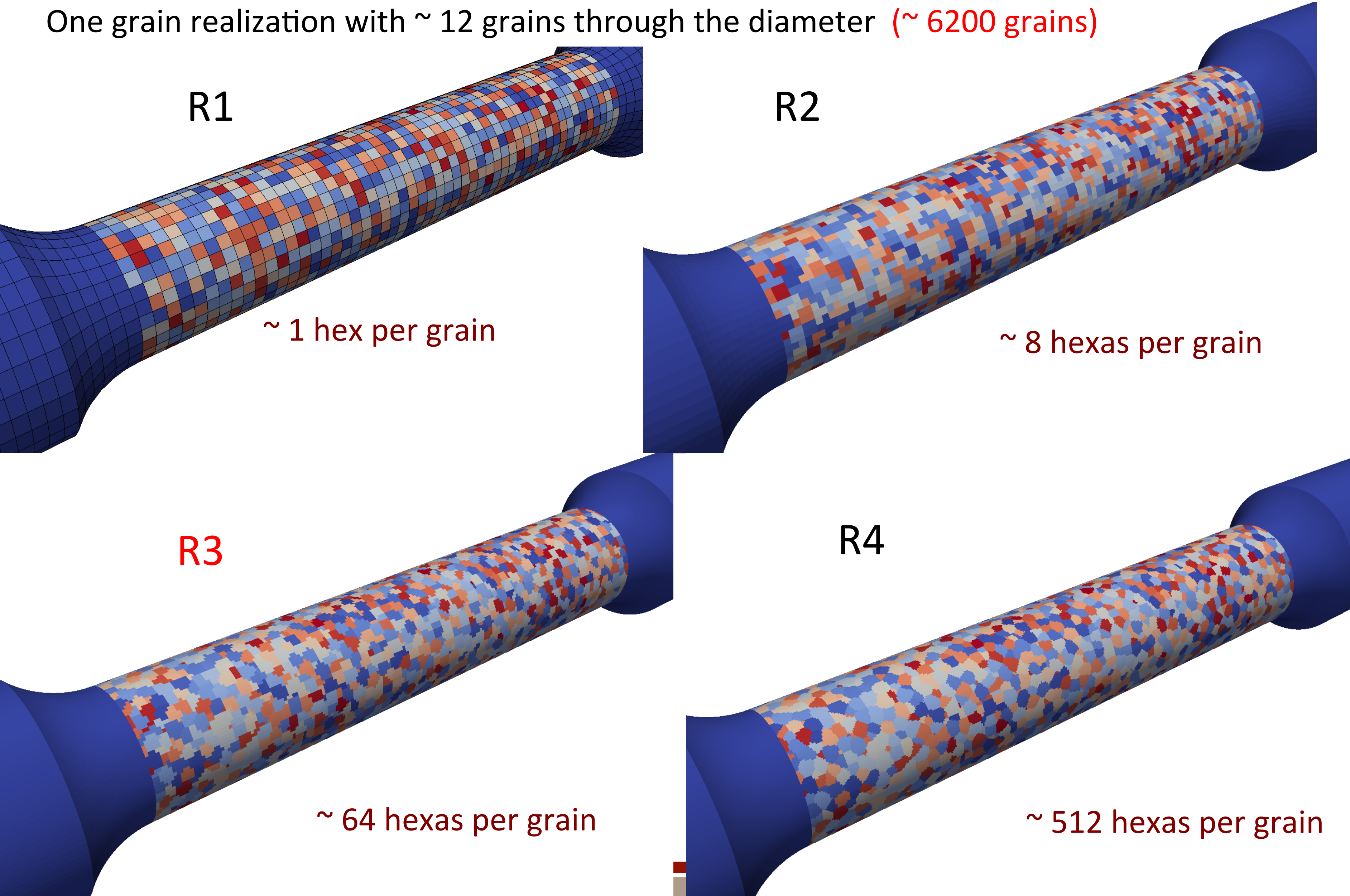


Microstructural overlay of hex mesh



Voronoi overlay of hierarchy of hex meshes

One grain realization with ~ 12 grains through the diameter (~ 6200 grains)



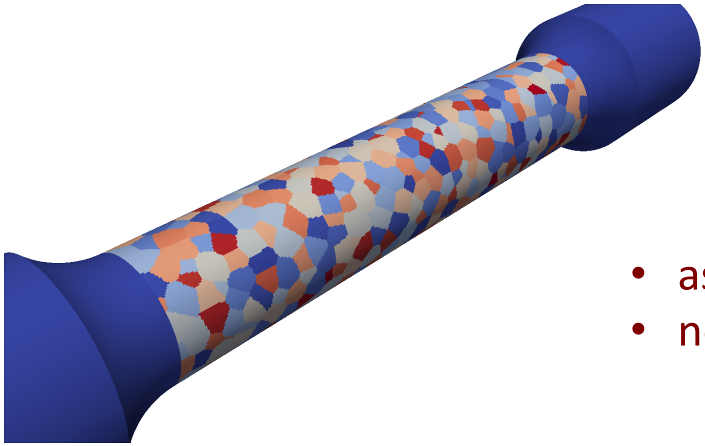
Stainless steel 304L single crystal elasticity constants (Ledbetter, 1984)

single crystal elastic constants (cubic symmetry)

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

anisotropy ratio,

$$A = \frac{2C_{12}}{C_{11} - C_{44}} = 3.5$$



- assume random crystallographic orientations
- no correlation between grains (no texture)

RPI crystal plasticity model

plastic velocity gradient: $$L^p = \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha P^\alpha$$ (sum over slip systems)

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

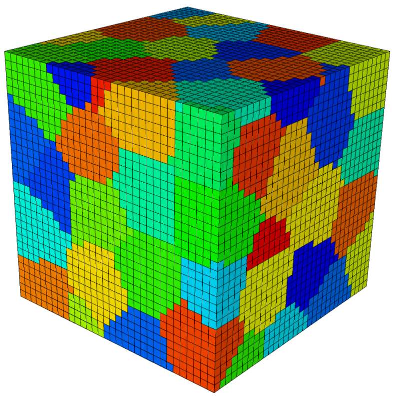
slip system slip rates: $$\dot{\gamma}^\alpha = \dot{\gamma}_o \frac{\tau^\alpha}{g^\alpha} \left| \frac{\tau^\alpha}{g^\alpha} \right|^{1/m-1}$$

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

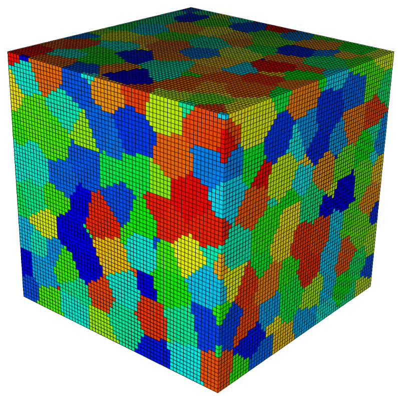
$$\gamma = \sum_{s=1}^{N} |\gamma^s|$$

How to get homogenized properties?

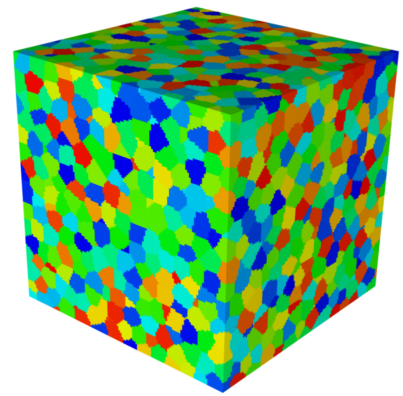
Convergence of stochastic volume elements (SVE) to representative volume element (RVE)



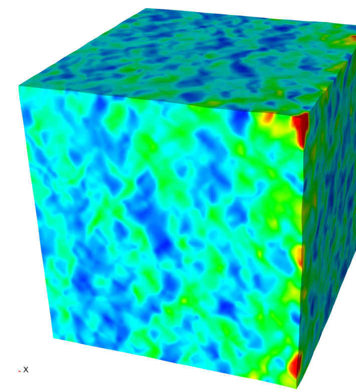
~ 4^3 grains



~ 8^3 grains



~ 16^3 grains



plastic response

Convergence to effective isotropic elastic properties

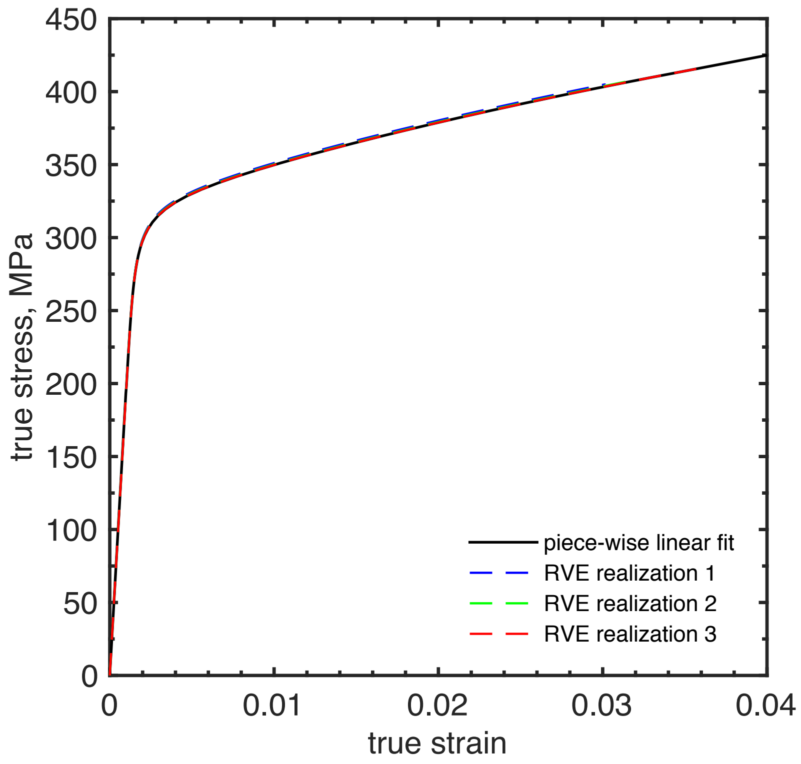
- mean of 100 simulations at each "grain level"
- rational function extrapolation to ∞

number of grains	apparent Young's Modulus (GPa)	apparent Poisson's ratio
~4^3 grains	185.2	0.307
~8^3 grains	190.5	0.301
~16^3 grains	193.9	0.298
~32^3 grains	195.7	0.296
∞	197.6	0.294

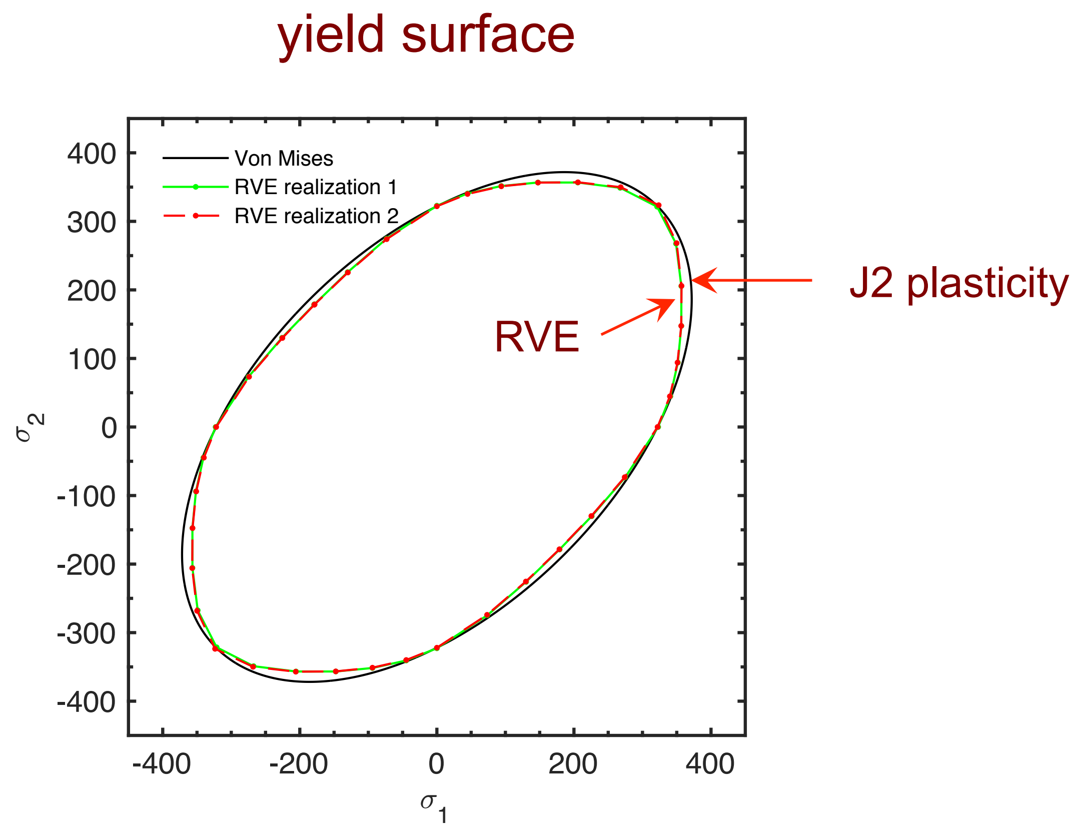
These values will be used as the homogenized, isotropic, elastic properties.

Effective plasticity model?

- Ideally, would use computational homogenization (FE^2) for nonlinear homogenization.
- Since this is not available, use a simple piece-wise linear hardening J2-plasticity model. This results, however, in a model-form error.

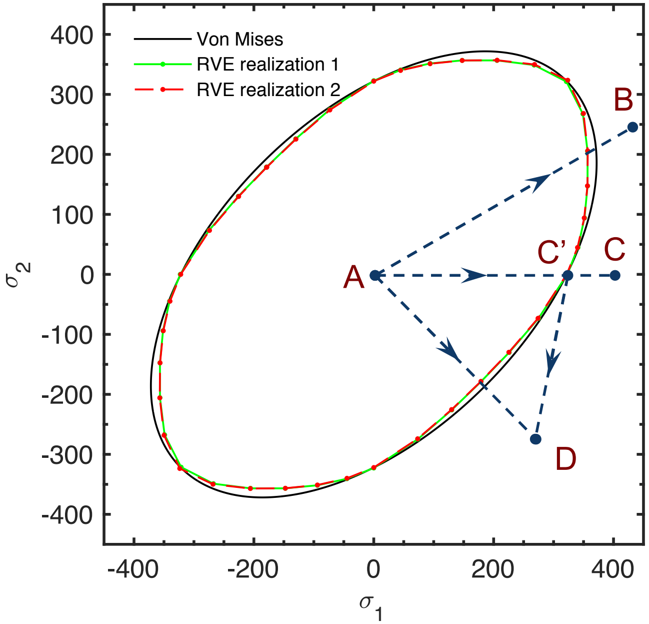


Model-form error – RVE vs. J2-plasticity



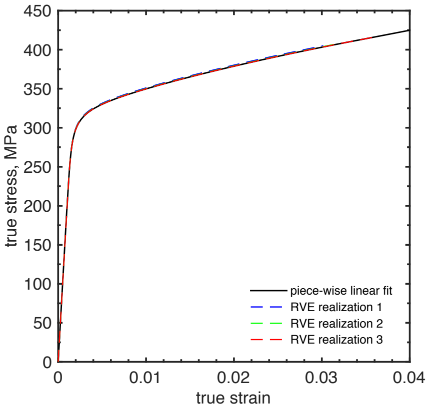
Model-form error – RVE vs. J2-plasticity

stress paths in principal-stress space



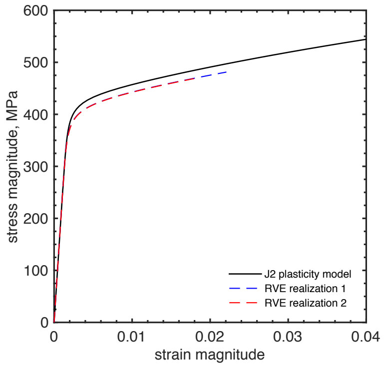
calibration

stress path A – C

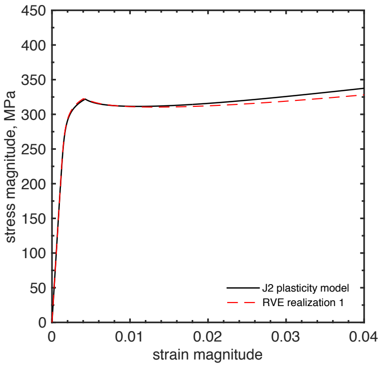


validation

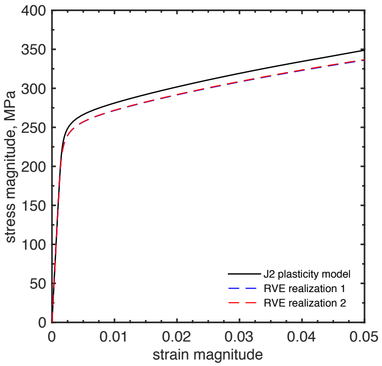
stress path A – B



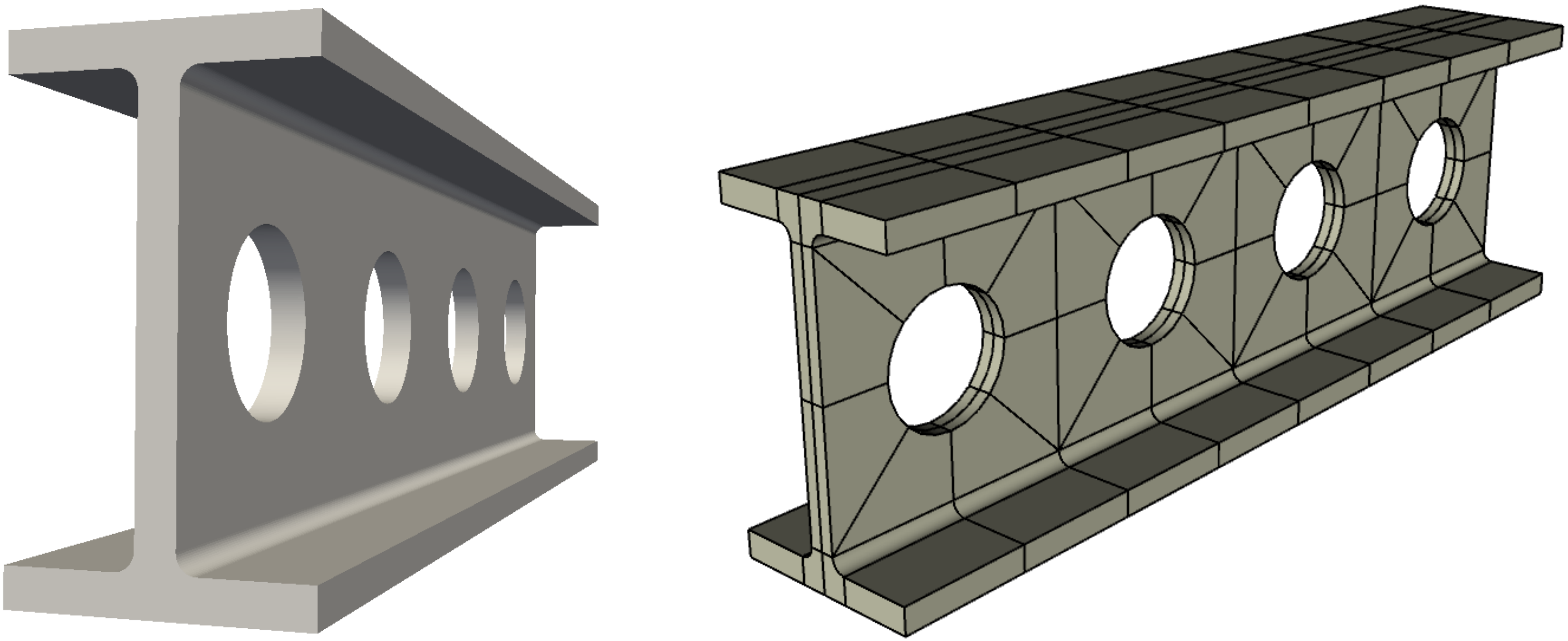
stress path A – C' – D



stress path A – D

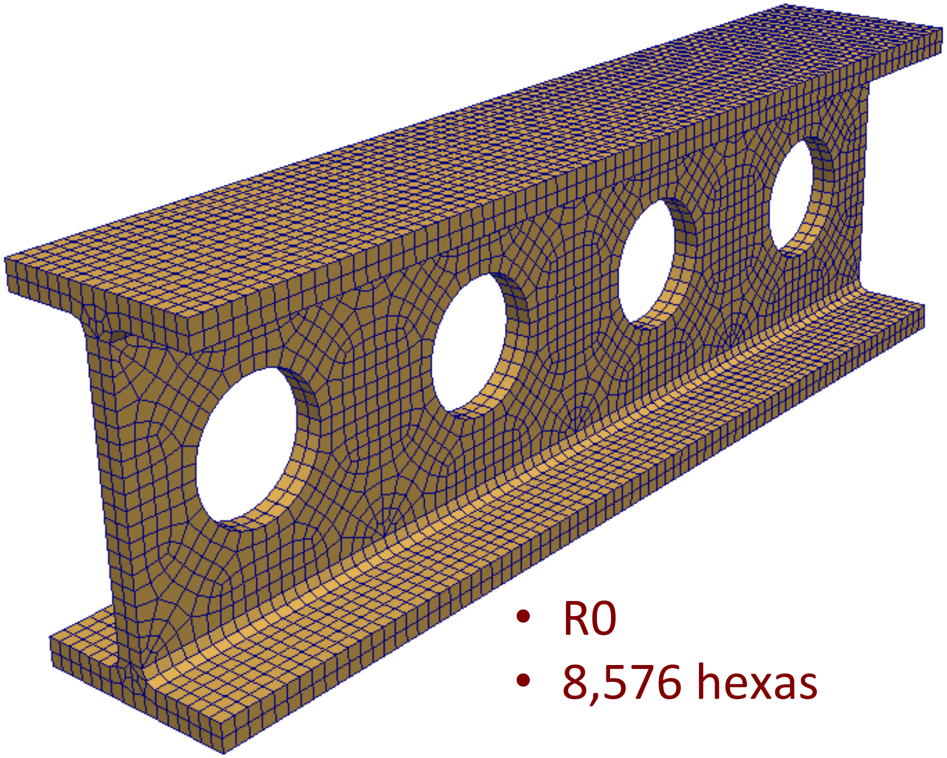


I-Beam example - elastic

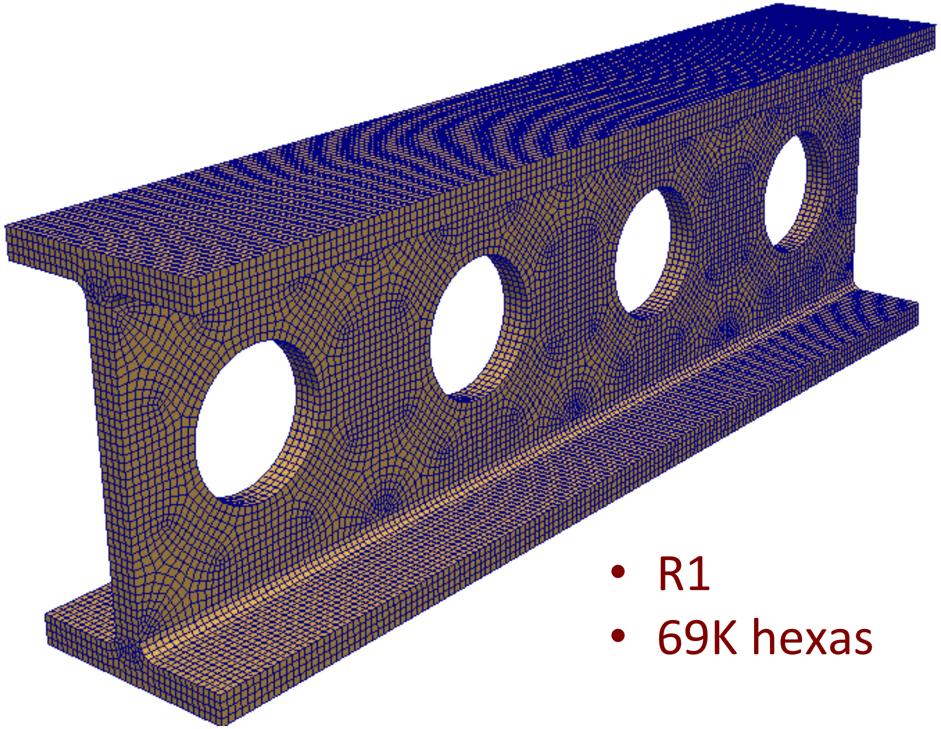


- tension
- bending
- torsion

Hierarchy of hexahedral meshes



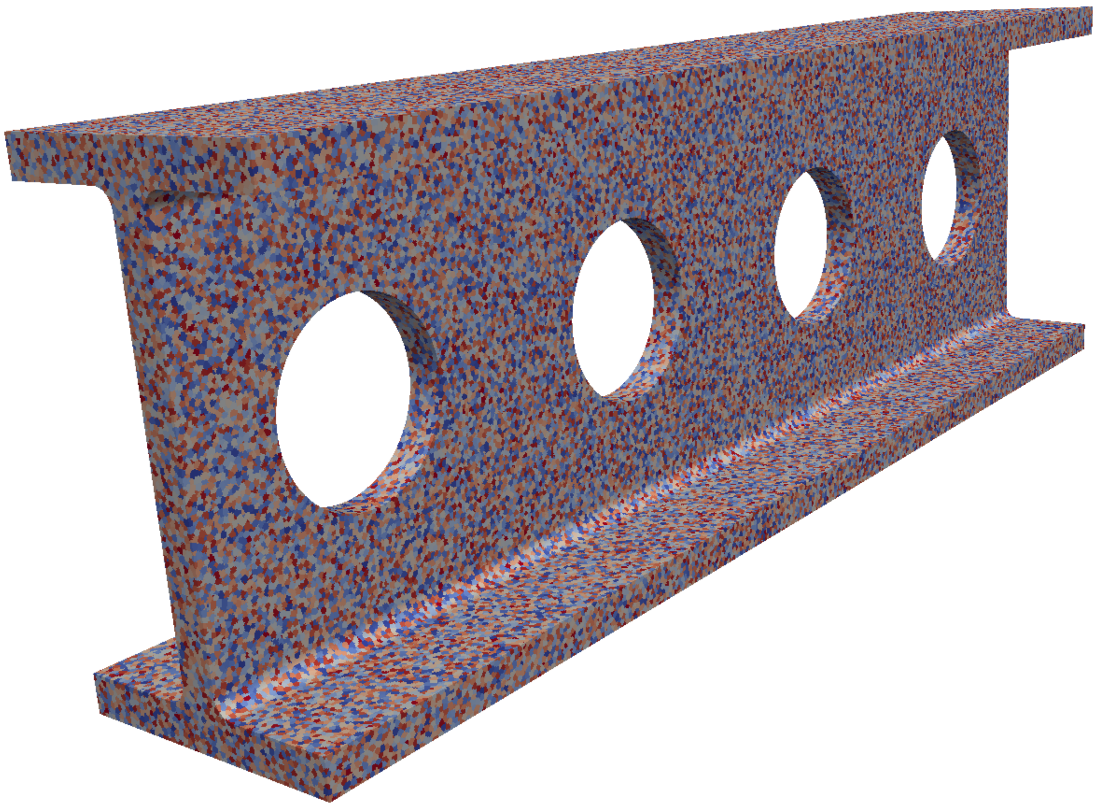
- R0
- 8,576 hexas

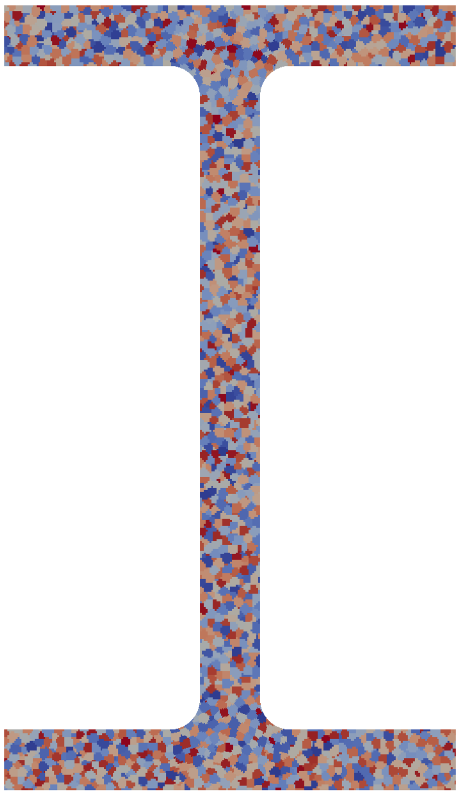


- R1
- 69K hexas

- R2, 549K hexas
- R3, 4.4M hexas
- R4, 35M hexas (~ 2000 cores, FETI solver)
- R5, 280M hexas (~ 20,000 cores, 3-level FETI)

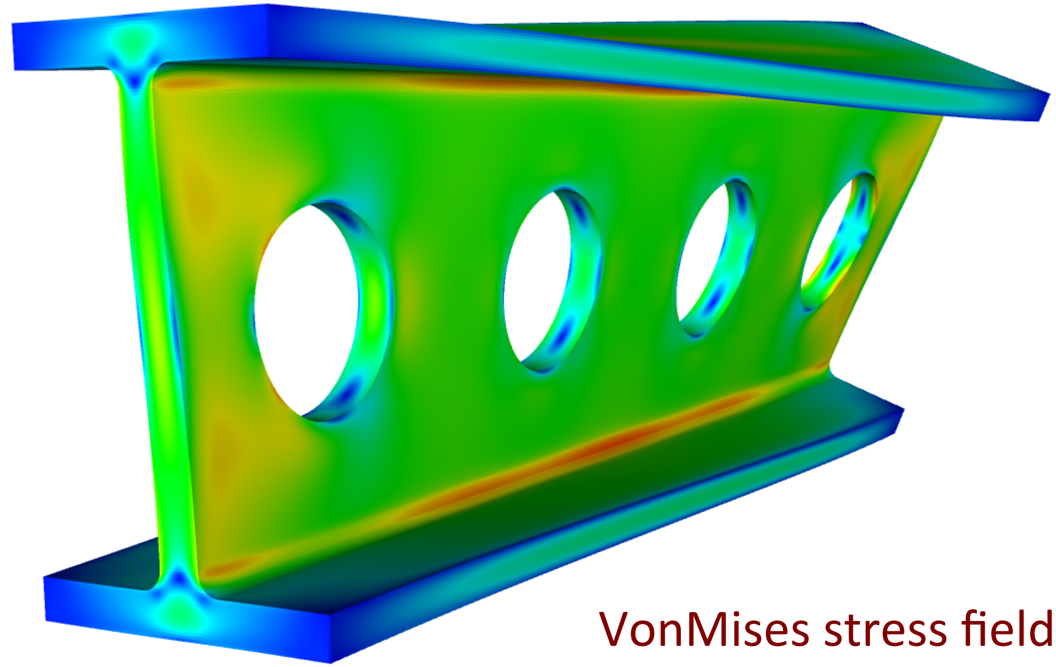
Thickness/grain ratio = 8



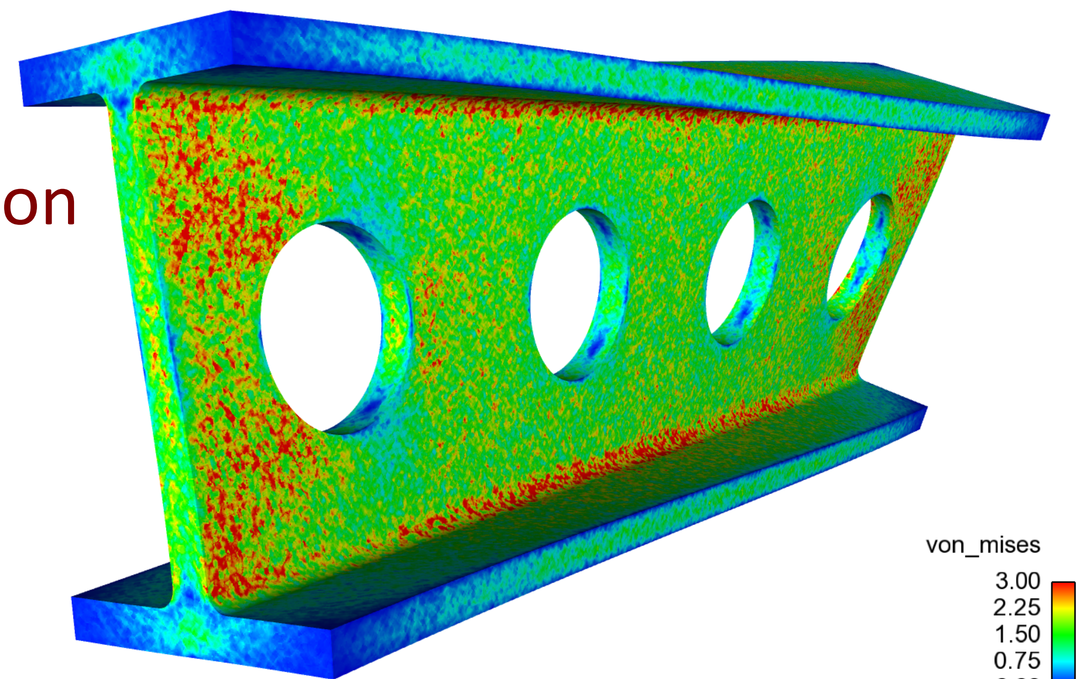


- uniformly random crystal orientations
- ~420,000 grains
- hex mesh overlay = R4 (35M elements)

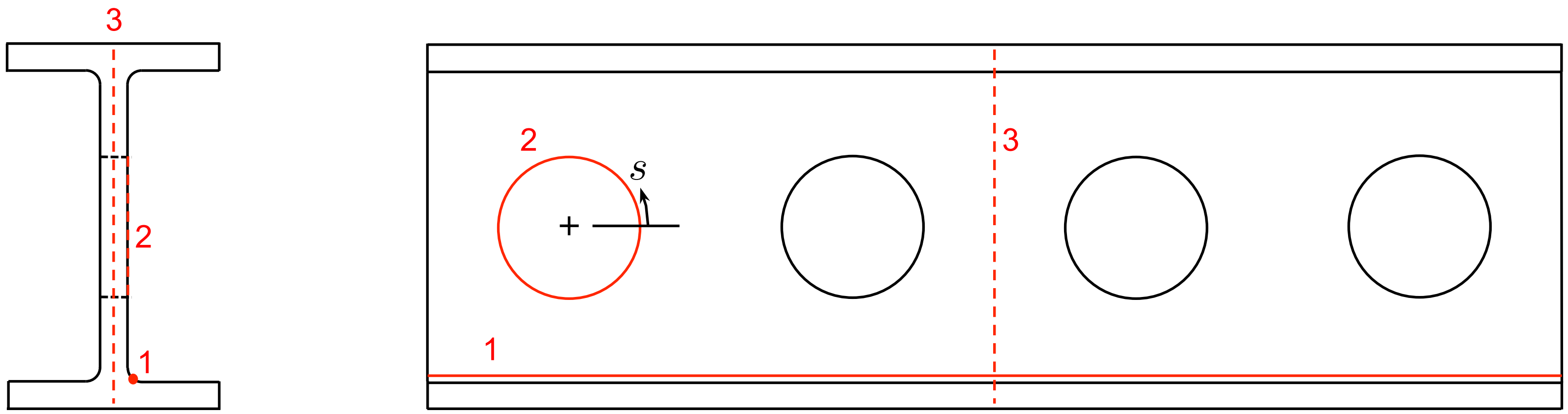
homogenized solution



direct numerical simulation



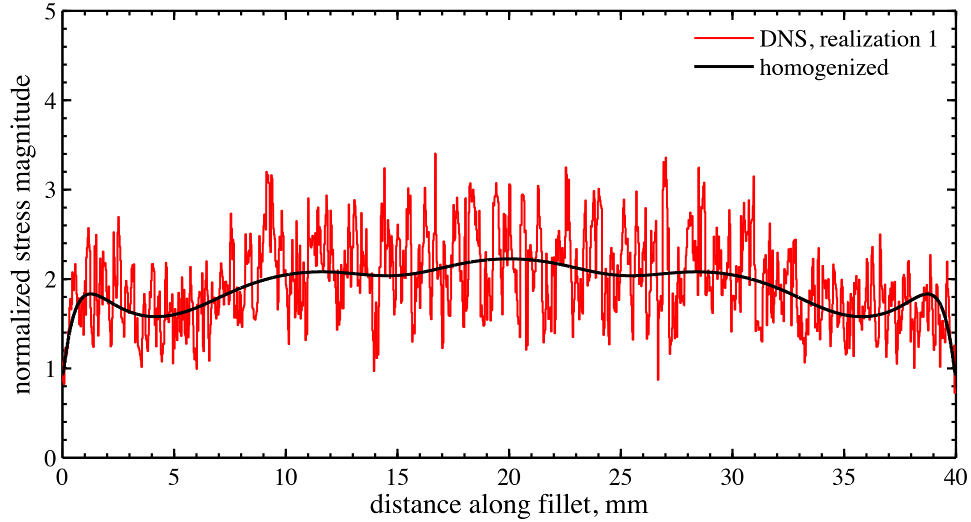
Stress extraction lines/curves



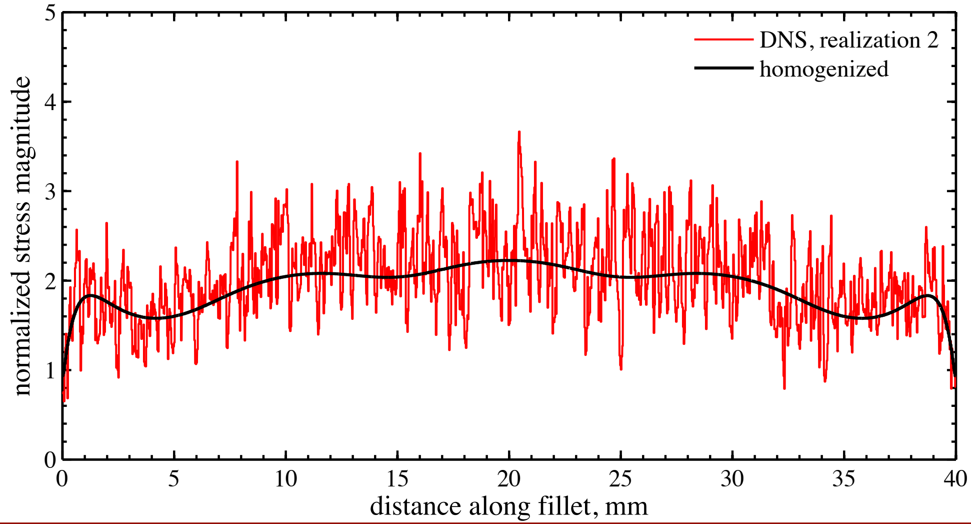
Homogenized solution vs. DNS

Stress magnitude along lower fillet

realization 1



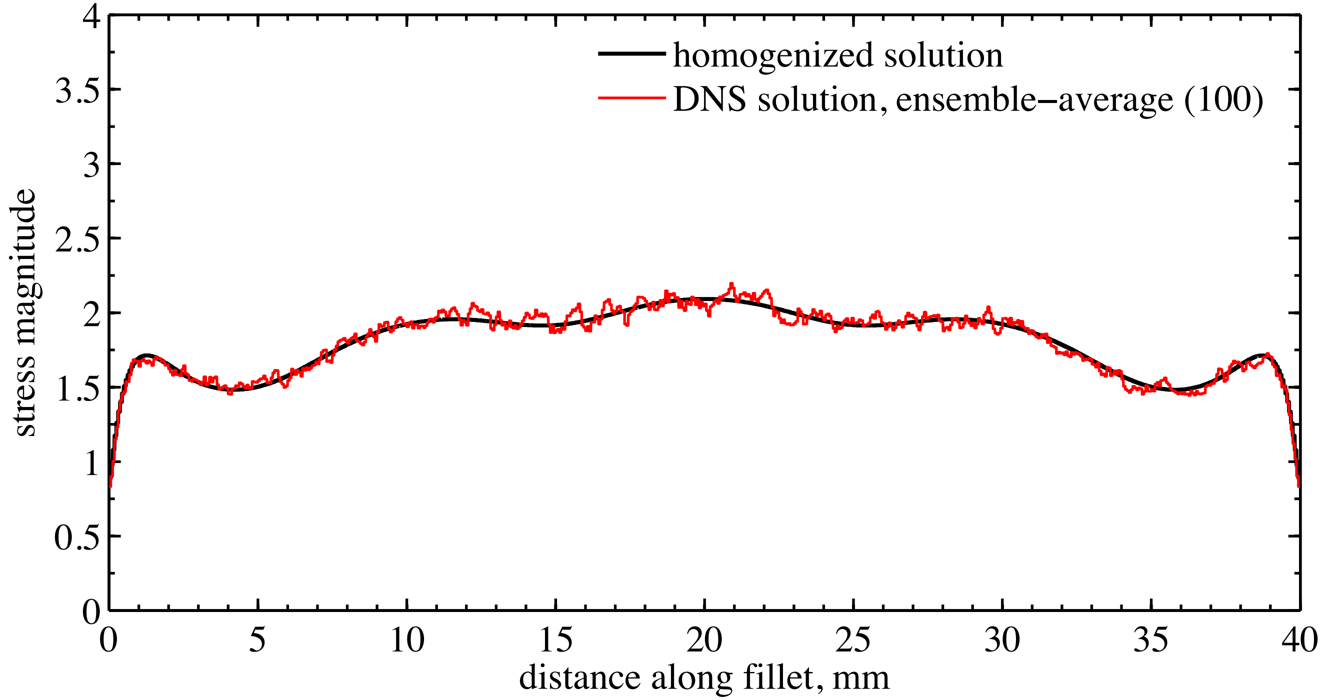
realization 2



Homogenized solution vs. ensemble average

Beran and McCoy (1970) showed that the governing equation for the mean field is **nonlocal**.

Stress magnitude along lower fillet

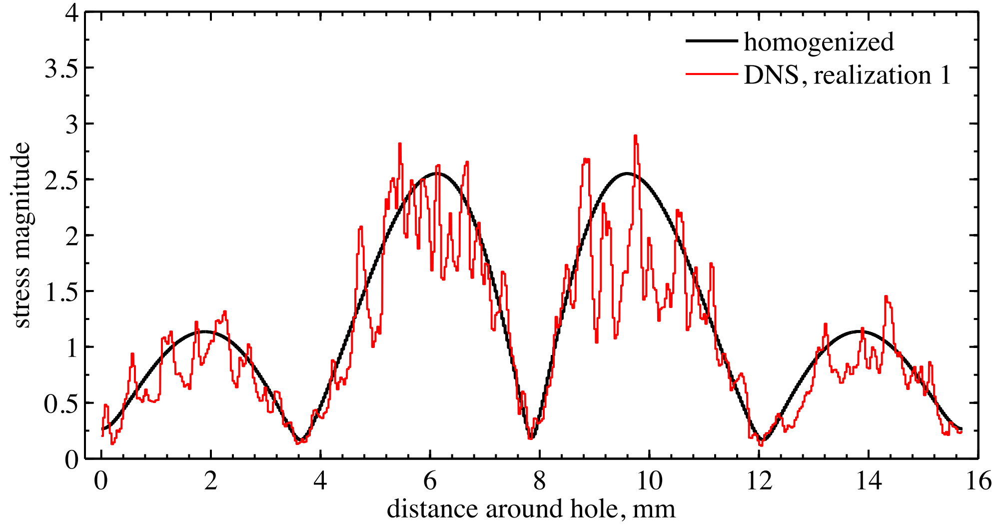


See no evidence for nonlocality here.

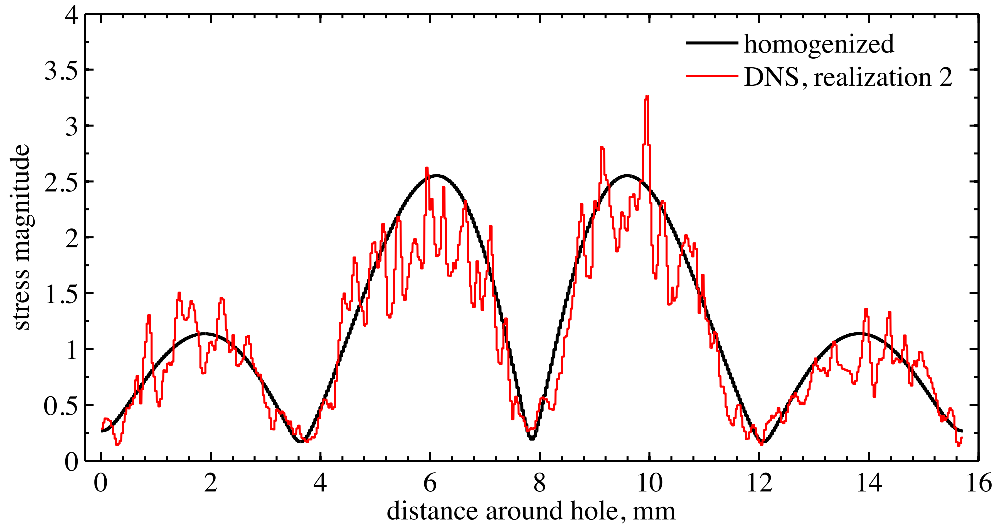
Homogenized solution vs. DNS

Stress magnitude around hole

realization 1



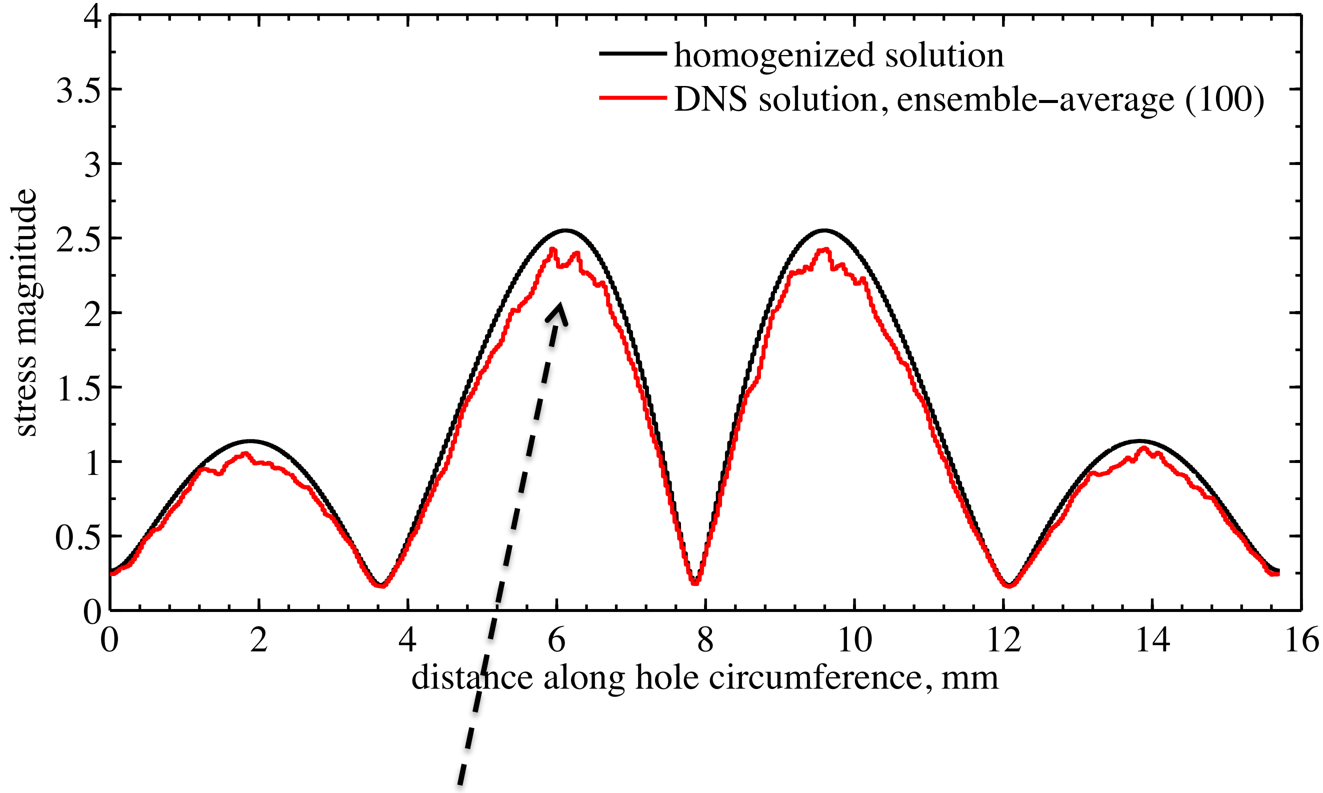
realization 2



Homogenized solution vs. ensemble average

al
tories

Stress magnitude around hole



100 realizations

See some evidence for nonlocality here.

3D moving average using Gaussian filter

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convolution

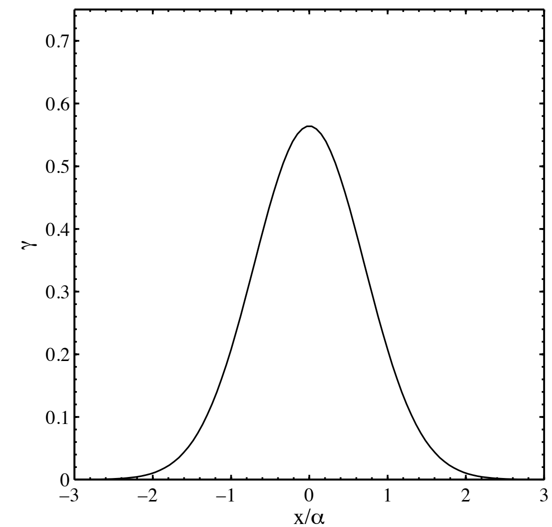
$$\hat{\sigma}_{ij}(\mathbf{x}) = \gamma_\alpha(\mathbf{x}) * \sigma_{ij}(\mathbf{x}) = \int_{\Omega_\infty} \gamma_\alpha(\mathbf{x}-\mathbf{y})\sigma_{ij}(\mathbf{y})d\mathbf{y}$$

$$\gamma_\alpha(\mathbf{x}-\mathbf{y}) = A\, e^{-\frac{||\mathbf{x}-\mathbf{y}||^2}{\alpha^2}}$$

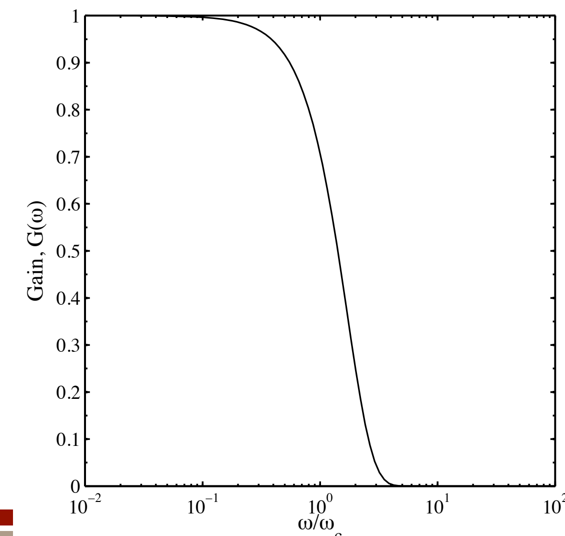
A = normalization constant to reproduce constant functions

cutoff frequency $\omega_c = \frac{\sqrt{2\ln 2}}{\alpha} = \frac{1.1774}{\alpha}$

Gaussian Kernel



Gain vs. spatial frequency



3D moving average using Gaussian filter

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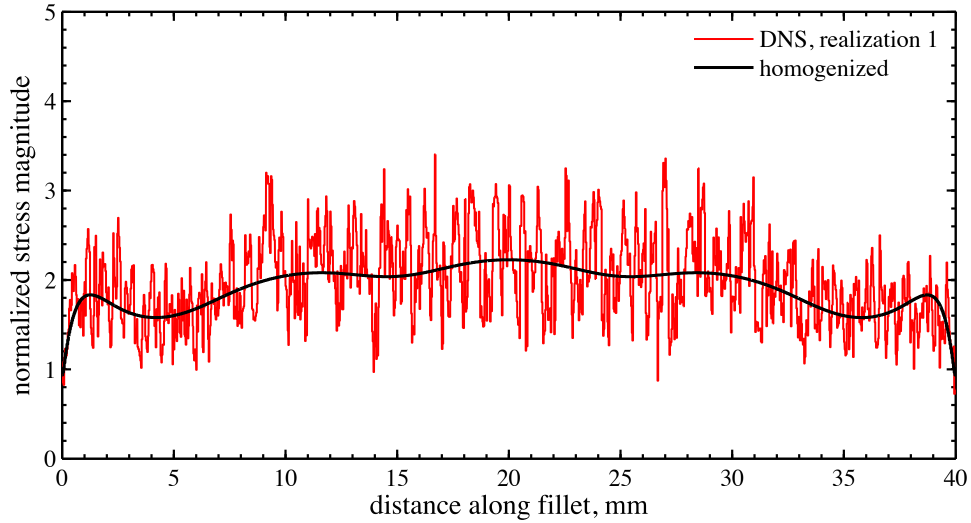
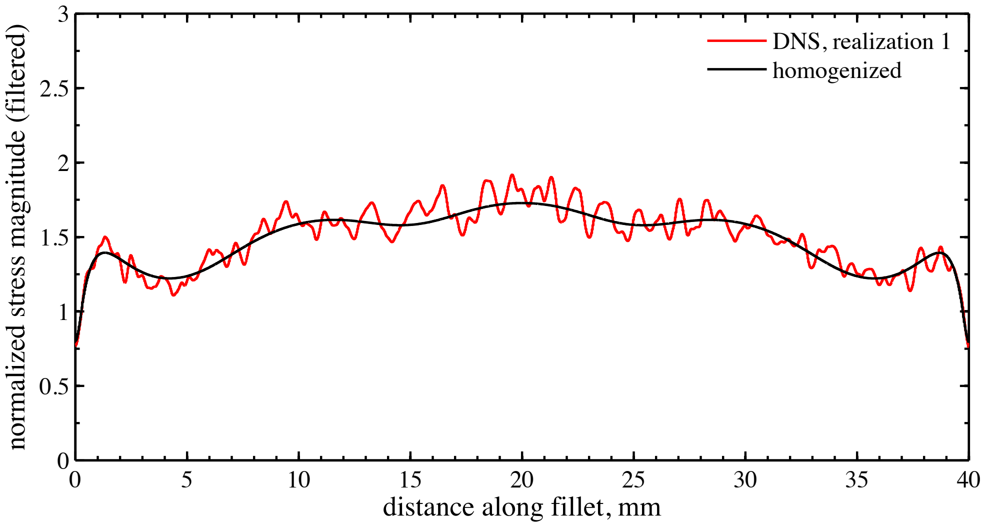
Stress magnitude along lower fillet

unfiltered



filtered

$\alpha = 0.125\,\mathrm{mm}$
(moving average over ~2x2x2 grains)

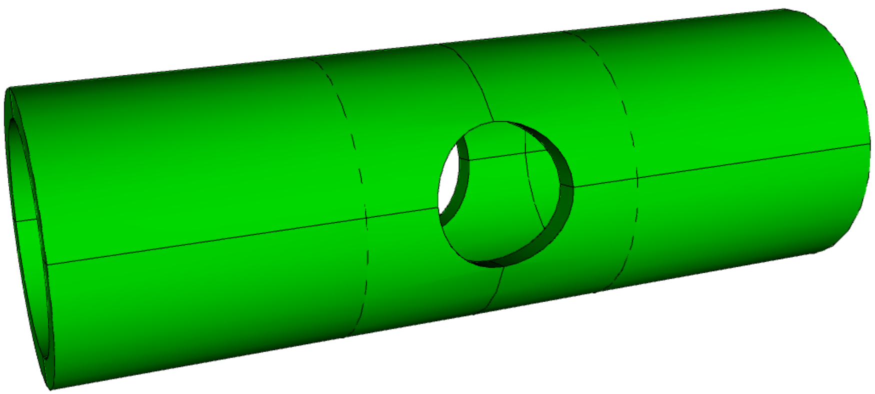


Homogenized solution is a surprisingly good approximation.

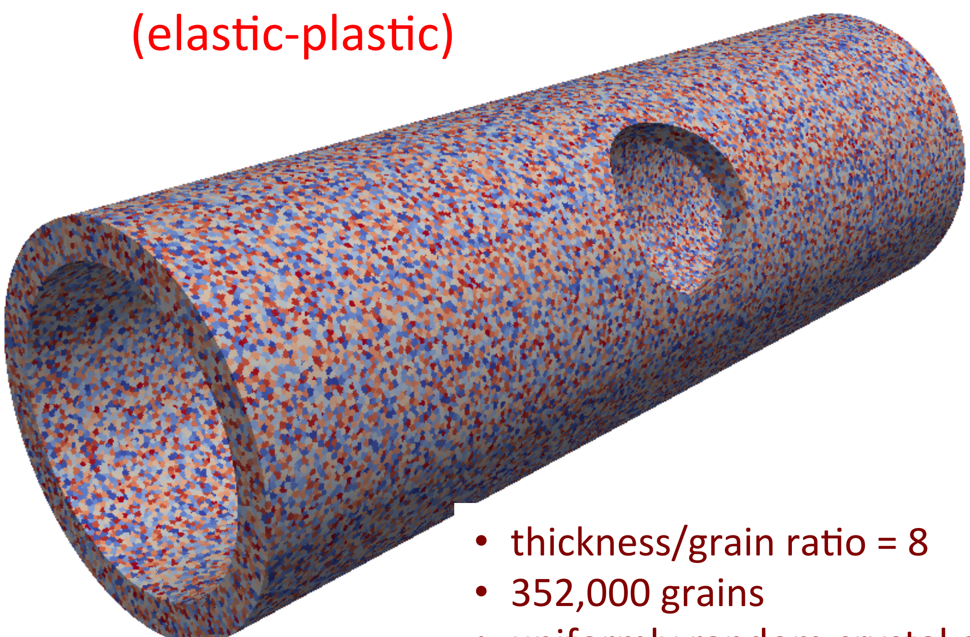
Summary (elastic results)

- Found little evidence of higher-order effects for this material and these BVPs. This is possibly due to the small correlation length inherent in the microstructure.
- Fluctuations (10-20%) on the length scale of several grains are present as evidenced by spatially filtered DNS results.
- What about plastic regime?

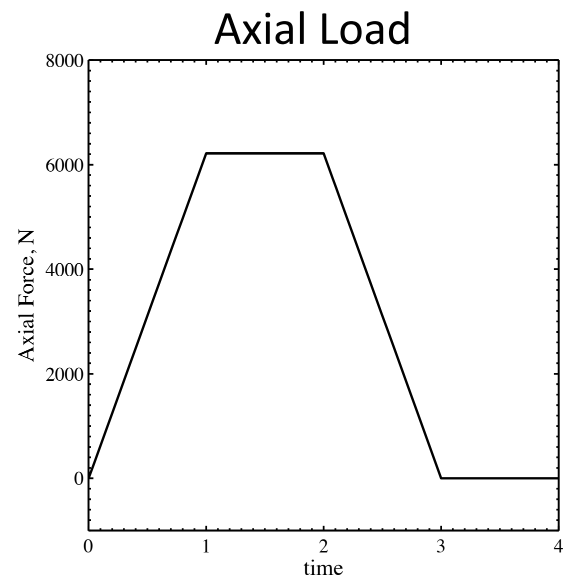
Plastic example: stainless-steel tube under combined tension-torsion

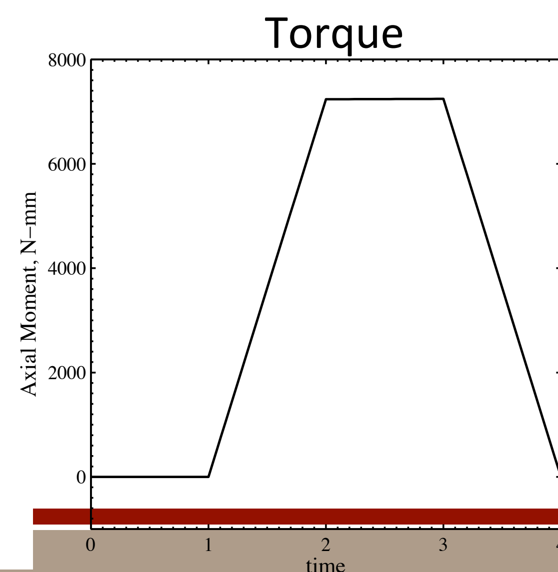


(elastic-plastic)

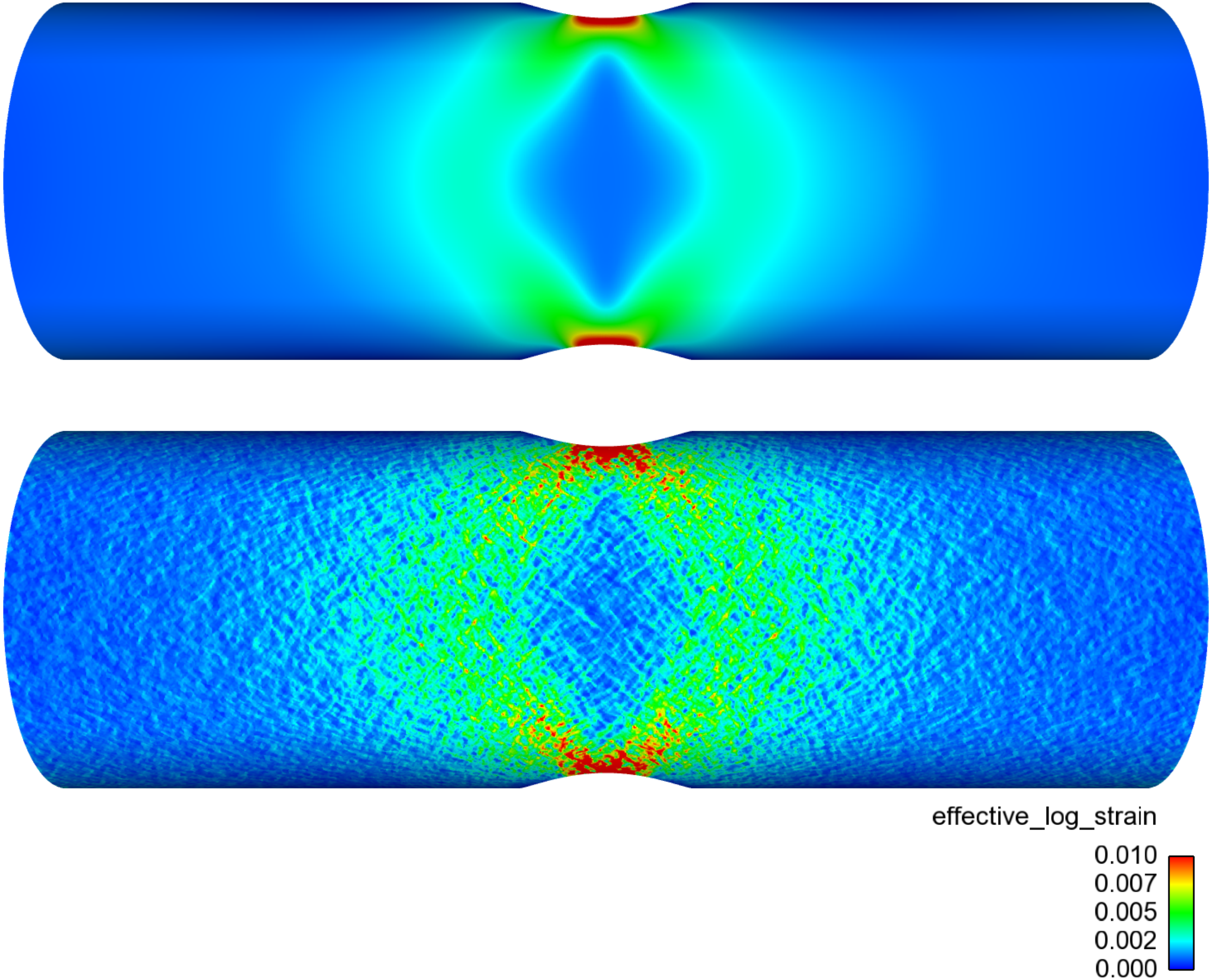


- thickness/grain ratio = 8
- 352,000 grains
- uniformly random crystal orientations

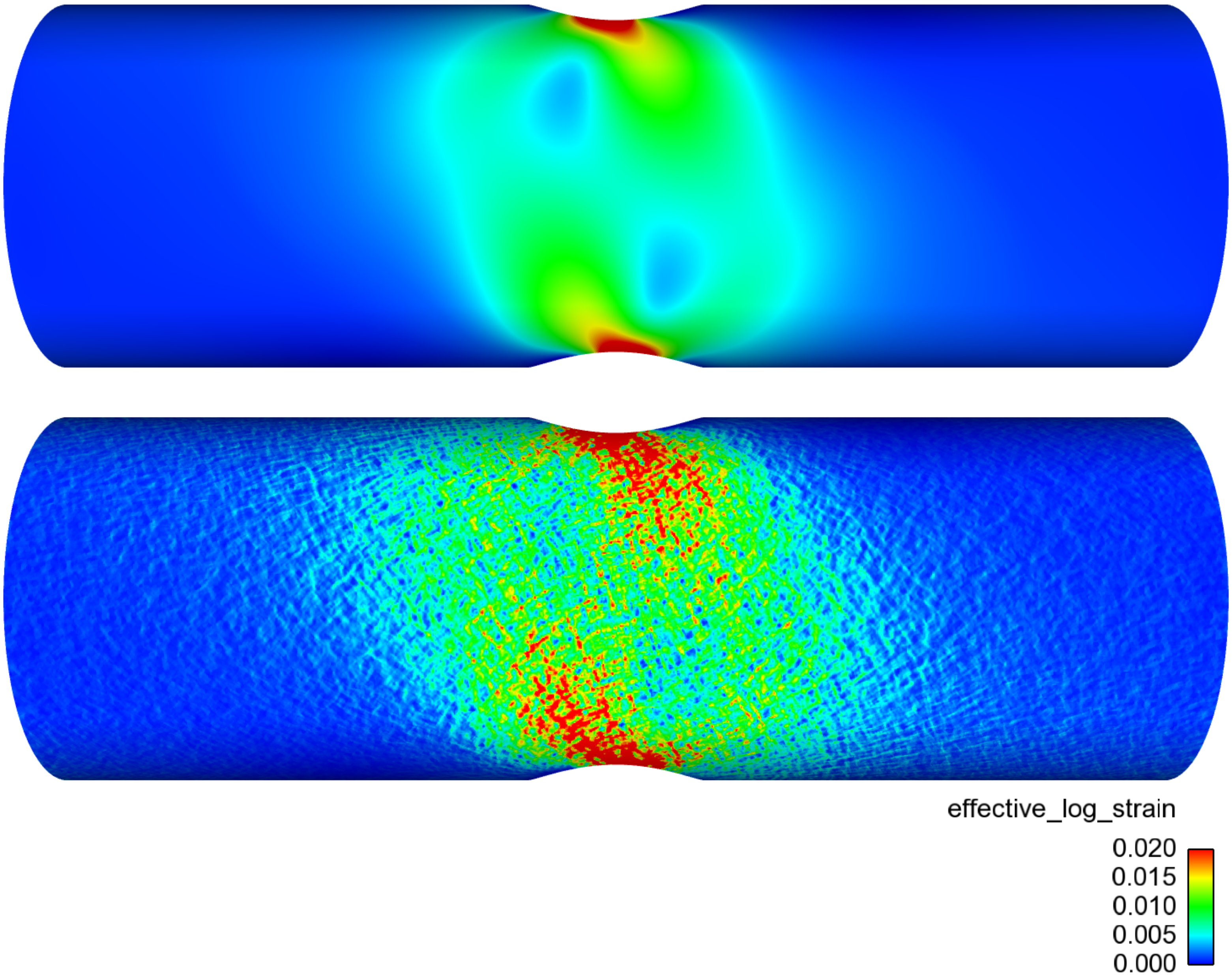




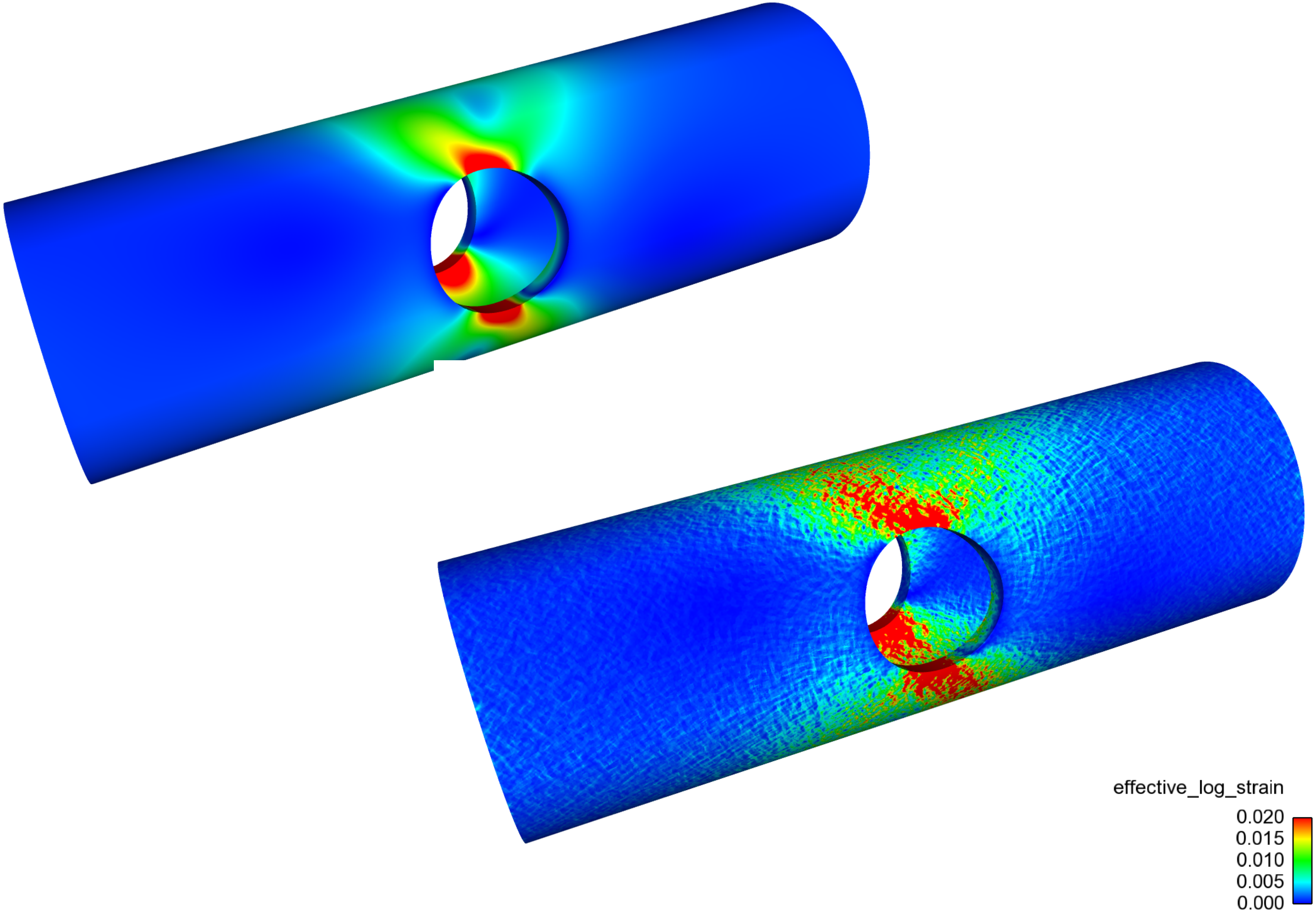
Axial Load Only



Axial load + torsion

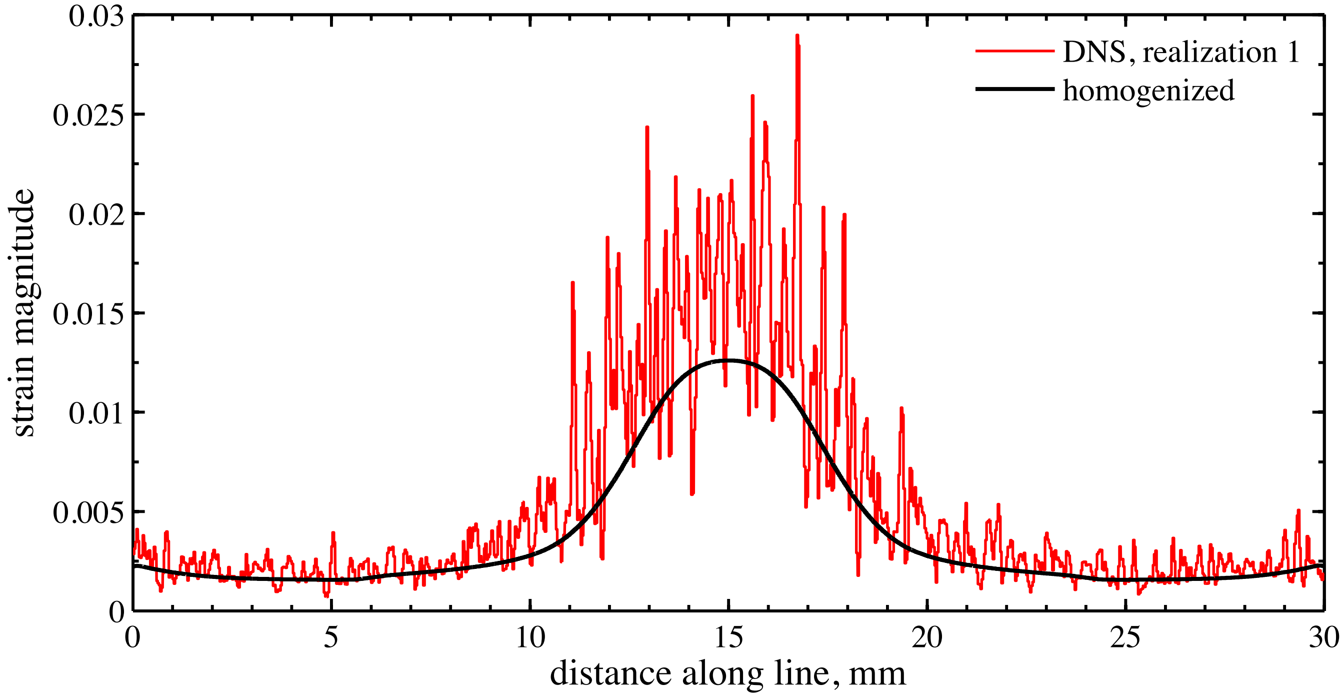


Strain under combined tension-torsion



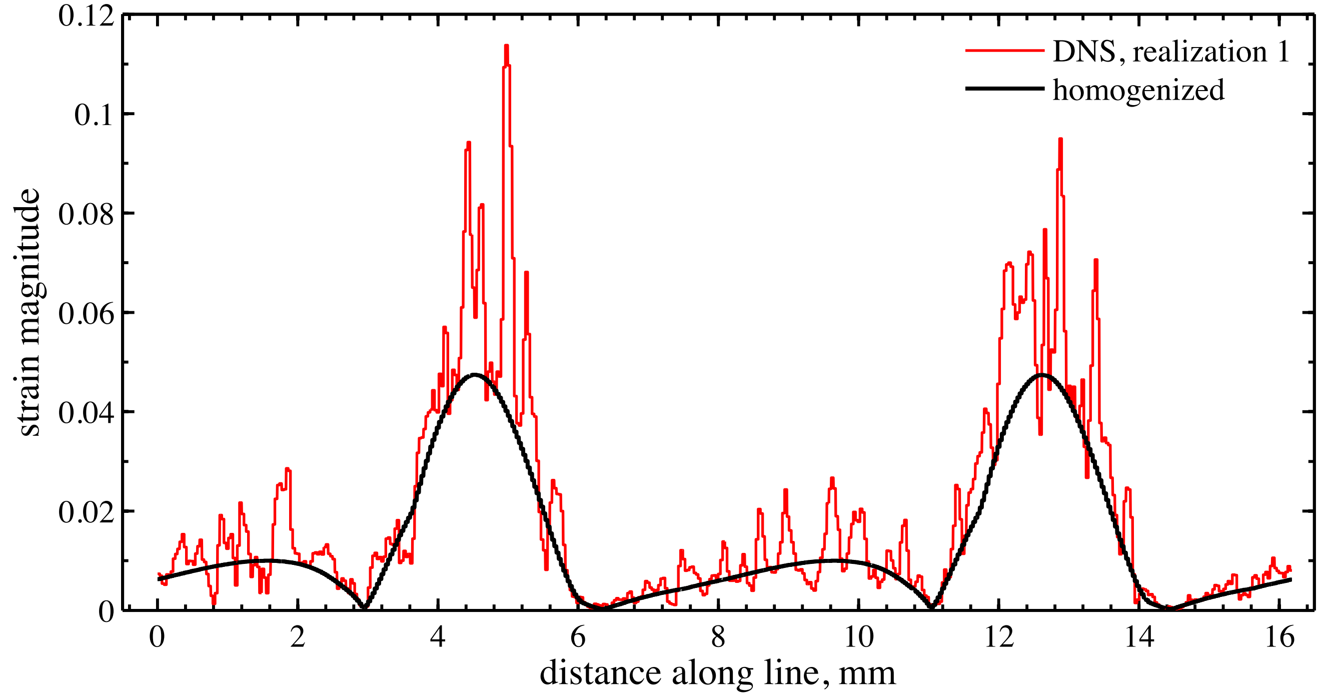
Strain magnitude along length of tube

midsection between holes, combined tension-torsion

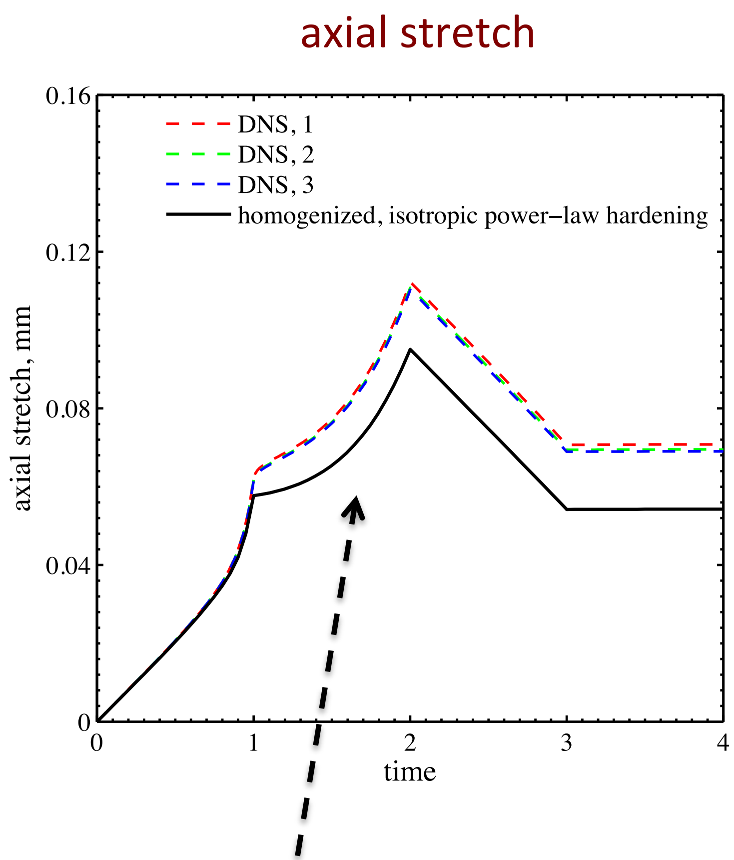


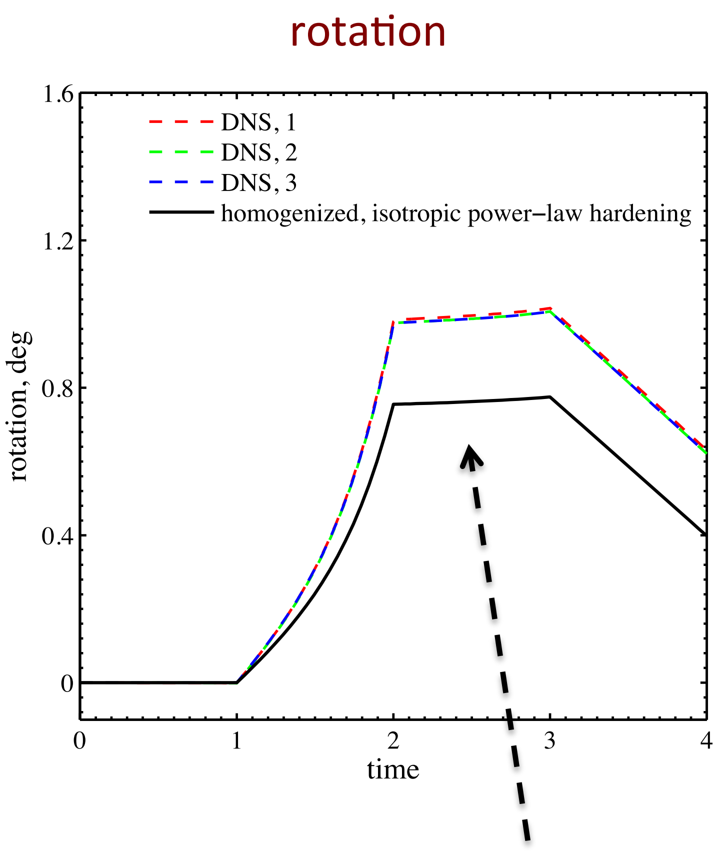
Strain magnitude around hole

inside circumference, combined tension-torsion



Global stretch and rotation of tube





Homogenized solution good in tension-only region but less accurate in combined tension-torsion.

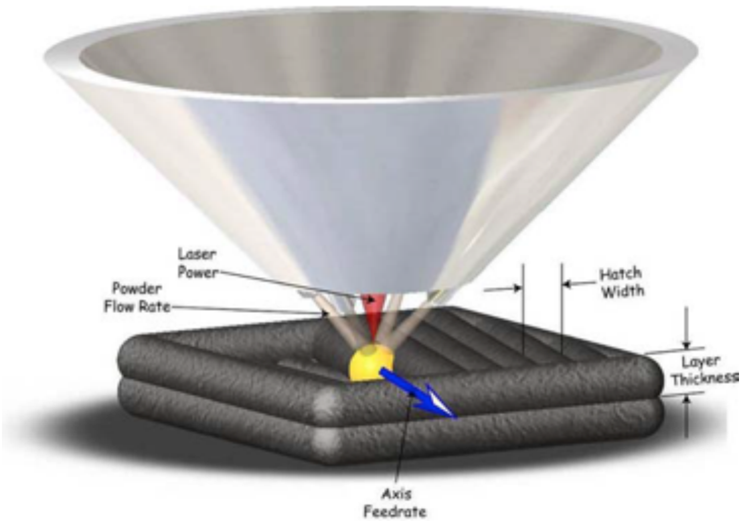
Summary (plastic results)

- See appreciable difference between a basic J2 plasticity model and DNS results.
- Need full FE^2 for true homogenization in the plastic regime.
- What about more complex microstructures, e.g. from additive?

Bishop, J., Emery, J., Field, R., Weinberger, C., Littlewood, D. 2015, "Direct numerical simulations in solid mechanics for understanding the macroscale effects of microscale material variability," *CMAME,* 287, pp. 262-289.

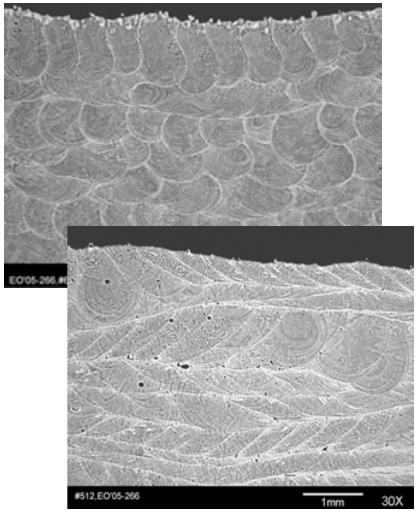
Application to additive manufacturing

Laser Engineered Net Shape (LENS)



Schematic of LENS™ laser-based deposition process

- LENS "hatch" structure results in a complex mesoscale structure.
- Classical assumption of scale-separation may no longer be applicable.

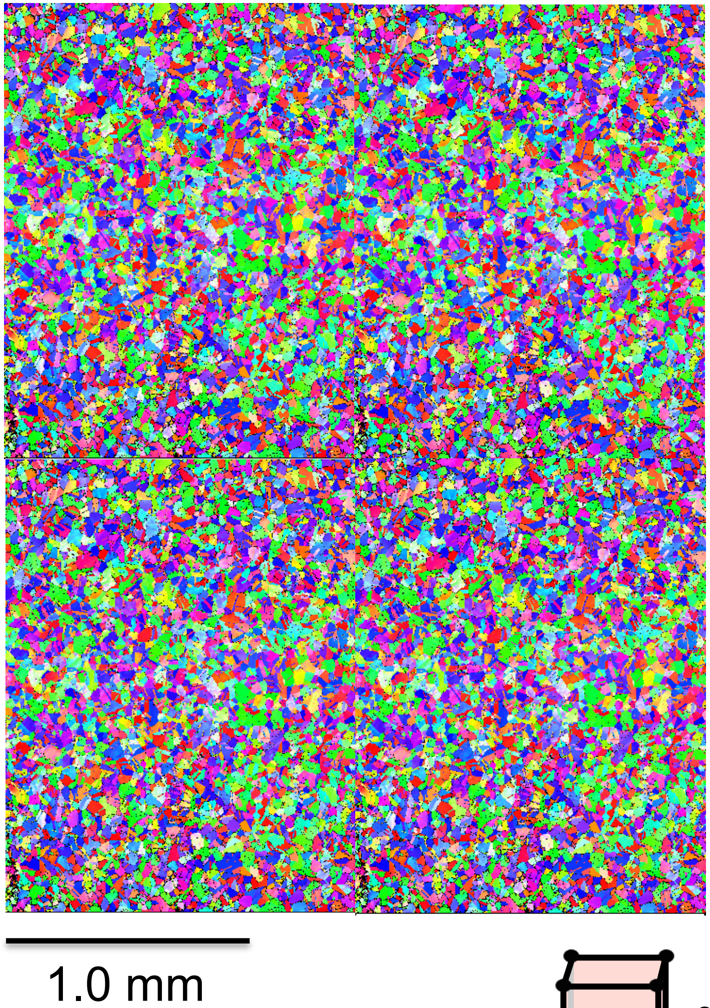


LENS mesostructure

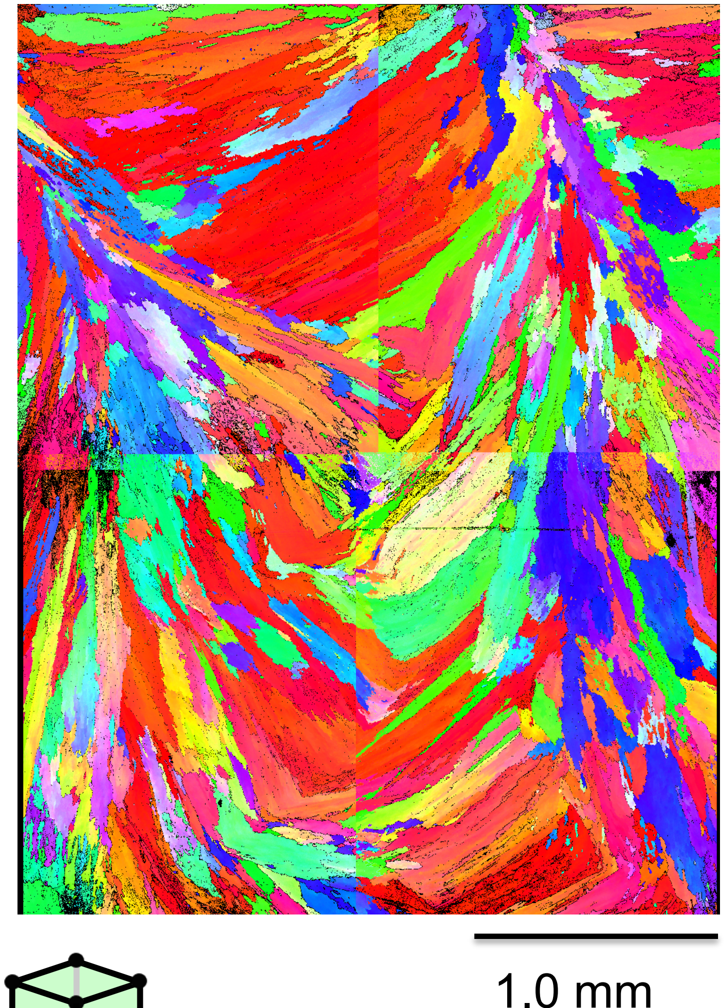
Microstructure: wrought vs. LENS

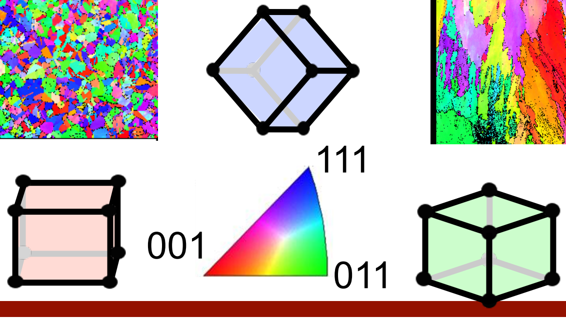
(Images shown at same scale.)

Wrought, SS 304L

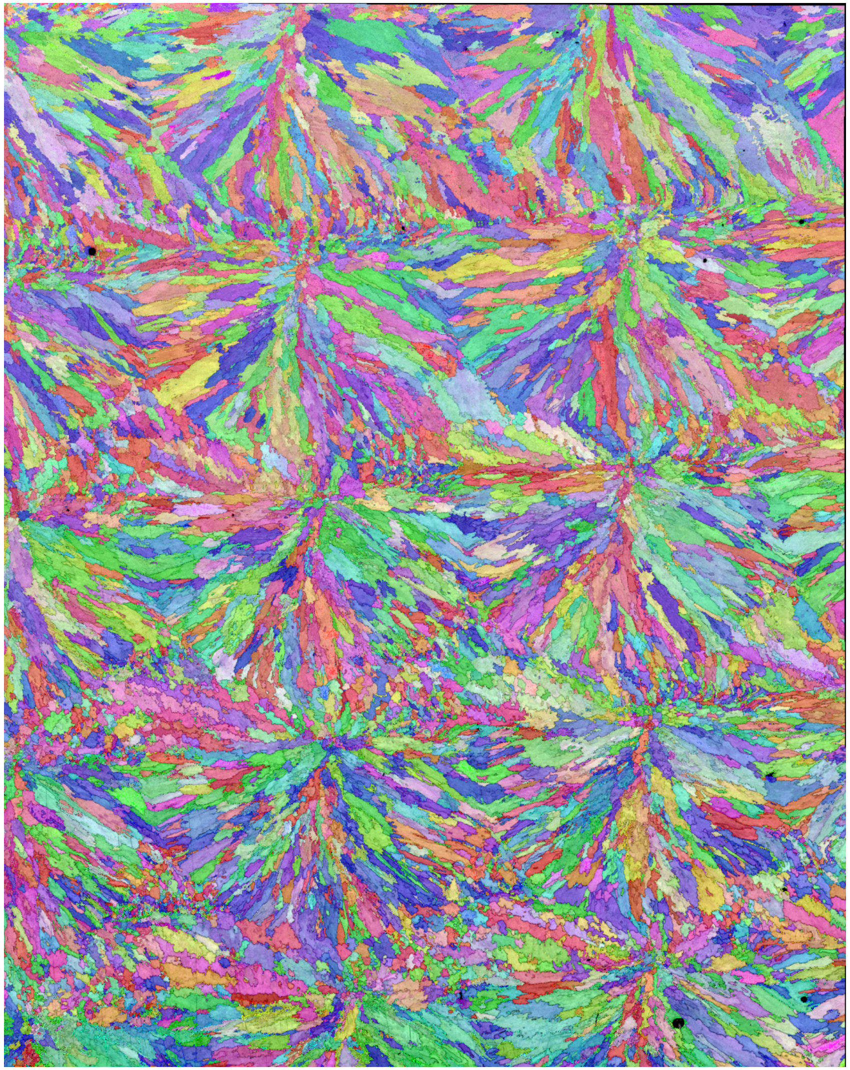


LENS, SS 304L, 3.8 kW





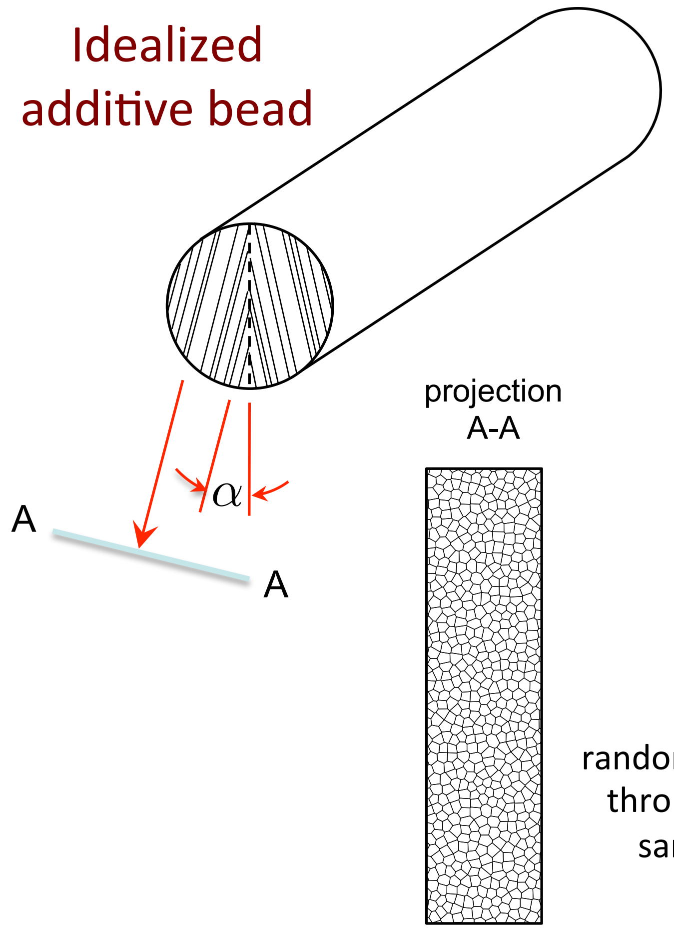
LENS microstructure



8 mm x 10 mm

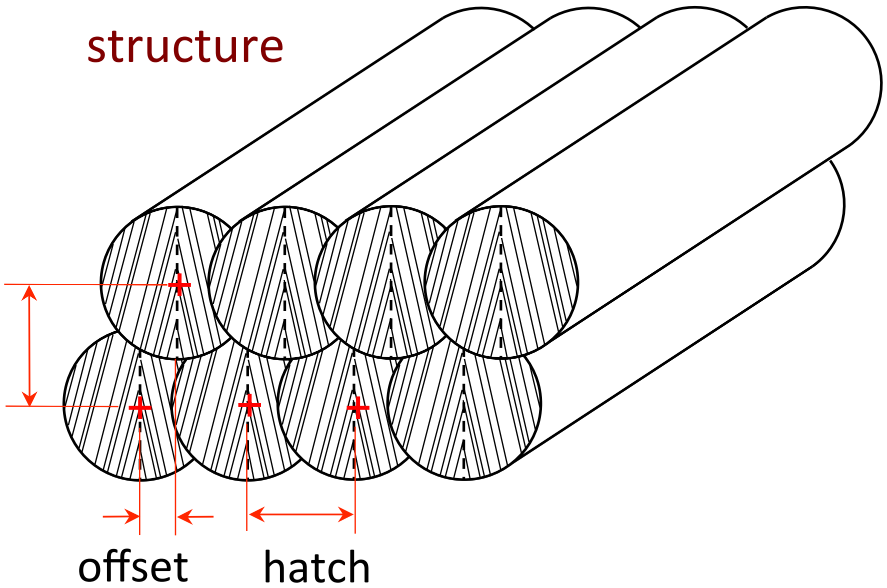
Idealized LENS microstructures

Idealized additive bead



random Voronoi through MPS sampling

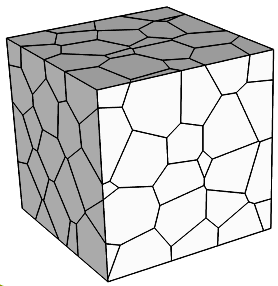
Idealized LENS structure

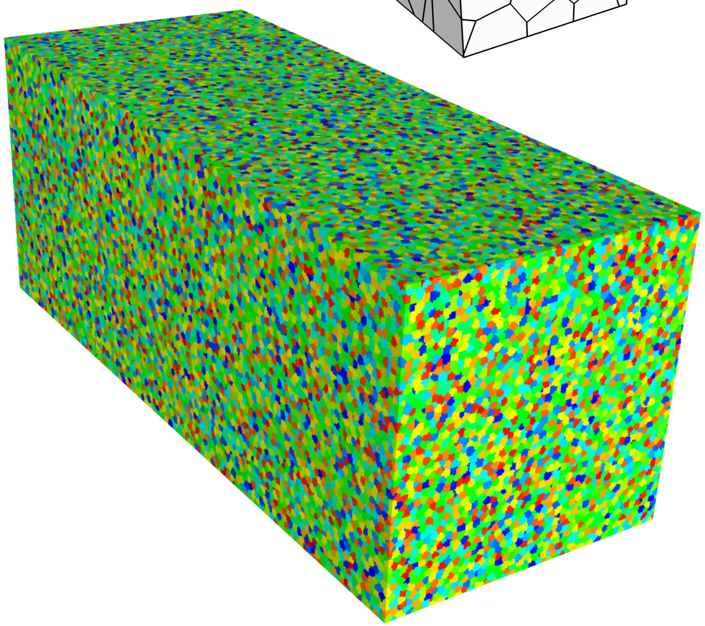


texture?

DNS modeling

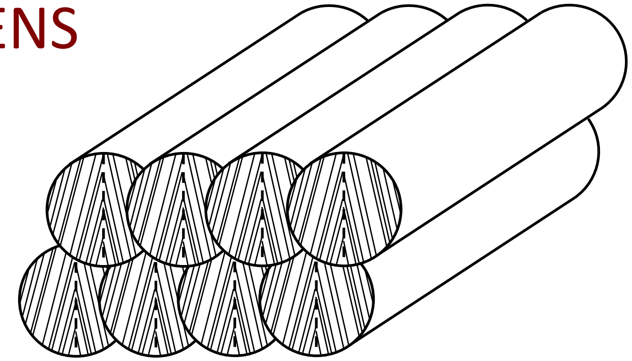
equiaxed



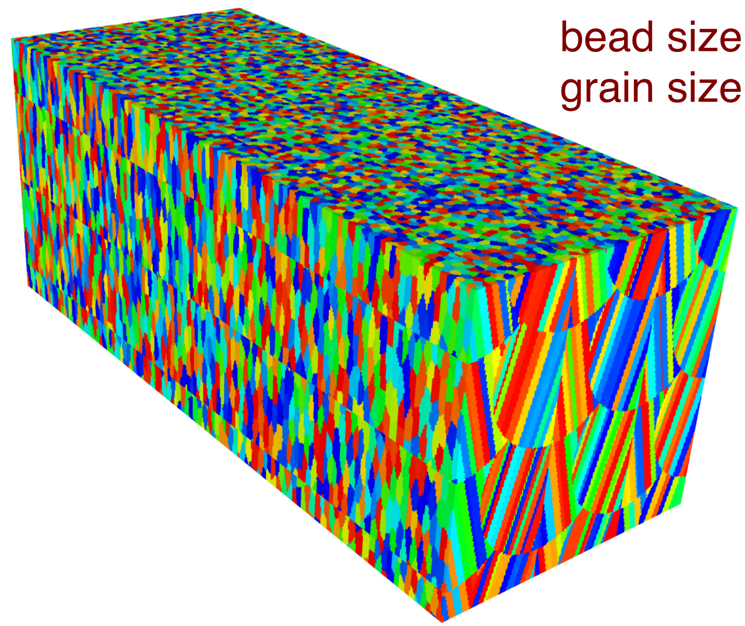


grain size = 40 microns

additive, LENS

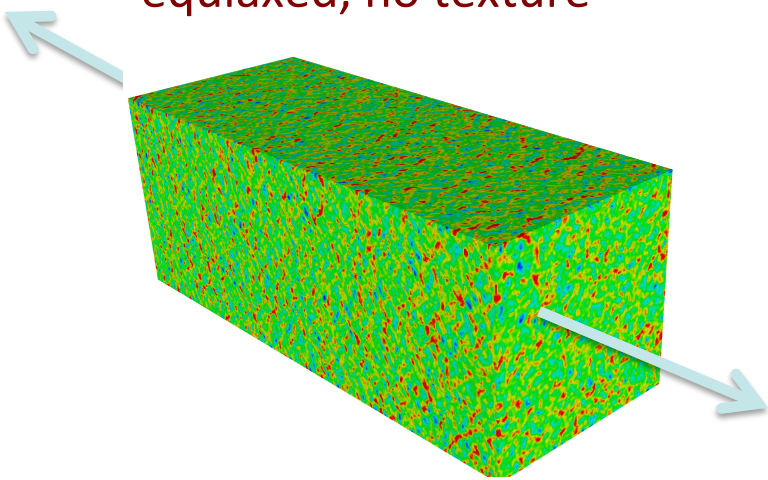


bead size = 1 mm
grain size = 40 microns

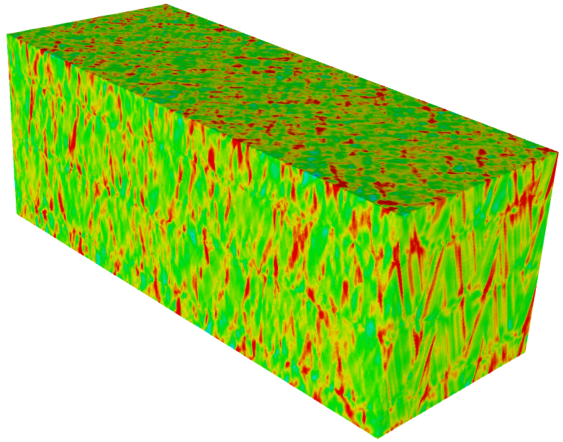


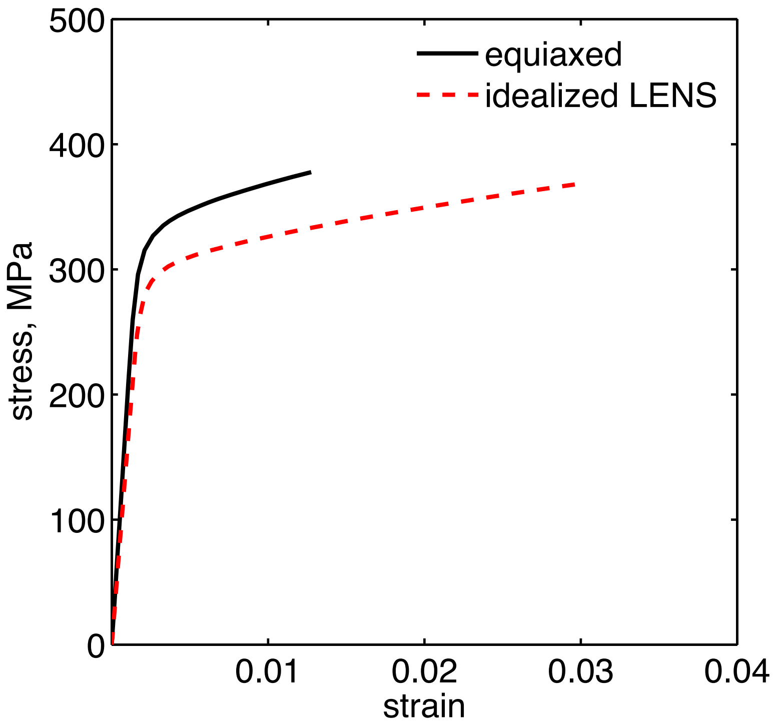
Engineering stress-strain

equiaxed, no texture



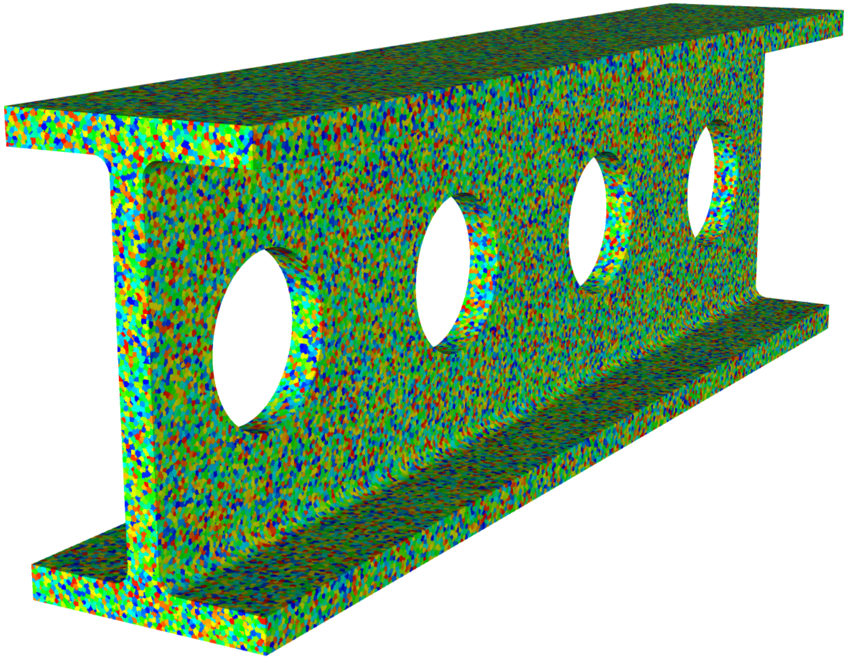
additive, LENS



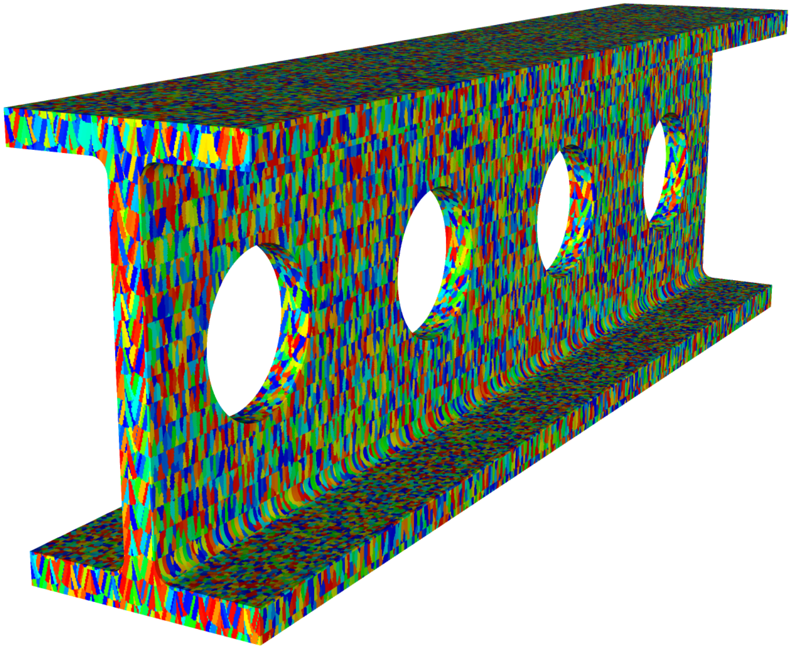


Idealized microstructures

equiaxed



LENS



Macroscopic stress field

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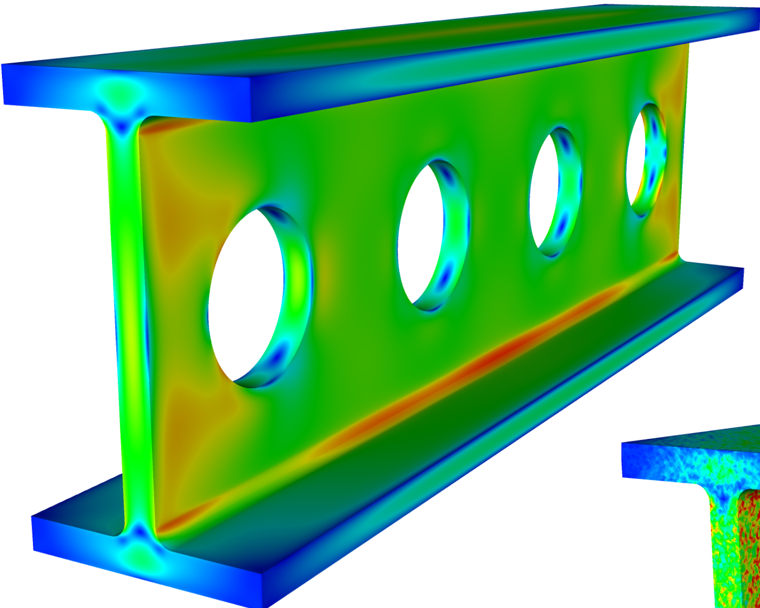
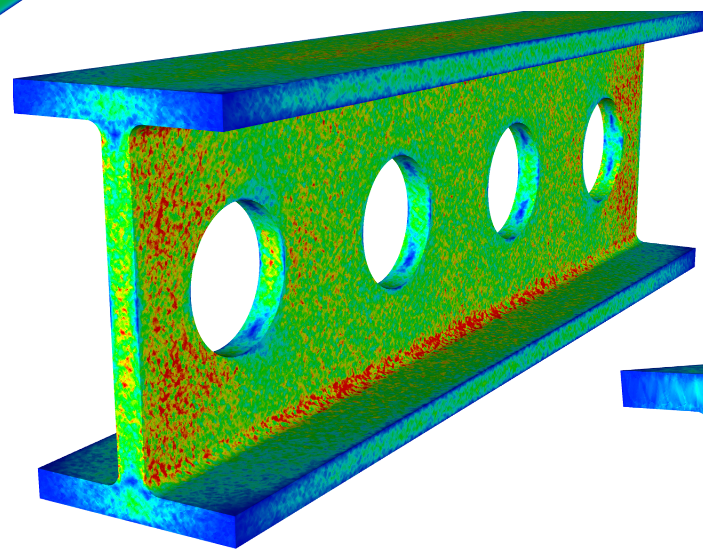
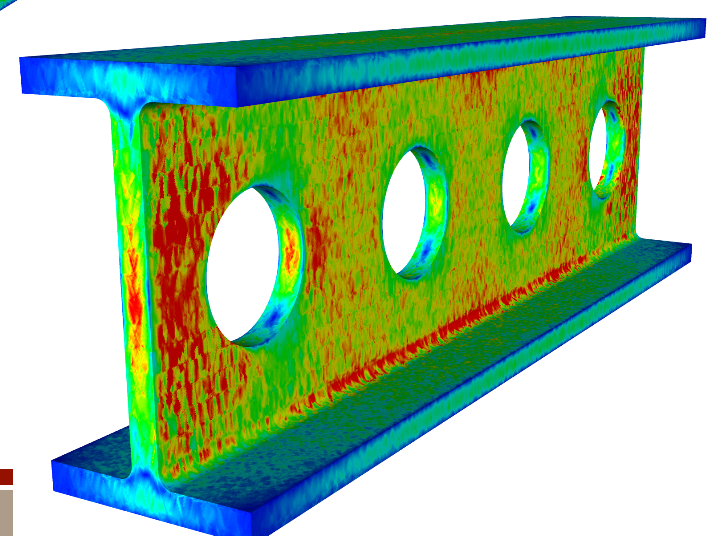


homogeneous, isotropic



equiaxed, no texture, isotropic



idealized LENS

Process modeling (Veena Tikare, SNL)

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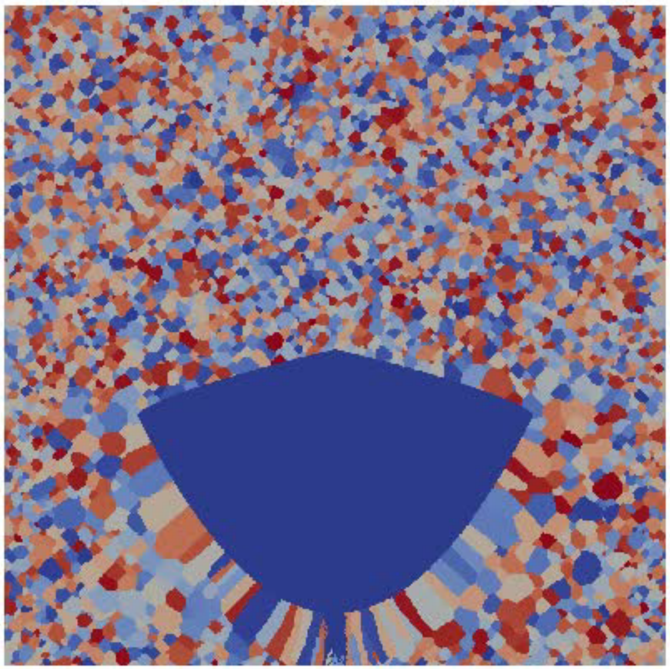
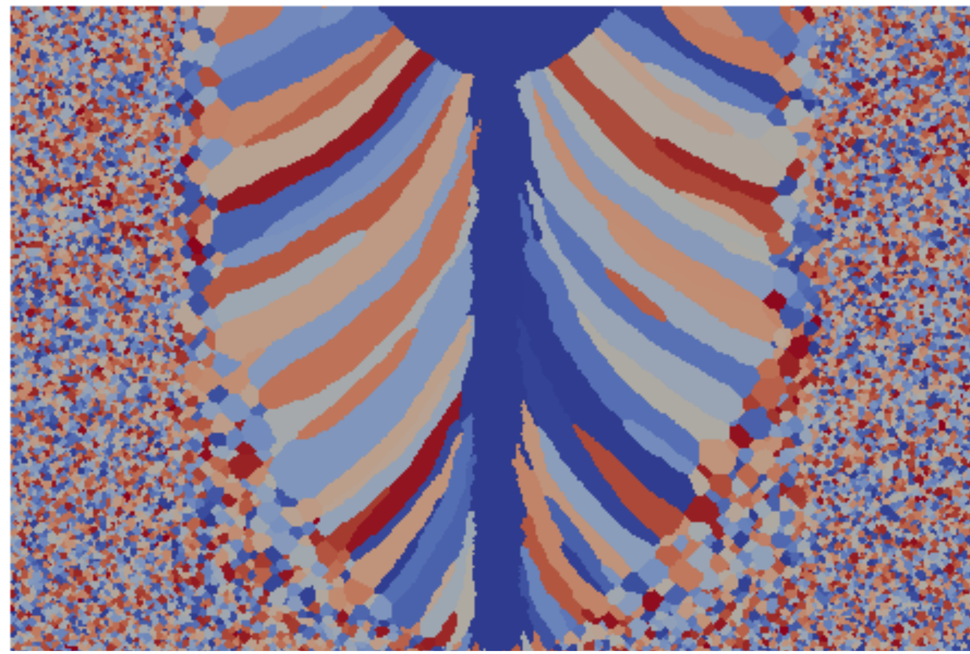
Future tie-in with process modeling:
grain growth simulation





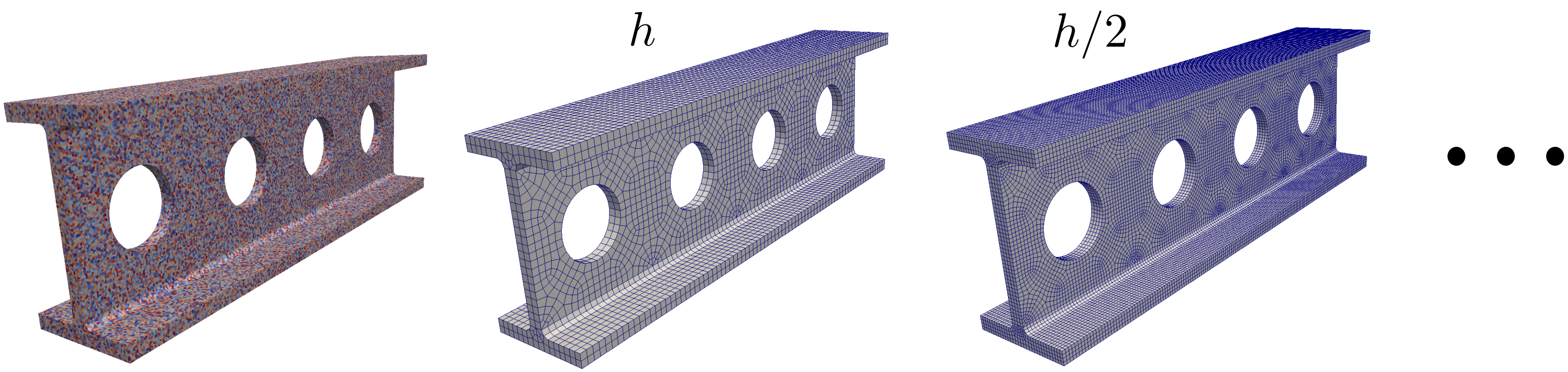
Kinetic Monte Carlo

Multiscale modeling using ‘geometric multigrid’ concepts

Miehe & Bayreuther, 2007
Fish & Belsky, 1995

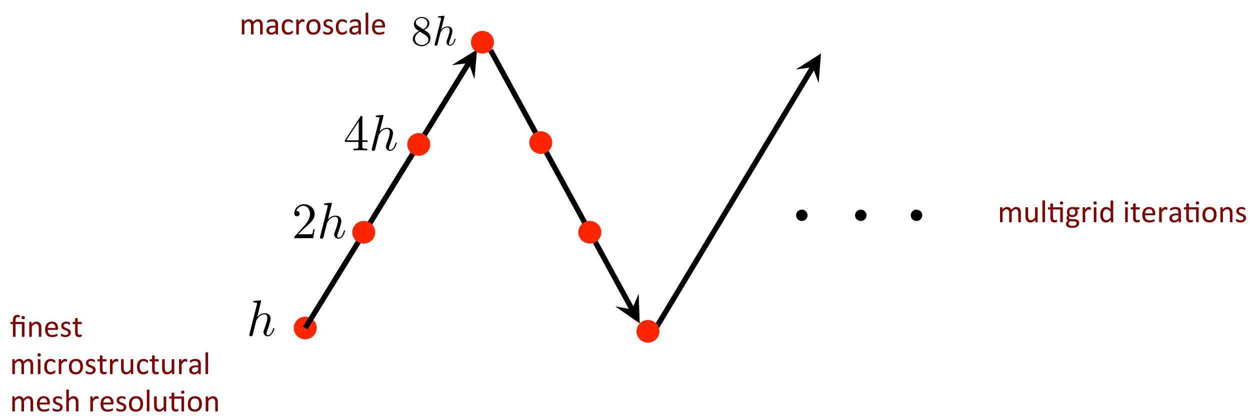
Multiscale multigrid solvers

- Key postulate: we have a fine scale representation/model that is predictive (e.g. microstructural model, crystal-plasticity model)
- Key idea: use geometric multigrid concepts to create a multiscale method (solver) that optimally obtains the “solution” at all scales
- No assumption of scale separation
- Applicable to linear or nonlinear problems
- Use goal-oriented error estimation to optimally create multigrid hierarchy
- Each grid represents a filtering of the fine-scale physics



We have a natural hierarchy of grids in our DNS approach.

Multigrid iterative V-cycle



$$A^h u^h = f^h$$

$$u^h = I_{2h}^h u^{2h}$$

submodeling based prolongation

$$I_h^{2h} = \left(I_{2h}^h\right)^T$$

Galerkin property

$$f^{2h} = I_h^{2h} f^h$$

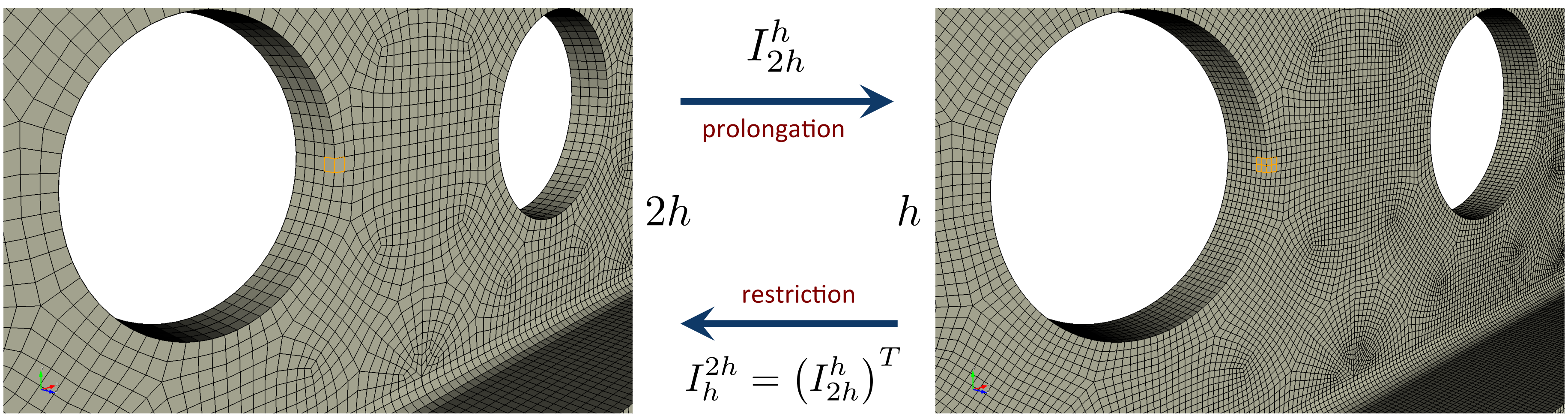
$$u^{2h} = I_h^{2h} u^h$$

$$A^{2h} = I_h^{2h} A^h I_{2h}^h$$

coarser grid operator

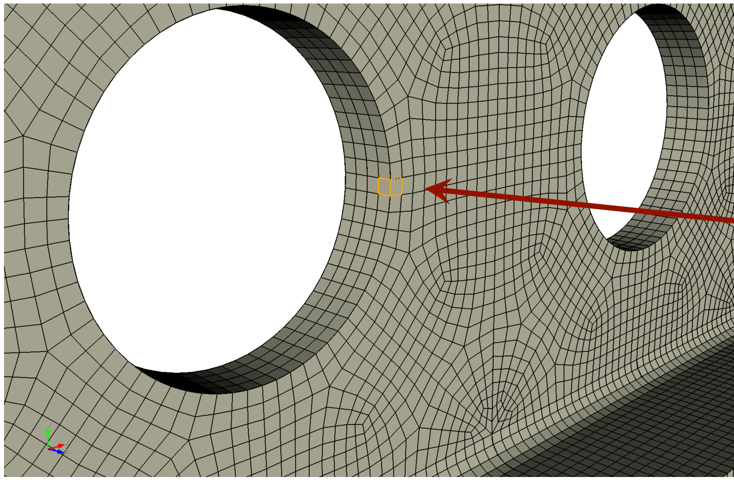
Intergrid transfer operators? I_{2h}^{h}

- Intergrid transfer operators (prolongation and restriction) are key elements of geometric multigrid methods.
- Due to material heterogeneity, can NOT use standard prolongation and restriction operators.
- Use ‘submodeling’ techniques to define prolongation operator (coarse to fine).
- Restriction operator (fine to coarse) is given by variational optimality condition.

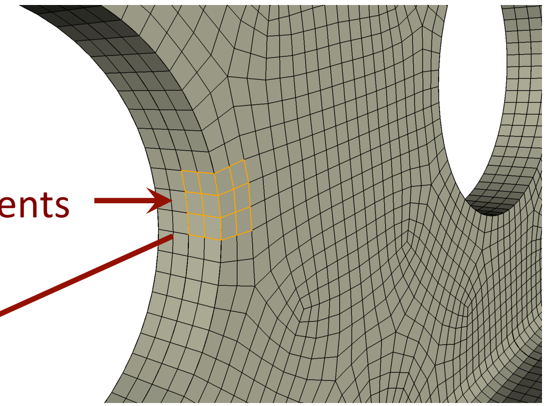


coarser grid $2h$ finer grid h

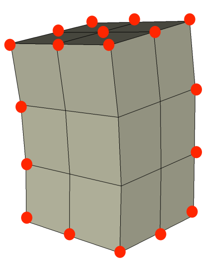
Construct I_{2h}^{h} using overlapping submodels



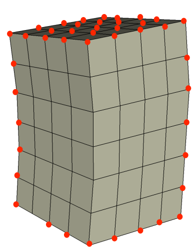
find attached elements

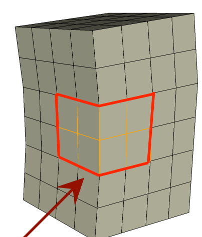


submodel



Apply displacement boundary conditions from coarse-scale model to finer-scale model





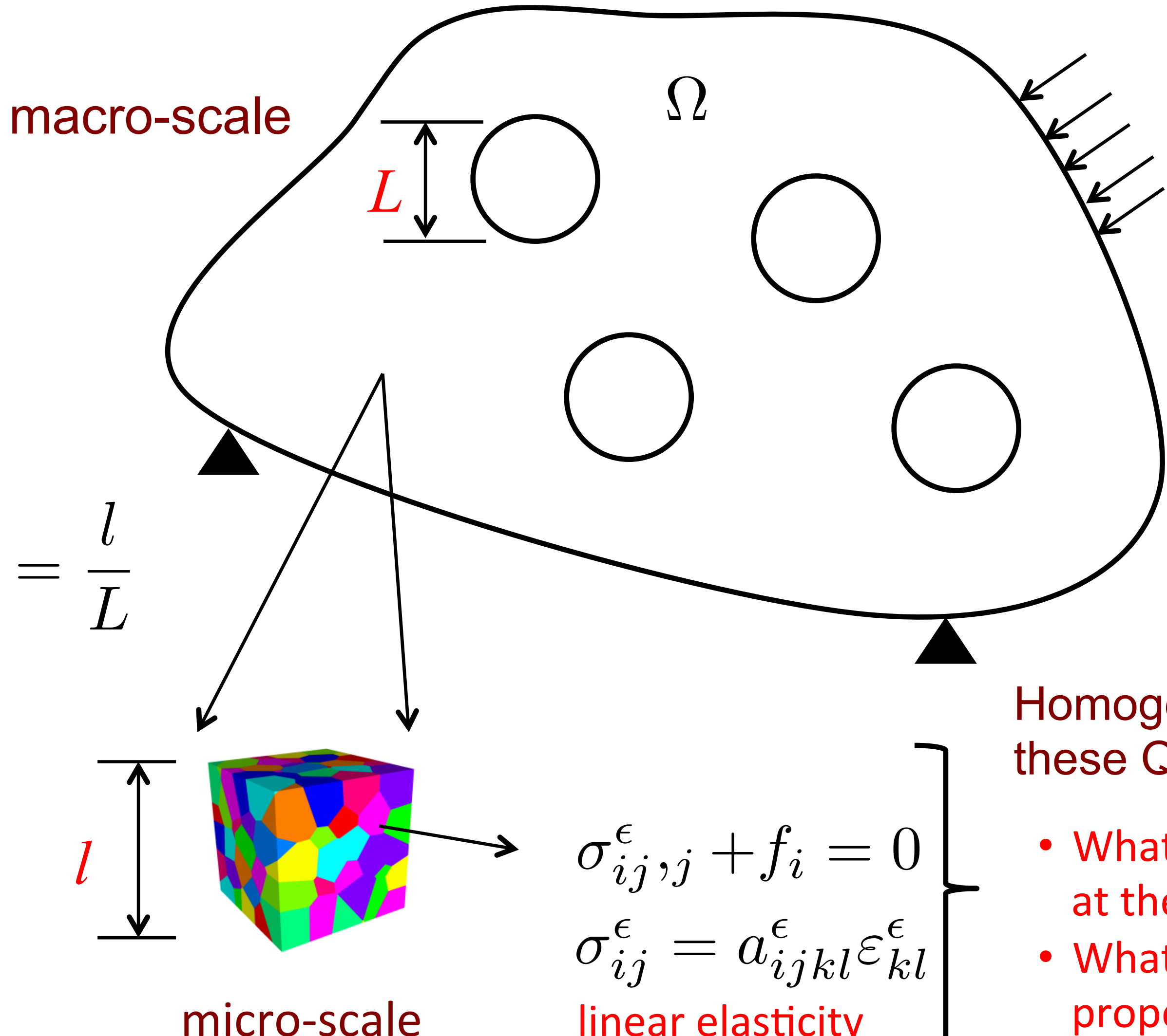
retained submodel results

- repeat submodeling to recover all of finer grid
- average results at interfaces

Thank you!

Extra

What about the Governing PDE?



$$\epsilon = \frac{l}{L}$$

$$\sigma^{\epsilon}_{ij},_j + f_i = 0$$

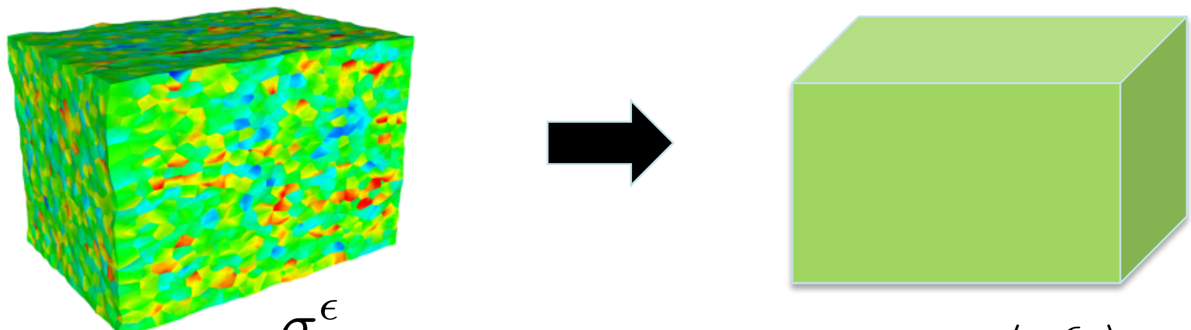
$$\sigma^{\epsilon}_{ij} = a^{\epsilon}_{ijkl}\varepsilon^{\epsilon}_{kl}$$

linear elasticity

Homogenization Theory Answers these Questions:

- What is the governing equation at the macroscale?
- What are the effective material properties?

Homogenization



σ_{ij}^{ϵ}

fine-scale fluctuations

$$\sigma_{ij} = \langle \sigma_{ij}^{\epsilon} \rangle$$

replaced with mean behavior

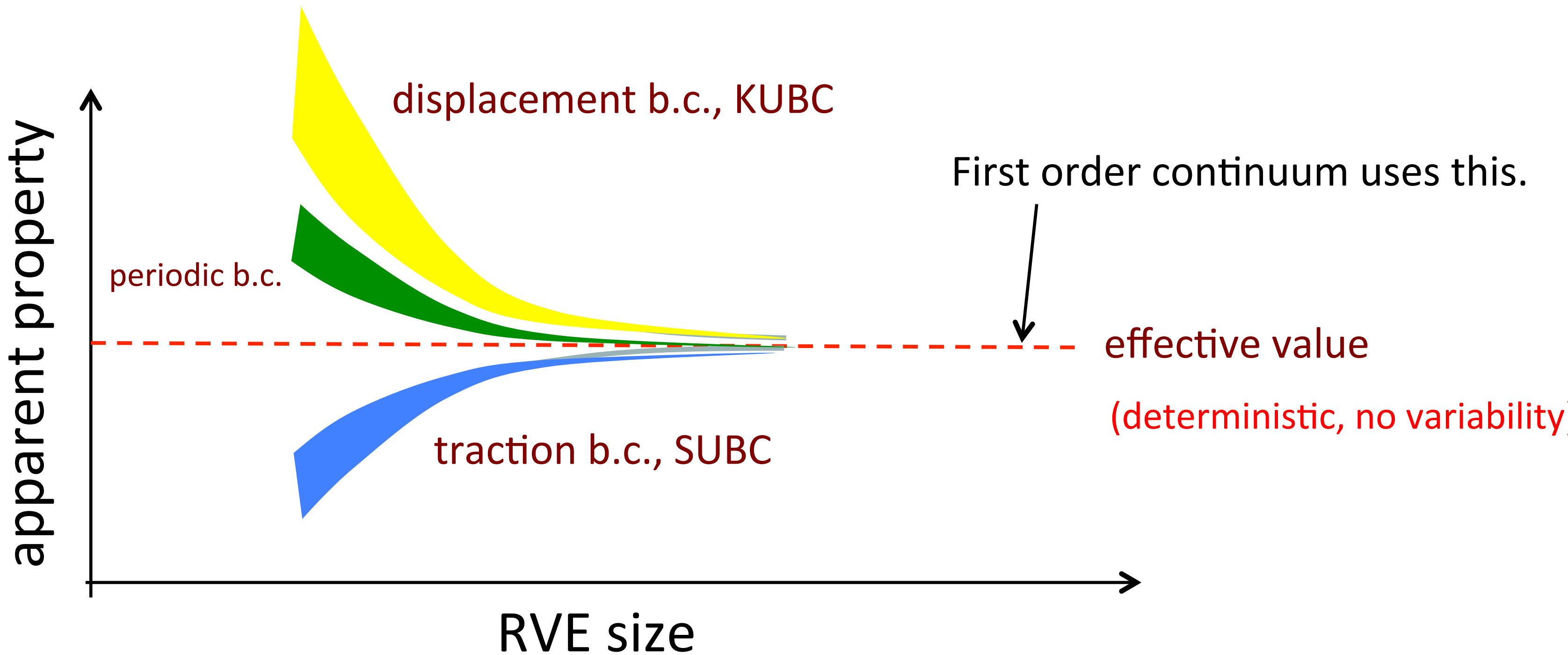
This equivalence is also satisfied energetically: $\sigma_{ij}\varepsilon_{ij} = \langle \sigma_{ij}^{\epsilon} \rangle \langle \varepsilon_{ij}^{\epsilon} \rangle$

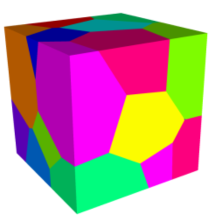
Constitutive models map average strain to average stress:

$$\varepsilon_{ij} = \langle \varepsilon_{ij}^{\epsilon} \rangle \longrightarrow \sigma_{ij} = \langle \sigma_{ij}^{\epsilon} \rangle$$

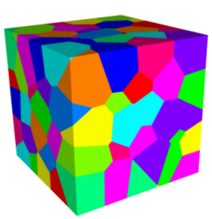
Apparent vs. Effective Material Properties

Huet, C. (1990)

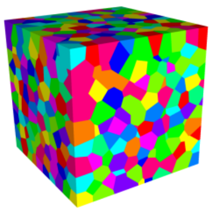




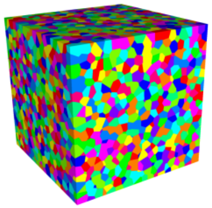
ε = 0.32



ε = 0.16



ε = 0.08



ε = 0.04

Apparent vs. Effective Material Properties

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Huet, C. (1990). "Application of variational concepts to size effects in elastic heterogeneous bodies." *Journal of the Mechanics and Physics of Solids,* 38(6): 813-841.

C = stiffness tensor

finite RVE, apparent

infinite RVE, effective

$$C_\sigma^{\text{app}}(\omega) \leq C \leq C_\varepsilon^{\text{app}}(\omega)$$

SUBC

stochastic

deterministic

KUBC

stochastic

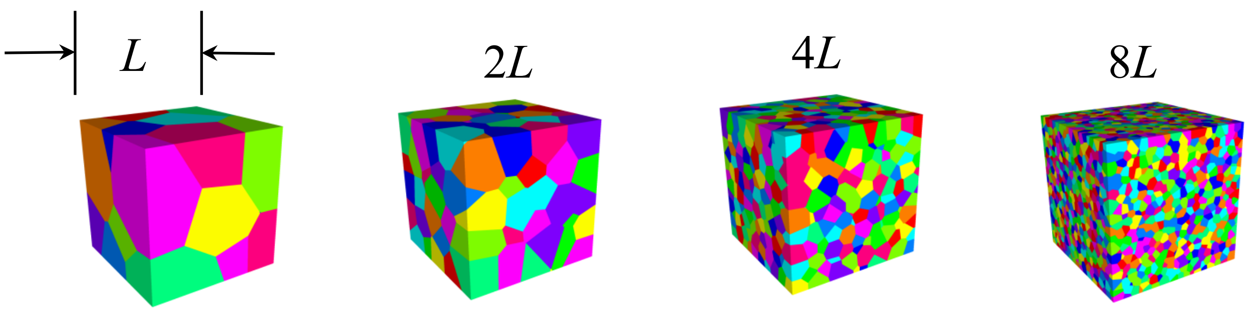
partial ordering defined in an energetic sense:

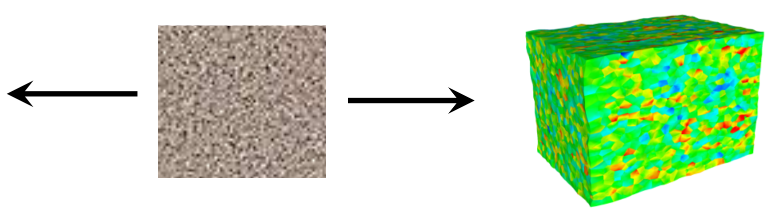
$B < A$ iff $\varepsilon : (A - B) : \varepsilon > 0$ for all $\varepsilon \neq 0$

Apparent vs. Effective Material Properties

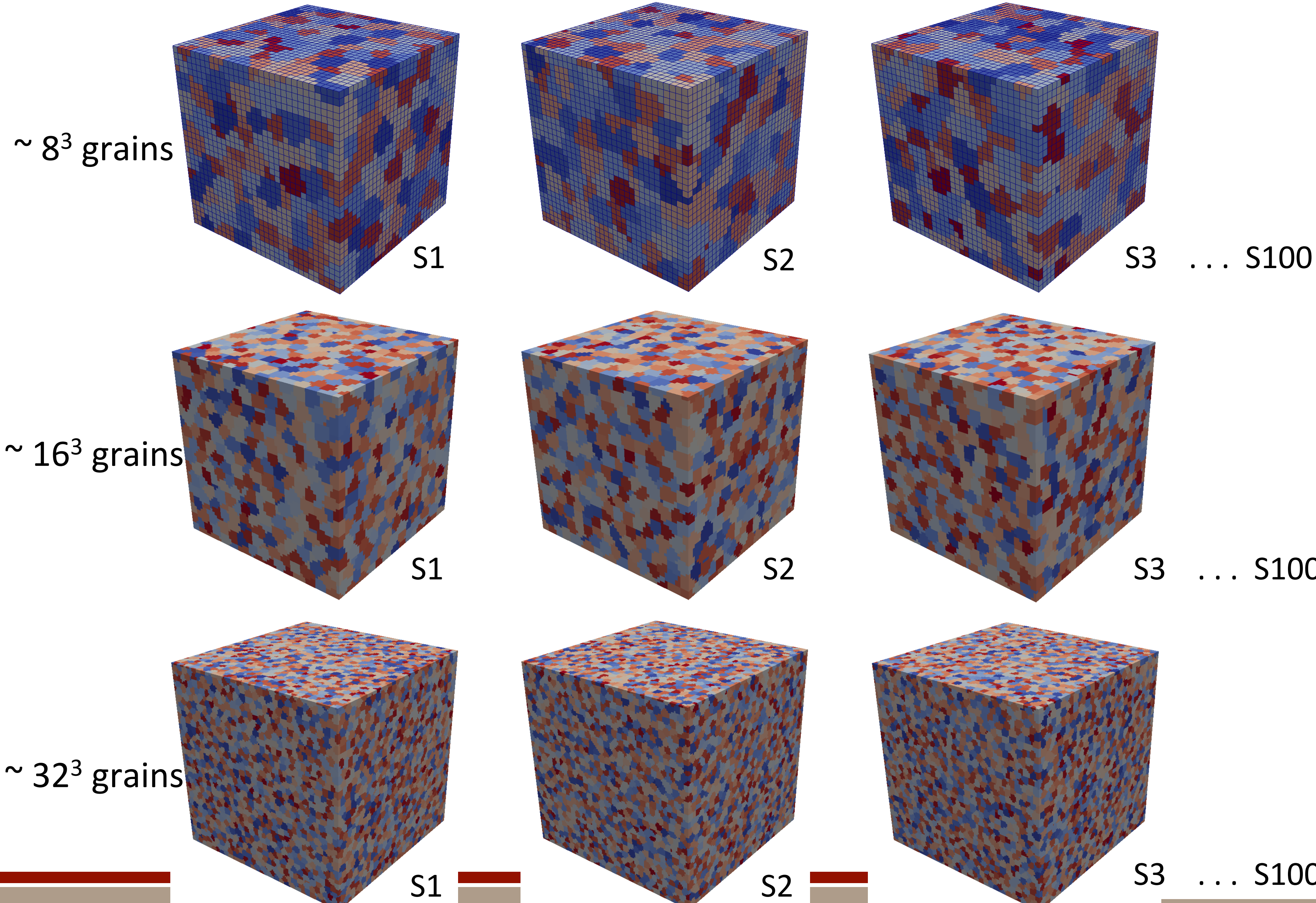
Huet, C. (1990). "Application of variational concepts to size effects in elastic heterogeneous bodies." *Journal of the Mechanics and Physics of Solids,* 38(6): 813-841.

$$C^{\mathrm{app}}_{\sigma,L} \leq C^{\mathrm{app}}_{\sigma,2L} \leq C^{\mathrm{app}}_{\sigma,4L} \leq \cdots \leq C^{\mathrm{app}}_{\sigma,\infty} = C$$



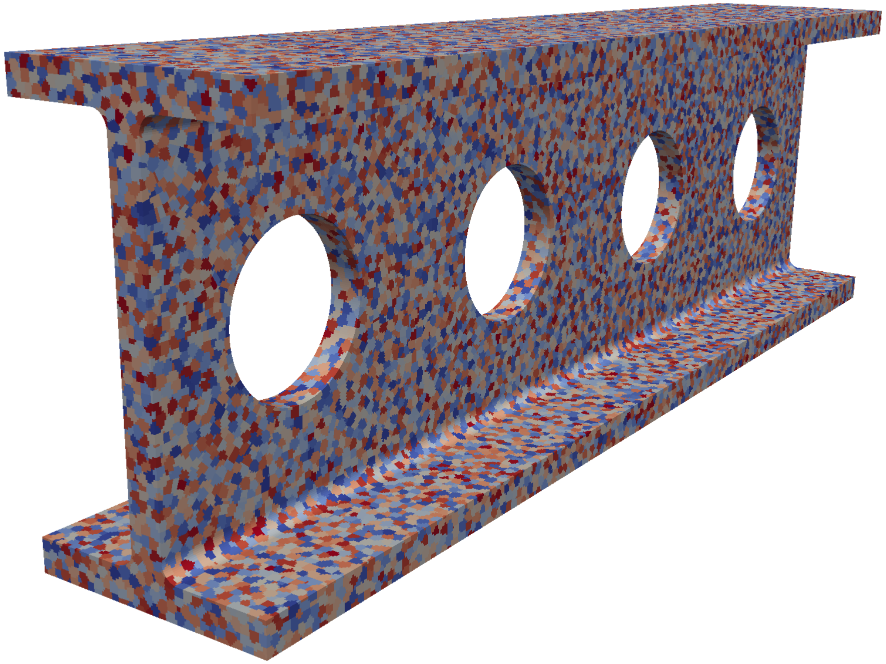


Stochastic Volume Elements

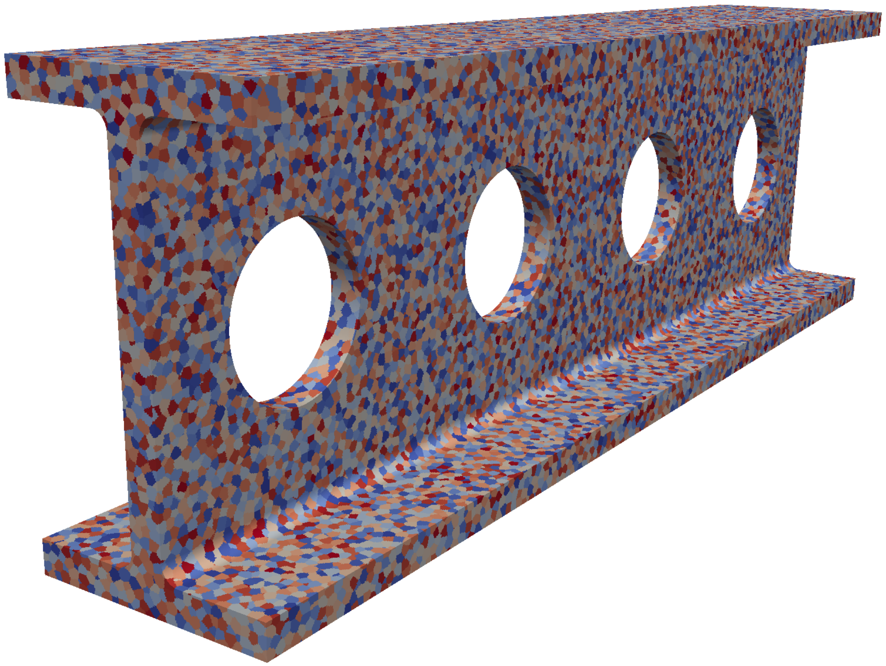


Effect of Mesh Refinement

thickness/grain ratio = 4



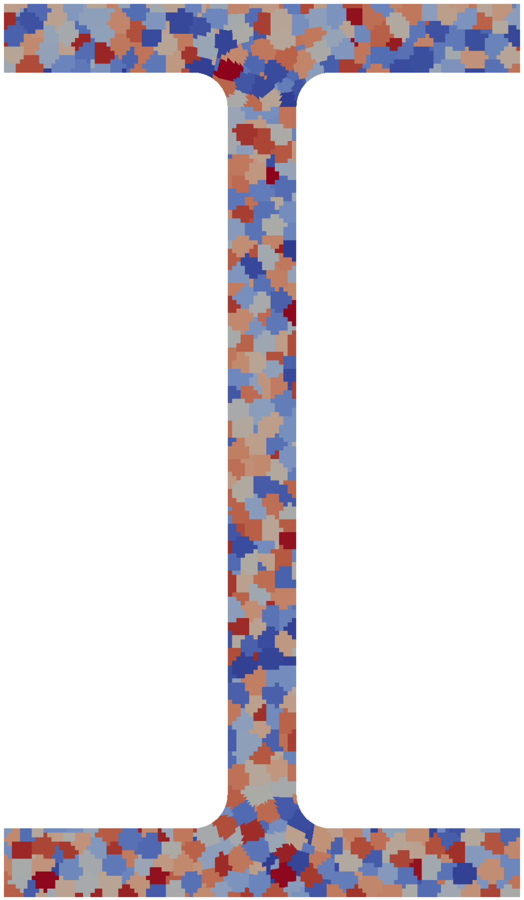
mesh refinement R3



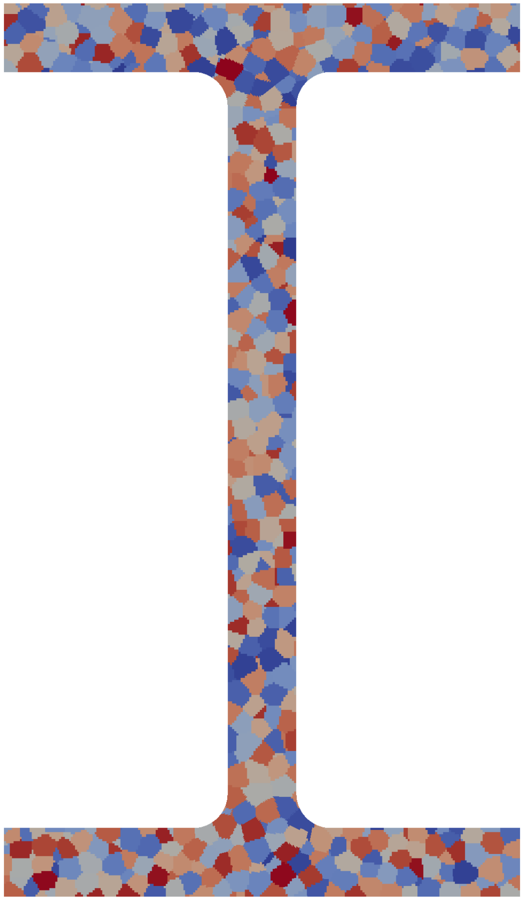
mesh refinement R4

Effect of Mesh Refinement

thickness/grain ratio = 4



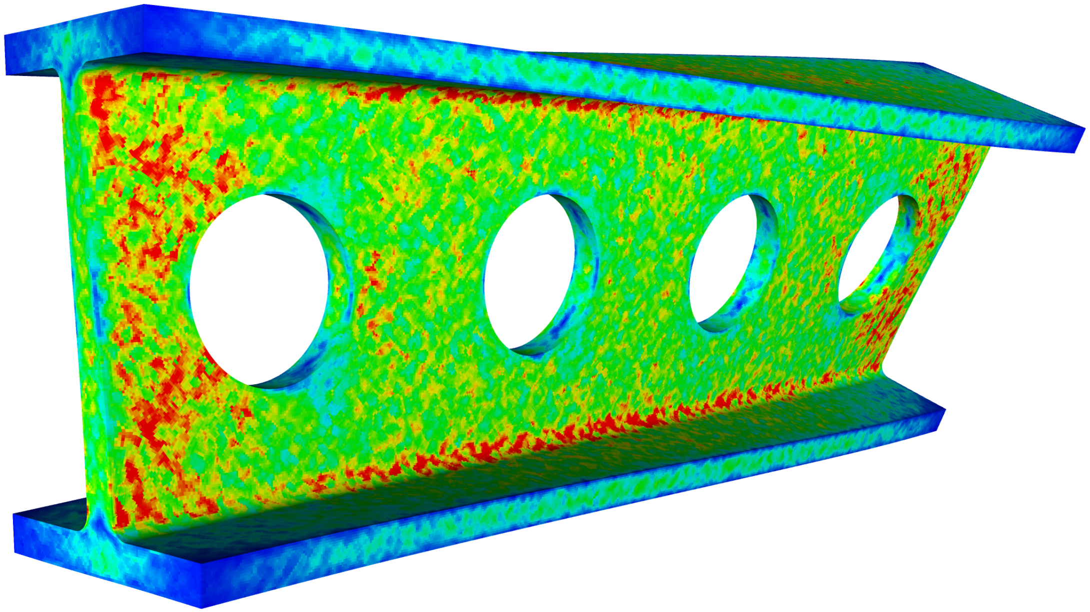
mesh refinement R3



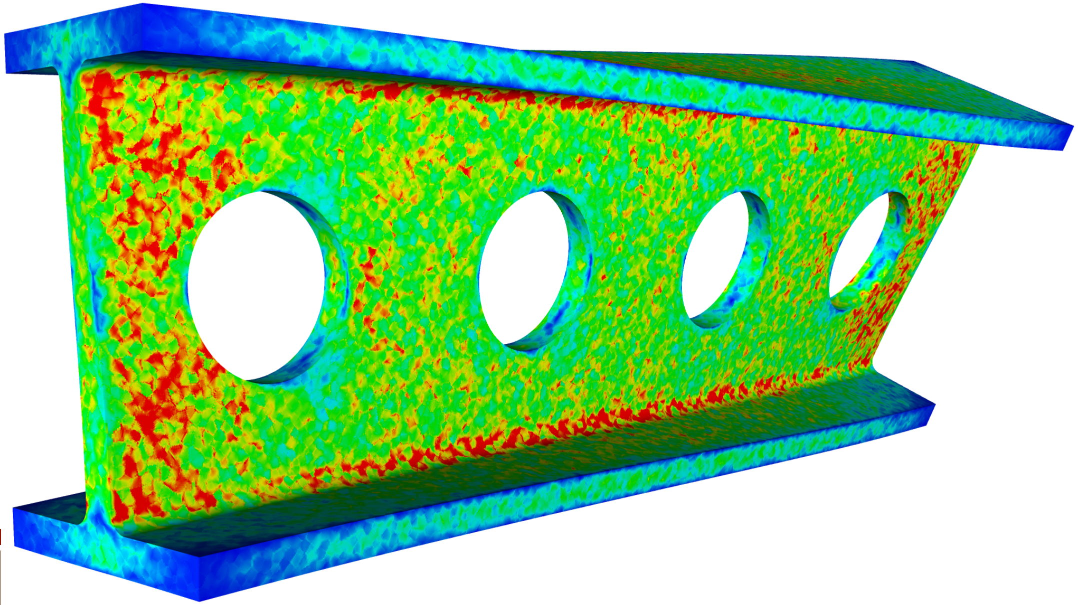
mesh refinement R4

Effect of Mesh Refinement

thickness/grain ratio = 4



mesh refinement R3



mesh refinement R4

Effect of Mesh Refinement

thickness/grain ratio = 4