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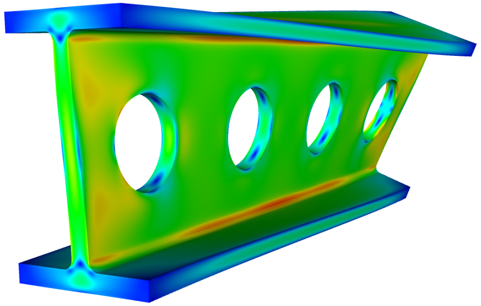

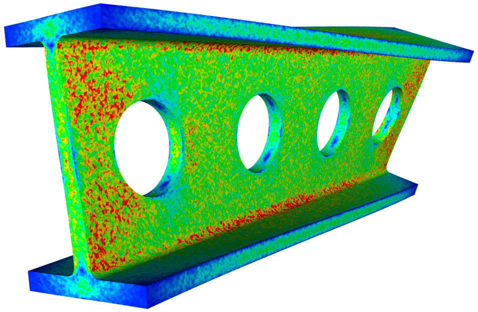

Homogenization and Material Variability

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Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Collaborators

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Amy Sun, Corbett Battaile, Jay Foulk, Brad Boyce

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Josh Robbins (1443): On the fruitfulness of using Mindlin's theory of a "continuum with microstructure."

Outline

1. Review of homogenization theory
    - apparent vs. effective material properties
    - weak convergence
    - Type 1 and Type 2 material variability
2. Direct numerical simulations and comparison to homogenized PDE solution
    - Voronoi microstructure
    - hexahedral mesh overlay
    - boundary value problems
3. Type 2 material variability in macroscale simulations: a path forward
    - Mindlin's continuum formulation
    - elastic formulation
    - nonlinear response via FE^2

Hierarchy of Continuum Models

(homogenization perspective)

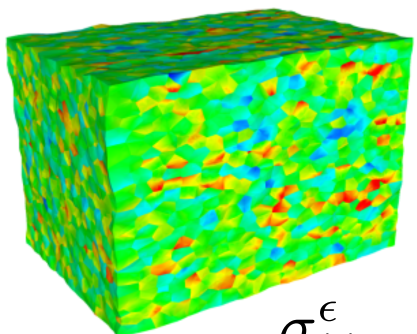
1. First-order continuum
   - microstructure is infinitesimally small
   - stored energy is a function of strain only
   - RVE size is infinite (very large compared to microstructure)
   - material properties can fluctuate only on a large scale (Type 1 material variability)
   - used in commercial FEA codes and Sierra

2. Second-order continuum
   - microstructure is small but finite
   - stored energy is a function of both strain and strain gradient (Mindlin, 1964)
   - RVE no longer exists, instead have a SVE (stochastic volume element; (Yin, 2008))
   - material properties are no longer *intrinsic* but are rather *extrinsic* (Huet, 1990)
   - material properties fluctuate on a small scale (Type 2 material variability)

3. Direct Numerical Simulation using Multiscale Mortars
   - each RVE is coupled through mortars with a multiscale basis obtained through first-order homogenization theory (Arbogast, 2007)

4. Direct Numerical Simulation

Homogenization



σ^{ϵ}_{ij}

fine-scale fluctuations

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

replaced with mean behavior

This equivalence is defined in an energy sense: $\sigma_{ij}\varepsilon_{ij} = \langle \sigma^{\epsilon}_{ij} \rangle \langle \varepsilon^{\epsilon}_{ij} \rangle$

Constitutive models map average strain to average stress:

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

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:

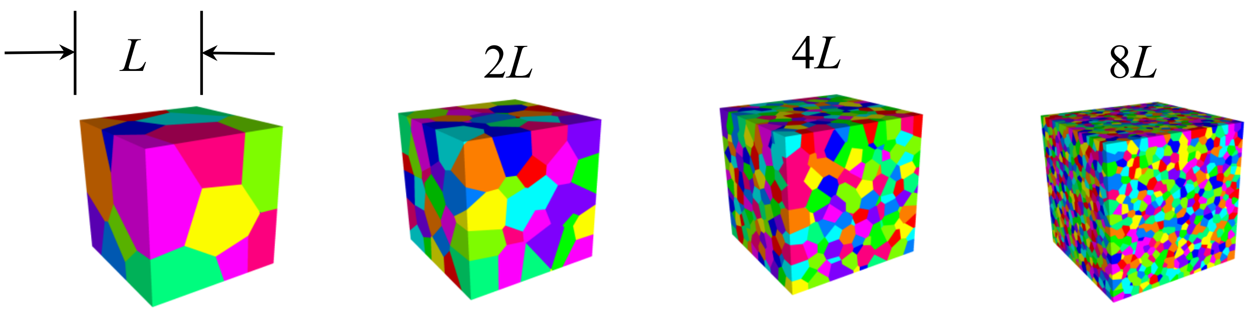
$B < A$ iff $\varepsilon : (A - B) : \varepsilon > 0$ for all $\varepsilon \neq 0$

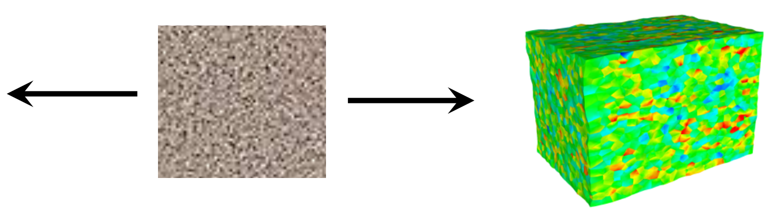
Apparent vs. Effective Material Properties

Sandia National Laboratories

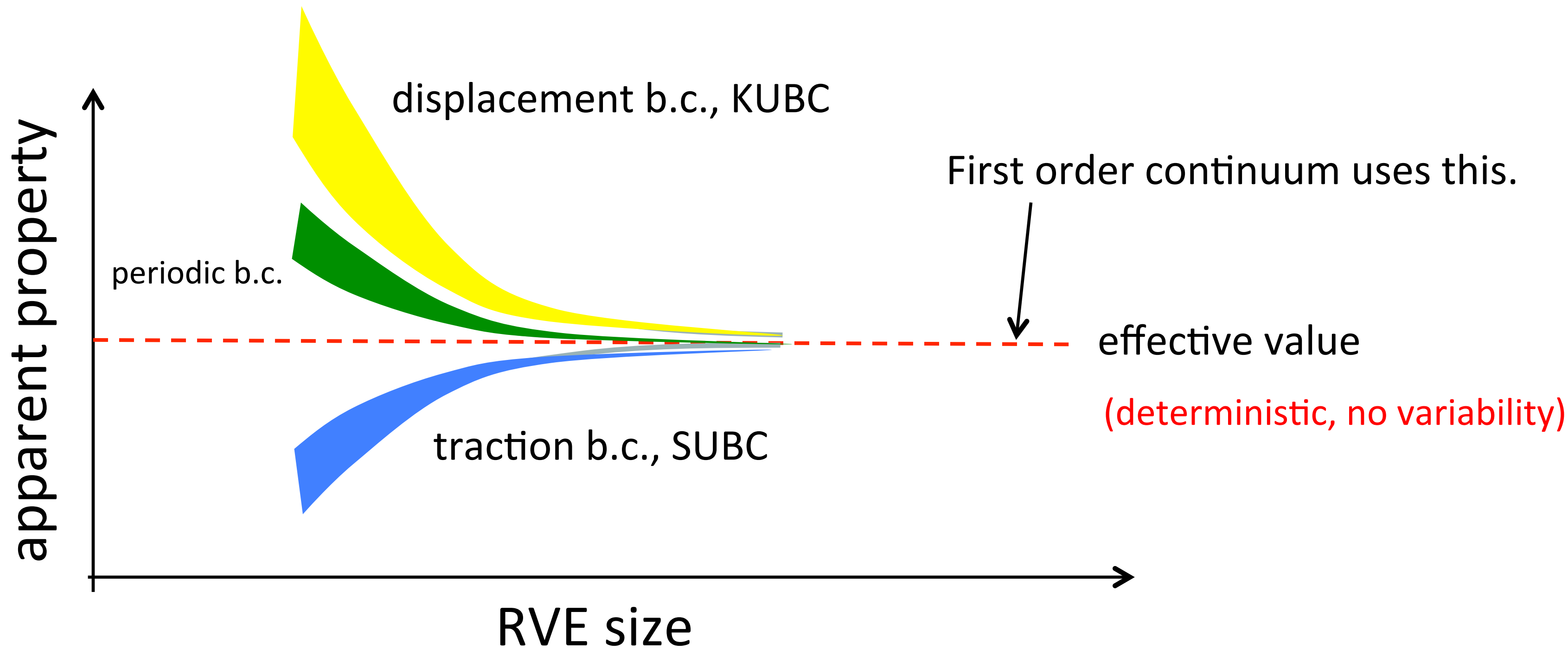
Huet, C. (1990). "Application of variational concepts to size effects in elastic heterogeneous bodies." *Journal of the Mechanics and Physics of Solids,* 38(6): 813-841.

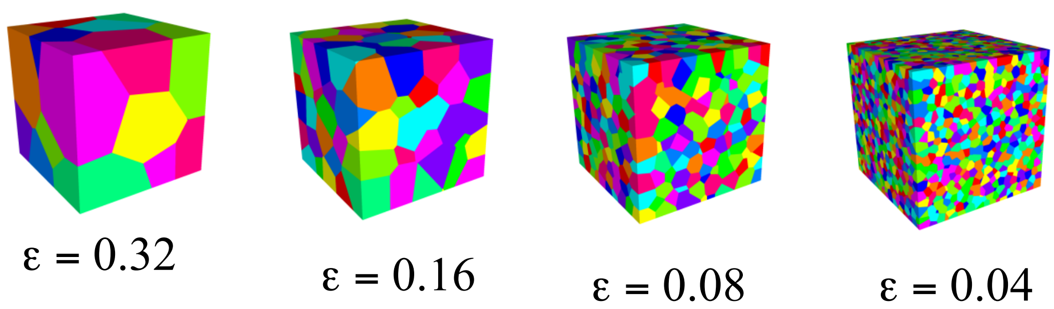
$$C^{\text{app}}_{\sigma,L} \leq C^{\text{app}}_{\sigma,2L} \leq C^{\text{app}}_{\sigma,4L} \leq \cdots \leq C^{\text{app}}_{\sigma,\infty} = C$$



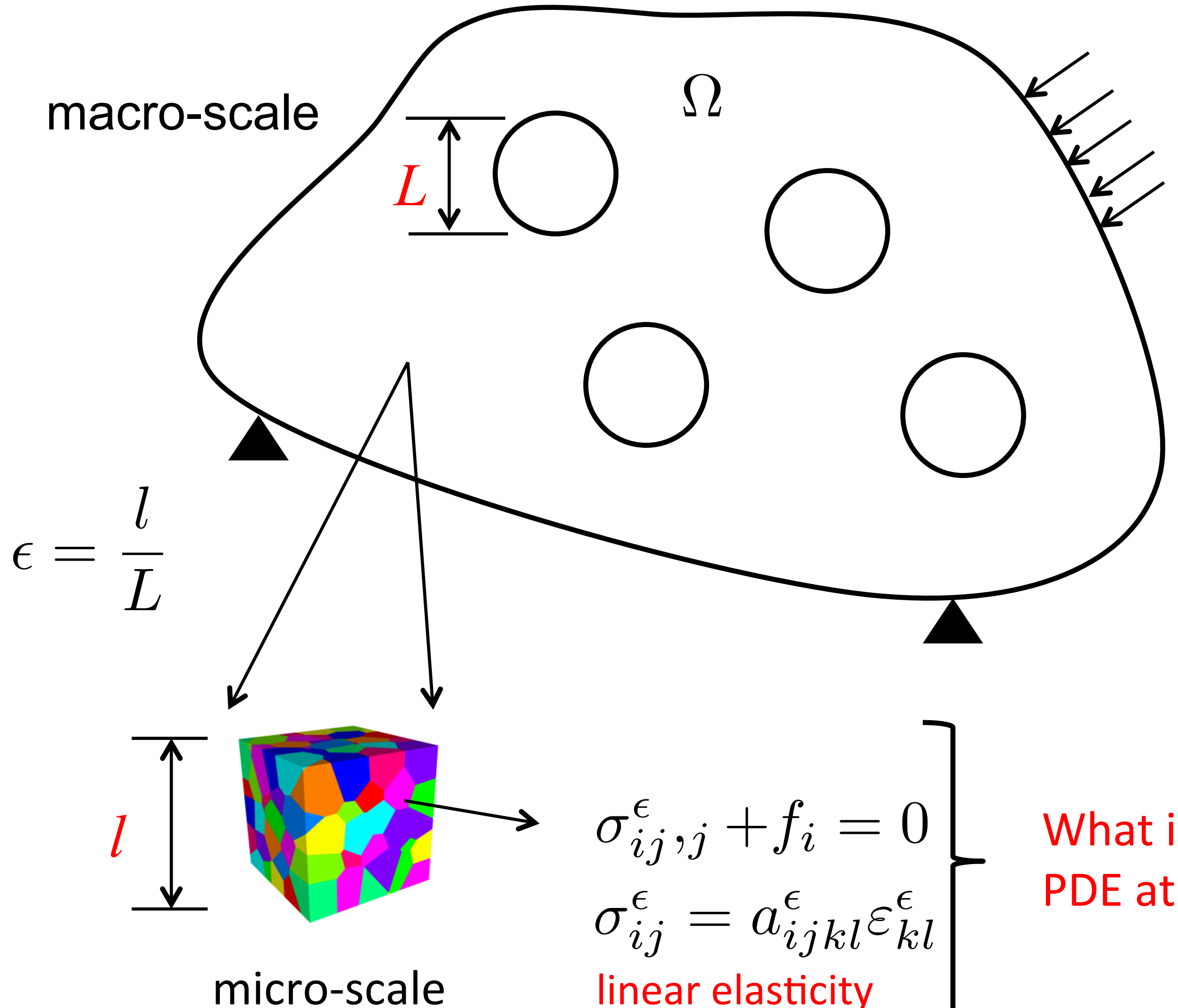


Apparent vs. Effective Material Properties





What about the Governing PDE?



$$\sigma^{\epsilon}_{ij},_j + f_i = 0$$
$$\sigma^{\epsilon}_{ij} = a^{\epsilon}_{ijkl}\varepsilon^{\epsilon}_{kl}$$

linear elasticity

What is the governing PDE at the macroscale?

Strong and Weak Convergence

A sequence of functions (u_n), $u_n \in L^2$ is **strongly** convergent to $u \in L^2$ if

$$\lim_{n\to\infty} \|u_n - u\|_{L^2} = 0$$

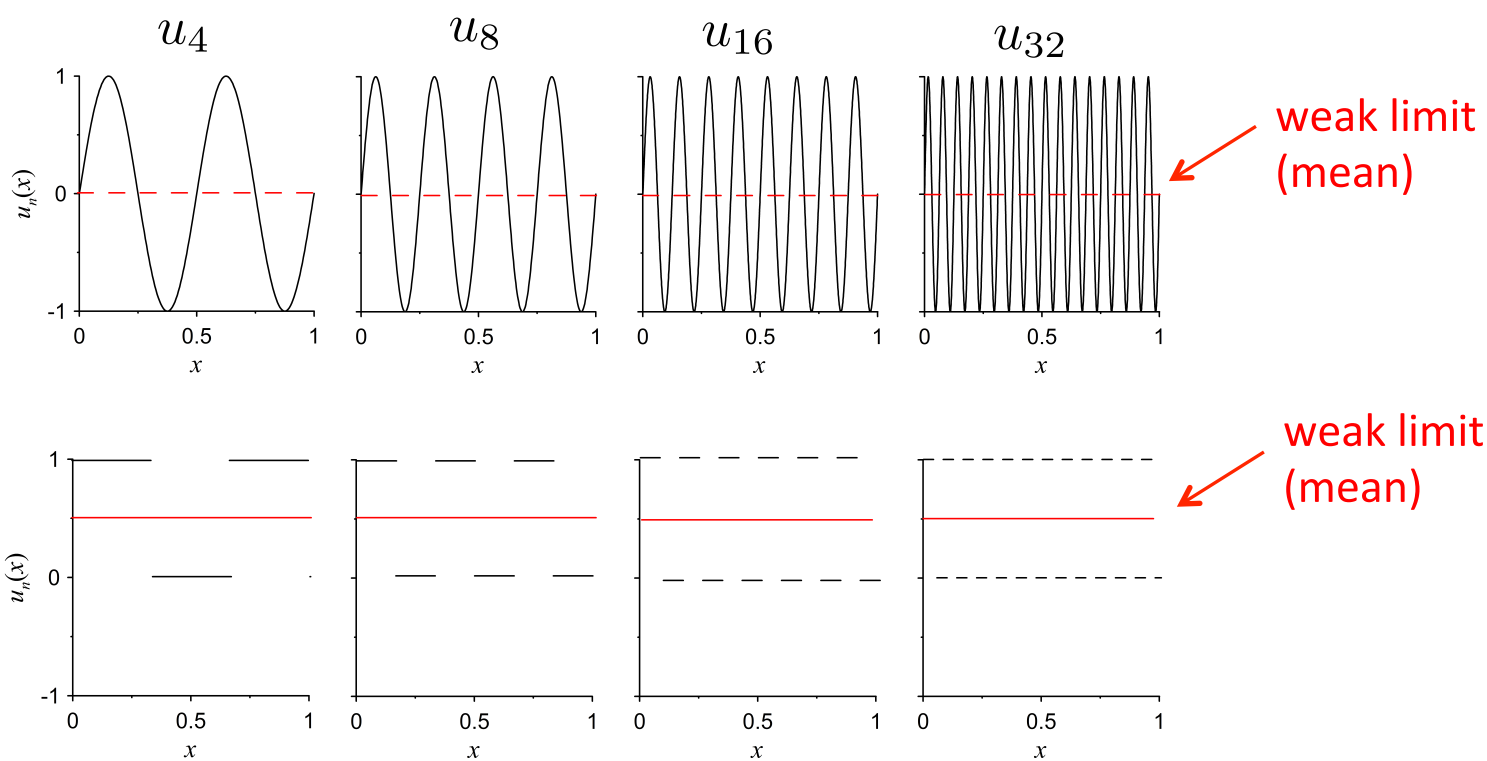
A sequence of functions (u_n), $u_n \in L^2$ is **weakly** convergent to $u \in L^2$ if

$$\lim_{n\to\infty} \langle u_n, v\rangle = \langle u, v\rangle \quad \text{for all } v \in L^2$$

These are the modes of convergence in which homogenization is defined.

Weak Convergence

Example: The sequence of functions $u_n = \sin(n\pi x)$ in $L^2[0,1]$ converges weakly to $u = 0$.



Theorem: Any sequence of periodic functions converges weakly to the mean as the period approaches zero.

Asymptotic Expansion

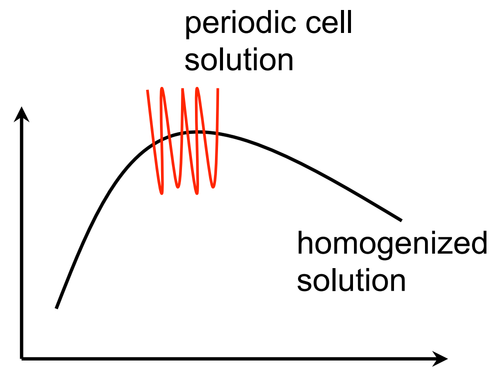
(Cioranescu and Donato, 1999, *An Introduction to Homogenization.*)

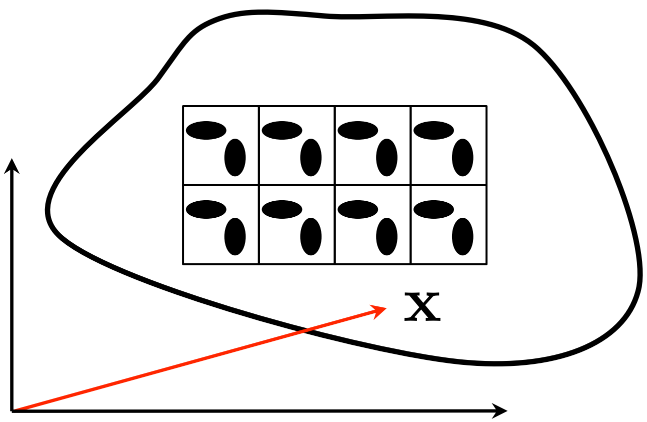
$$\mathbf{u}^{\epsilon}(\mathbf{x}) = \mathbf{u}_0(\mathbf{x},\mathbf{y}) + \epsilon\mathbf{u}_1(\mathbf{x},\mathbf{y}) + \epsilon^2\mathbf{u}_2(\mathbf{x},\mathbf{y}) + \cdots$$

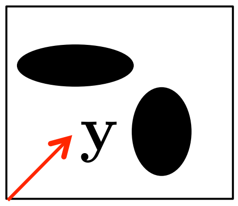
$\mathbf{u}_j(\mathbf{x},\mathbf{y})$ are periodic in $\mathbf{y}$

$\mathbf{y} = \mathbf{x}/\epsilon$ is the `fast' variable

$\mathbf{x}$ is the `slow' variable







Linear Homogenization Results

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$$\mathbf{u}^{\epsilon}(\mathbf{x}) = \mathbf{u}_0(\mathbf{x},\mathbf{y}) + \epsilon \mathbf{u}_1(\mathbf{x},\mathbf{y}) + \epsilon^2 \mathbf{u}_2(\mathbf{x},\mathbf{y}) + \cdots$$

substitute

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

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

RESULT: $$\mathbf{u}^{\epsilon}(\mathbf{x}) = \mathbf{u}_0(\mathbf{x}) - \epsilon \chi(\mathbf{y}) \cdot \nabla \mathbf{u}_0 + \epsilon^2 \theta(\mathbf{y}) : \nabla\nabla \mathbf{u}_0 + \cdots$$

homogenized solution does not depend upon ϵ!

first-order corrector

second-order corrector

Observations:

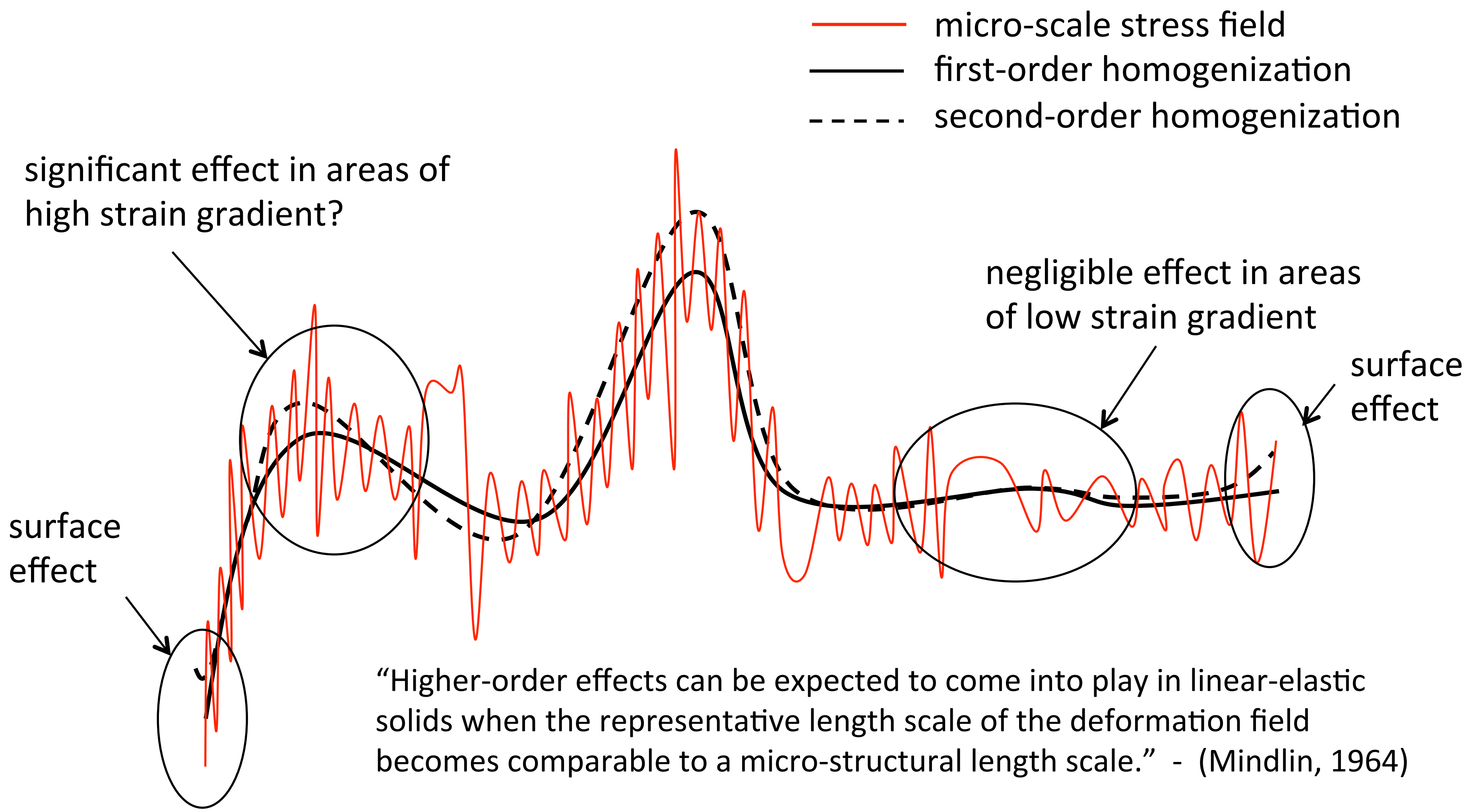
- In the limit as $\epsilon \to 0$, get a first-order continuum (homogenized).
- For $\epsilon \neq 0$ need gradient terms (higher-order continuum)

Linear Homogenization Results

(Cioranescu and Donato, 1999, *An Introduction to Homogenization*.)

$$\mathbf{u}^{\epsilon} \to \mathbf{u} \ \text{ strongly in } \ L^2$$
$$\mathbf{u}^{\epsilon} \to \mathbf{u} \ \text{ weakly in } \ H^1$$
$$\sigma^{\epsilon} \to \sigma \ \text{ weakly in } \ L^2$$
$$W^{\epsilon} \to W \ \text{ strongly in } \ \Re$$

Homogenization



"Higher-order effects can be expected to come into play in linear-elastic solids when the representative length scale of the deformation field becomes comparable to a micro-structural length scale." - (Mindlin, 1964)

Identify Two Types of Material Variability

1. spatial variability of homogenized material constants (Type 1)
   - size of microstructure $\varepsilon = 0$
   - first-order homogenization, first-order PDE
   - spatial correlation at the macro-scale
   - elastic isotropy assumption holds regardless of scale
2. higher-order terms in the PDE itself (Type 2)
   - micro-structure is finite $\varepsilon \neq 0$
   - higher-order PDE
   - spatial correlation at the micro-scale only
   - anisotropic fluctuations

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    - elastic formulation
    - nonlinear response via FE^2

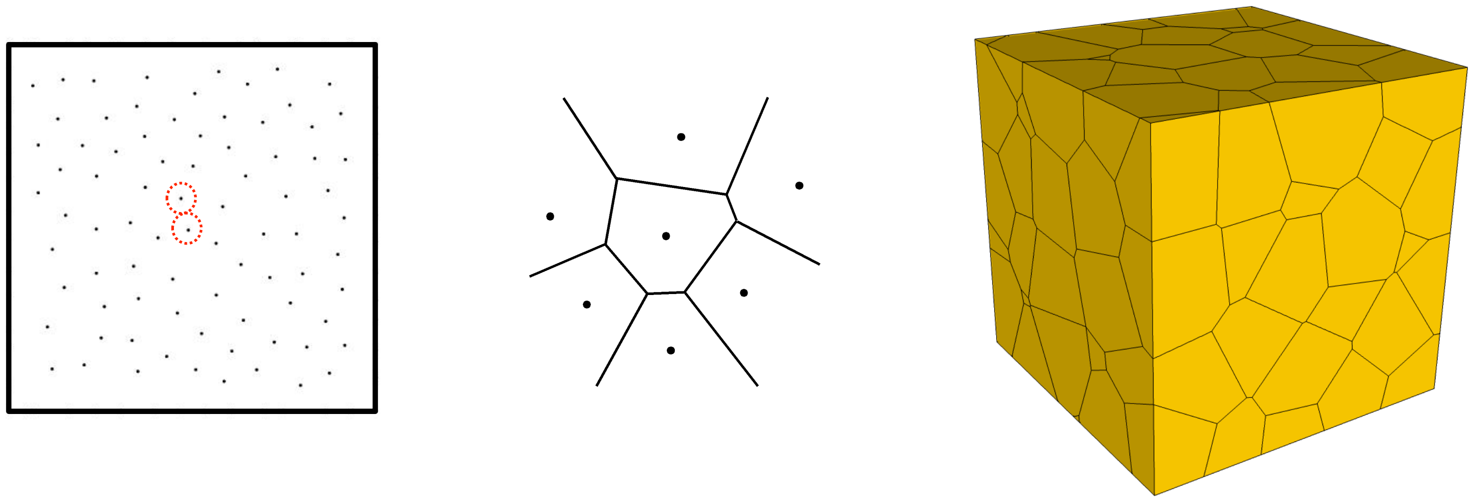
Goals

- 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 incomplete first-order homogenization.
- Propose/investigate a higher-order continuum theory for Type-2 material variability.

DNS Solutions

- Use Voronoi grains structures resulting from maximal Poisson sampling.
- Use the RPI crystal plasticity model (Dave Littlewood, John Emery)
- Overlay Voronoi grains onto an independent hexahedral mesh of the structure.

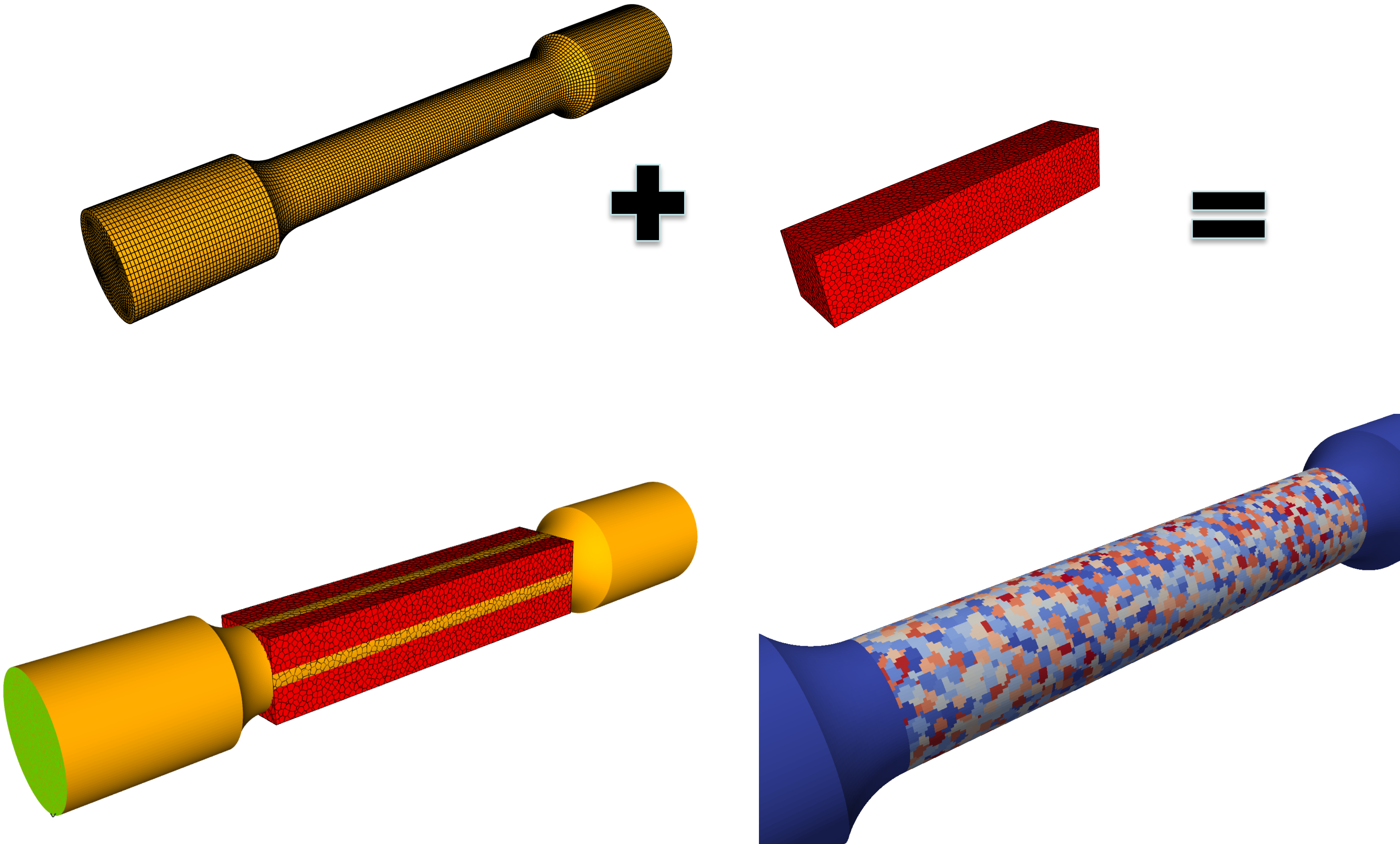
Voronoi Microstructure from MPS Seeding



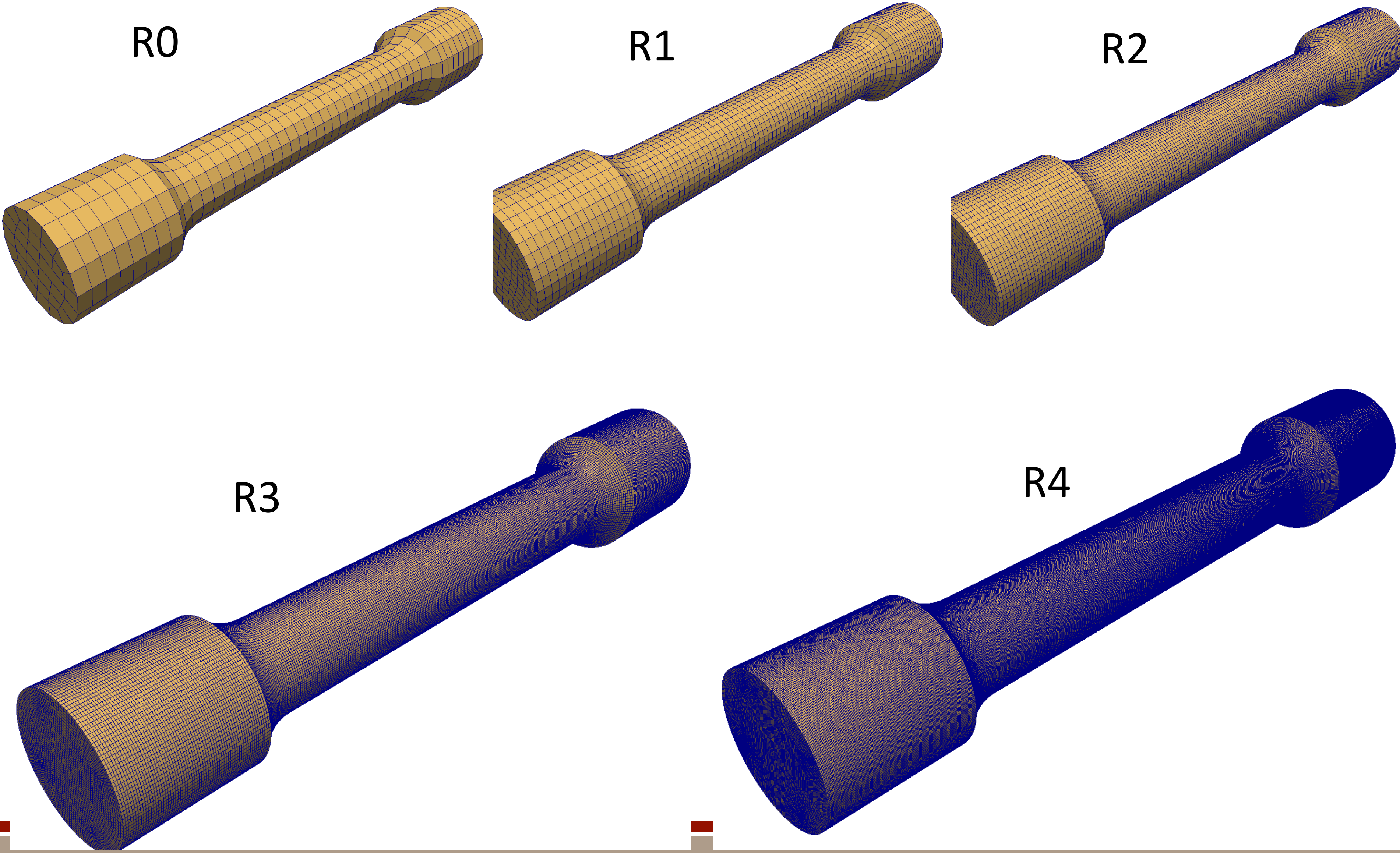
Maximal Poisson Sampling

- constraint on min. dist.
- seed until ‘max’ packing
- Ebeida/Mitchell Algorithm (1400)

Voronoi Overlay of Hexahedral Mesh

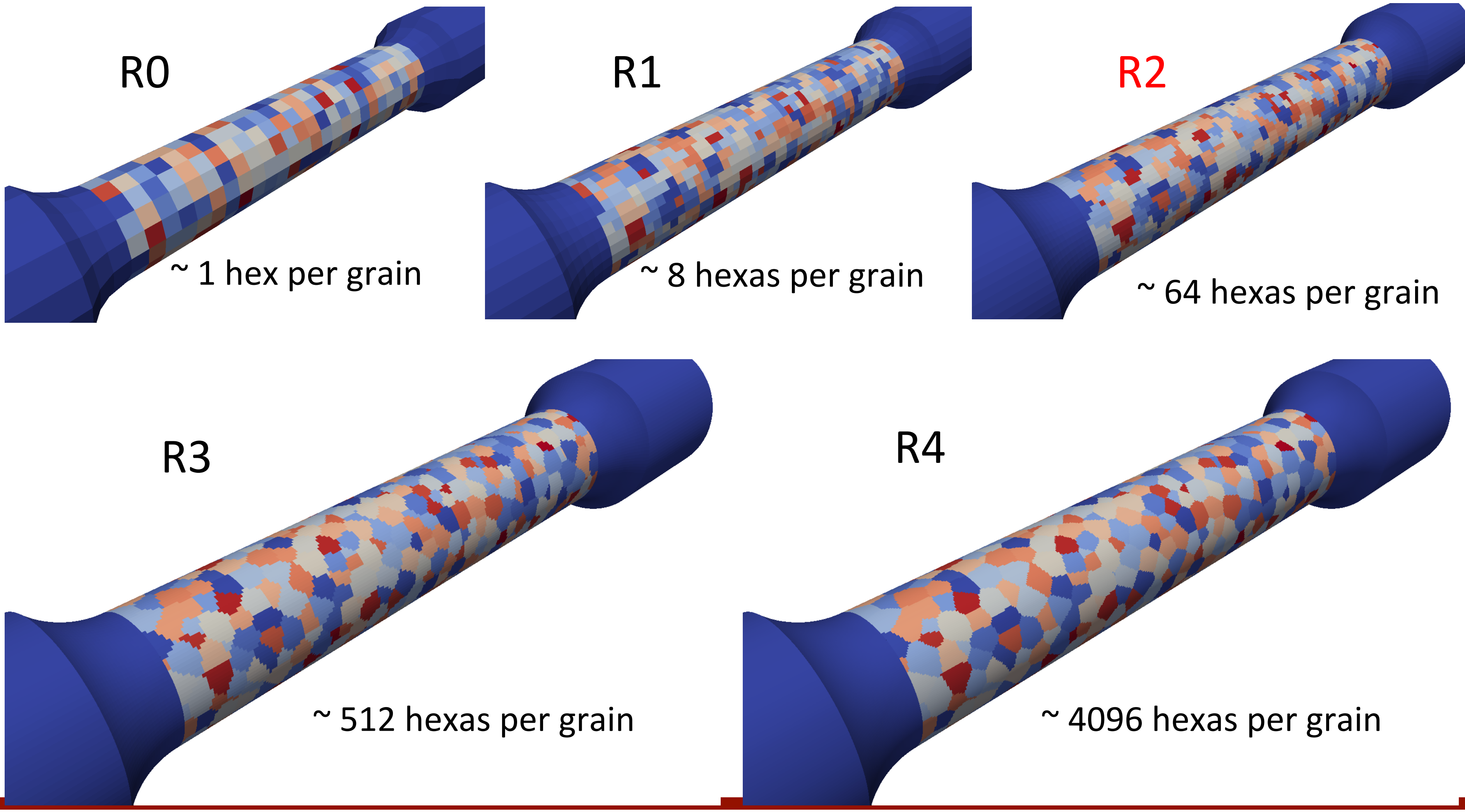


Hierarchy of Hexahedral Meshes



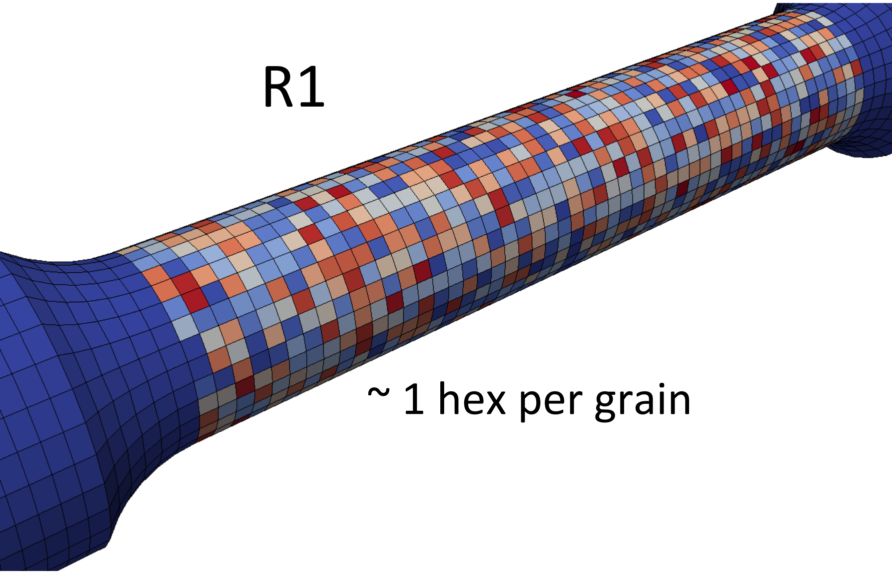
Voronoi Overlay of Hierarchy of Hexahedral Meshes

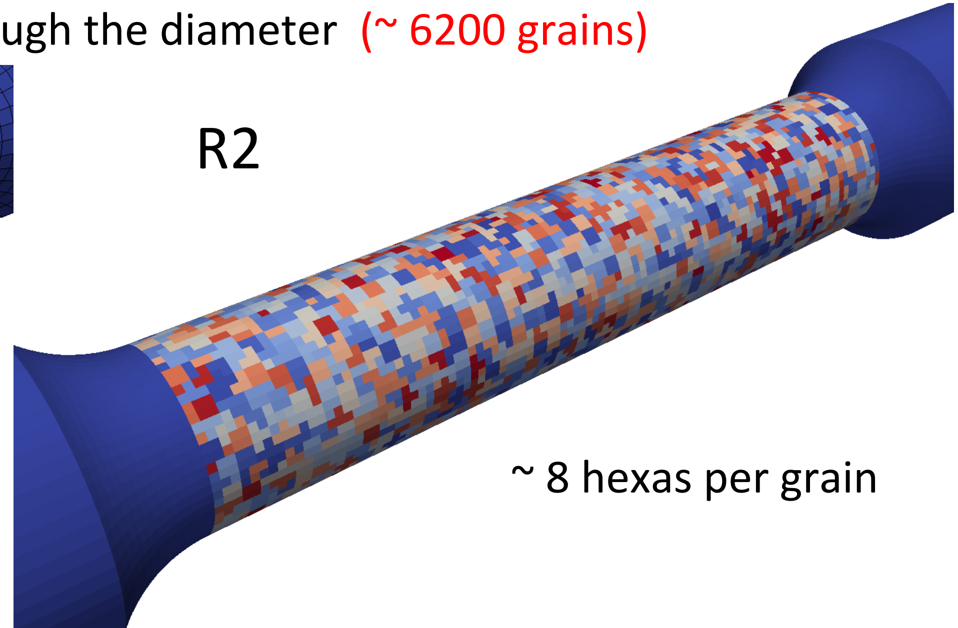
- One grain realization with ~ 6 grains through the diameter (~ 940 grains)
- Hierarchy of hexahedral meshes
- Pixelation decreases with mesh refinement

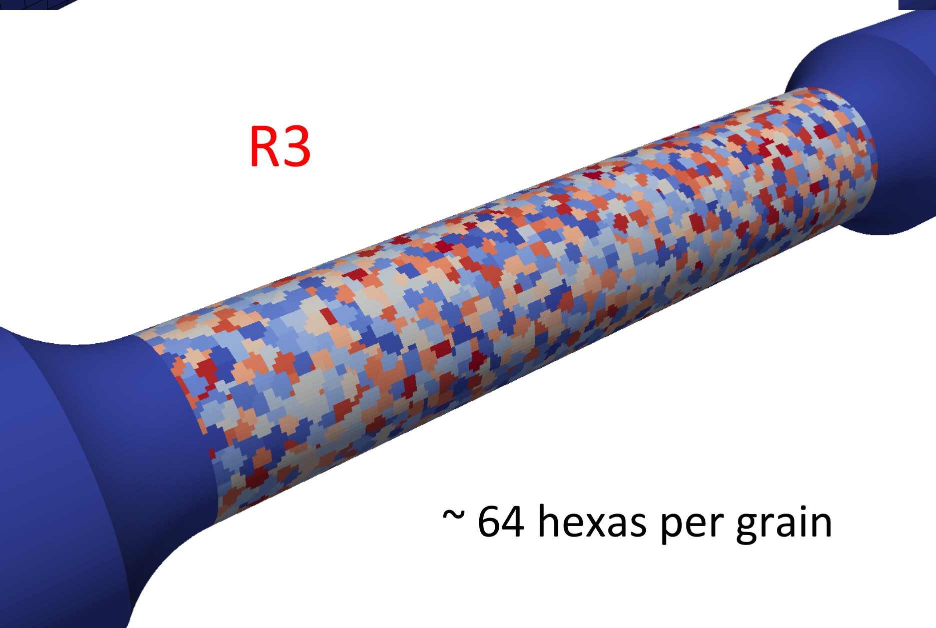


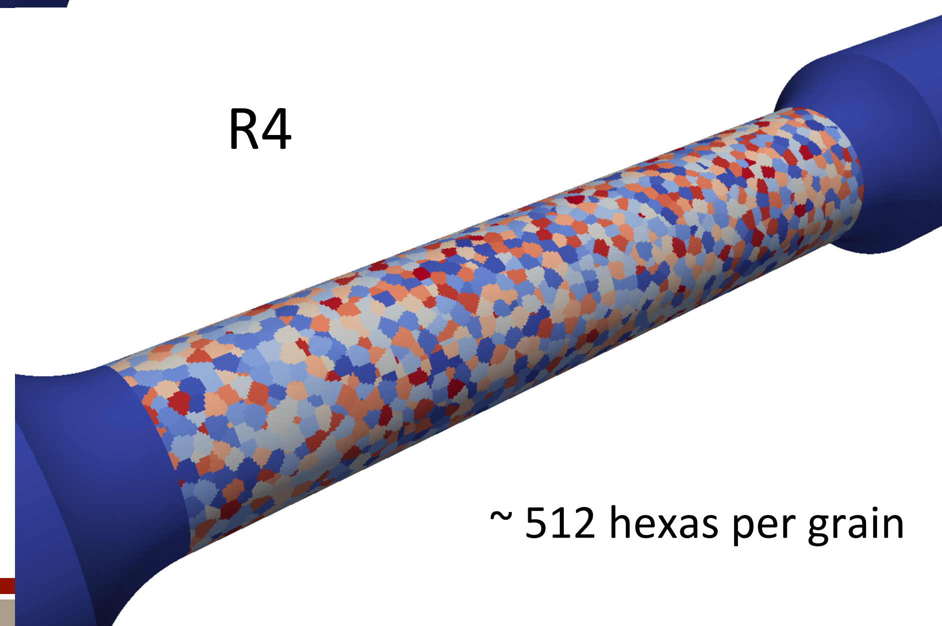
Voronoi Overlay of Hierarchy of Hexahedral Meshes

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









304L Single Crystal Elasticity Constants

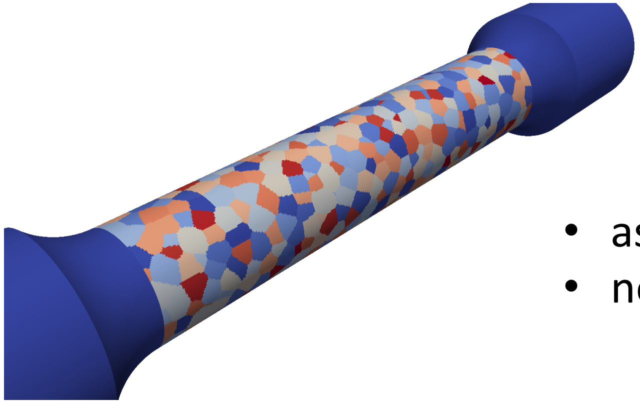
(Ledbetter, 1984)

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

(Dave Littlewood, John Emery, Chris Weinberger)

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

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

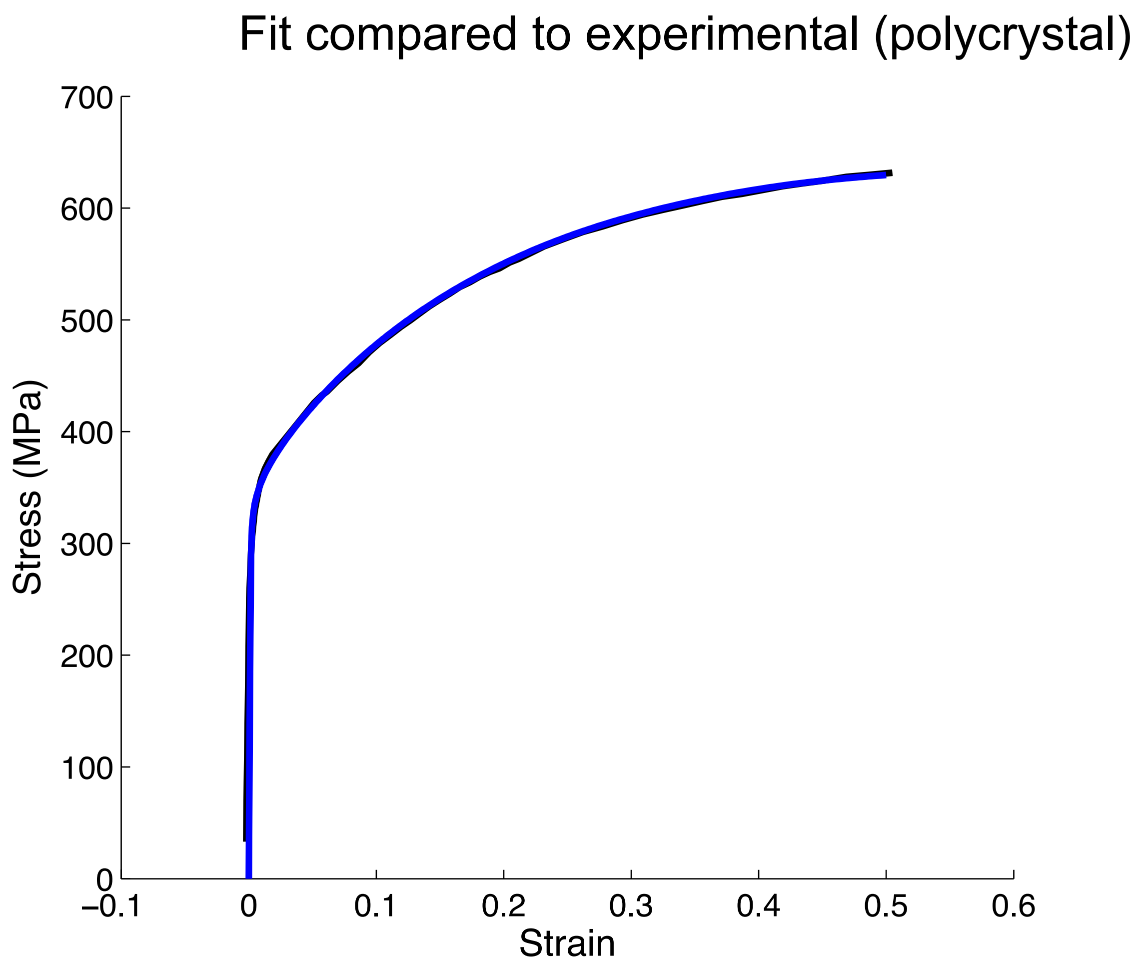
slip system slip rates: $\dot{\gamma}^\alpha = \dot{\gamma}_o \frac{\tau^\alpha}{g^\alpha} \left| \frac{\tau^\alpha}{g^\alpha} \right|^{1/m-1}$

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

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

Fit to 304L

(Chris Weinberger)



Fit parameters

$$\tau_o = 130$$

$$g_{so} = 230$$

$$G_o = 465$$

Uniaxial Tension, Displacement Control

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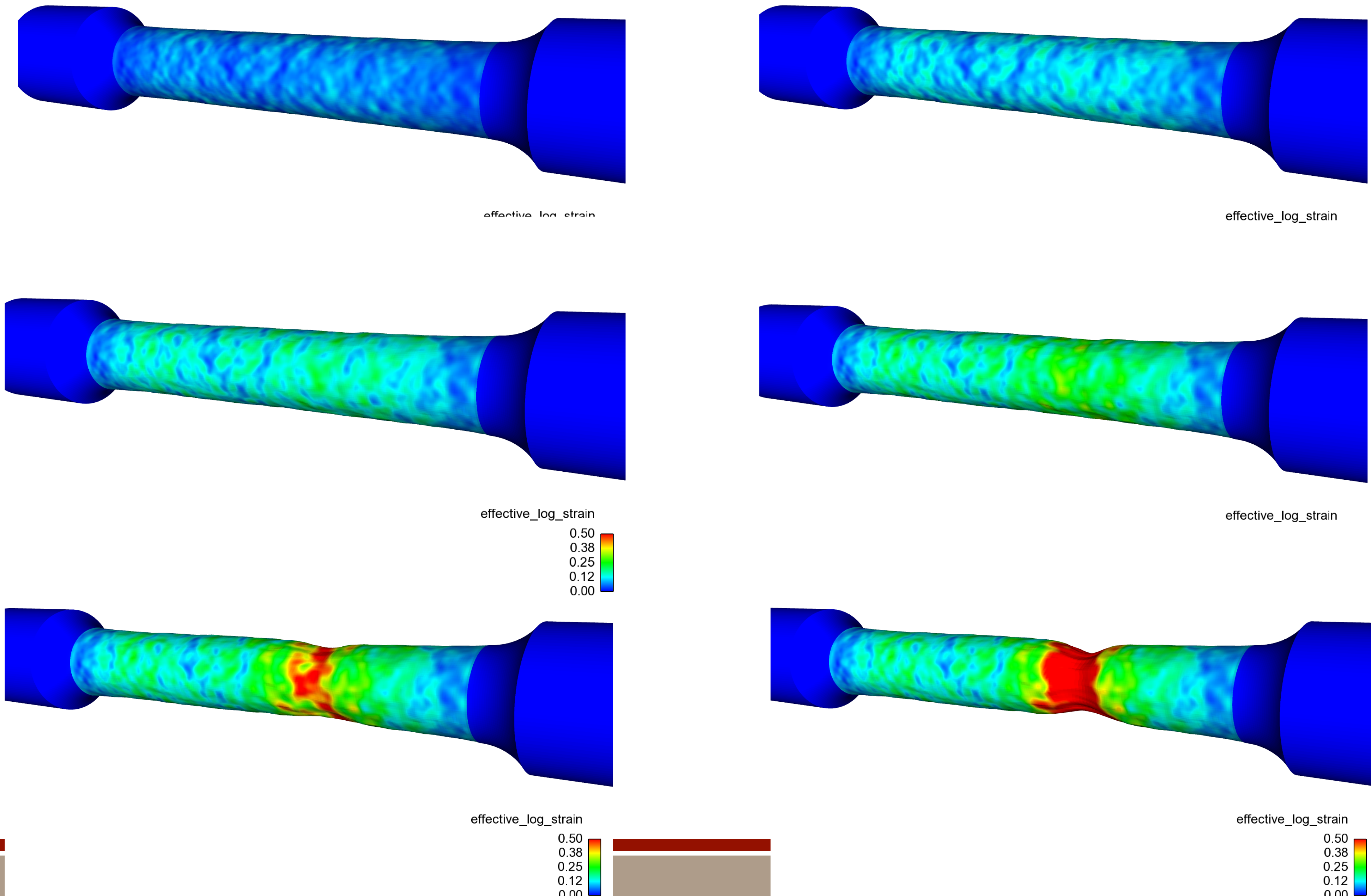
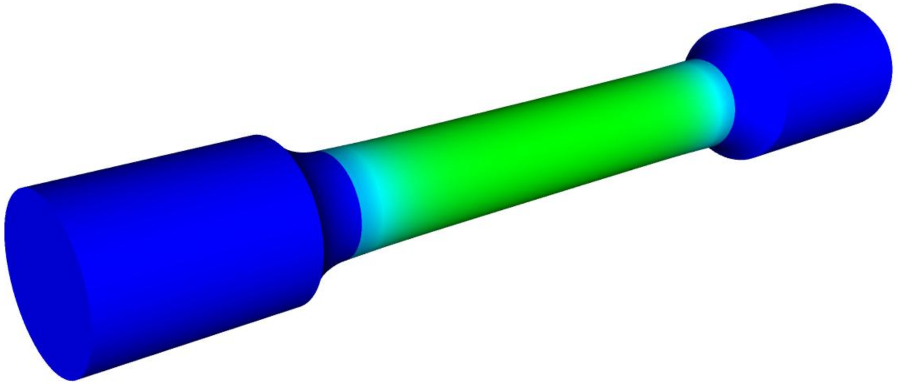
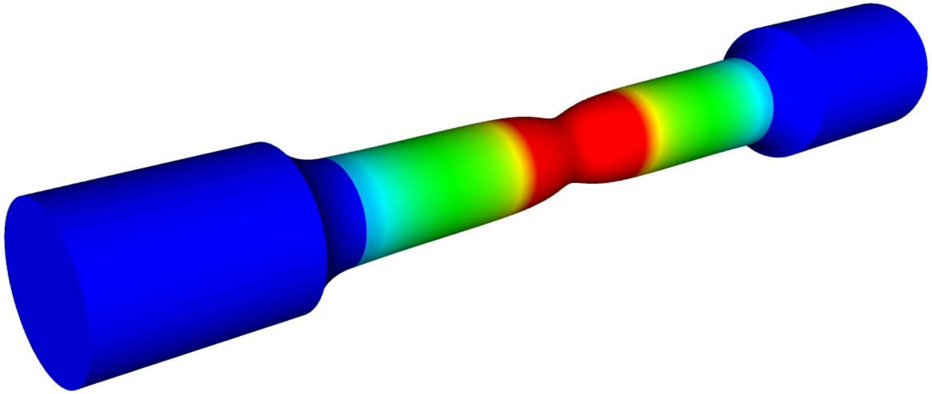
~ 12 grains across diameter, R3 mesh



Compare with Homogenized PDE (No Variability)

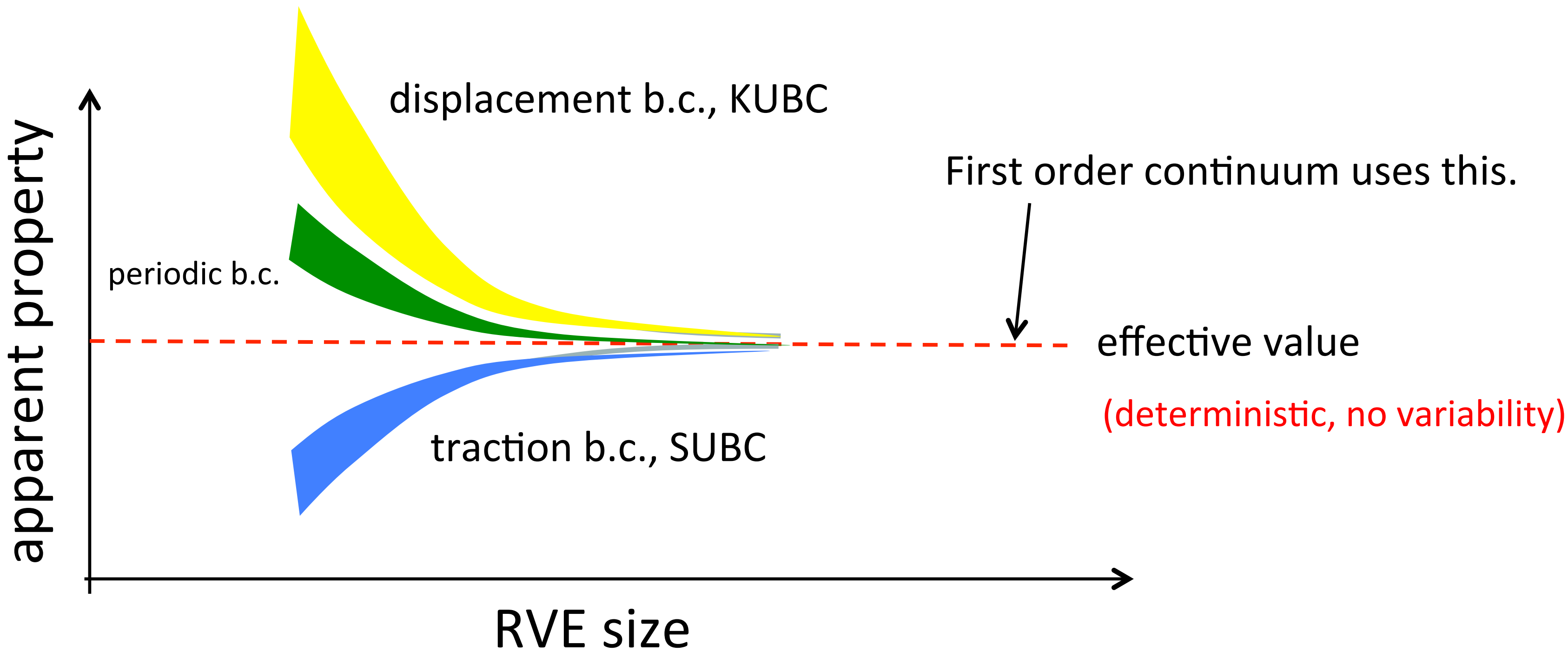


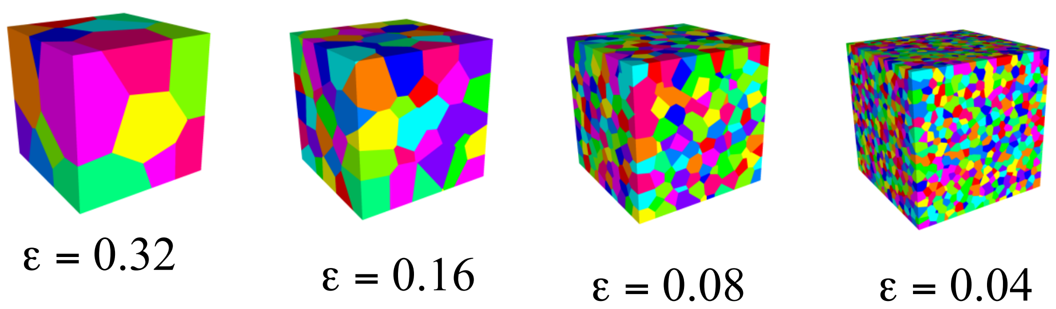
before necking



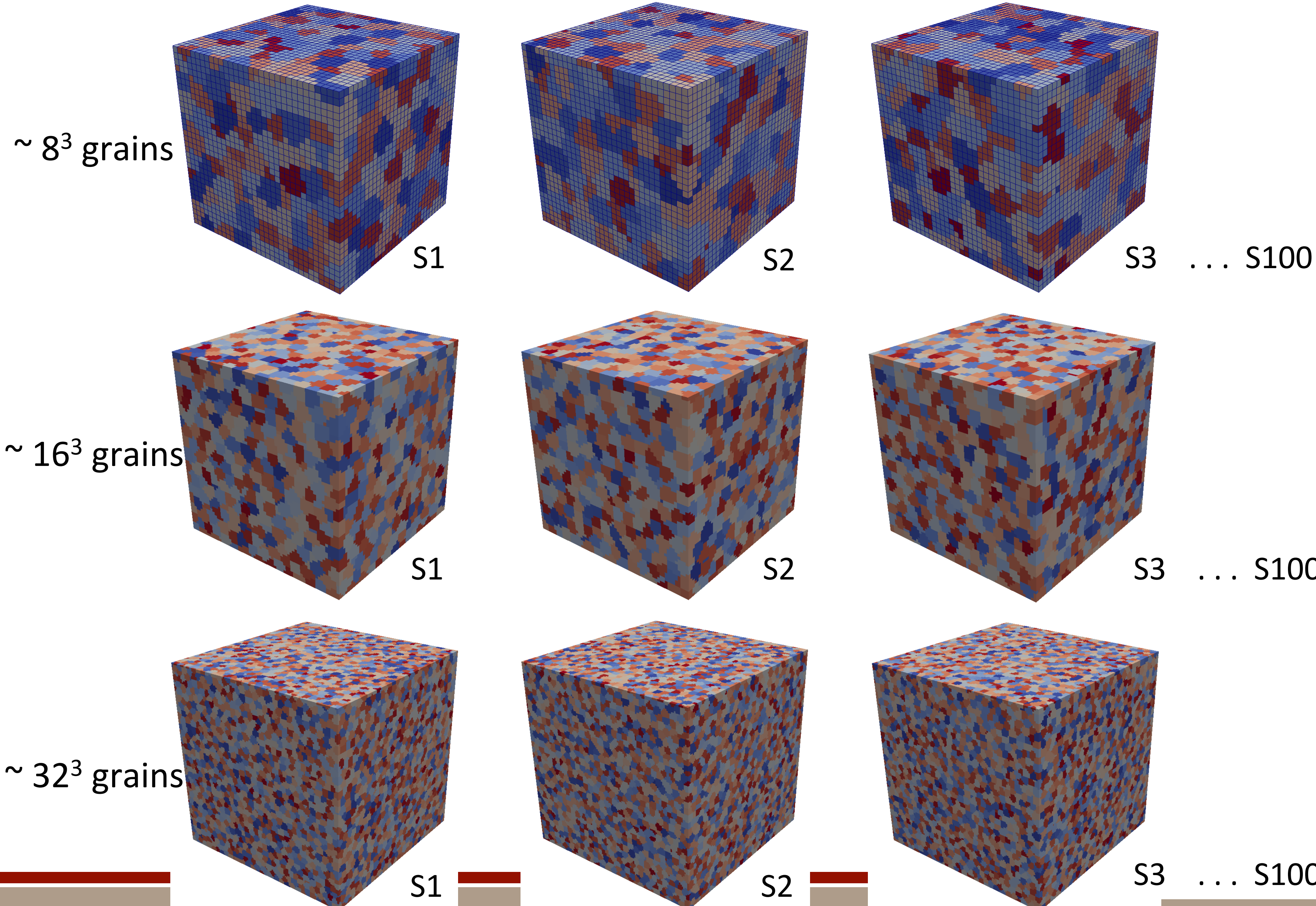
- symmetric
- neck is exactly at center

Apparent vs. Effective Material Properties





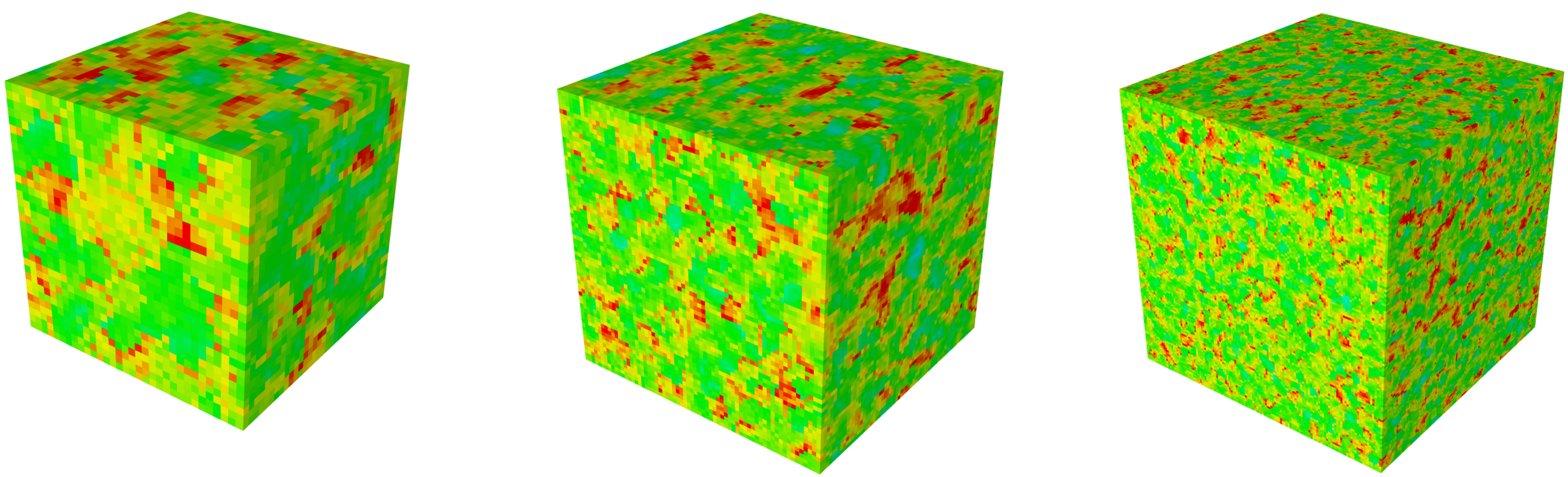
Stochastic Volume Elements



Stochastic Volume Elements

- traction boundary conditions corresponding to uniaxial stress state
- ideally would use periodic boundary conditions (couldn't get working in Adagio)
- recover average strain field
- calculate apparent moduli
- 100 realizations at each grain level
- take average

Von Mises stress field



~ 8^3 grains

~ 16^3 grains

~ 32^3 grains

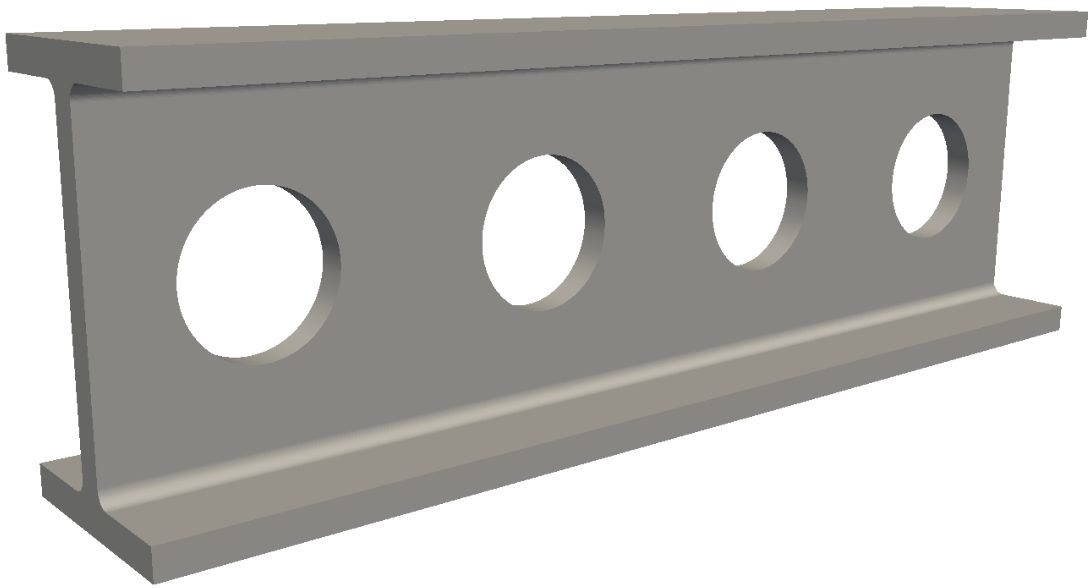
Convergence to Effective Isotropic Properties

- mean of 100 simulations at each “grain level”
- rational function extrapolation to ∞
- first order convergence rate

number of grains	apparent Young’s Modulus (GPa)	apparent Poisson’s ratio
~8^3 grains	177.2	0.317
~16^3 grains	180.6	0.312
~32^3 grains	182.4	0.310
∞	184.1	0.309

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

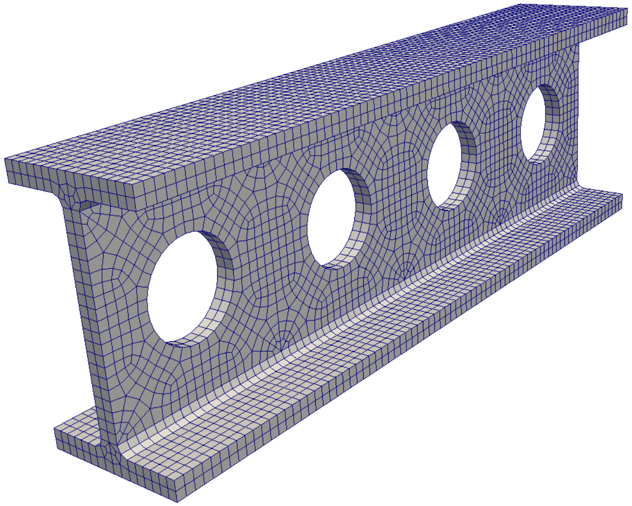
I-Beam Example



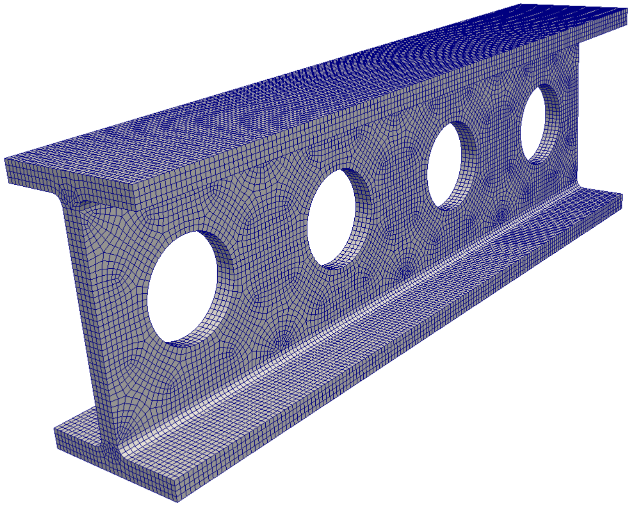
- tension
- bending
- torsion

- Study statistics of direct numerical simulations
- Compare to homogenized solution
- Look for evidence of Type 2 material variability

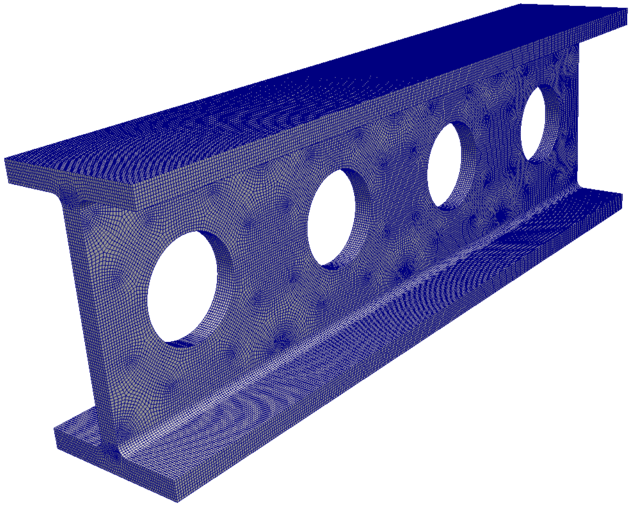
Hierarchy of Hexahedral Meshes



- R0
- 8,576 hexas



- R1
- 69K hexas

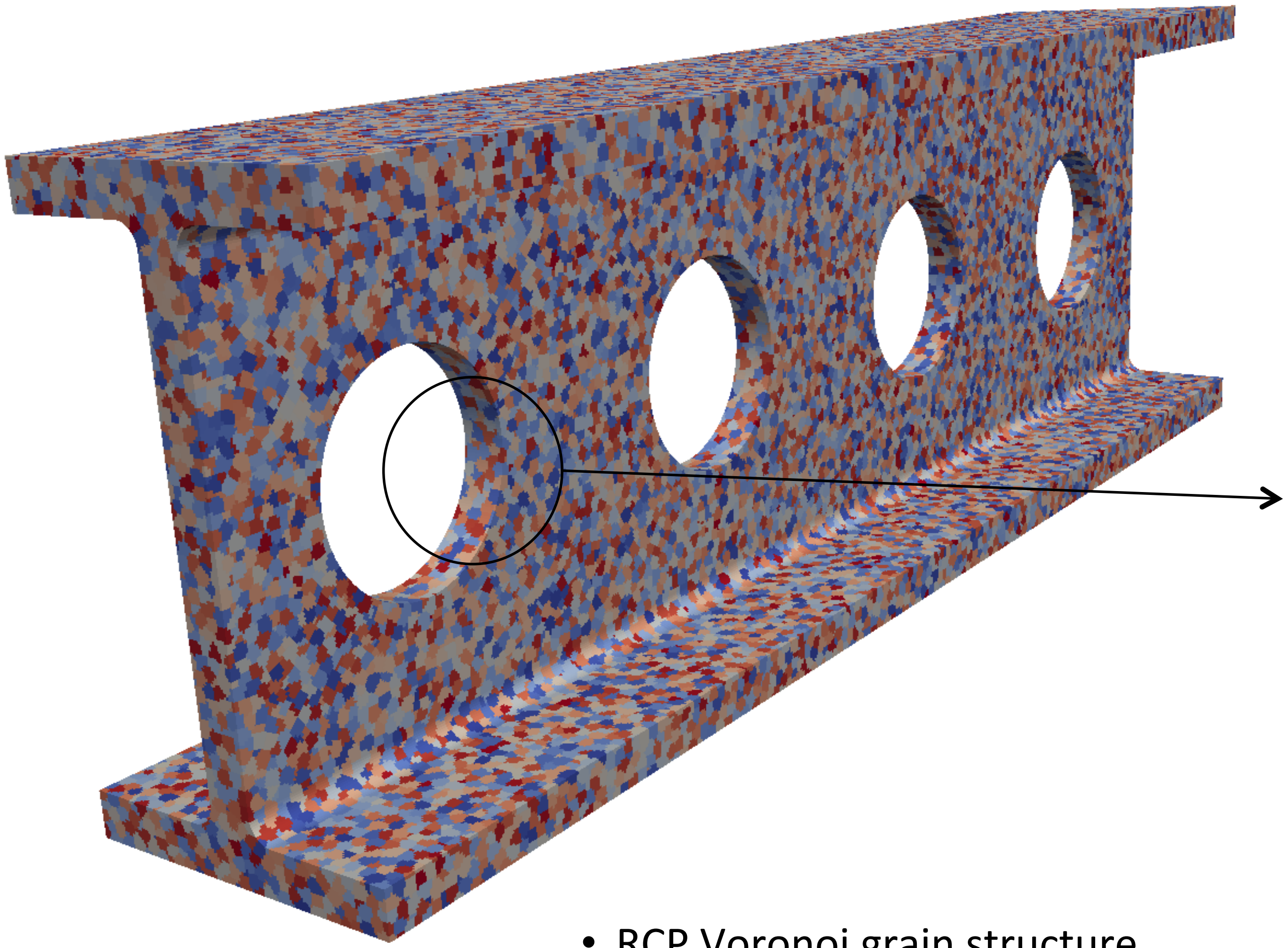


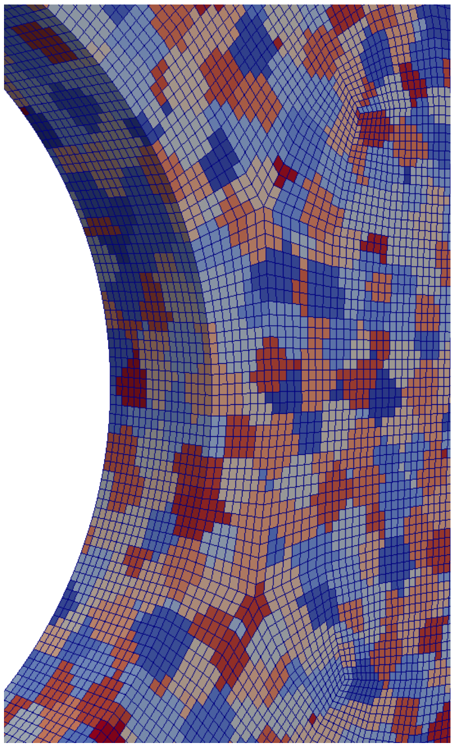
- R2
- 549K hexas

- R3
- 4.4M hexas

- R4
- 35M hexas

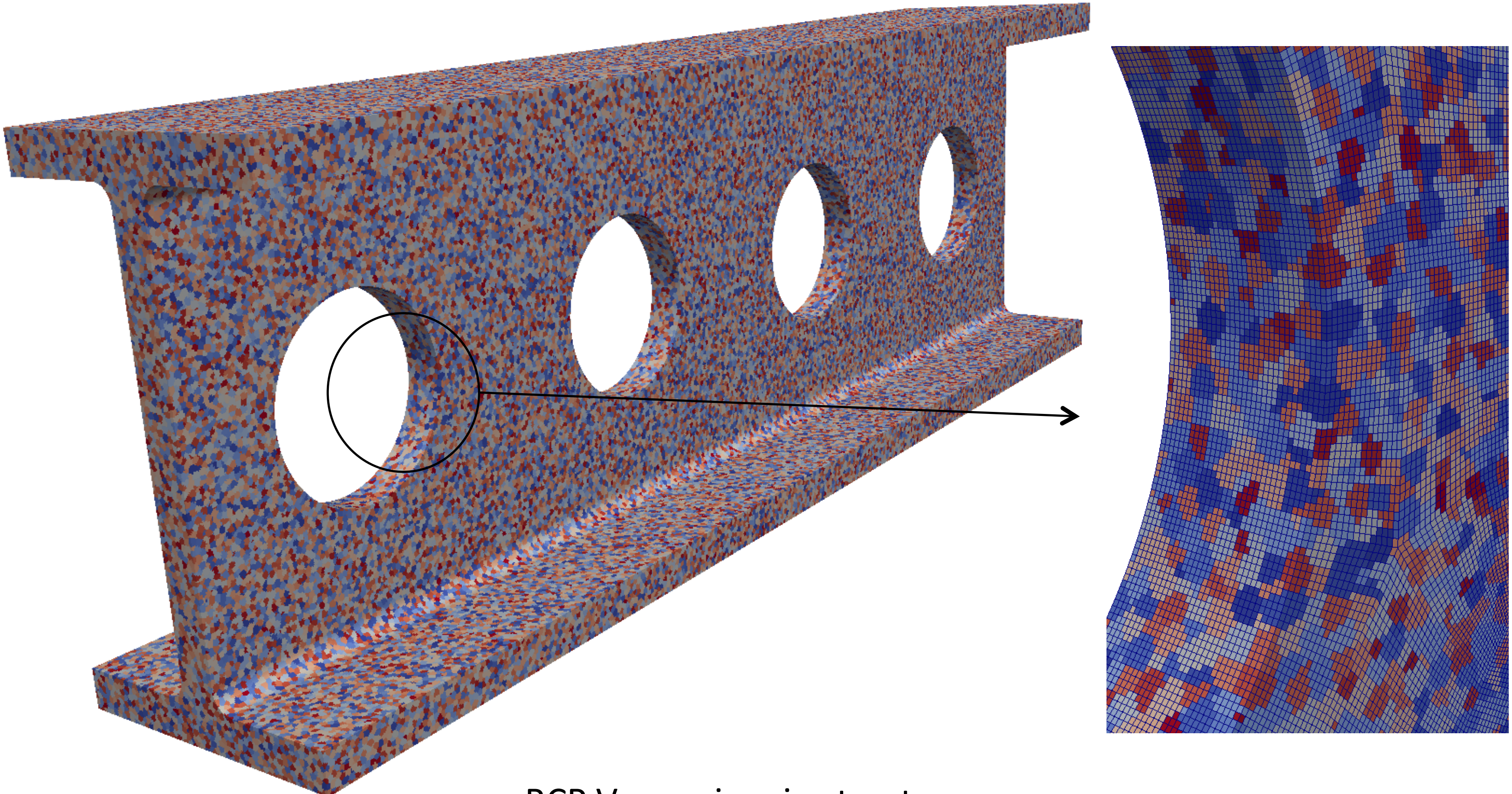
Thickness/grain ratio = 4





- RCP Voronoi grain structure
- 60K grains
- hex mesh overlay = R3 (4.4M elements)

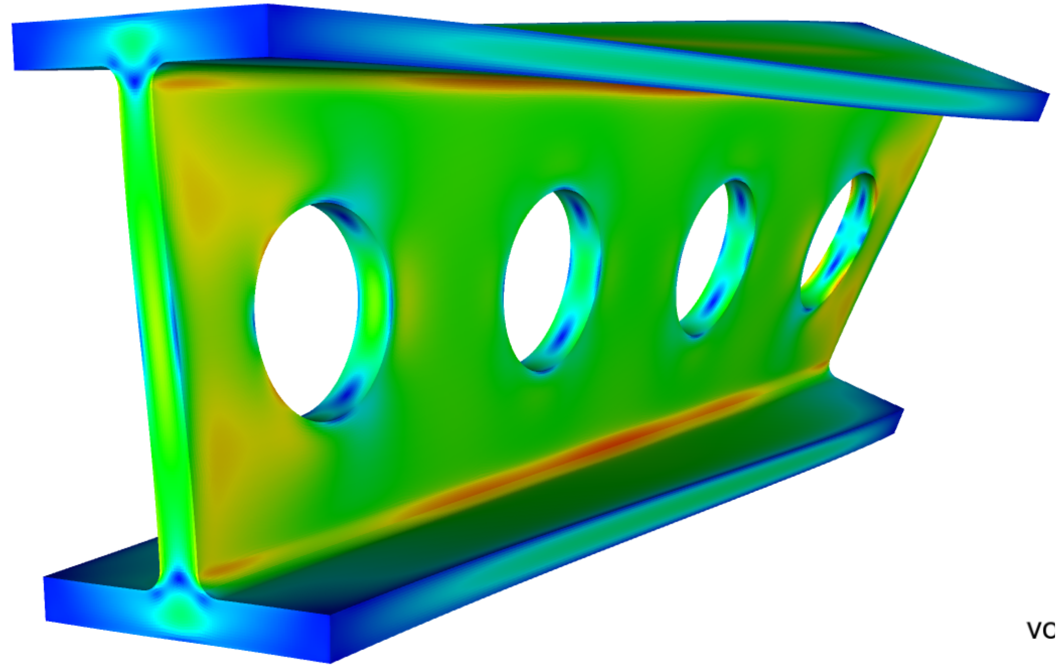
Thickness/grain ratio = 8



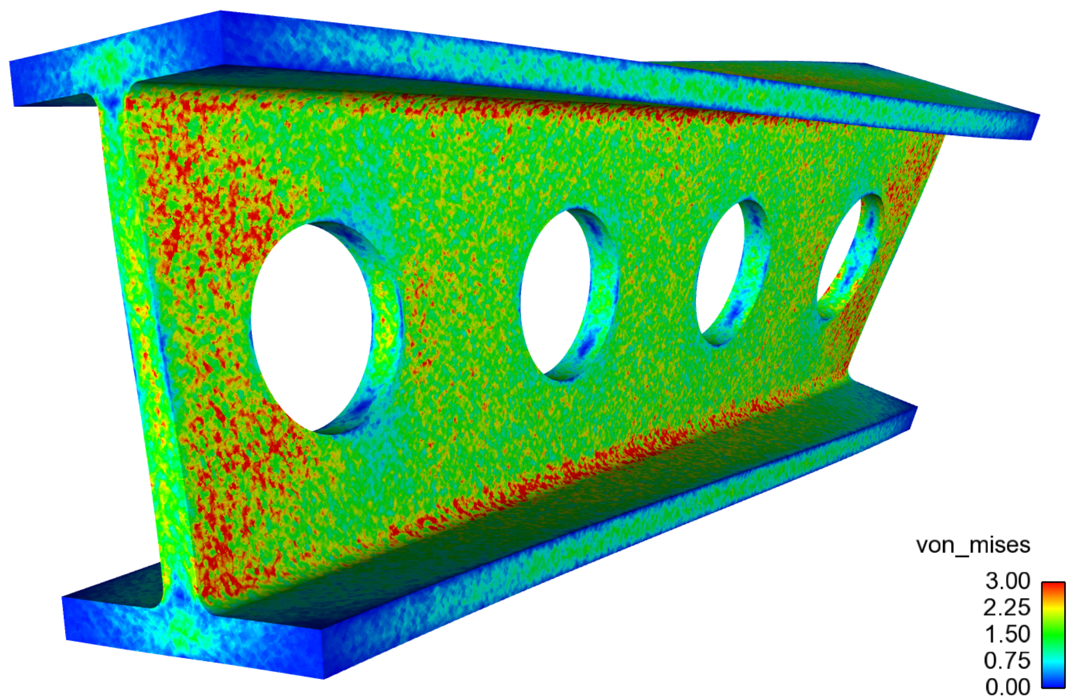
- RCP Voronoi grain structure
- 420K grains
- hex mesh overlay = R4 (35M elements)

Thickness/grain ratio = 8

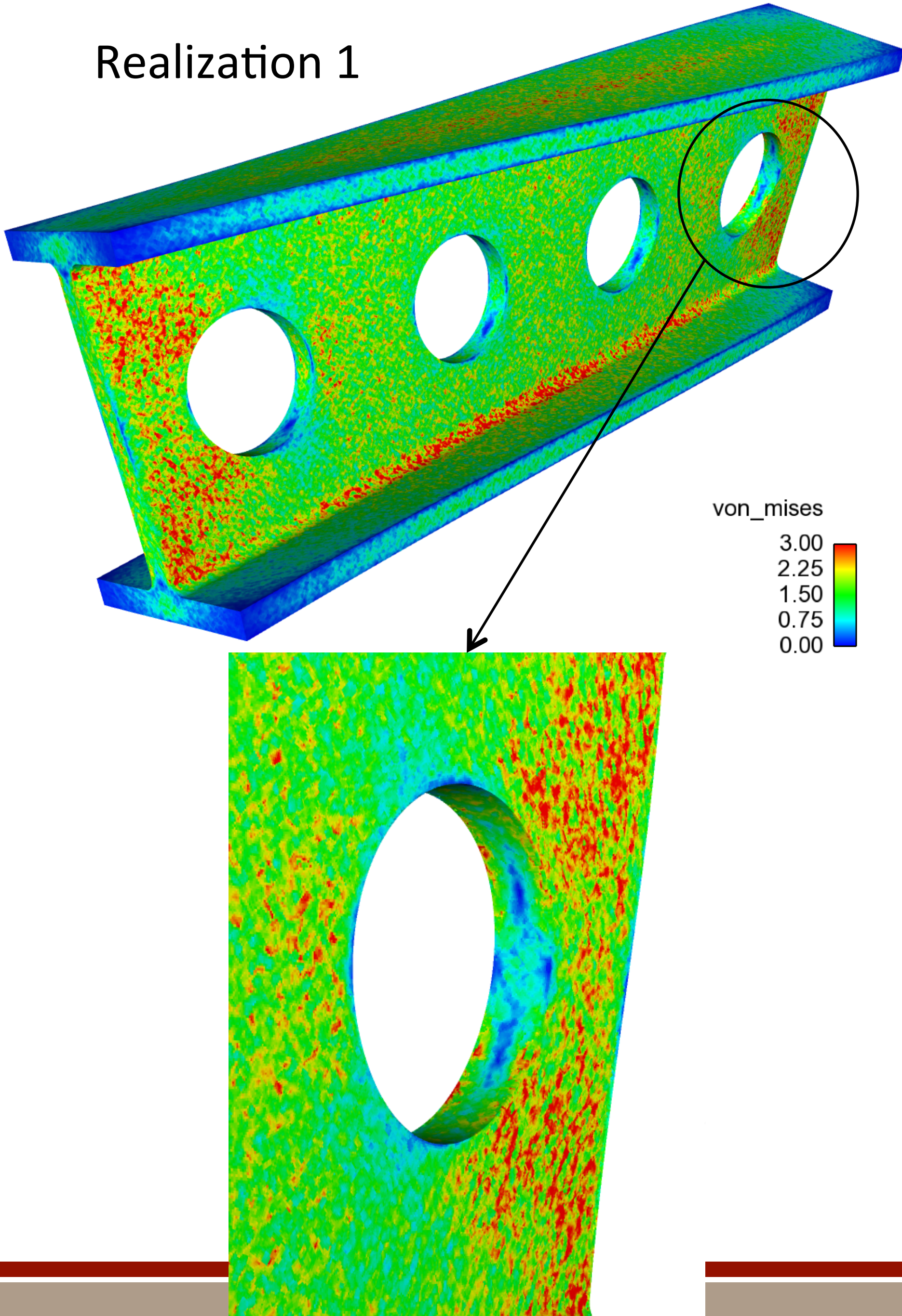
VM stress field, Homogenized



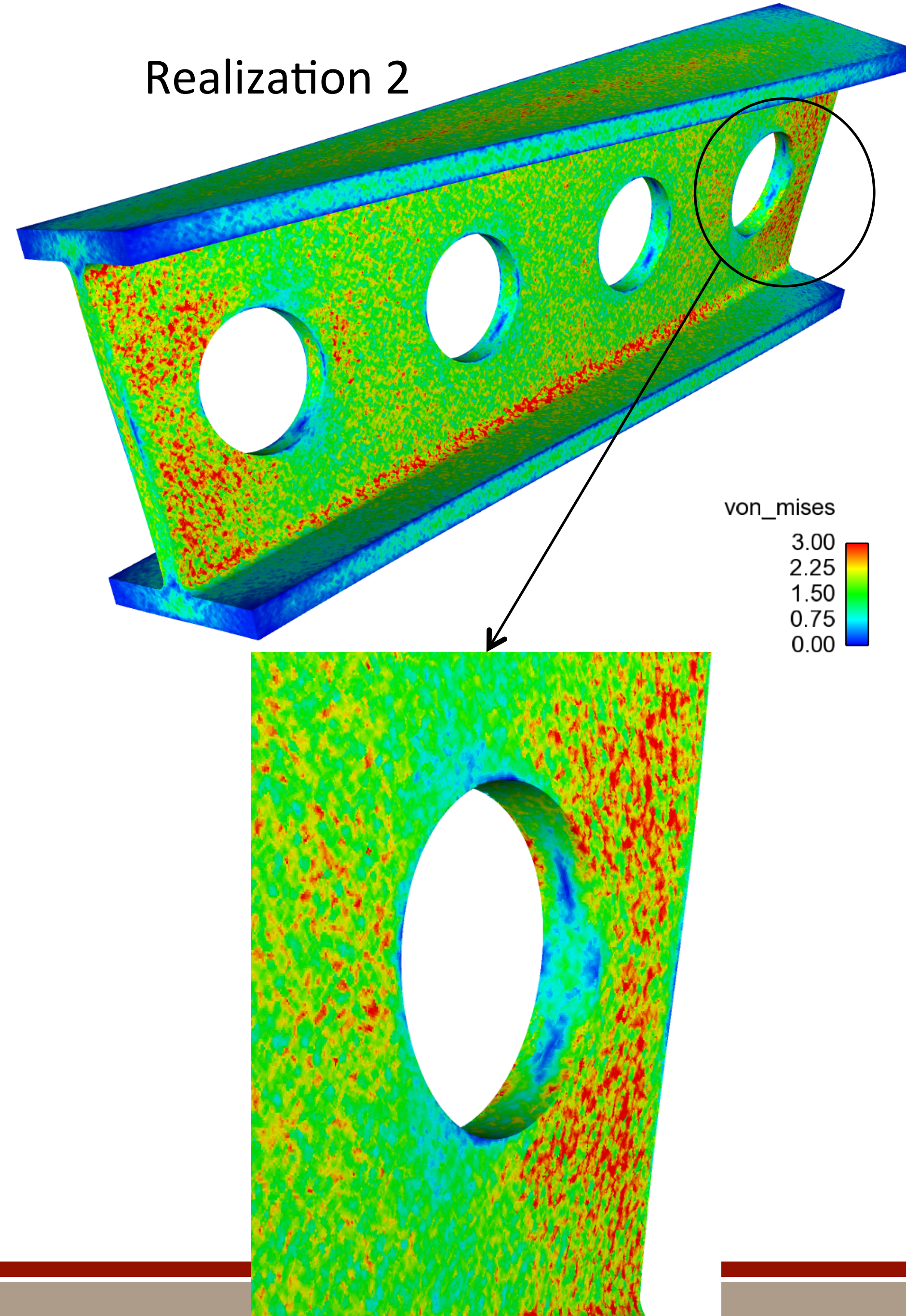
VM stress field, DNS



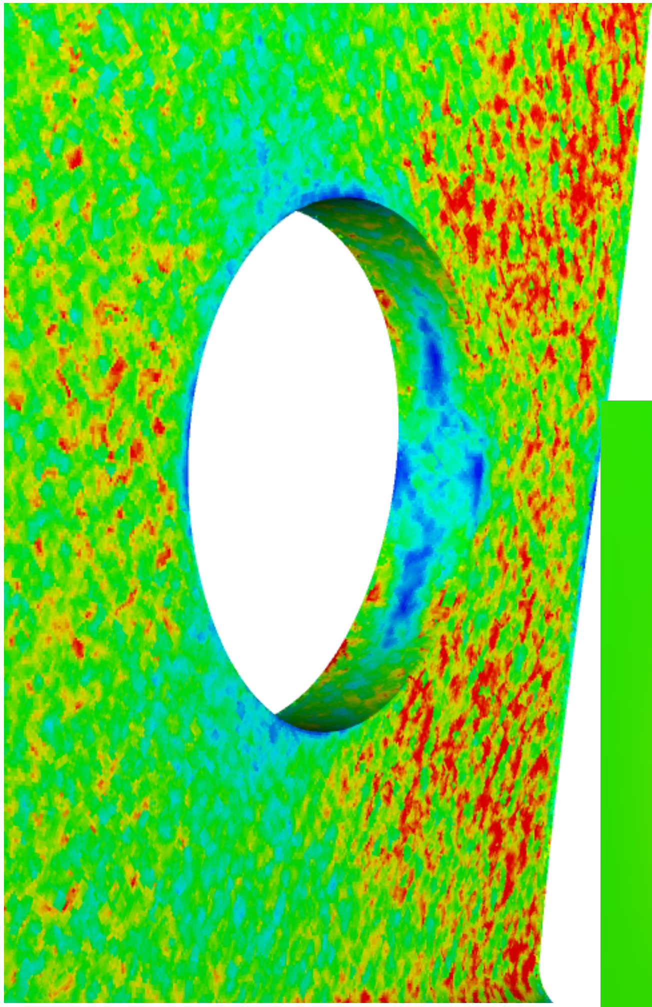
Realization 1



Realization 2

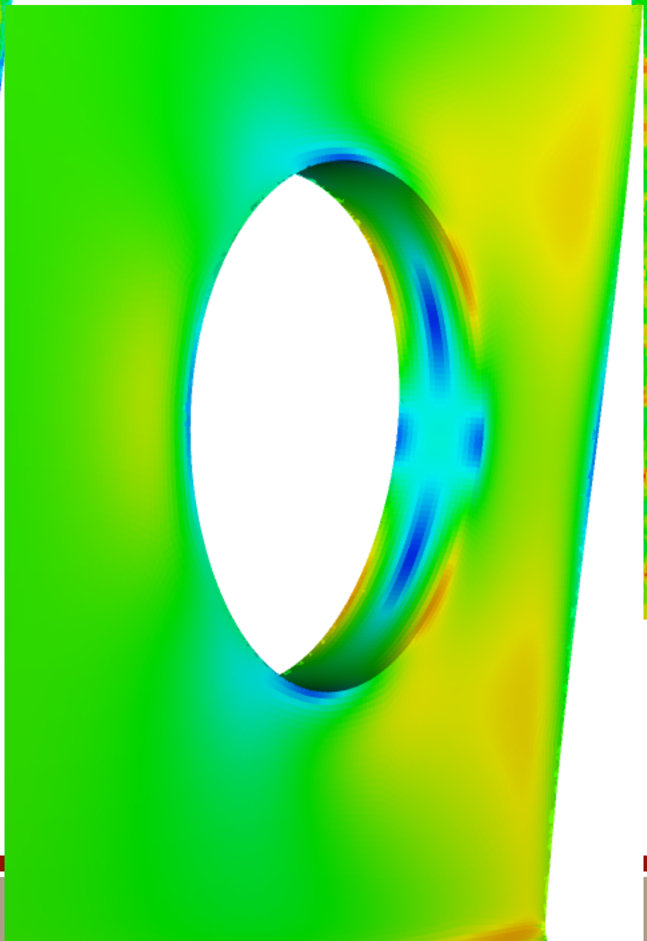


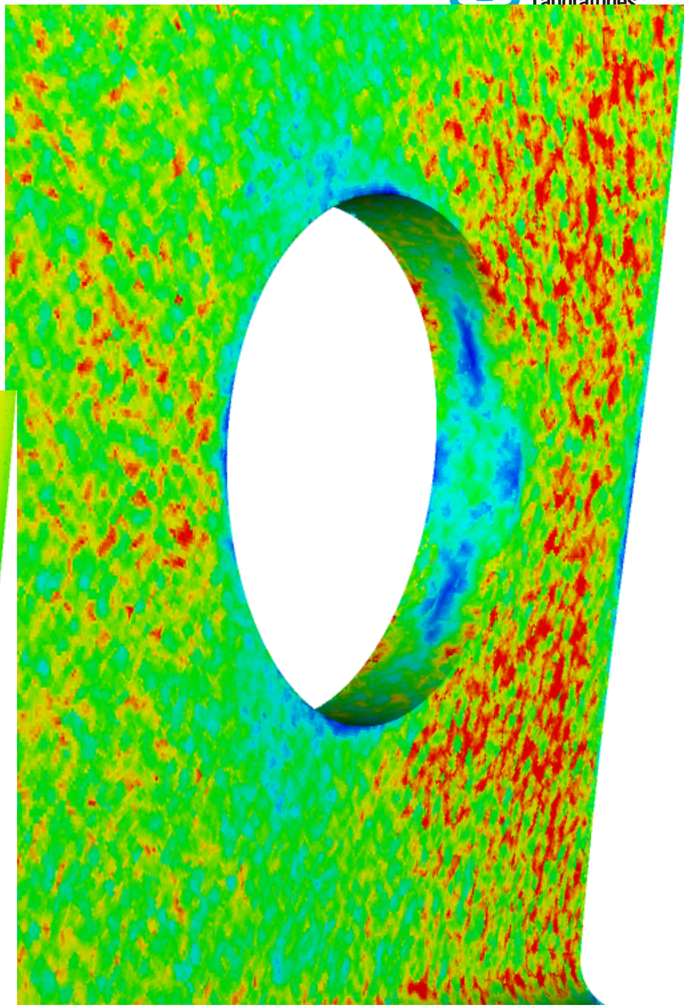
Symmetry Breaking



Realization 1

Homogenized solution



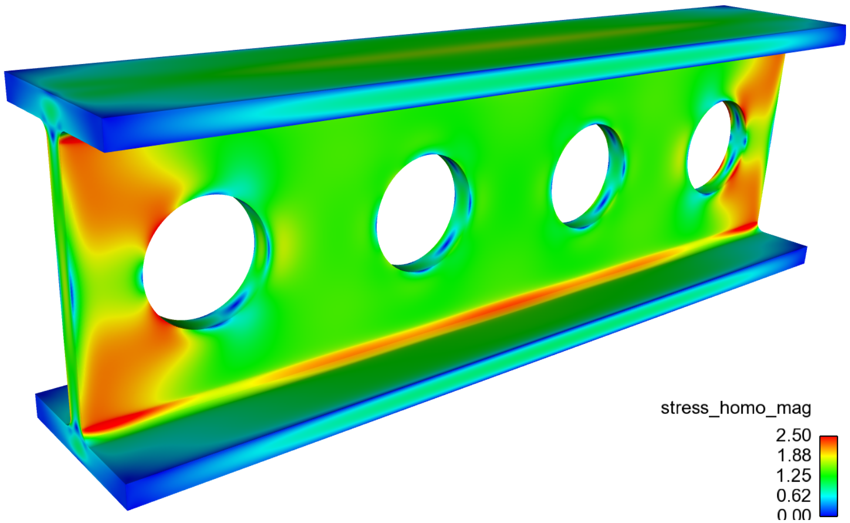


Realization 2

Ensemble Results

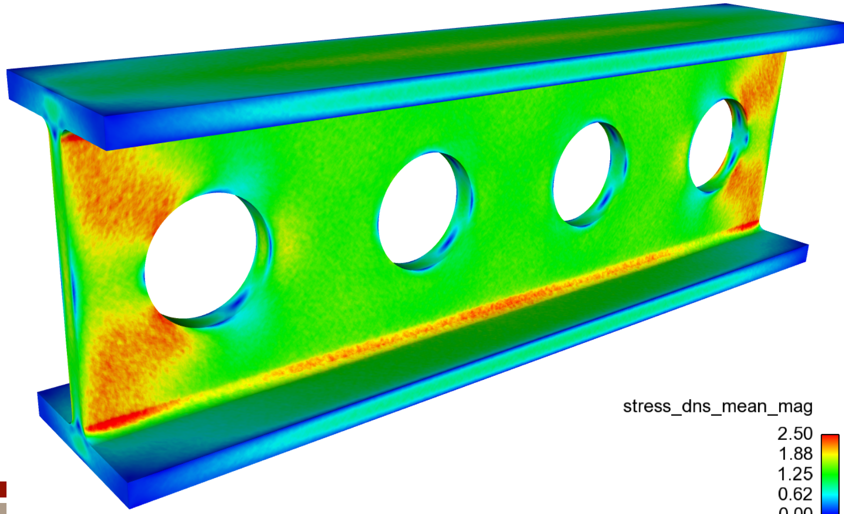
- 100 realizations for thickness/grain ratio = 4
- 62 realizations for thickness/grain ratio = 8
- magnitude of ensemble average stress tensor
- standard deviation of stress ensemble
- magnitude of difference of ensemble average stress tensor and homogeneous solution
- projection of DNS solutions to coarse scale mesh and repeat

Ensemble Results, 62 Realizations

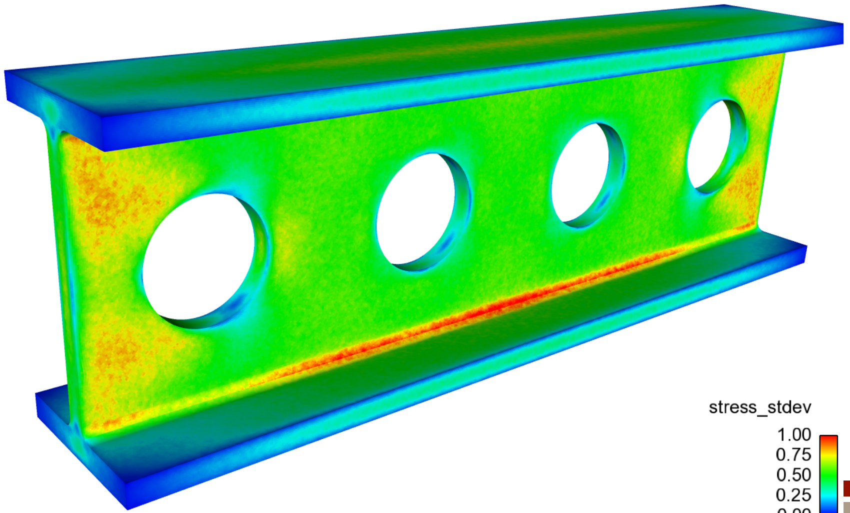


homogeneous solution
(stress magnitude)

DNS
(magnitude of ensemble average stress)



DNS
(stress standard deviation)



Ensemble Results minus Homogeneous

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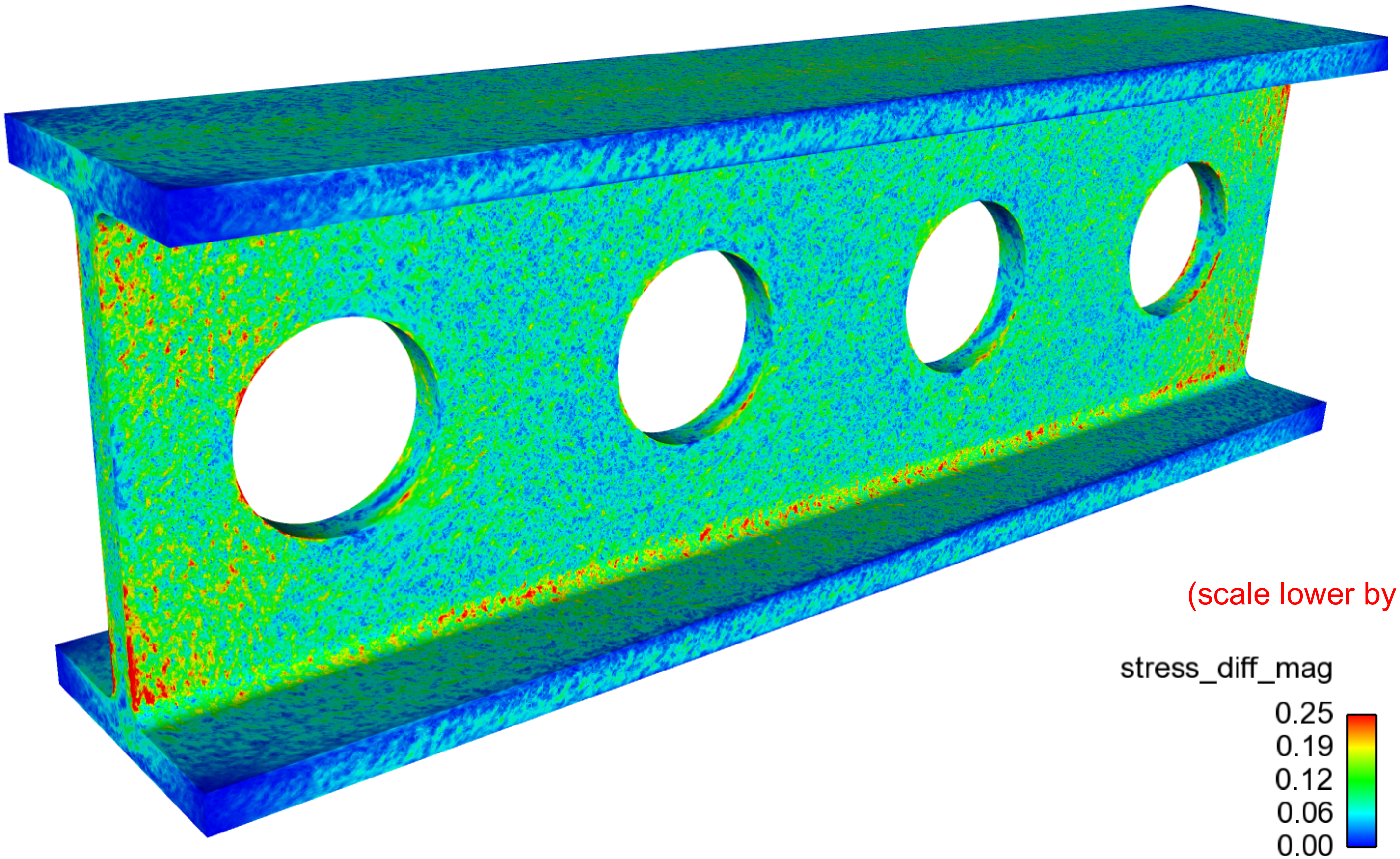
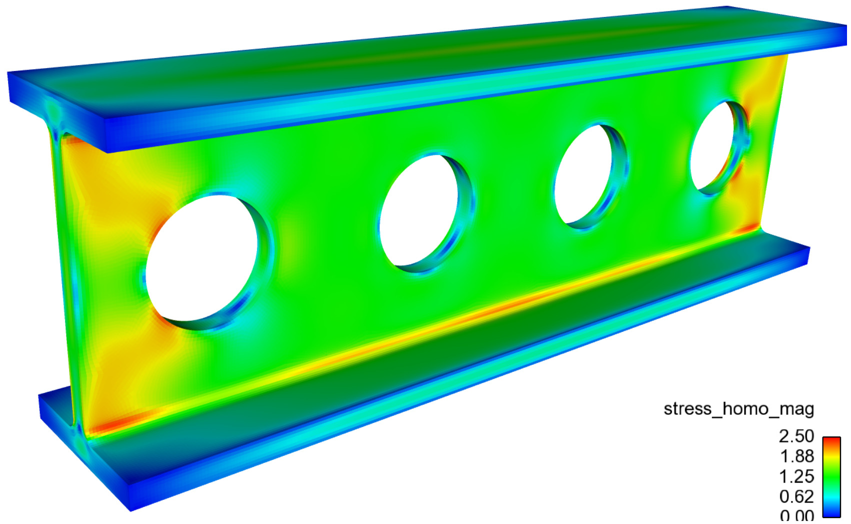


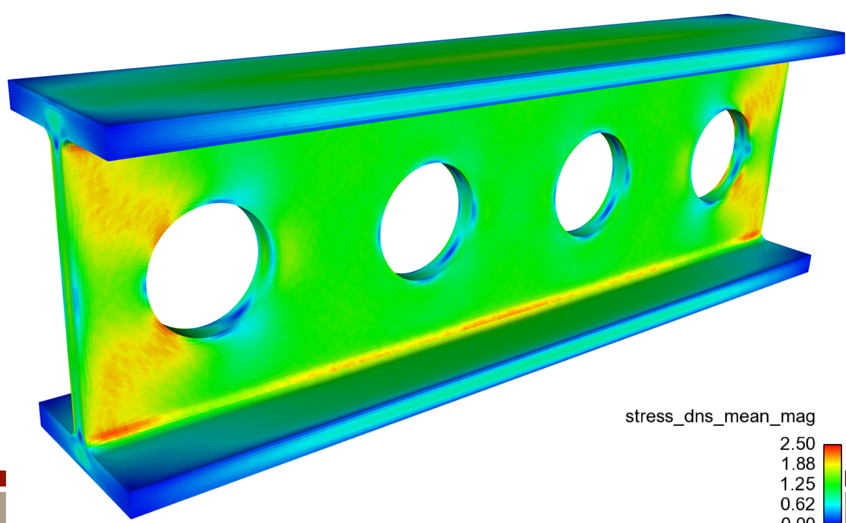
magnitude (ensemble average stress – homogeneous stress)

Projection/Average to Coarse Mesh, R2

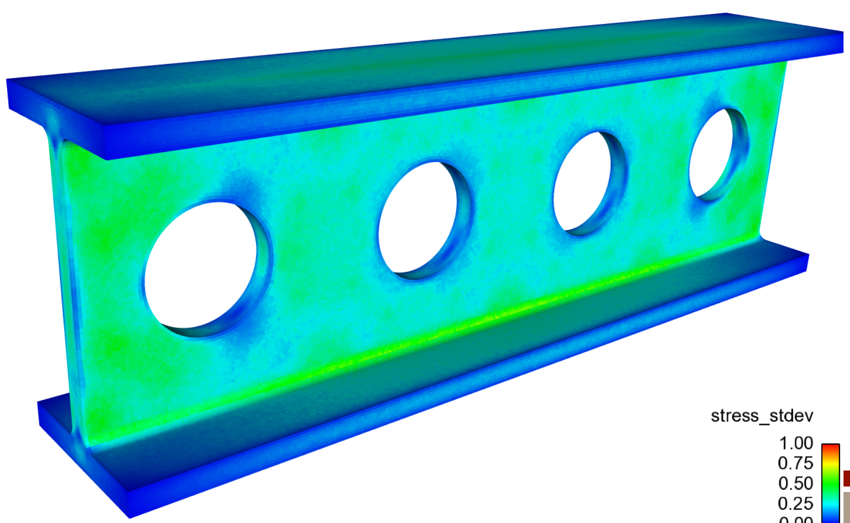


homogeneous solution
(stress magnitude)

DNS
(magnitude of ensemble average stress)

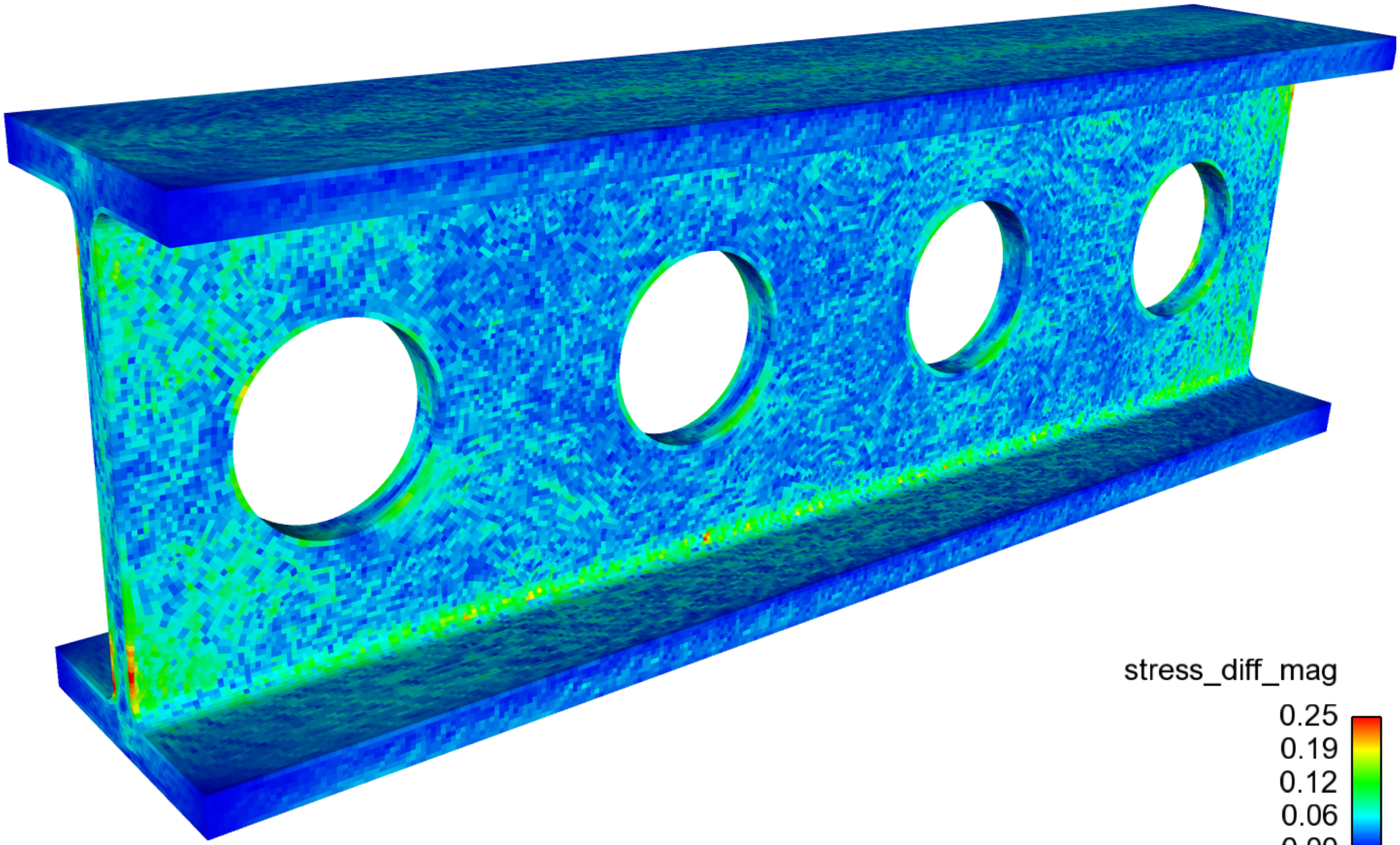


DNS
(stress standard deviation)



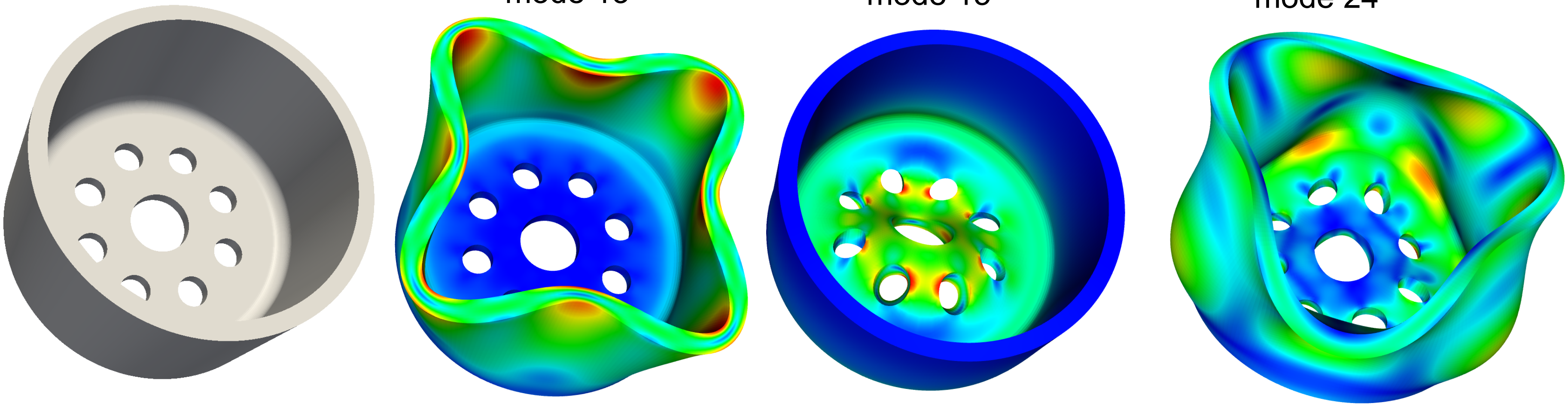
Ensemble Results minus Homogeneous

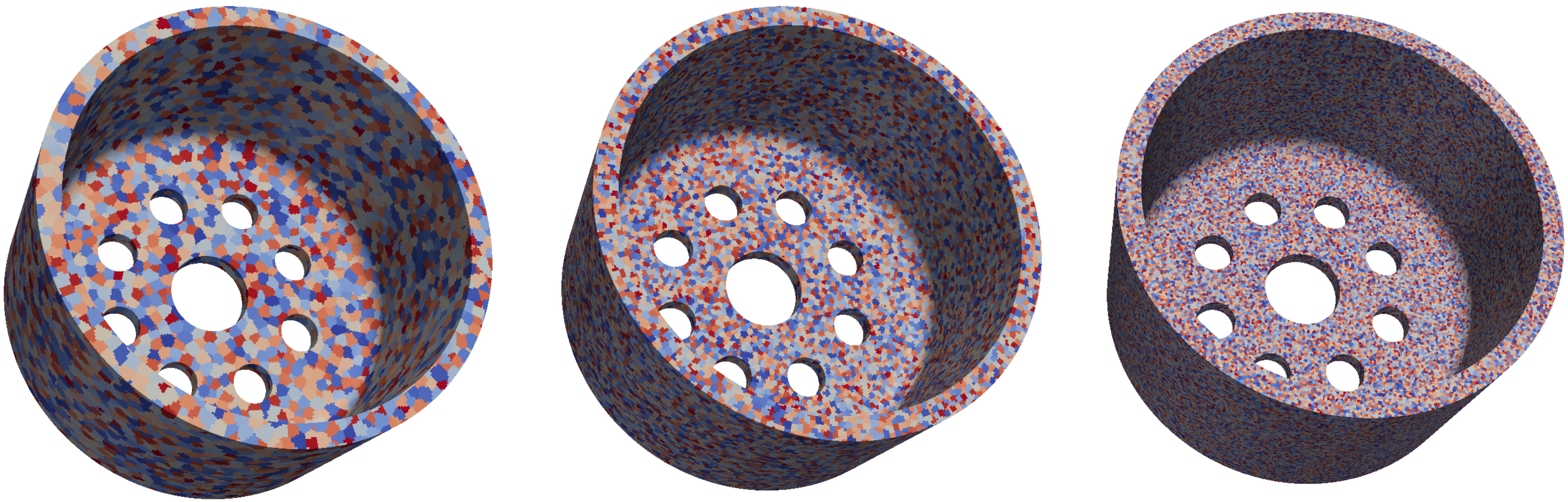
Projection/Average to Coarse Mesh, R2



Direct Numerical Simulation, Structural Dynamics

idealized part | mode 13 | mode 15 | mode 24





- 2 grains across wall thickness
- ~8600 grains

- 4 grains across wall thickness
- ~53K grains

- 4 grains across wall thickness
- ~53K grains

Outline

1. Review of homogenization theory
    - apparent vs. effective material properties
    - weak convergence
    - Type 1 and Type 2 material variability
2. Direct numerical simulations and comparison to homogenized PDE solution
    - Voronoi microstructure
    - hexahedral mesh overlay
    - boundary value problems
3. Type 2 material variability in macroscale simulations: a path forward
    - Mindlin's continuum formulation
    - elastic formulation
    - nonlinear response via FE^2

A Path Forward for Including Microscale Variability in Macroscale Models

- Homogenization theory indicates that for finite microstructure, strain gradient effects are present (strain energy depends on both strain and strain gradient).
- Additionally, expect to see a “size effect”, even for homogeneous fields, at the macroscale (“apparent” material properties described by Huet, 1990).
- Several strain-gradient continuum formulations
- Following Josh Robbins lead, going to explore the use of Mindlin’s micromorphic formulation (1964). (Josh Robbins, org 1443, LDRD, “Micromorphic Continua for High Fidelity Physics Models”)
- Mindlin, 1964, “Microstructure in Linear Elasticity”
- Mindlin’s formulation allows existing H^1 FEA formulations to be used, but with extra nodal degrees of freedom.
- much recent work by W.K. Liu’s group at NU for modeling localization phenomena

Mindlin’s Micromorphic Continuum Formulation

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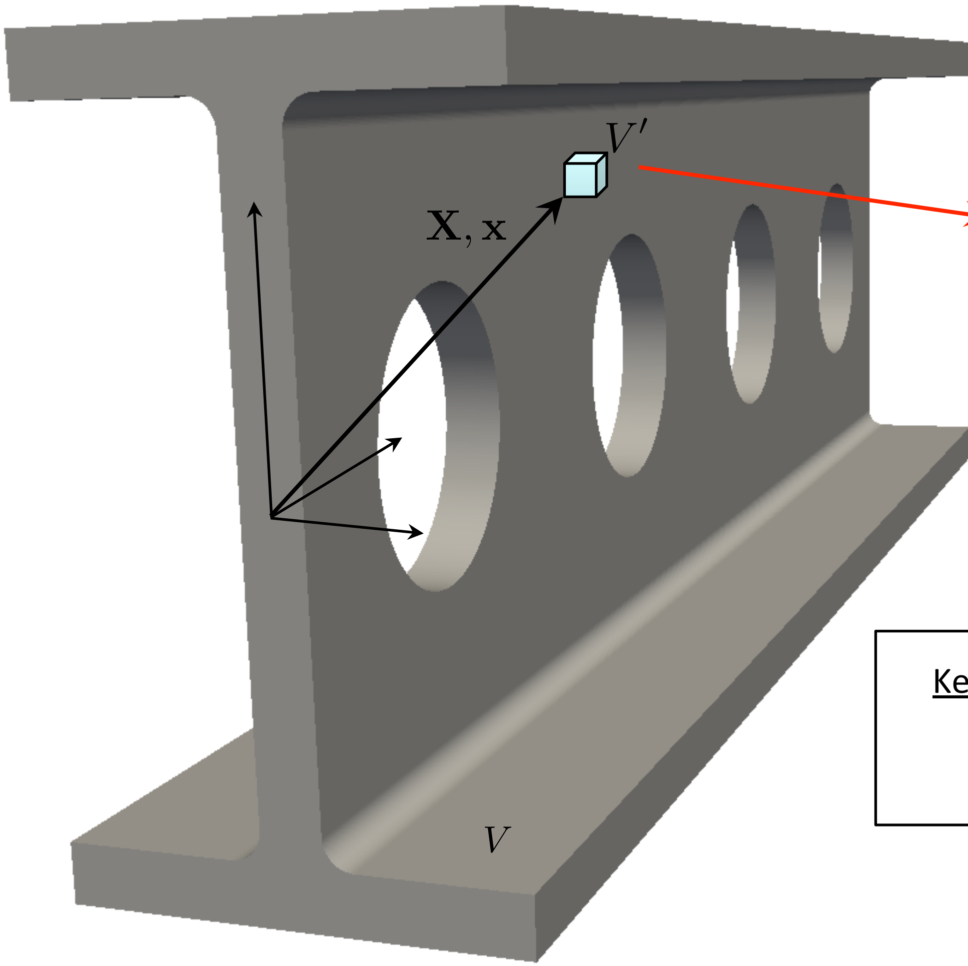
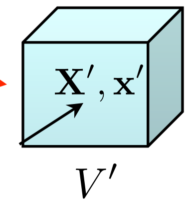
(Mindlin, 1964, “Micro-structure in Linear Elasticity,” *Archive for Rational Mechanics and Analysis*, v 16, 51-78.)





Embedded in each material particle, there is assumed to be a “micro-volume” V'

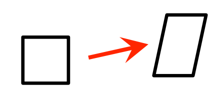
macro-displacement, $\mathbf{u} = \mathbf{x} - \mathbf{X}$

micro-displacement, $\mathbf{u}' = \mathbf{x}' - \mathbf{X}'$

$$\mathbf{u} = \mathbf{u}(\mathbf{x})$$
$$\mathbf{u}' = \mathbf{u}'(\mathbf{x}, \mathbf{x}')$$

<u>Key Approximation</u>: Approximate $\mathbf{u}'$ as linear on V'.

$$u'_i \approx x'_j \, \psi_{ji}$$



micro-deformation $\psi_{ij} = \dfrac{\partial u'_j}{\partial x'_i}$

Micro-deformation $\mathbf{\Psi}(\mathbf{x})$ is constant on V' but varies on macro-scale V.

Mindlin's Micromorphic Continuum Formulation

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relative deformation $\gamma_{ij} = u_{j,i} - \psi_{ij}$ (not symmetric)

macro-gradient of the micro-deformation $\chi_{ijk} = \dfrac{\partial \psi_{jk}}{\partial x_i}$ (no minor symmetry)

macro-strain $\varepsilon_{ij} = \dfrac{1}{2}(u_{i,j} + u_{j,i})$ (infinitesimal displacements)

strain energy	$W = W(\varepsilon_{ij}, \gamma_{ij}, \chi_{ijk})$

Cauchy stress $\sigma_{ij} = \dfrac{\partial W}{\varepsilon_{ij}}$ (symmetric)

relative stress $\tau_{ij} = \dfrac{\partial W}{\gamma_{ij}}$ (not symmetric)

double stress $\mu_{ijk} = \dfrac{\partial W}{\chi_{ijk}}$ (no minor symmetry)

Mindlin's Micromorphic Continuum Formulation

(Mindlin, 1964, "Micro-structure in Linear Elasticity," *Archive for Rational Mechanics and Analysis*, v 16, 51-78.)

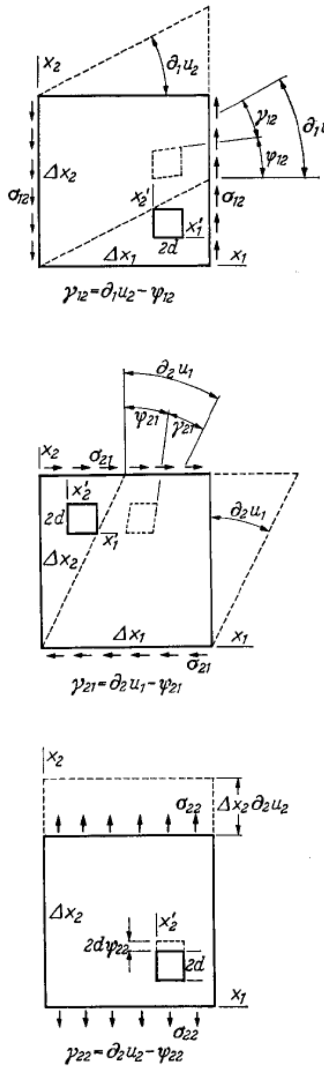


Fig. 1. Typical components of relative stress σ_{ij}, displacement-gradient $\partial_i u_j$, micro-deformation ψ_{ij} and relative deformation γ_{ij}

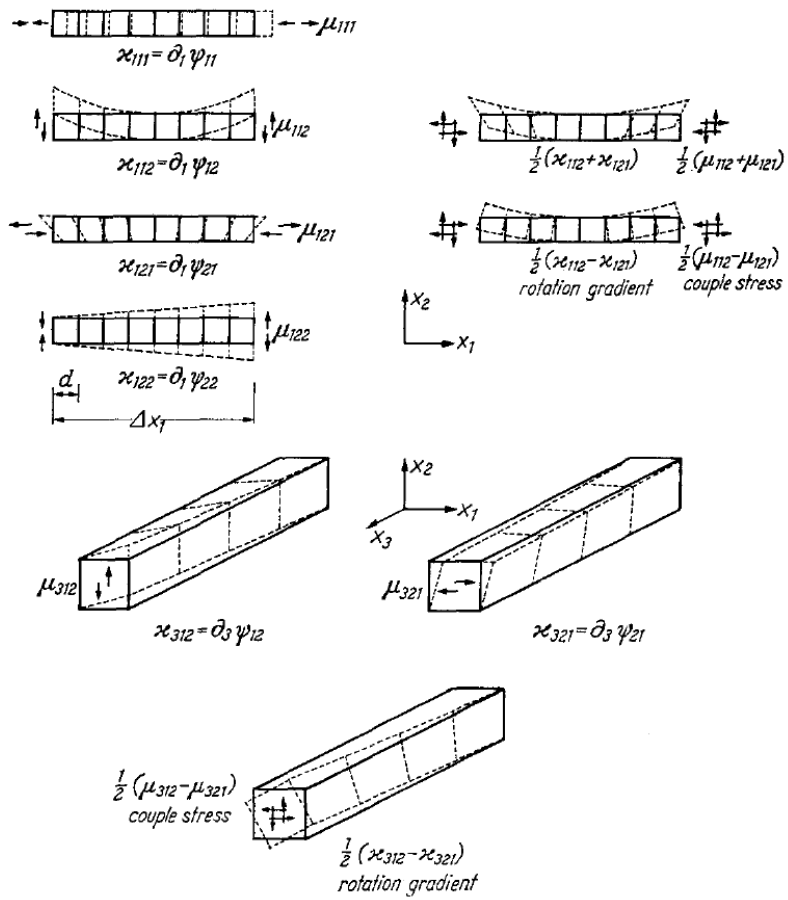


Fig. 2. Typical components of double stress μ_{ijk} and gradient of micro-deformation $\varkappa_{ijk}$

Linear Elastic

$$\left\{ \begin{array}{c} \sigma \\ \tau \\ \mu \end{array} \right\} = \left[\begin{array}{ccc} C & G & F \\ G & B & D \\ F & D & A \end{array} \right] \left\{ \begin{array}{c} \varepsilon \\ \gamma \\ \chi \end{array} \right\}$$

- displacement based finite element formulation
- nodal variables are $\mathbf{u}$ (3) and ψ_{ij} (9)
- use same shape functions but with 12 d.o.f. per node

What about material variability?

standard stiffness matrix (deterministic)

all others are random

$$\begin{Bmatrix} \sigma \\ \tau \\ \mu \end{Bmatrix} = \begin{bmatrix} C & G & F \\ G & B & D \\ F & D & A \end{bmatrix} \begin{Bmatrix} \varepsilon \\ \gamma \\ \chi \end{Bmatrix}$$

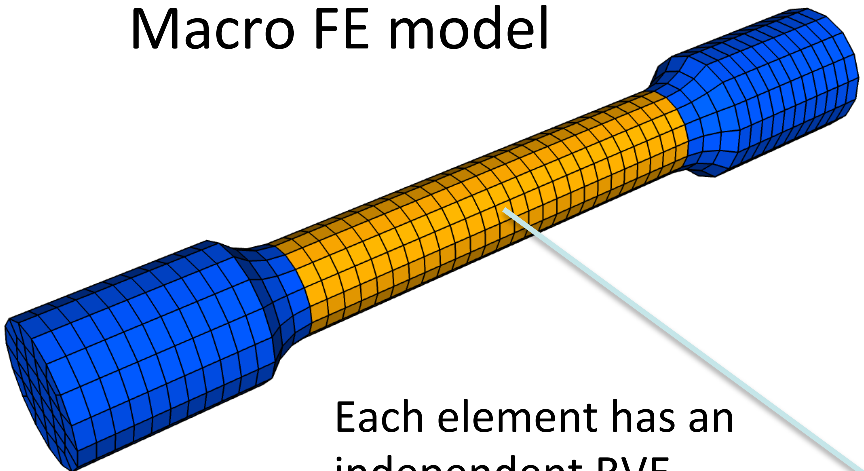
- For polycrystalline material variability, take G, F, B, D, A to be random matrices.
- The random matrices are a function of sampling volume V' .
- Take this sampling volume to be a function of the finite-element volume.
- The random matrices are generally anisotropic.
- As $V' \to \infty$, the microstructural fluctuations should disappear.

**** Need to stay in weak form (no strong form). ****

Homogenized Simulation via FE^2

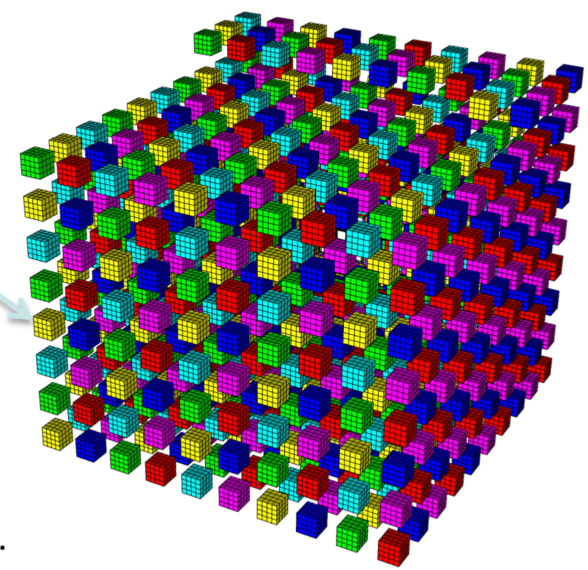
(to be compared with direct simulation)

Macro FE model



Each element has an independent RVE.

RVE array



(This RVE array is for testing Sierra/SM capability.)

Challenges:

- RVE needs to be as small as possible for efficiency.
- RVE needs to be as large as possible to give effective properties.
- RVE mesh needs to be sufficiently refined.
- Number of RVEs grows with mesh refinement in macro model.
- Robustness of CPFE models.

Summary

- Difference between Apparent and Effective material properties
- Homogenization theory based on concept of weak convergence
- Use Direct Numerical Simulations of macroscale boundary value problems containing microstructure to investigate incomplete first-order homogenization.
- Propose using Mindlin's micromorphic continuum theory to model Type-2 material variability
- Will probably need to use FE^2 approaches to model nonlinear micromorphic continua.