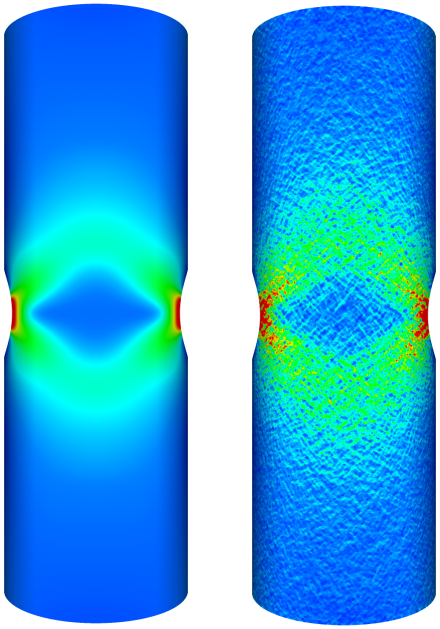
SAND2016-1002C



Direct numerical simulations of grain-scale crystal plasticity in engineering components

Corbett Battaile, Joe Bishop, John Emery
Sandia National Laboratories
Albuquerque, NM

International Symposium on Plasticity
January 7 2015

Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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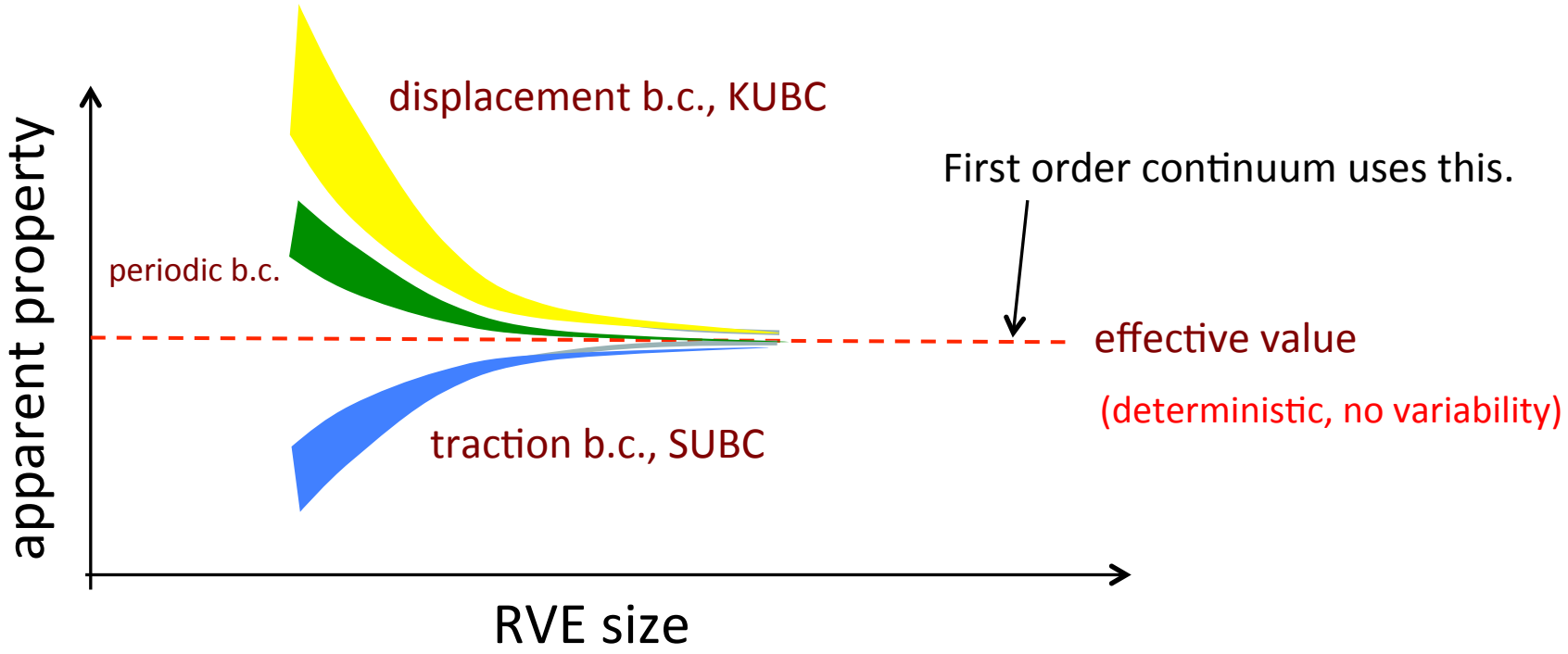
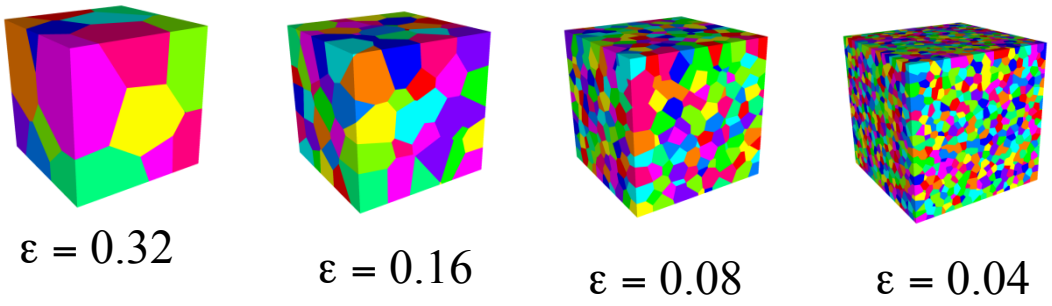
Apparent vs. effective material properties

Huet, C., 1990, *JMPS,* 38, 813-841.





Convergence to effective isotropic elastic properties

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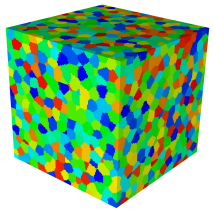

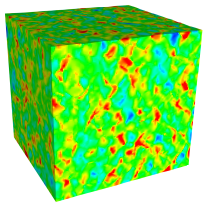

- mean of 100 simulations at each "grain level"
- rational function extrapolation to ∞

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.

Crystal plasticity model

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K. Matous, A. Maniatty, 2004, *IJNME*

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

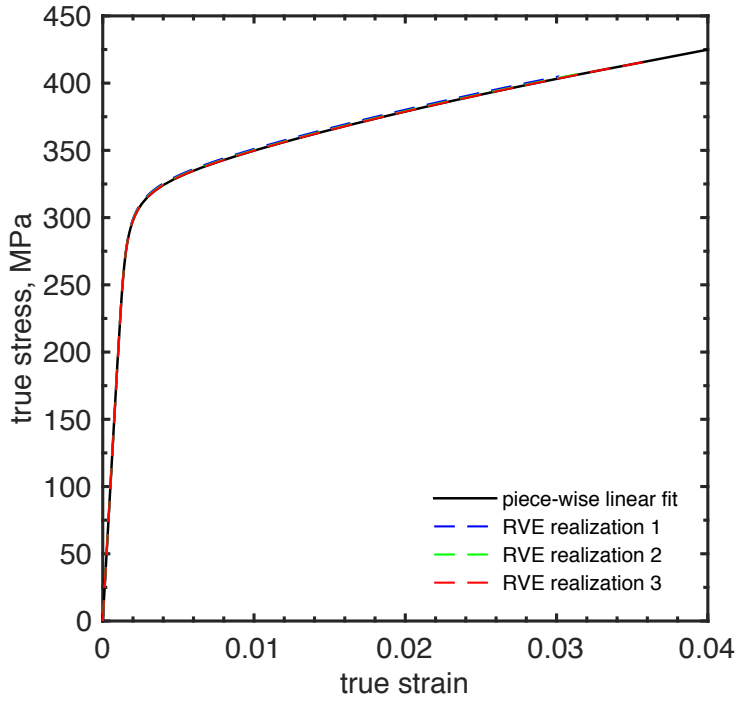
slip system hardening: $g = g_o + (g_{so} - g_o) \left[1 - \exp\left(-\frac{G_o}{g_{so} - g_o} \gamma \right) \right]$ $\gamma = \sum_{s=1}^{N} |\gamma^s|$

Not considering:

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

Effective macro-scale 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.
- Ideally, would use a macroscale viscoplasticity model (next step).



Model-form error – RVE vs. J2-plasticity

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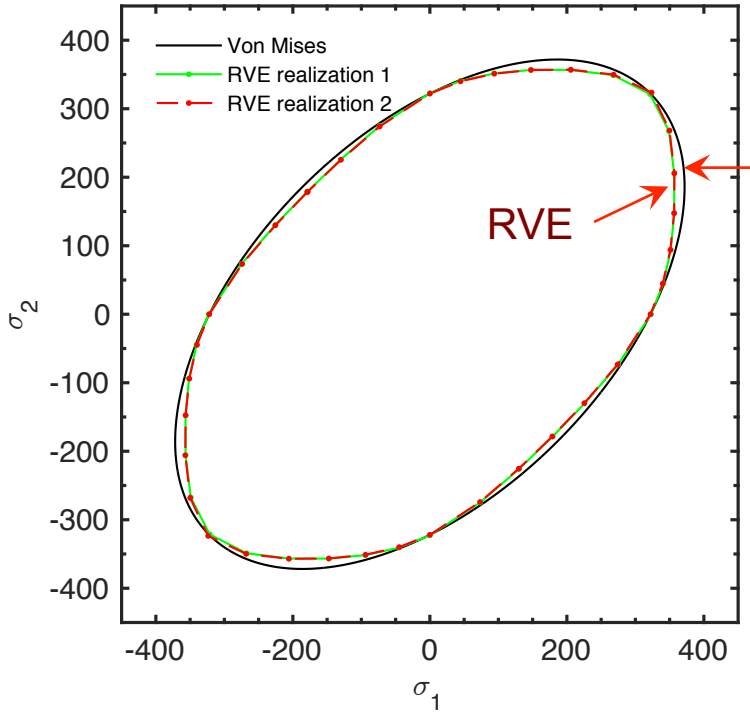
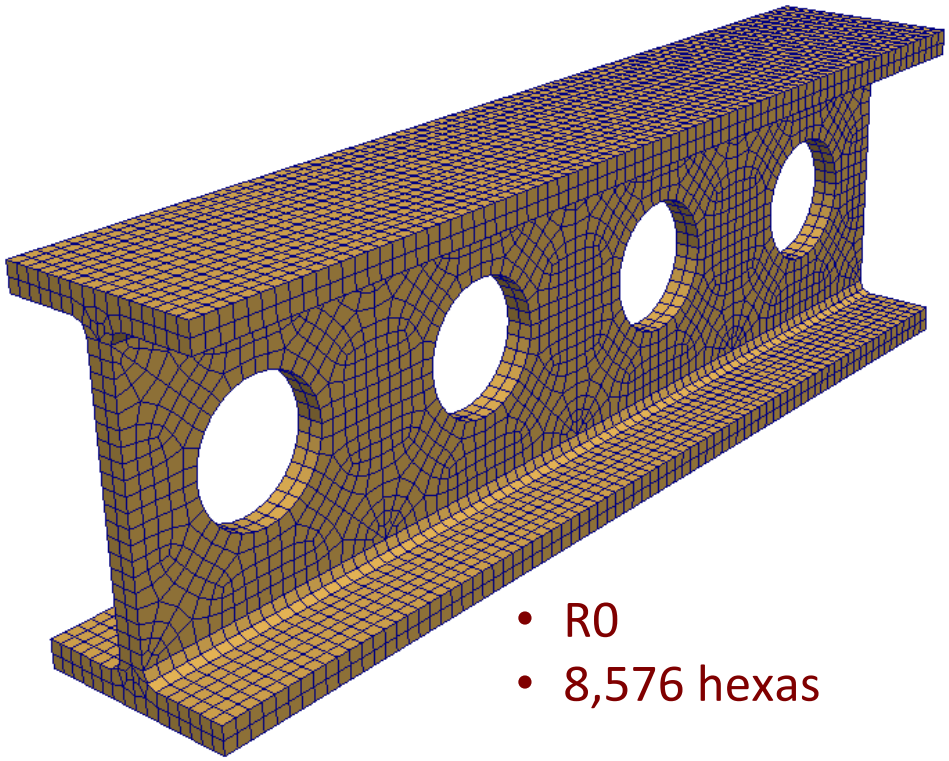
yield surface



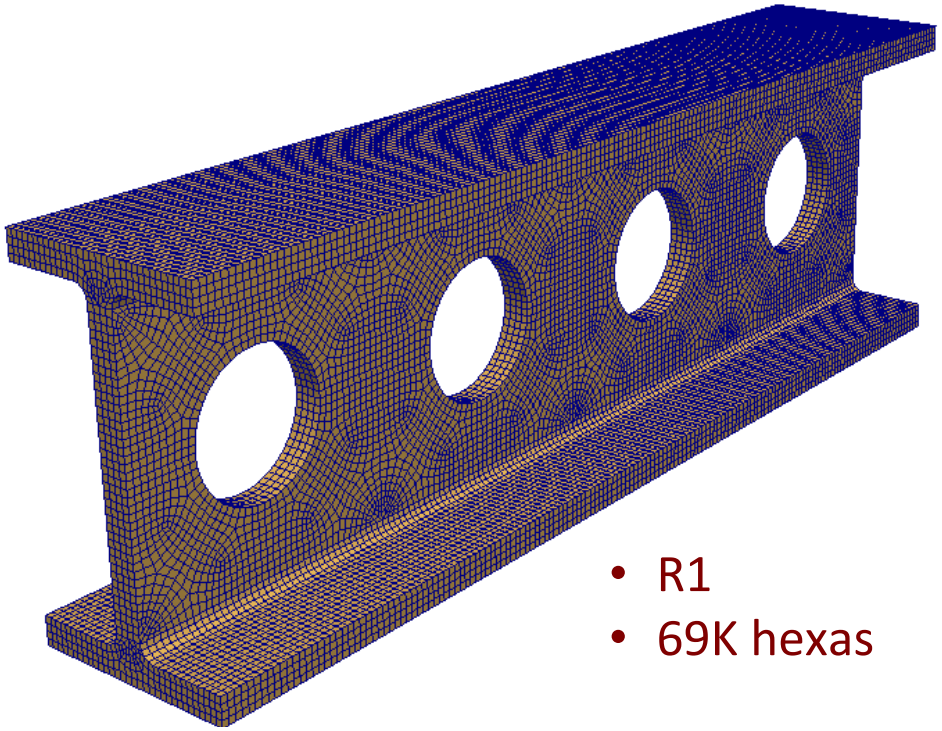
RVE

J2 plasticity

Hierarchy of hexahedral meshes



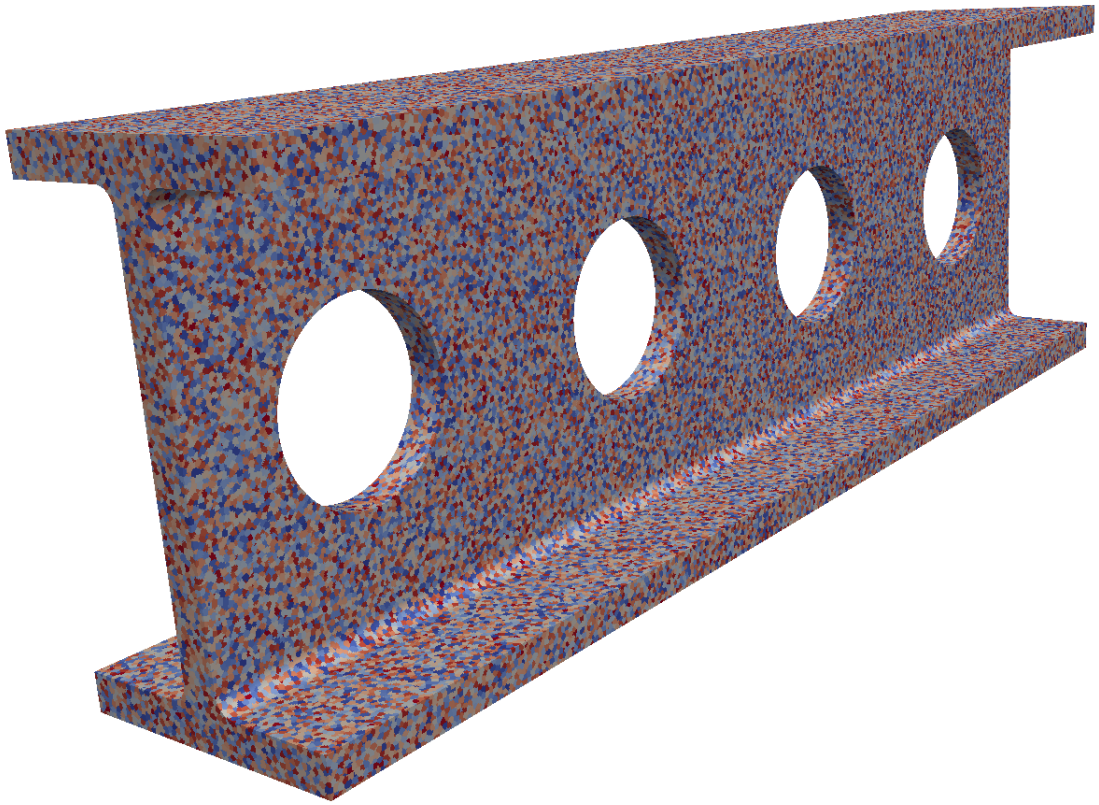
- R0
- 8,576 hexas

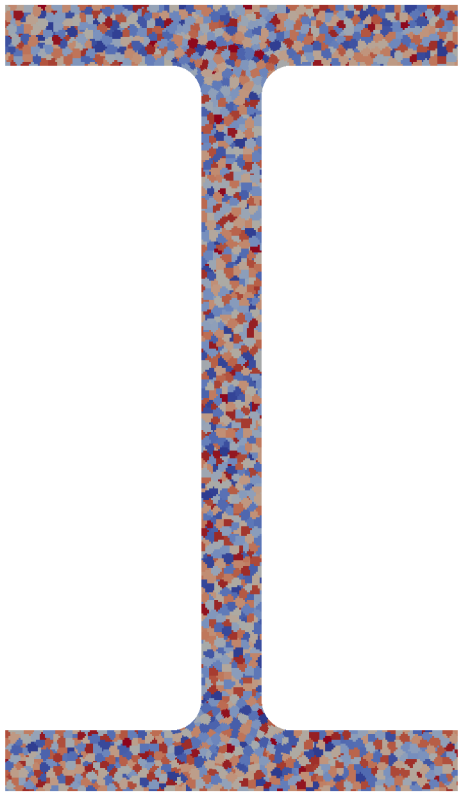


- R1
- 69K hexas

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

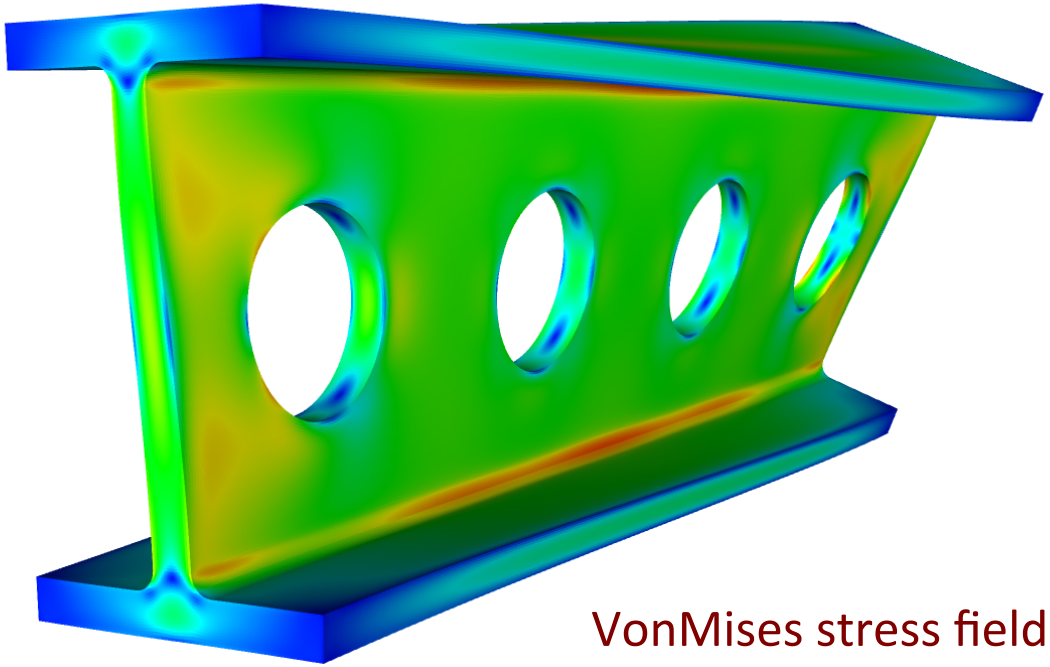
Thickness/grain ratio = 8





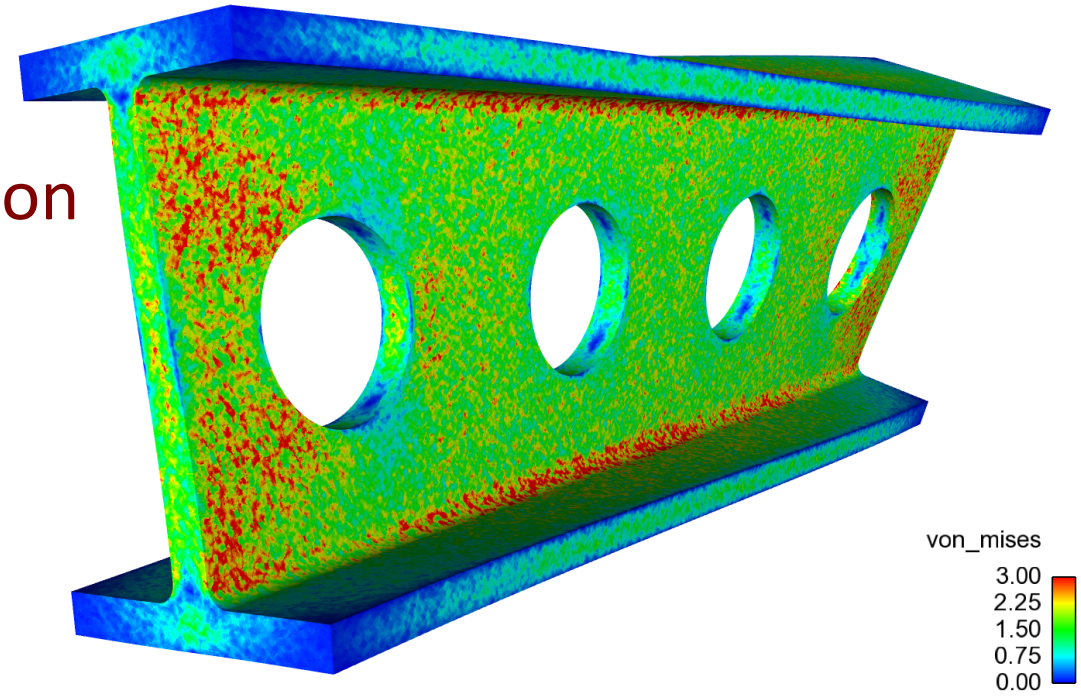
- uniformly random crystal orientations
- ~420,000 grains
- hex mesh overlay = R4 (35M elements)

homogenized solution

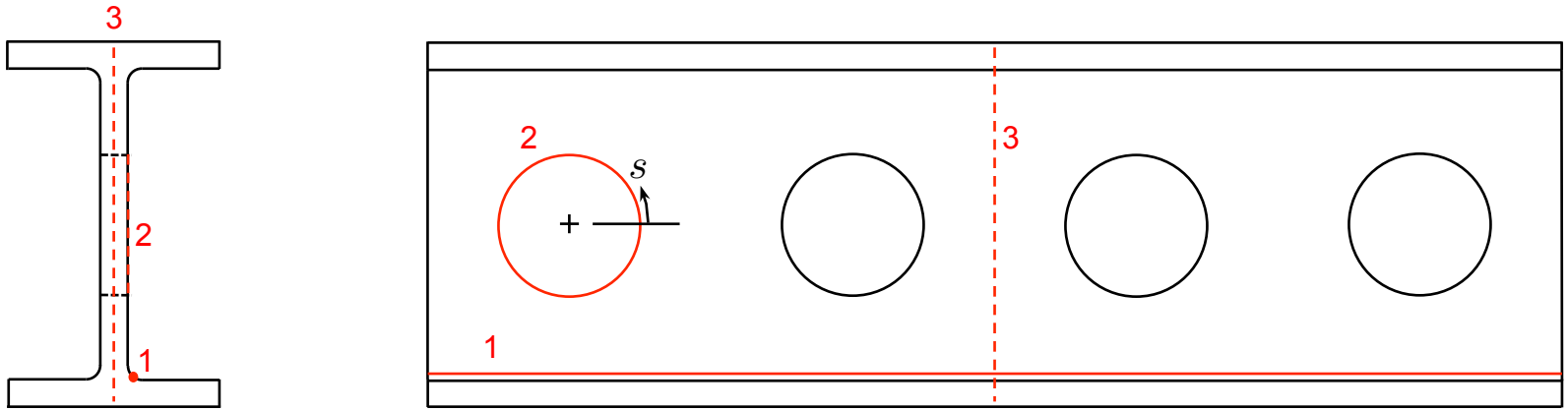


VonMises stress field

direct numerical simulation



Stress extraction lines/curves



Homogenized solution vs. DNS

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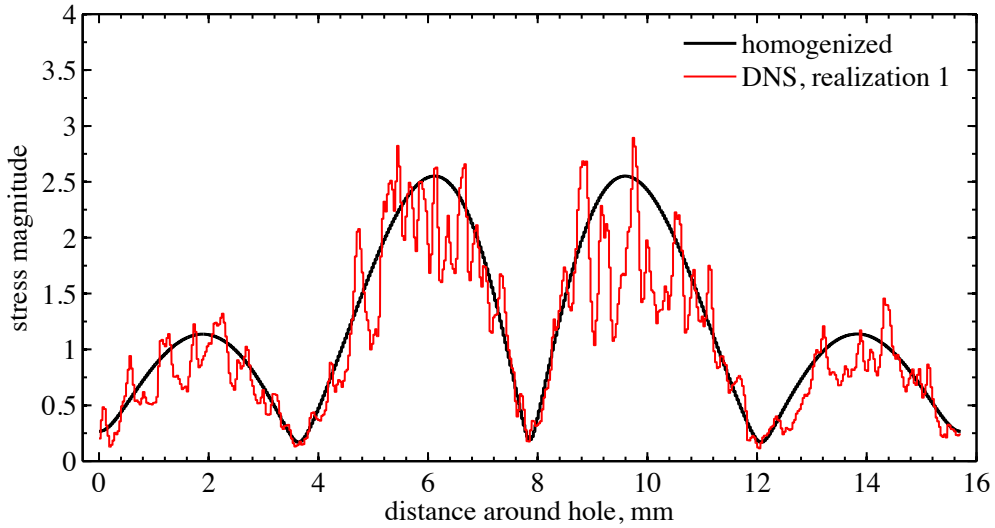
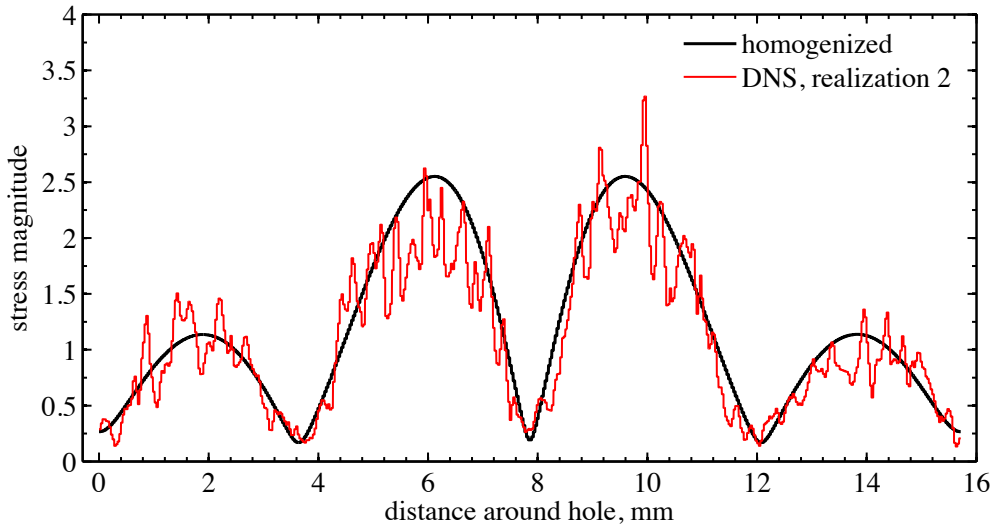
Stress magnitude around hole

realization 1



realization 2



Homogenized solution vs. DNS

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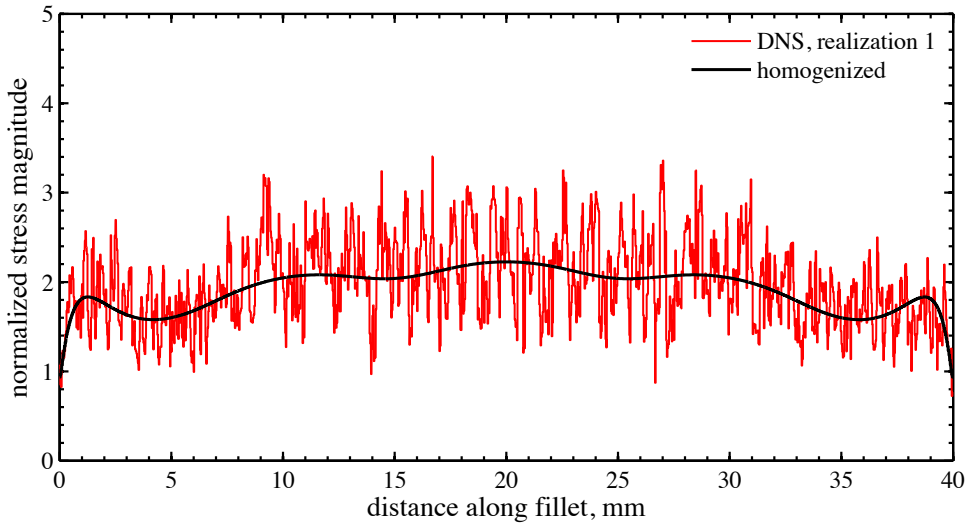
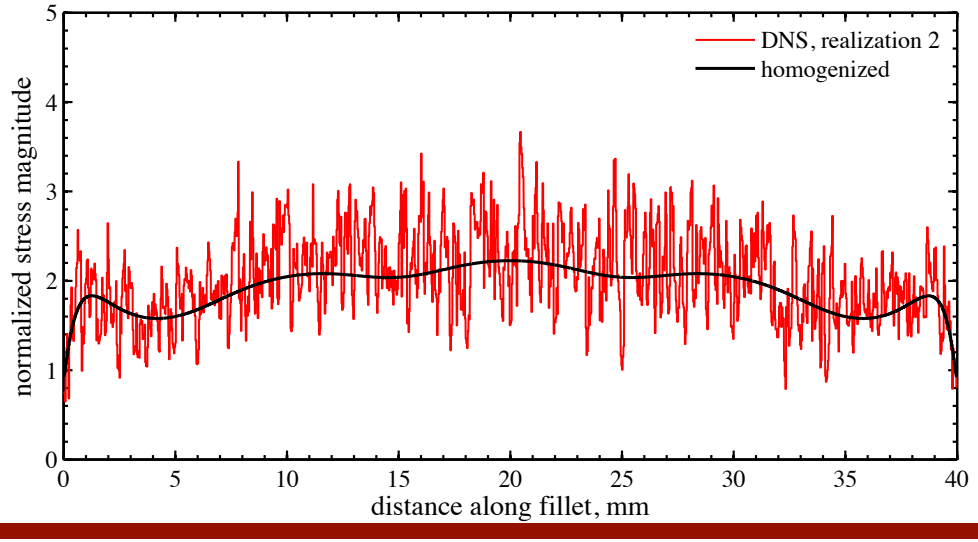
Stress magnitude along lower fillet

realization 1



realization 2



3D moving average using Gaussian filter

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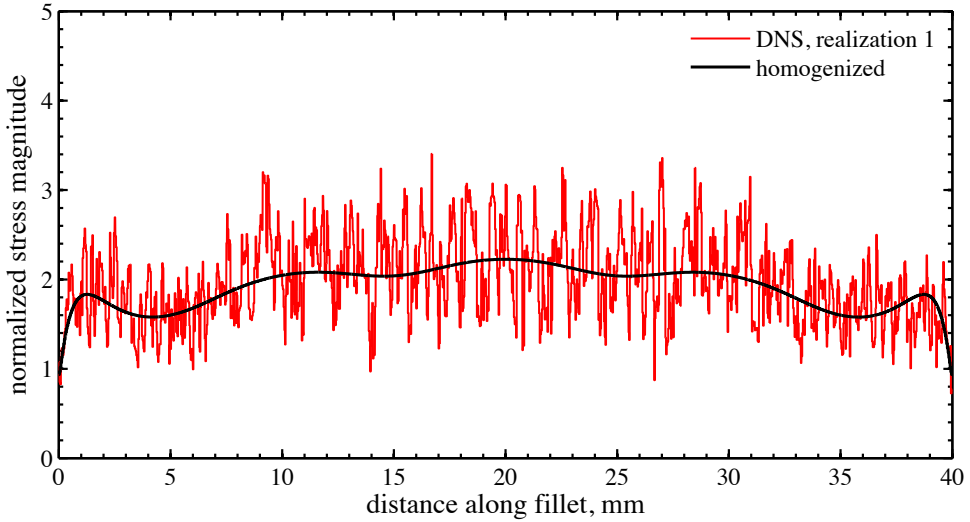
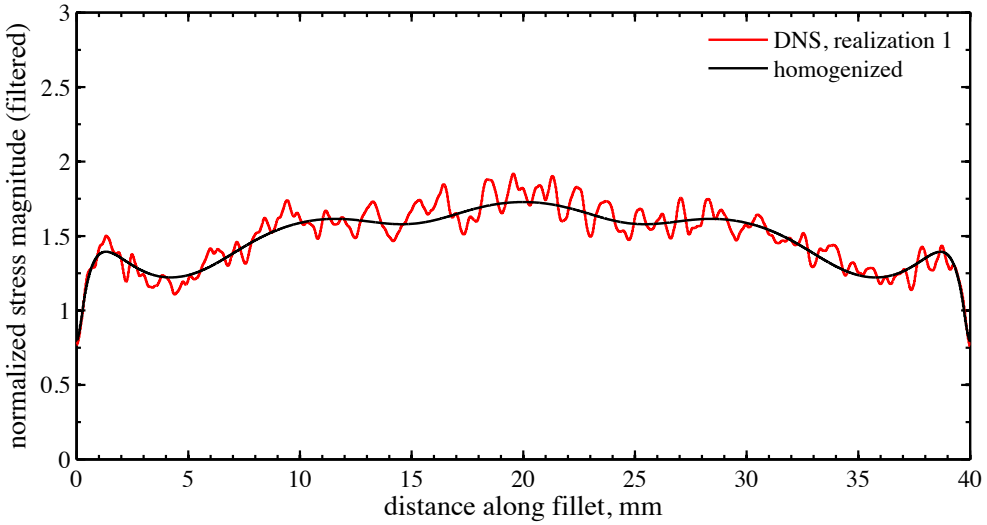
unfiltered

Stress magnitude along lower fillet



filtered

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



Homogenized solution is a surprisingly good approximation.

Summary (elastic results)

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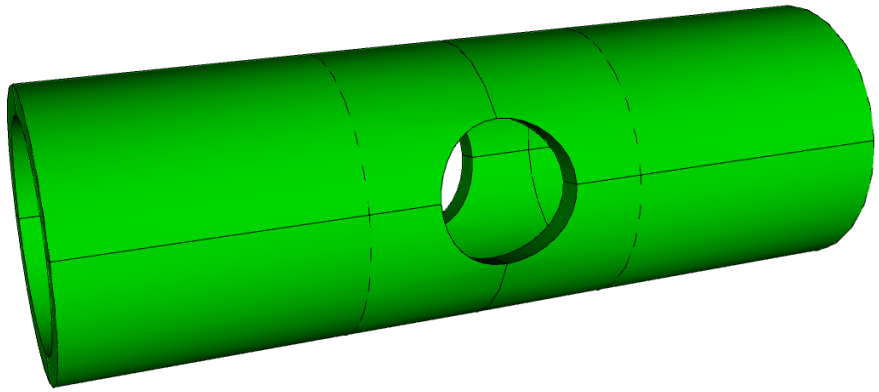
- Found little evidence of higher-order effects for this material and these BVPs. This is possibly due to the small correlation length inherent in the microstructure.
- Fluctuations (10-20%) on the length scale of several grains are present as evidenced by spatially filtered DNS results.
- What about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

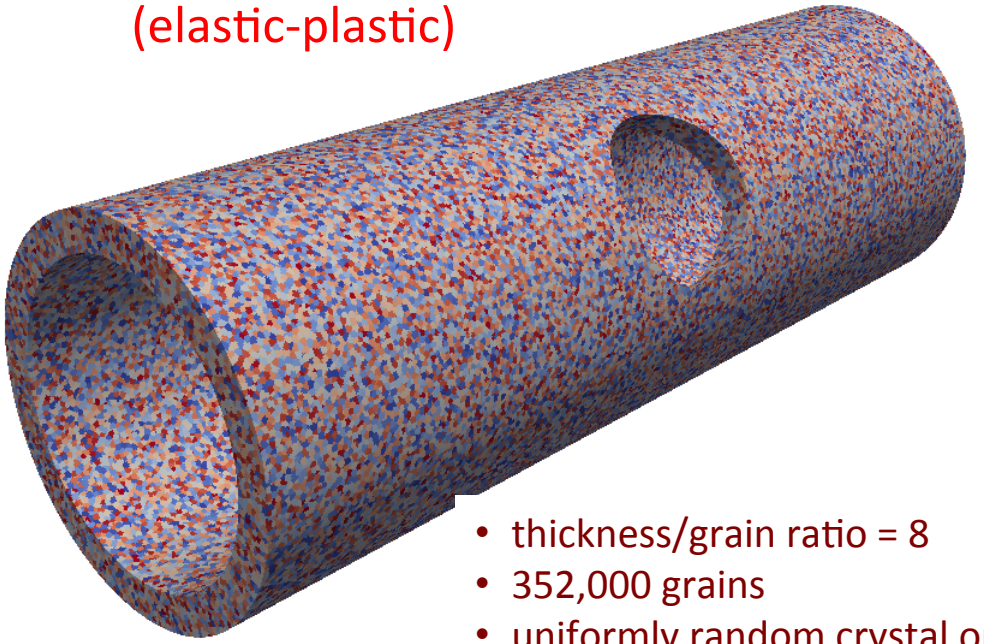
Bishop, J., Emery, J., Field, R., Weinberger, C., Littlewood, D. 2015, "Direct numerical simulations in solid mechanics for understanding the macroscale effects of microscale material variability," *CMAME,* 287, pp. 262-289.

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

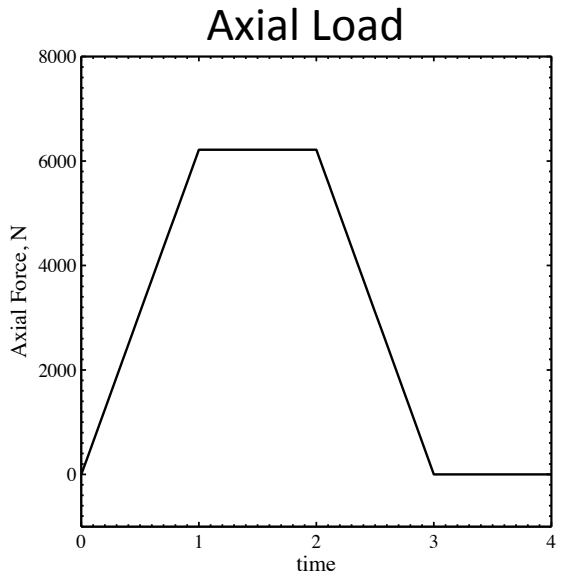
Sandia National Laboratories

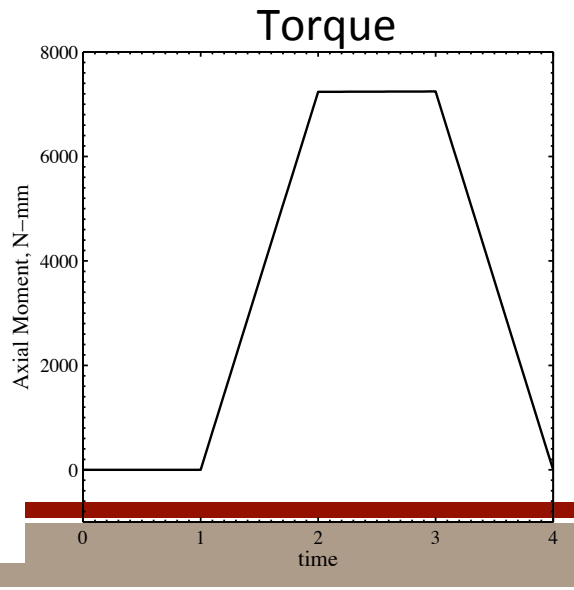


(elastic-plastic)

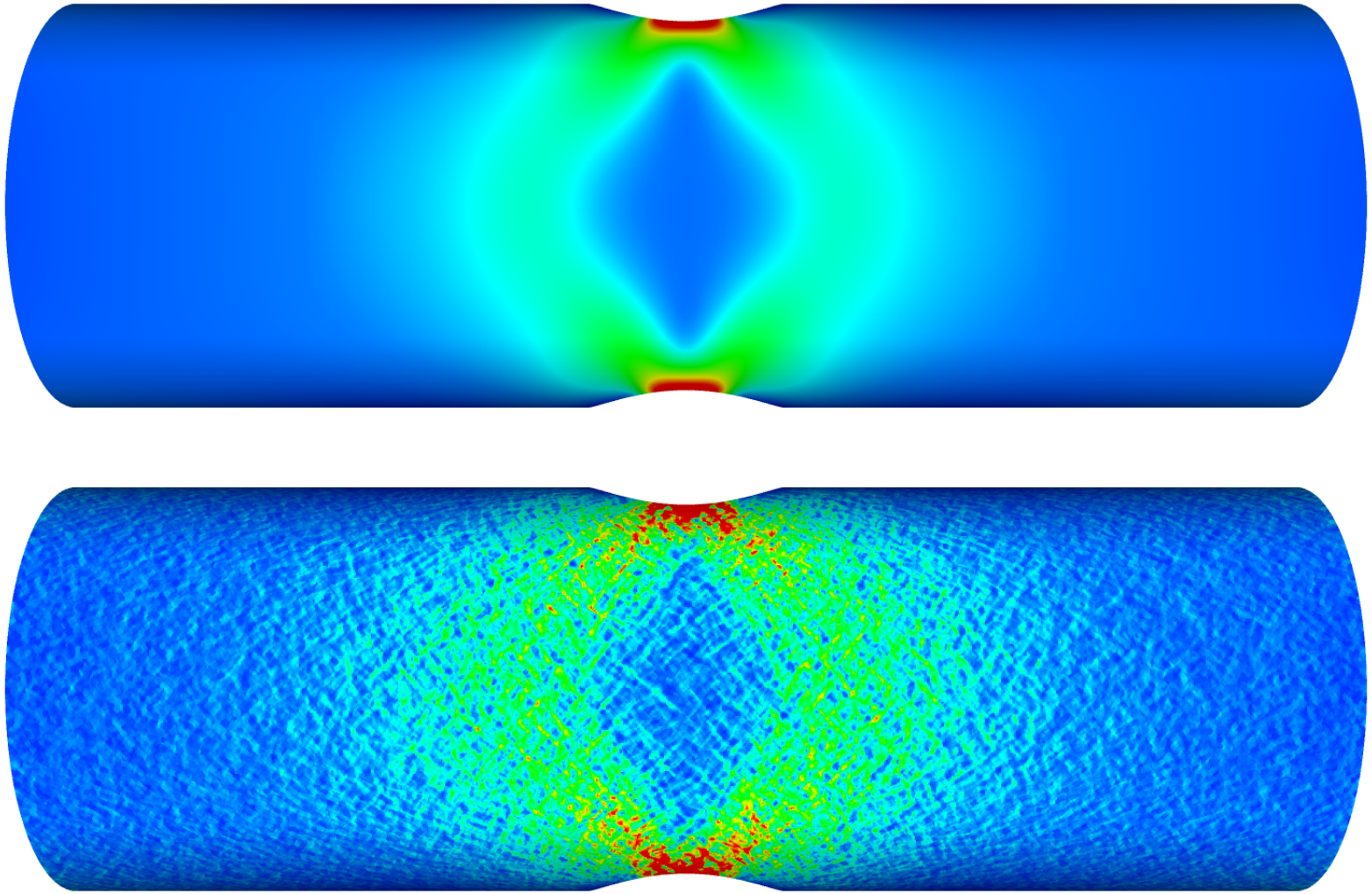


- thickness/grain ratio = 8
- 352,000 grains
- uniformly random crystal orientations

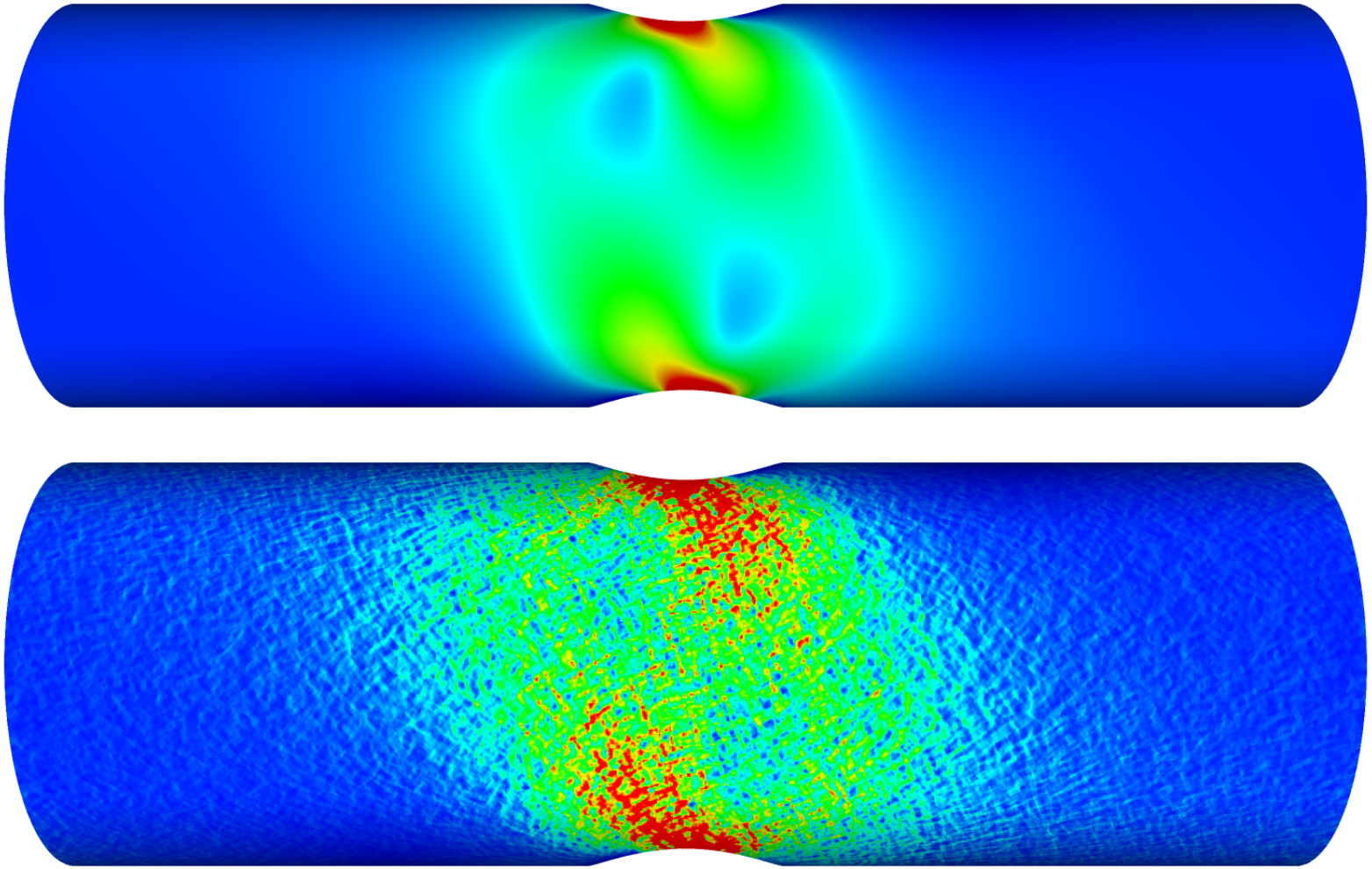




Axial Load Only

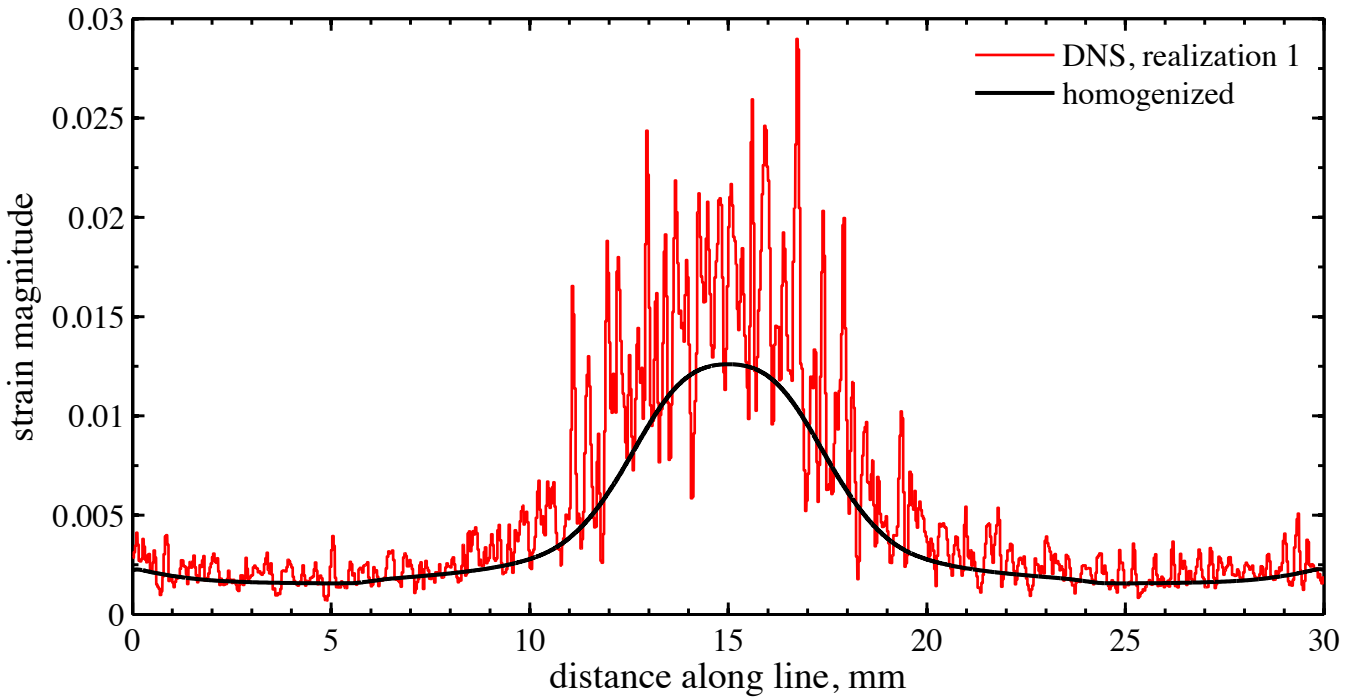


Axial load + torsion



Strain magnitude along length of tube

midsection between holes, combined tension-torsion



Strain magnitude around hole

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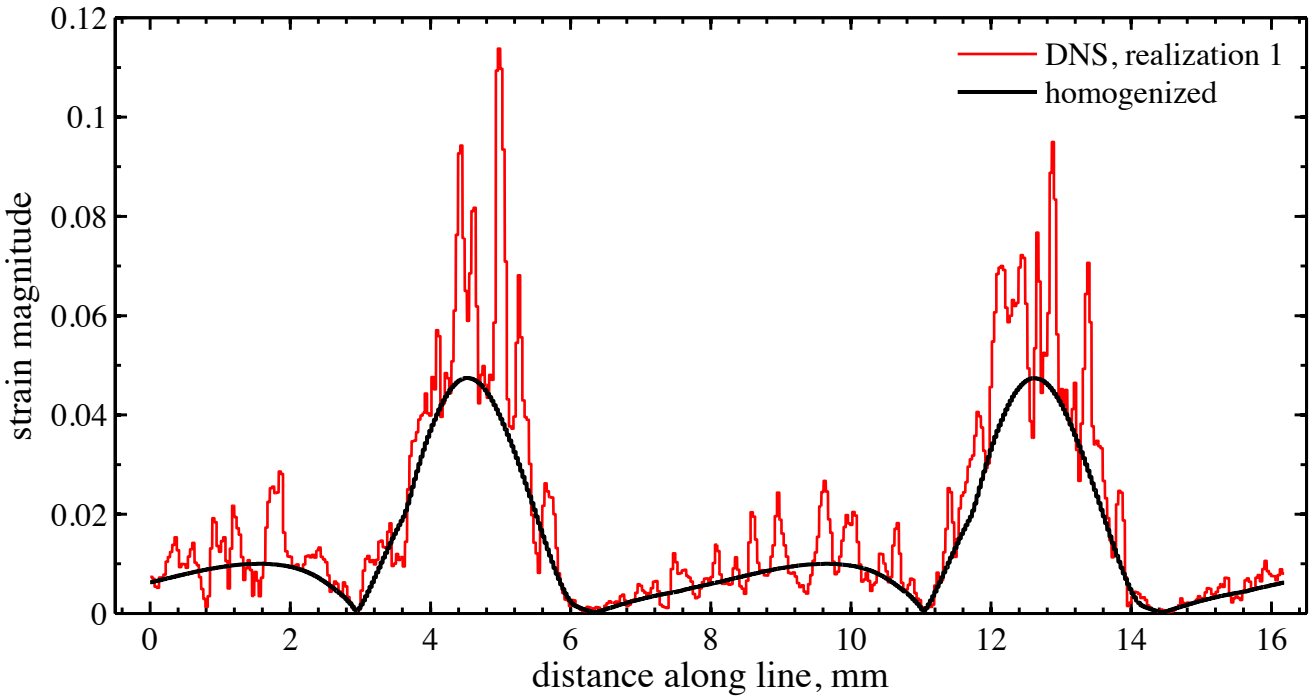
inside circumference, combined tension-torsion



Global stretch and rotation of tube

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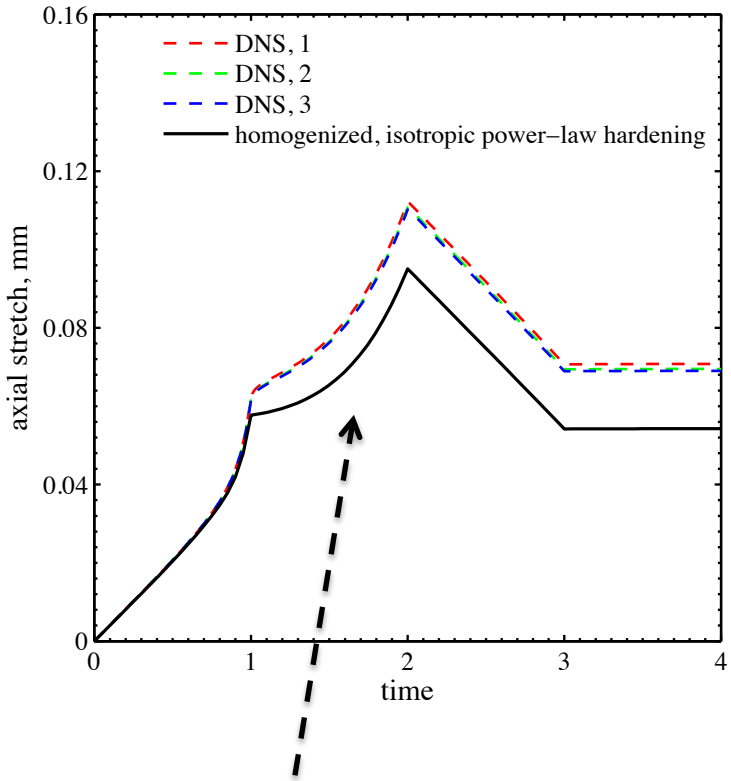
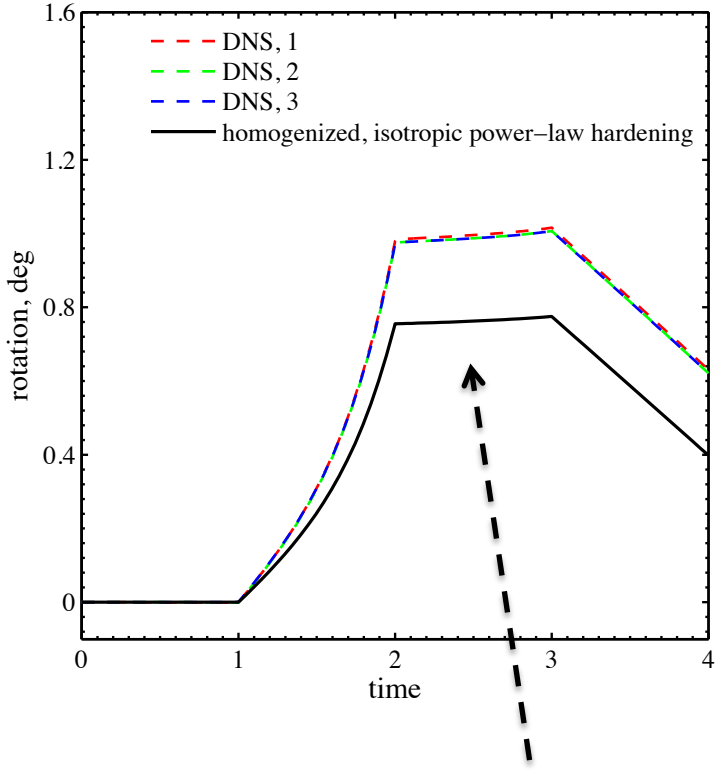
axial stretch



rotation



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

Summary (plastic results)

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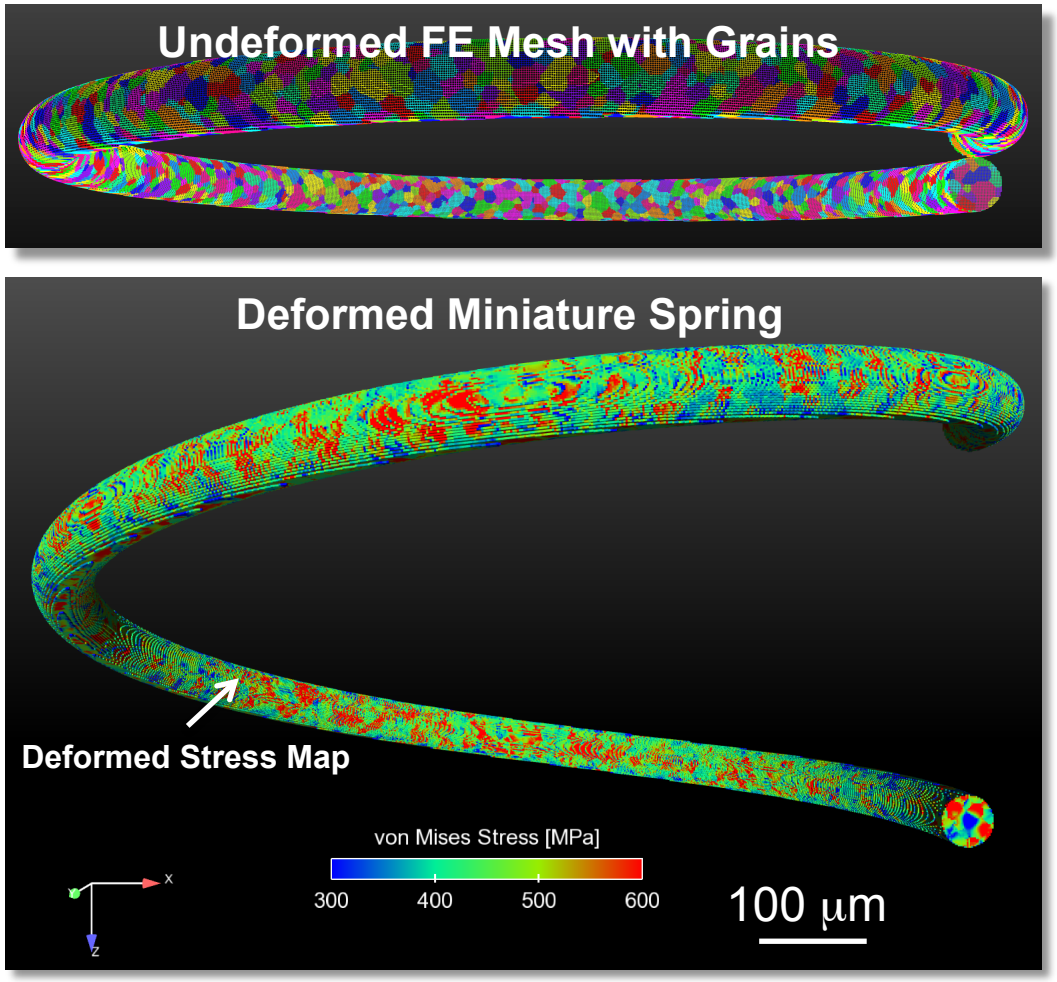
- See appreciable difference between a basic J2 plasticity model and DNS results.
- Need full FE^2 for true homogenization in the plastic regime.
- What about more complex microstructures, texture, spatial correlation, rate-dependence?

Deformation of a Micro-Spring



Stress variations in a miniature Inconel X750 spring microstructure.

Spring Properties

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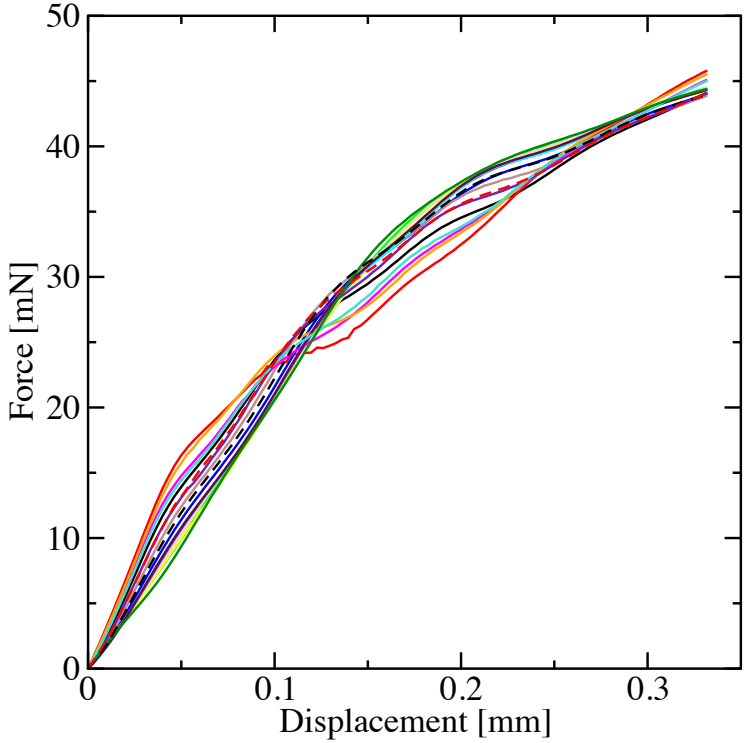
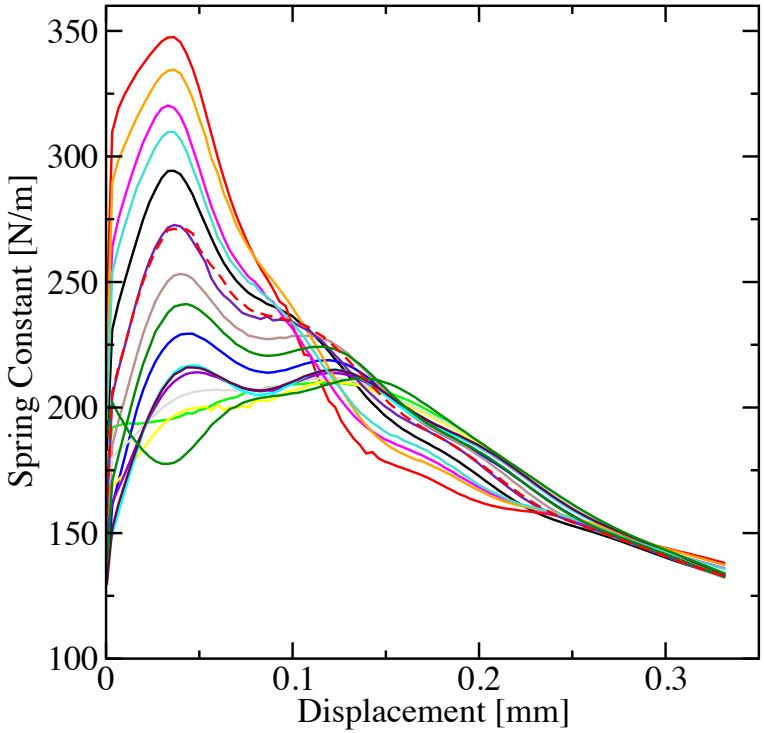
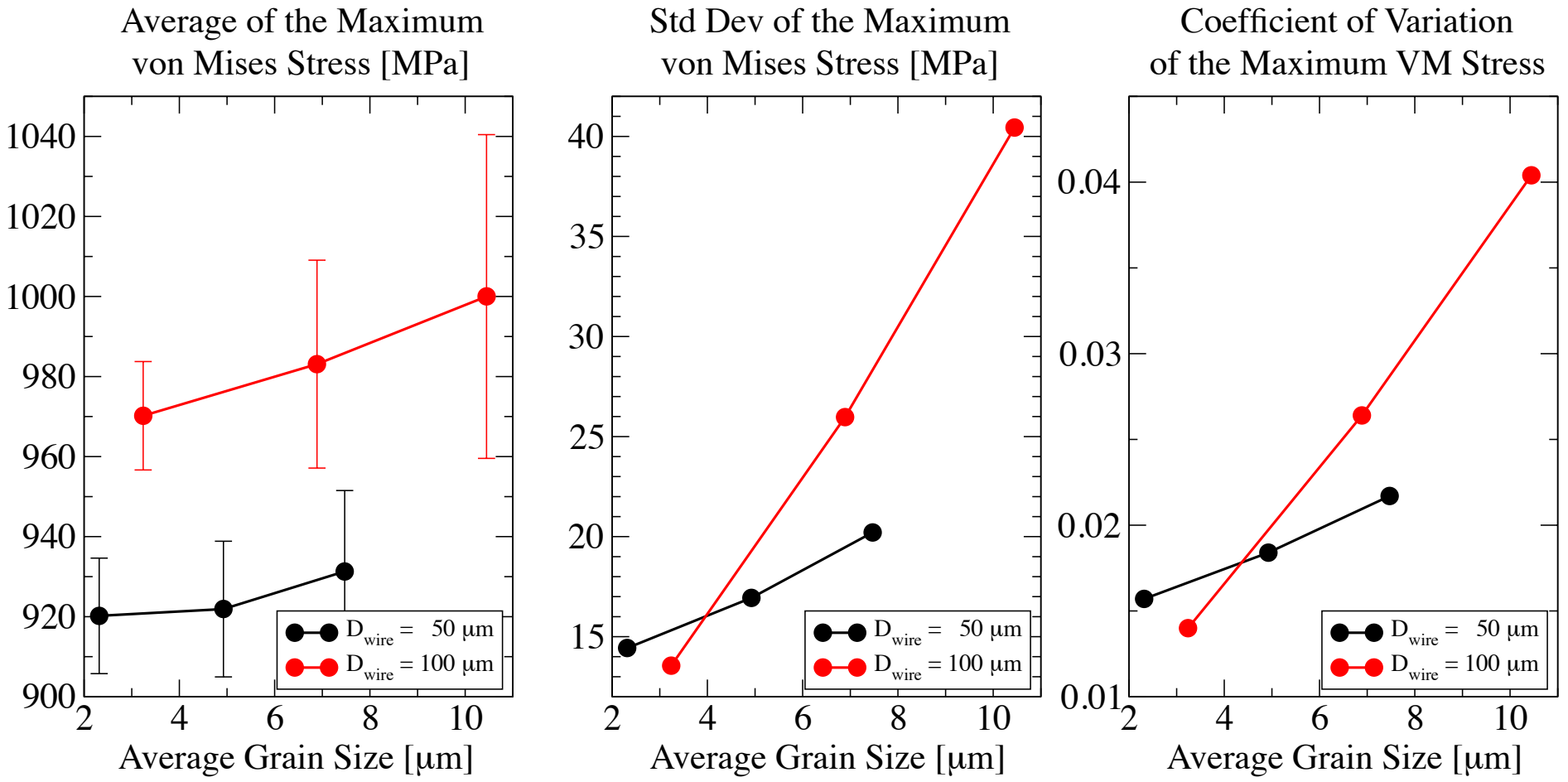
50 μm wire diameter, 2.317 μm grains

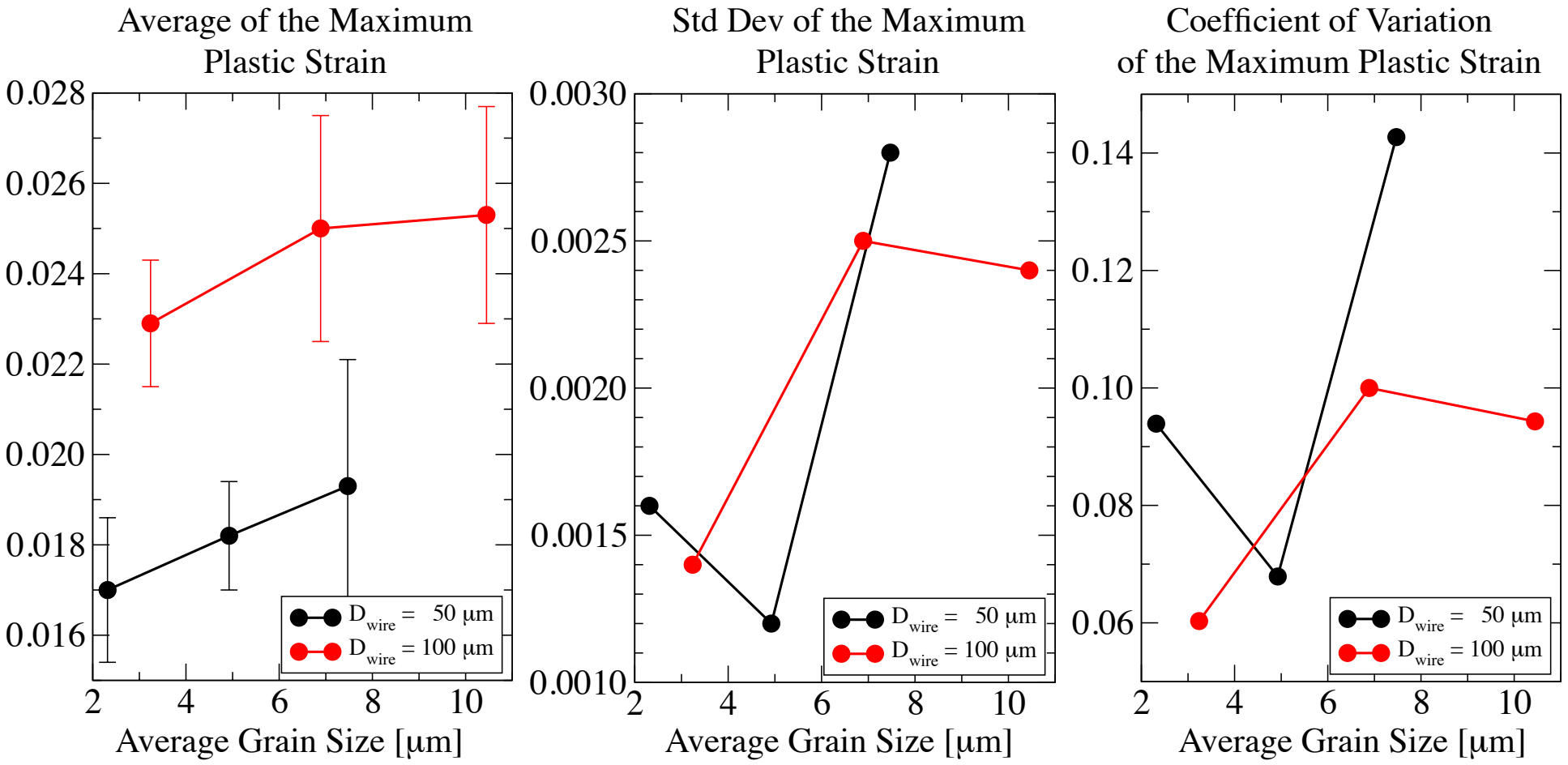




Micro-Springs Max Stress Statistics



Micro-Springs Max Strain Statistics



Summary

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- We are using Direct Numerical Simulations in solid mechanics to understand material variability and errors in homogenization theory.
- See some evidence of surface-effects in elastic results of I-beam.
- Investigated the model-form error in using a macroscale J2-plasticity model, in comparison with DNS (crystal plasticity).
- Investigated model-form error and impact on engineering quantities of interest.
- We are using DNS to explore impact of microstructure for additively manufactured structures.

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Extra

Strain-rate dependence

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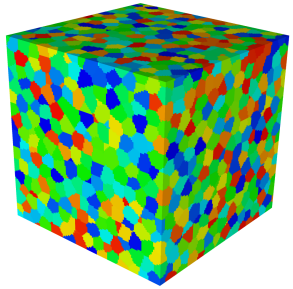
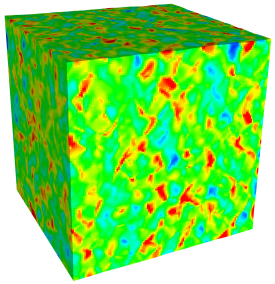
RVE response

- strain control
- uniaxial stress

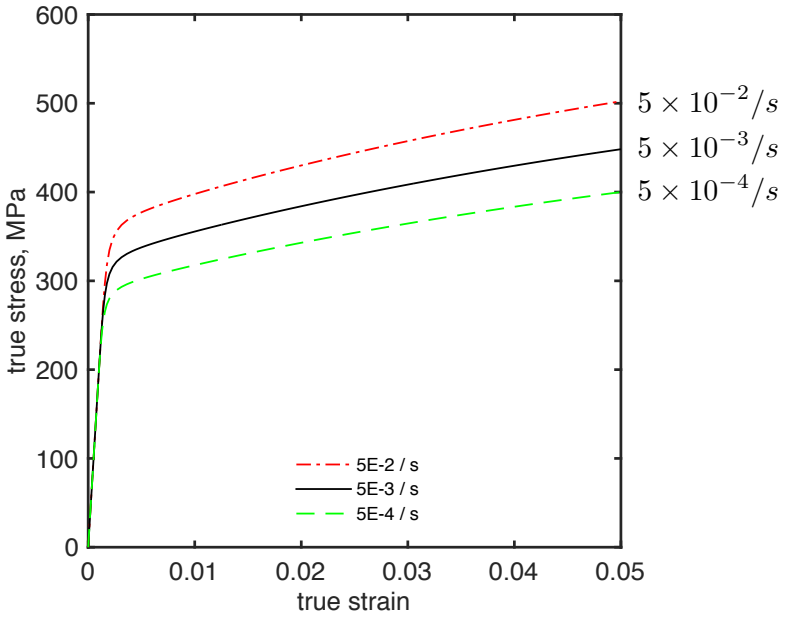


~ 16^3 grains



plastic response

strain-rate dependence



Model-form error – RVE vs. J2-plasticity

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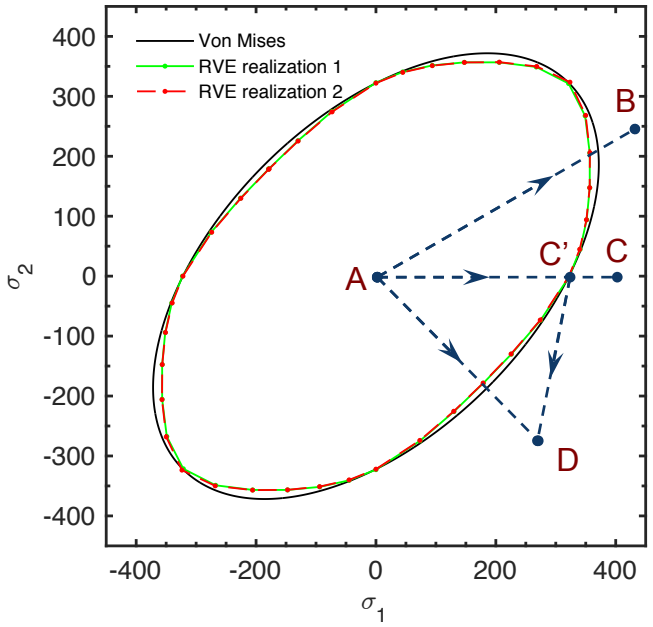
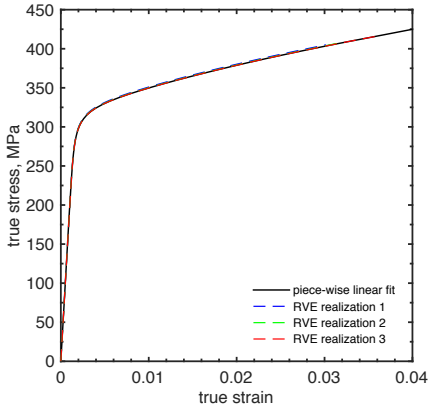
stress paths in principal-stress space



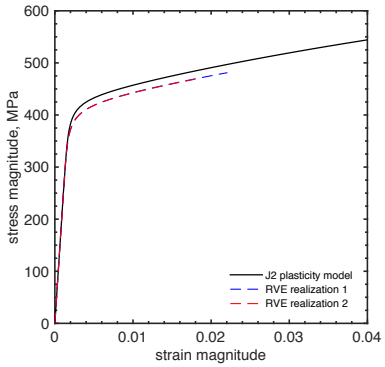
calibration

stress path A − C

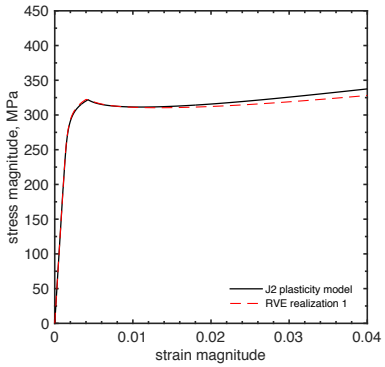


validation

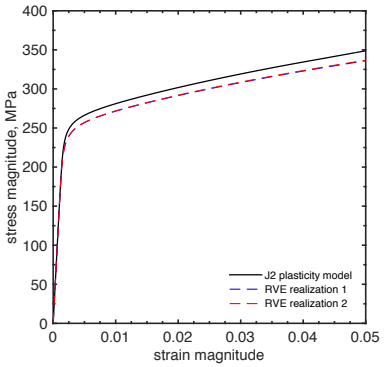
stress path A − B



stress path A − C' − D



stress path A − D



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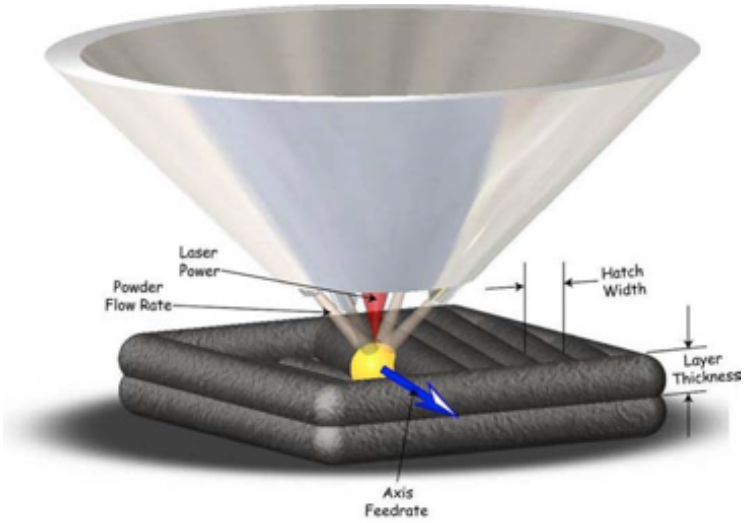
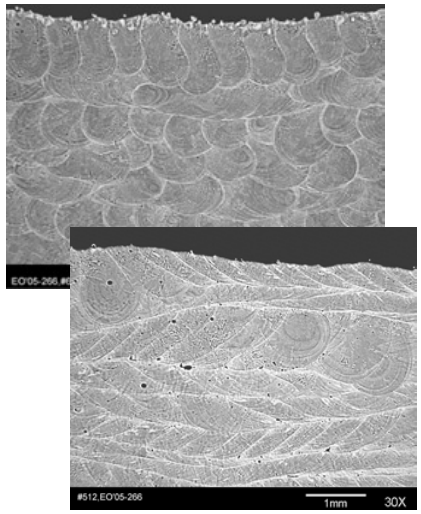
Application to additive manufacturing

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.



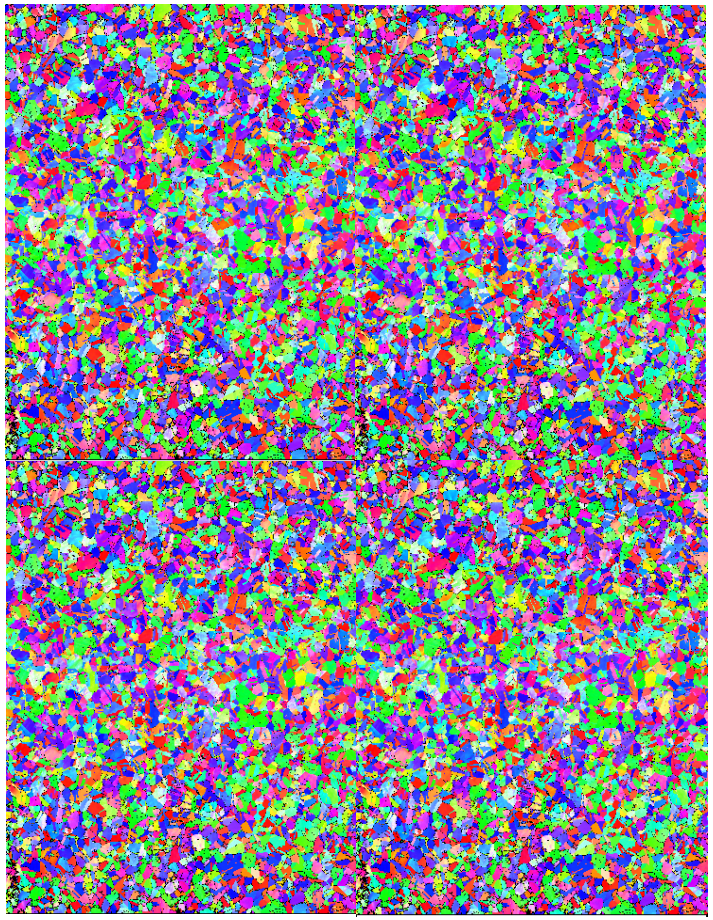
LENS mesostructure

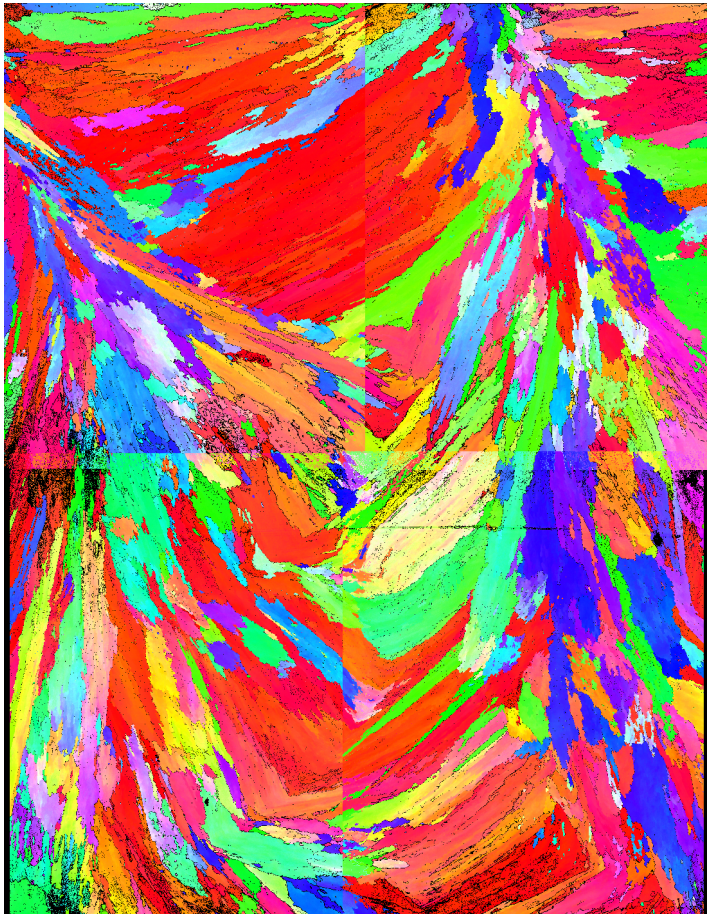
Microstructure: wrought vs. LENS

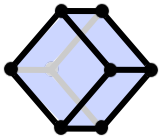
Wrought, SS 304L

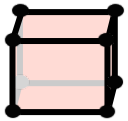
(Images shown at same scale.)

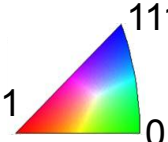
LENS, SS 304L, 3.8 kW

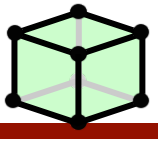








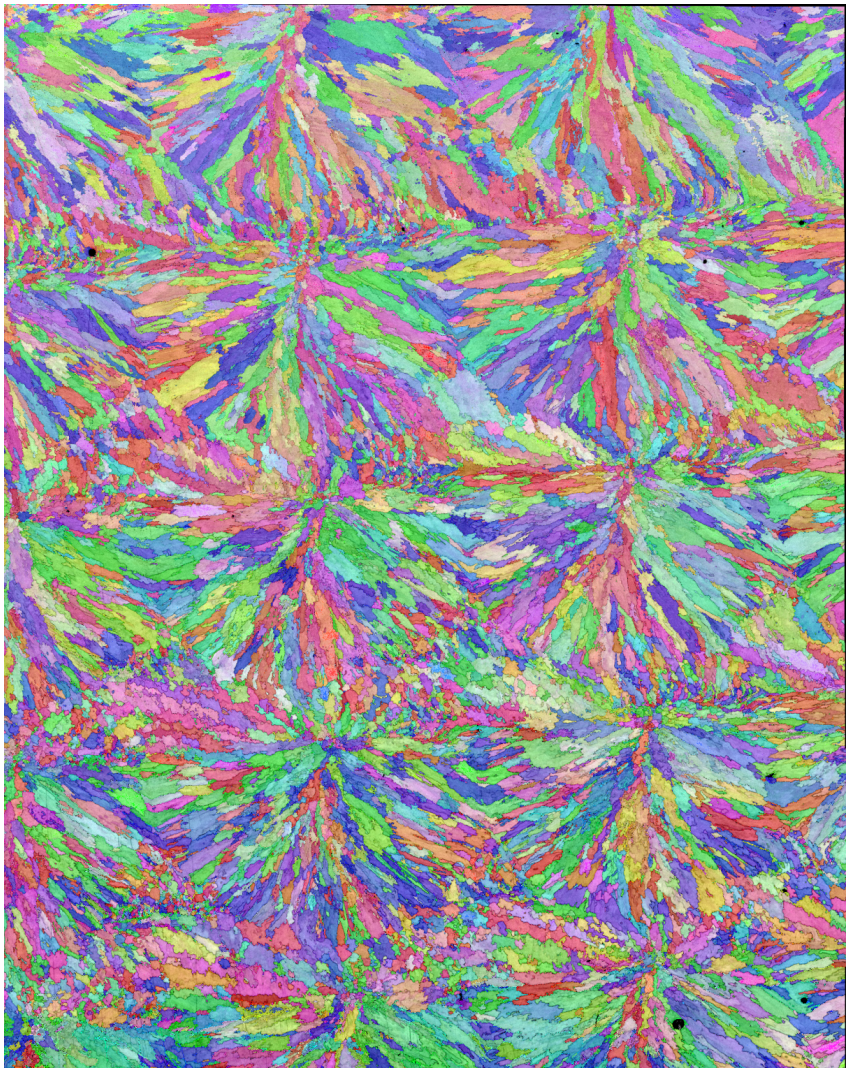




1.0 mm

1.0 mm

LENS microstructure



8 mm x 10 mm

Idealized LENS microstructures

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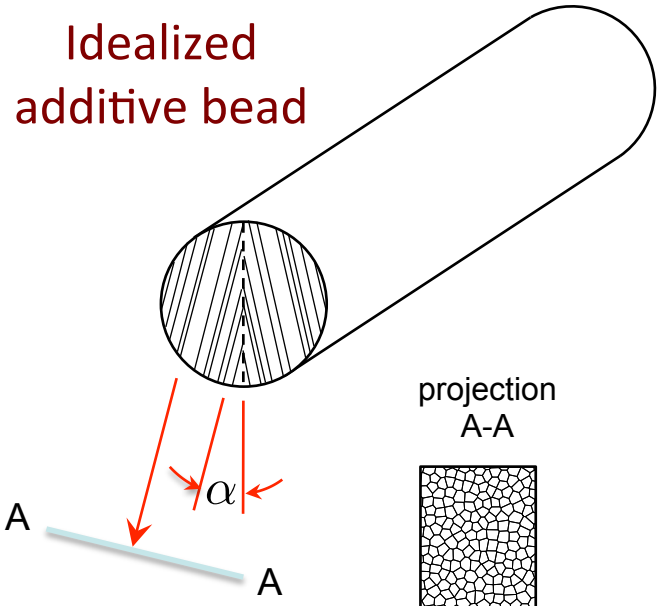
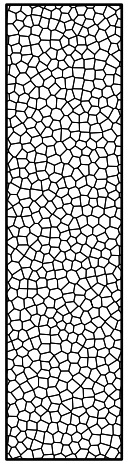
Idealized additive bead

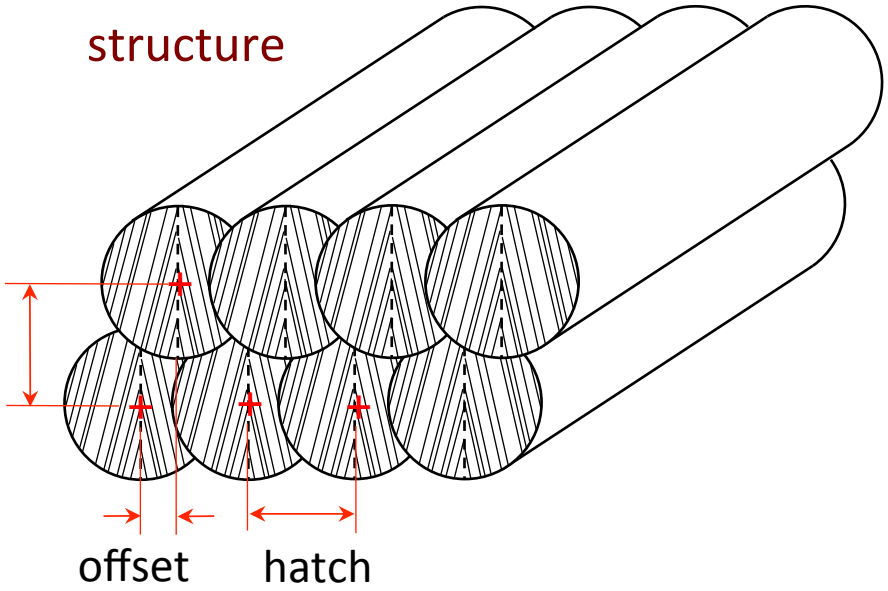


projection A-A



random Voronoi through MPS sampling

Idealized LENS structure



texture?

DNS modeling

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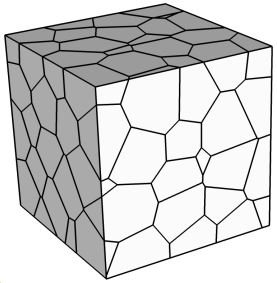
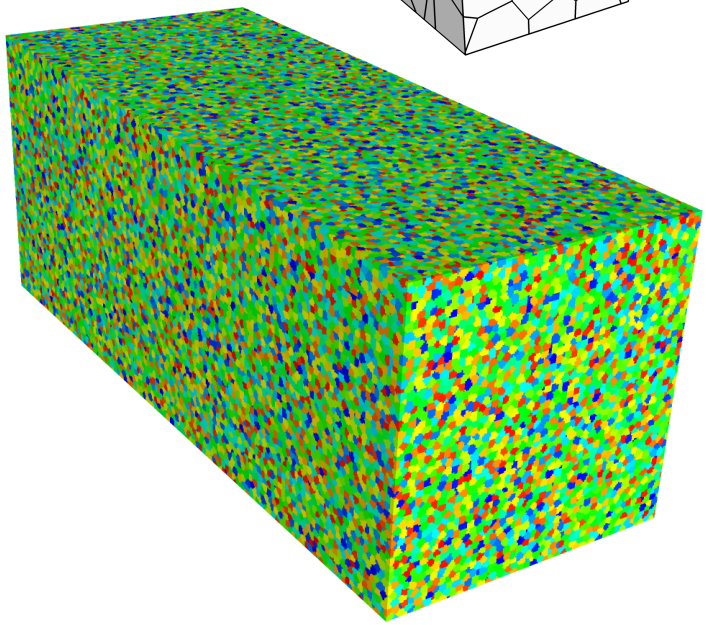
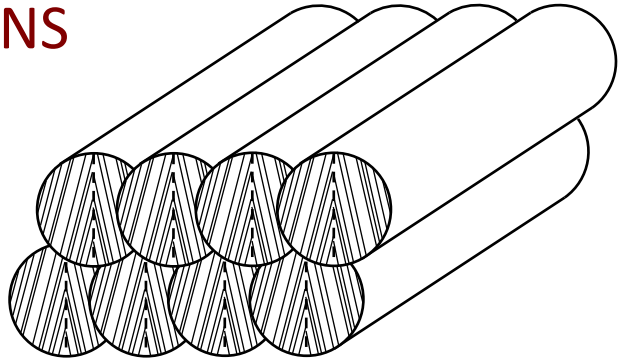
equiaxed



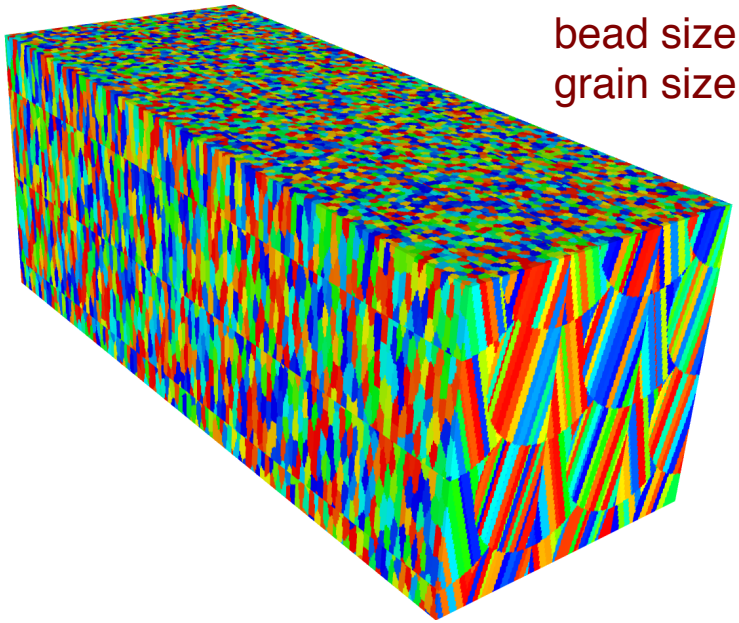


grain size = 40 microns

additive, LENS



bead size = 1 mm
grain size = 40 microns



Engineering stress-strain

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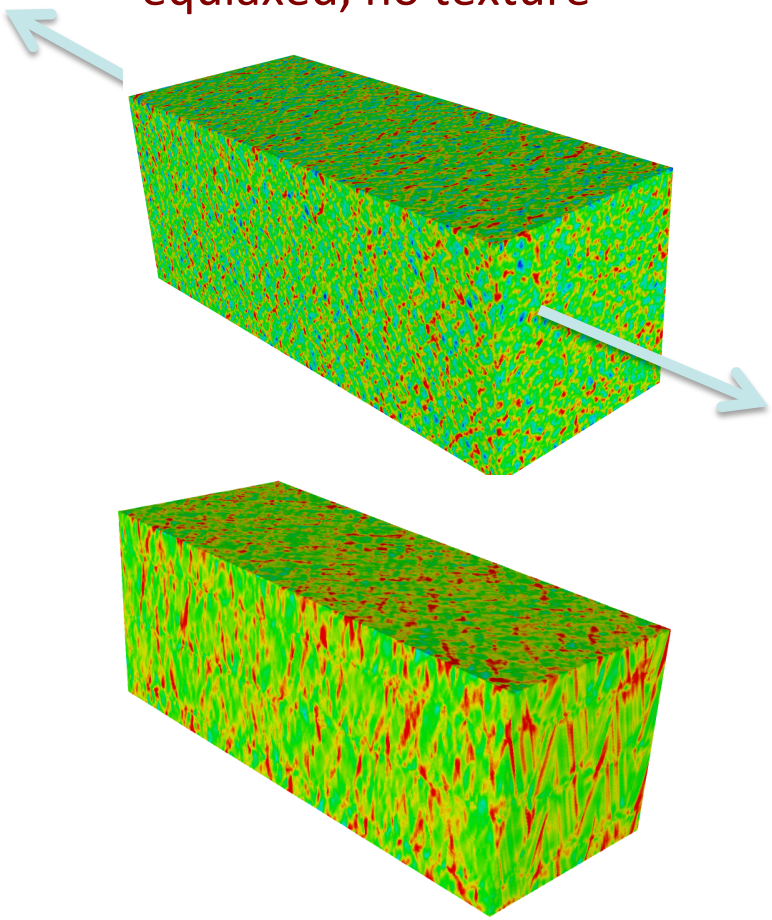
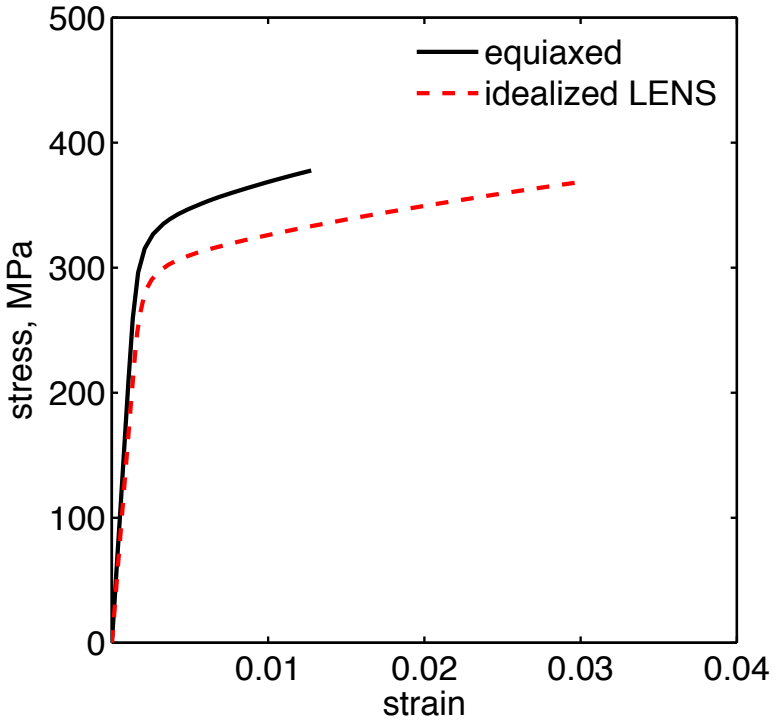
equiaxed, no texture



additive, LENS



Idealized microstructures

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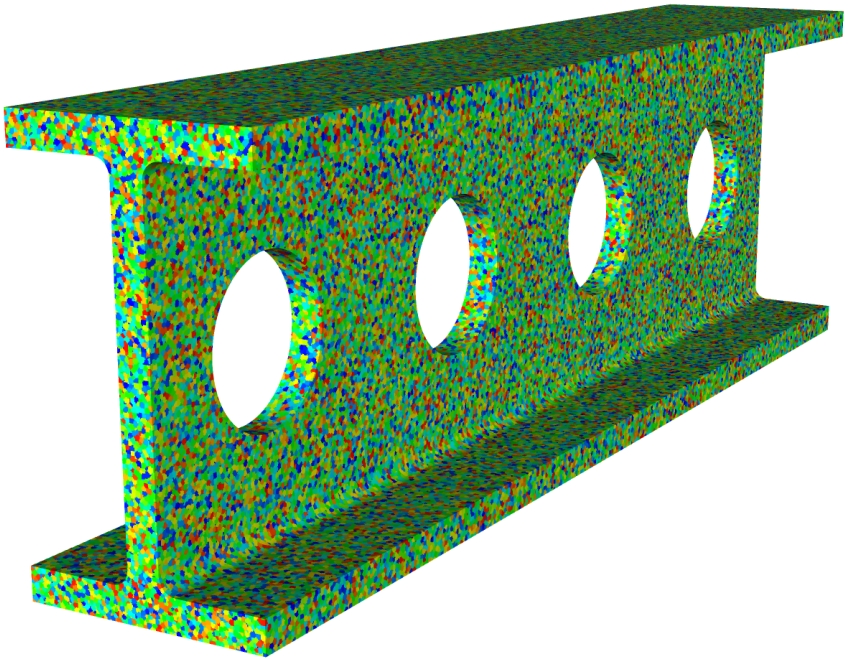
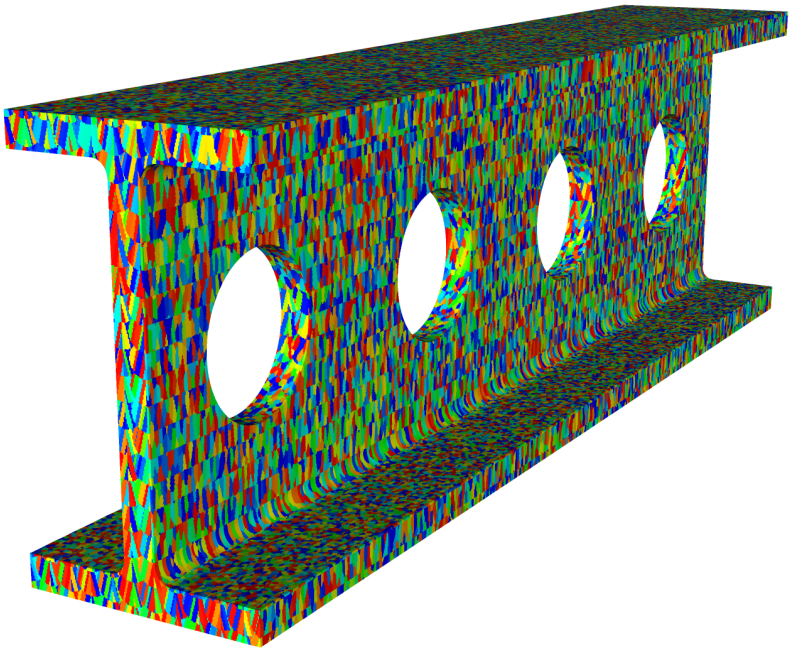
equiaxed



LENS



Macroscopic stress field

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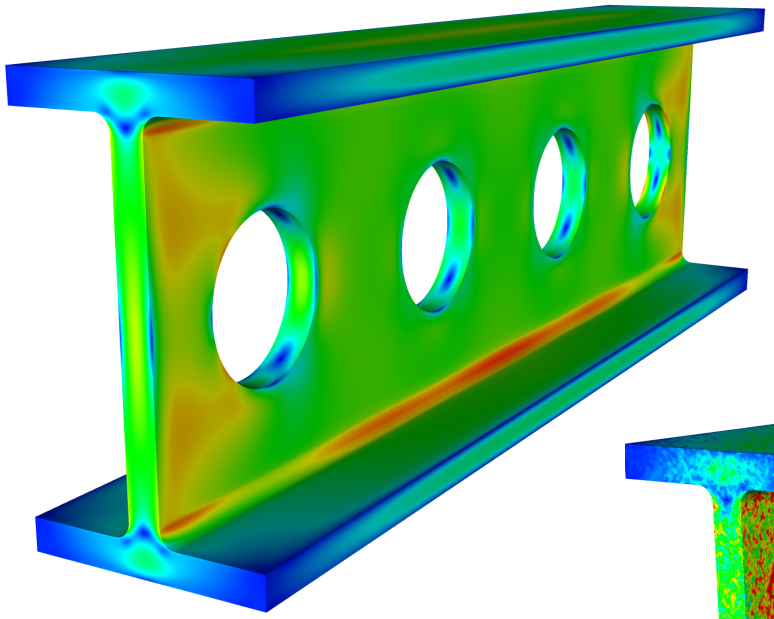
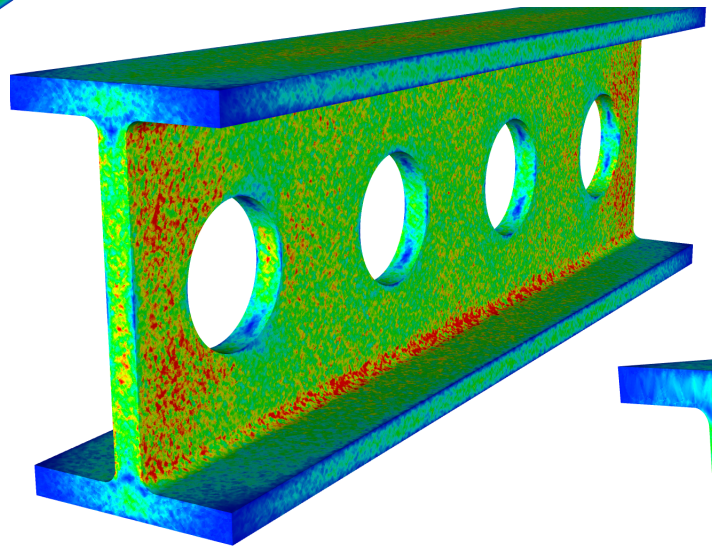
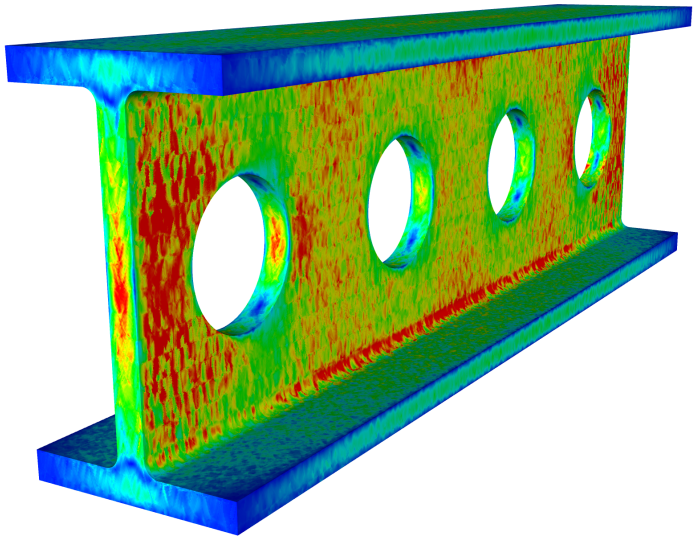


homogeneous, isotropic

equiaxed, no texture, isotropic



idealized LENS



Process modeling

(Veena Tikare, SNL)

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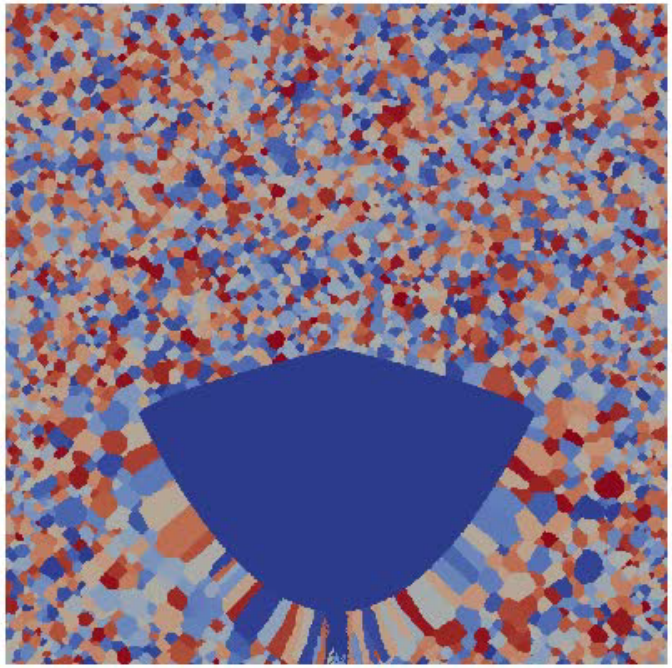
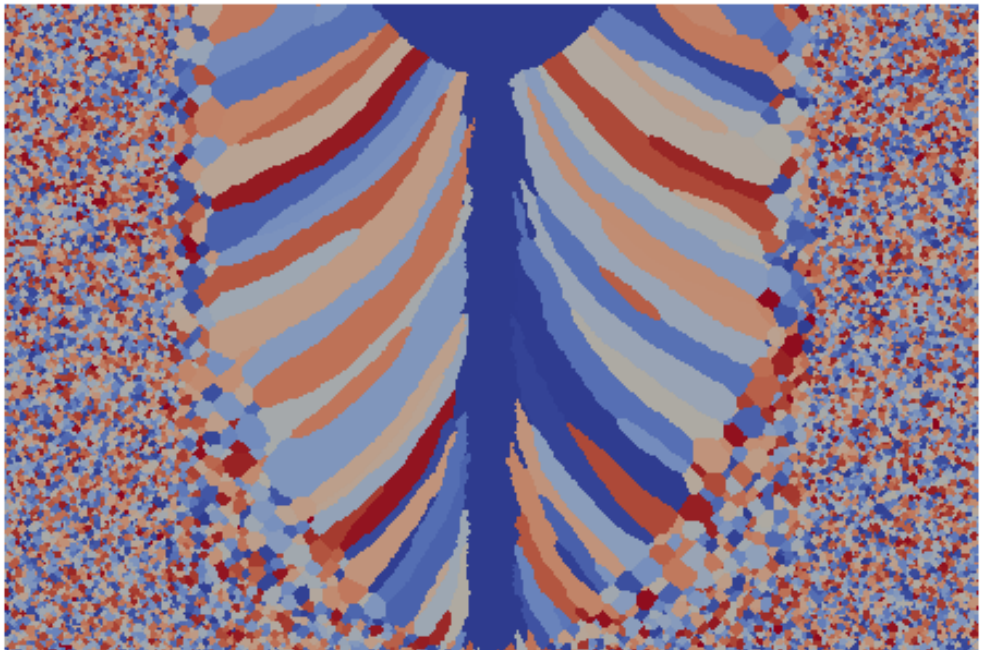
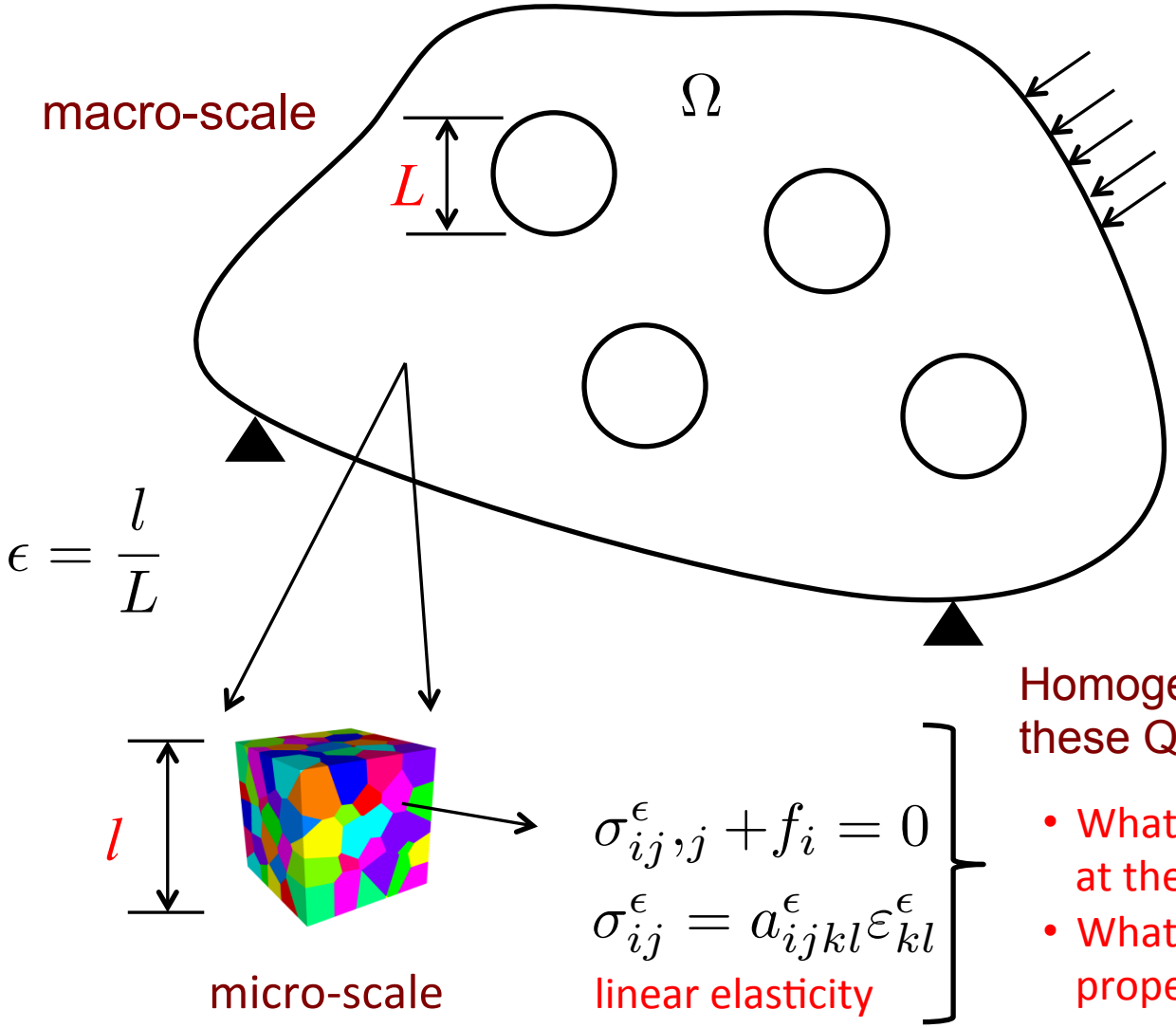
Future tie-in with process modeling:
grain growth simulation





Kinetic Monte Carlo

What about the Governing PDE?

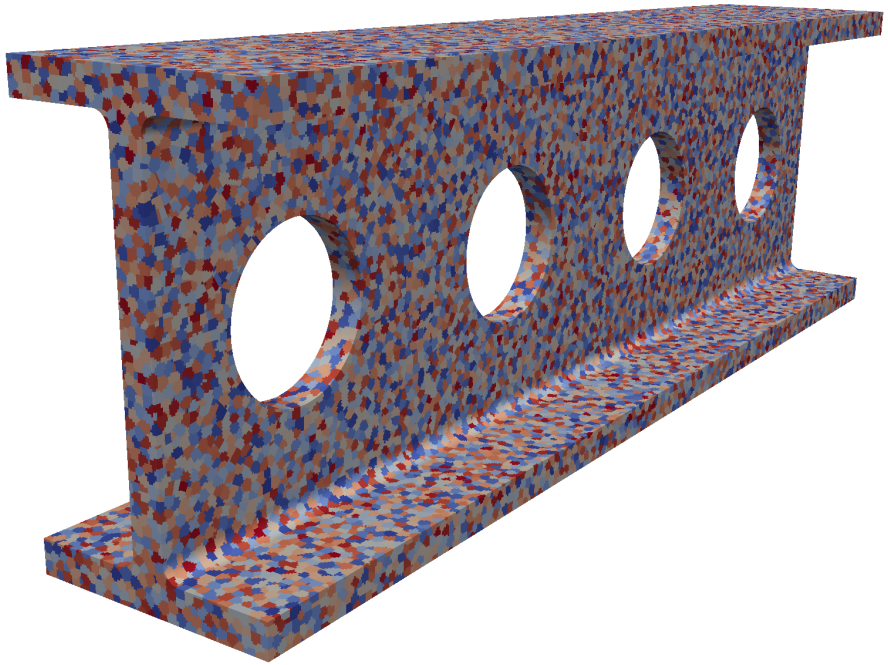


Homogenization Theory Answers these Questions:

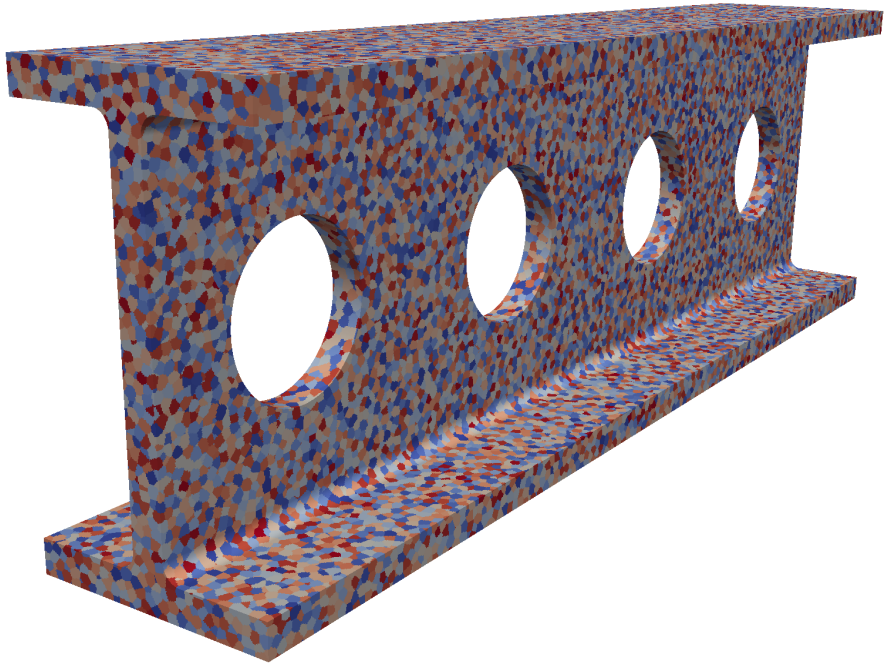
- What is the governing equation at the macroscale?
- What are the effective material properties?

Effect of Mesh Refinement

thickness/grain ratio = 4



mesh refinement R3



mesh refinement R4

Effect of Mesh Refinement

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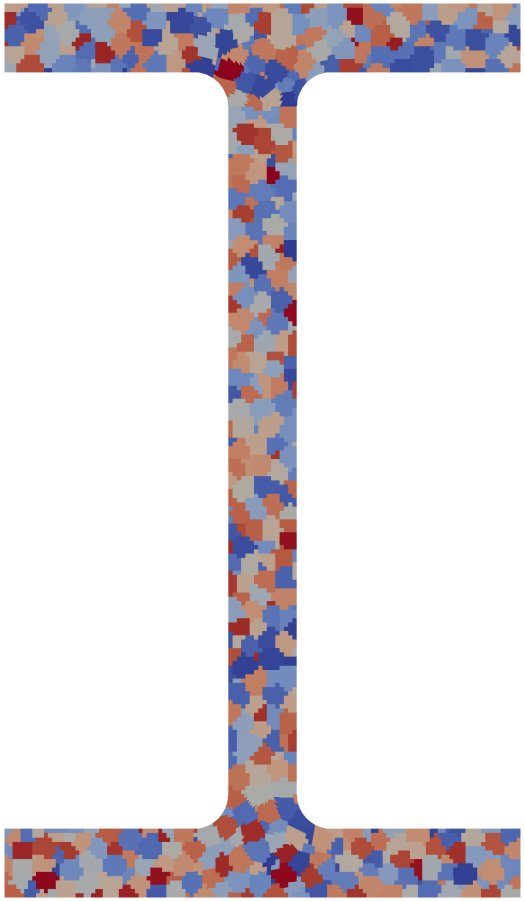
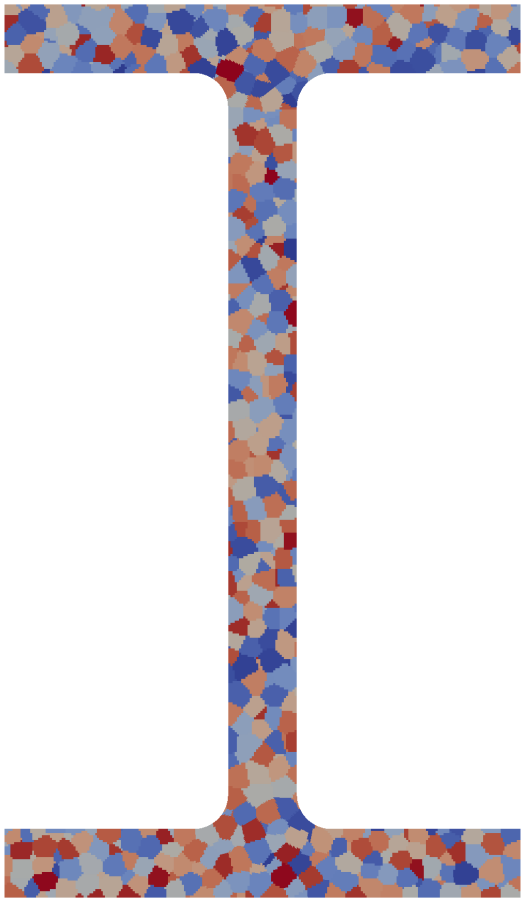
thickness/grain ratio = 4



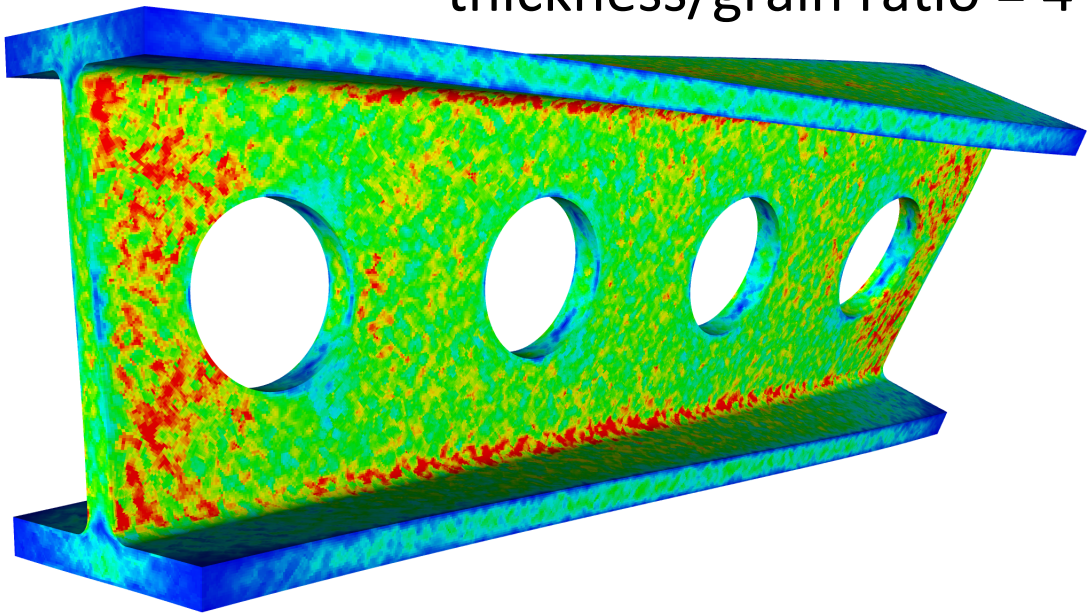
mesh refinement R3



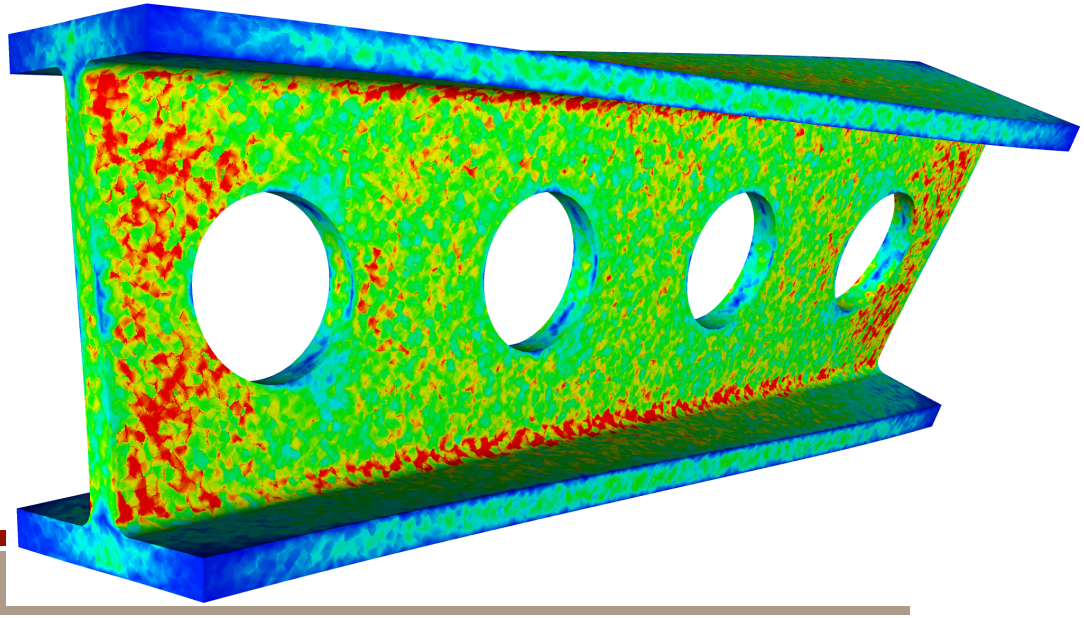
mesh refinement R4

Effect of Mesh Refinement

thickness/grain ratio = 4



mesh refinement R3



mesh refinement R4

Effect of Mesh Refinement

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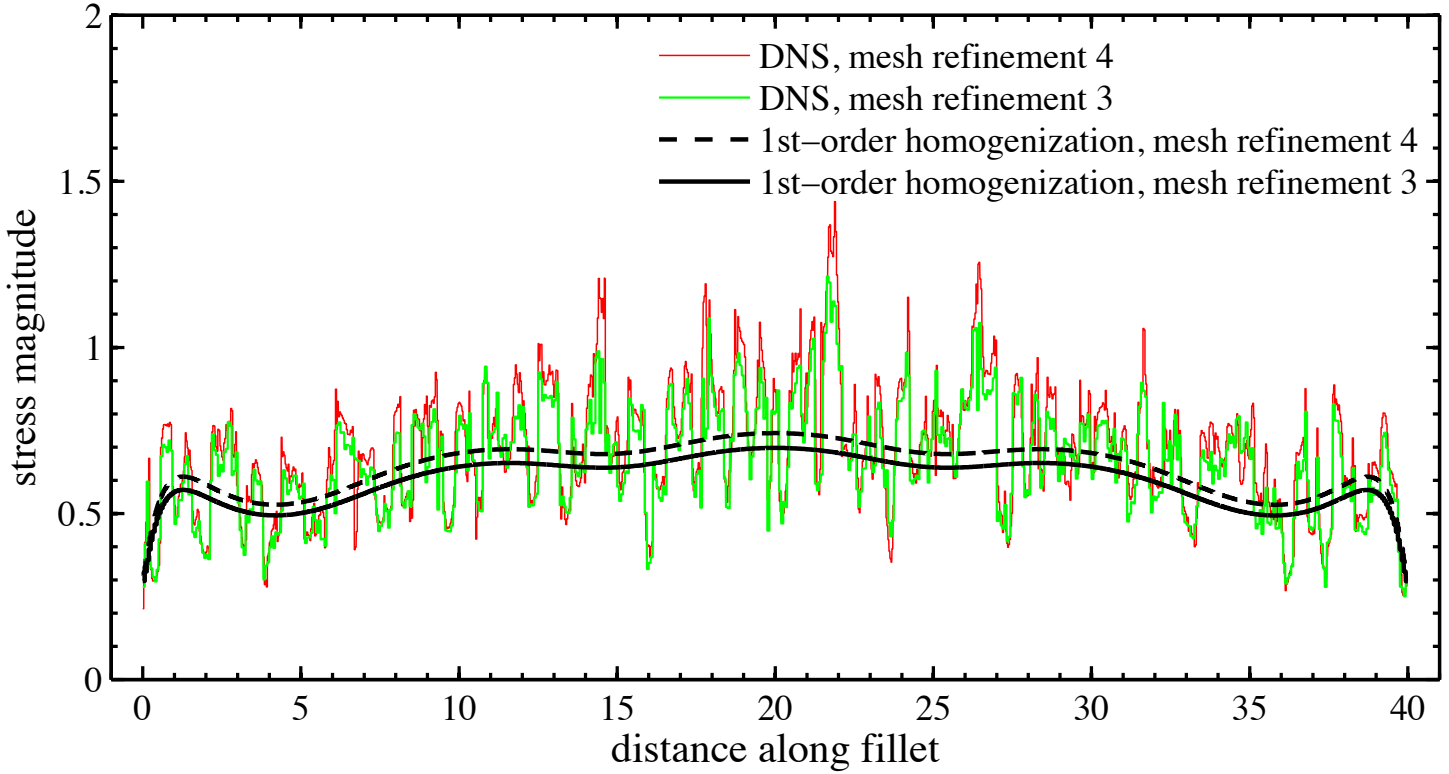
thickness/grain ratio = 4



Homogenized solution vs. ensemble average

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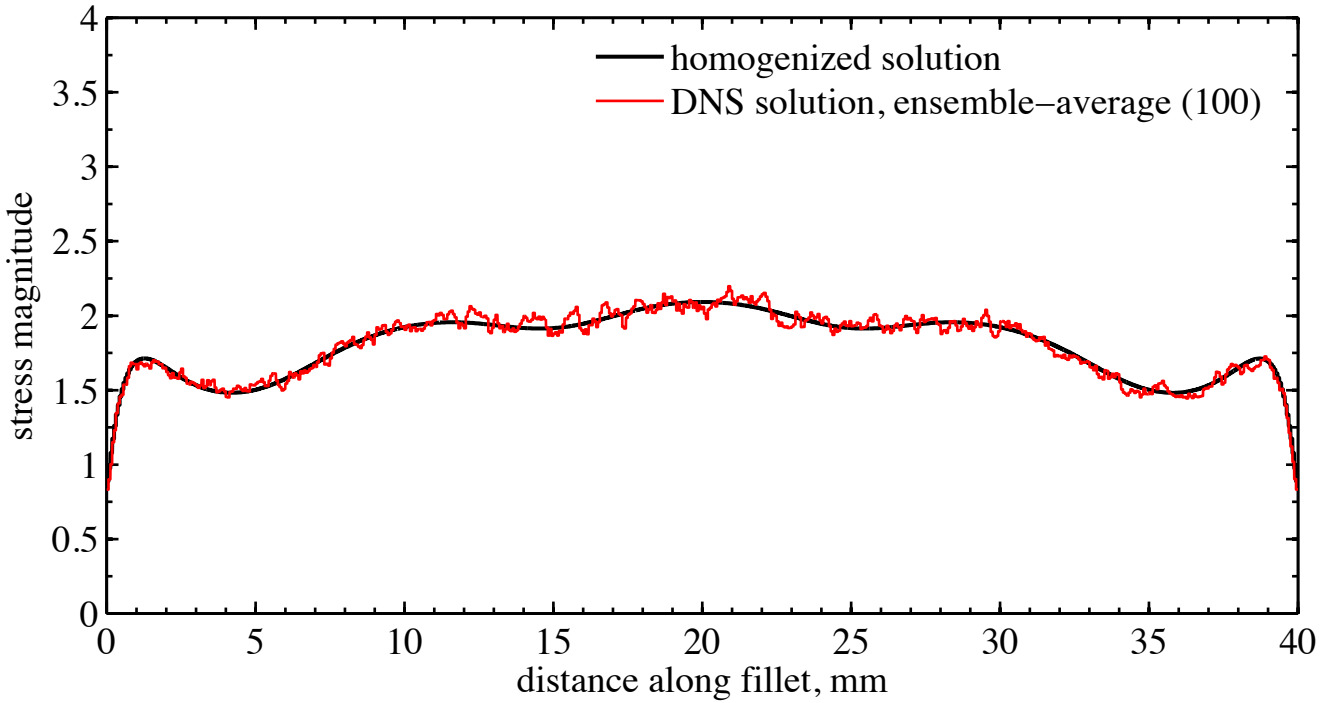
Beran and McCoy (1970) showed that the governing equation for the mean field is **nonlocal**.

Stress magnitude along lower fillet



See no evidence for nonlocality here.

Homogenized solution vs. ensemble average

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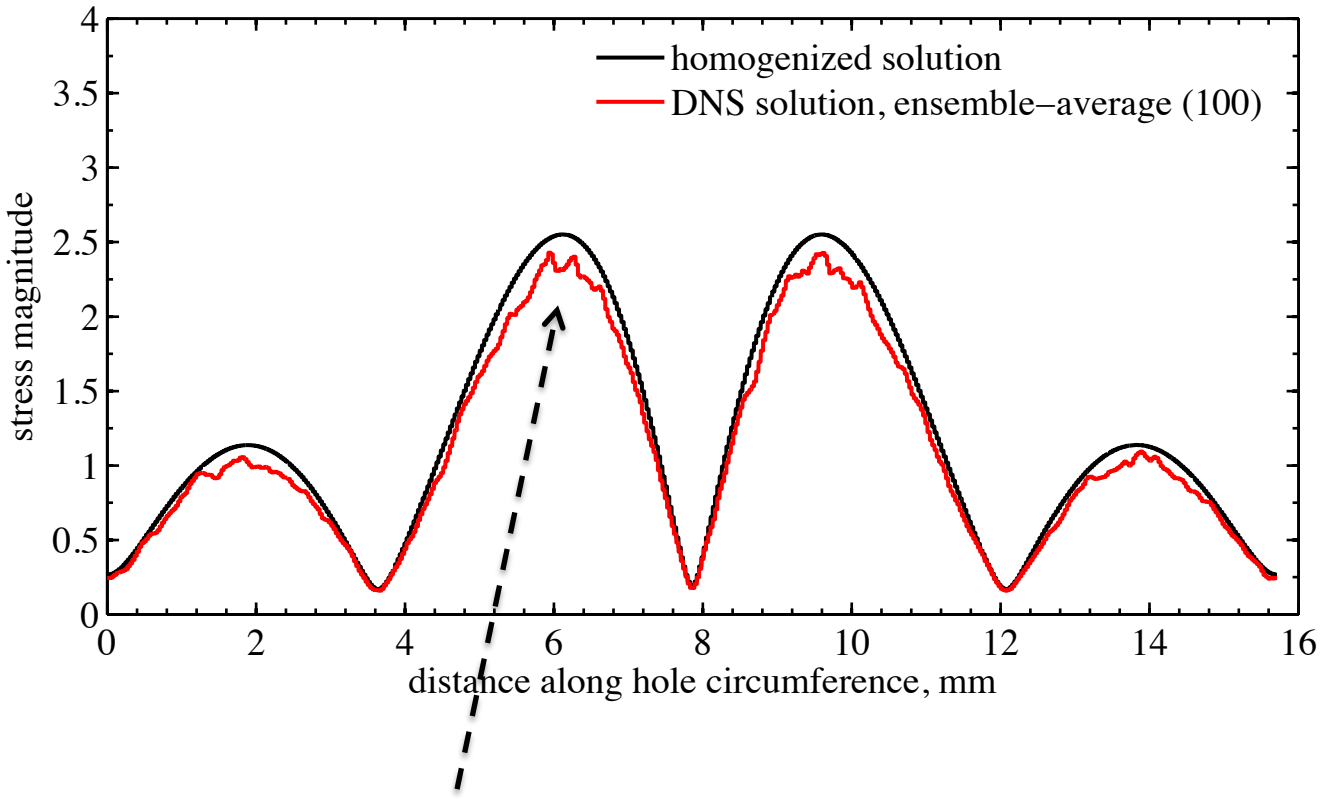
Stress magnitude around hole



100 realizations

See some evidence for nonlocality here.

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

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

SUBC

stochastic

deterministic

KUBC

stochastic

partial ordering defined in an energetic sense:

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