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Investigating mesh sensitivity and polycrystalline RVEs in crystal plasticity finite element simulations

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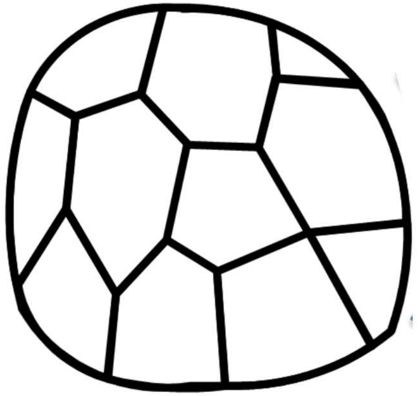
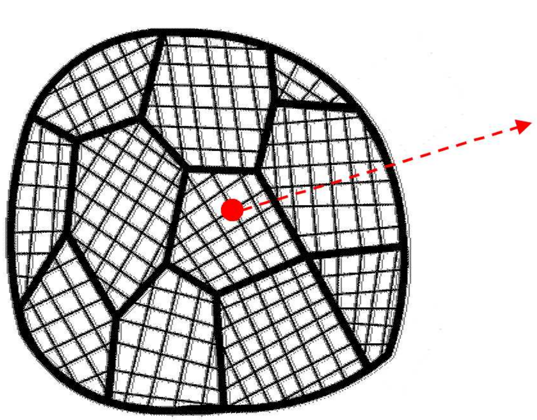
Crystal Plasticity-Finite Element (CP-FE) method



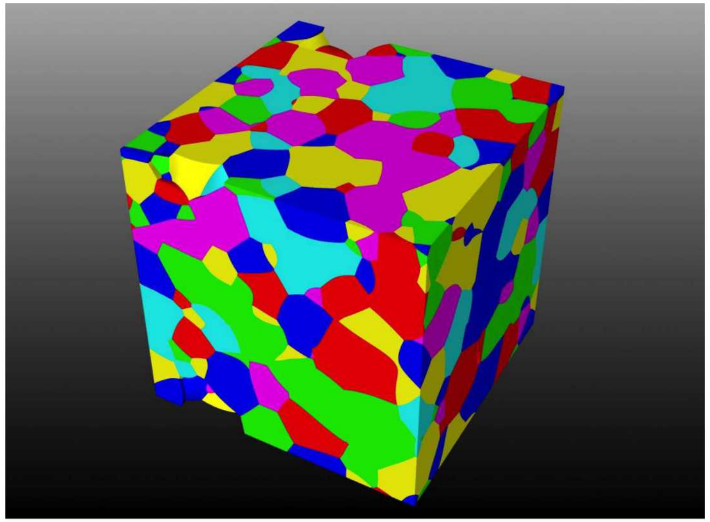
Polycrystalline body



FE discretization

Single crystal constitutive equations

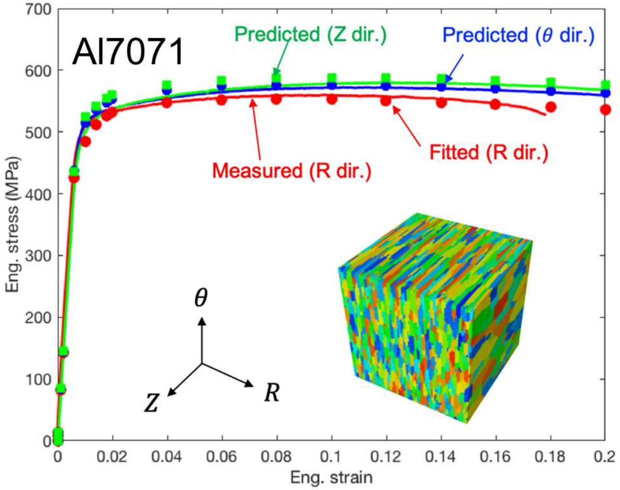
$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha} \left(\frac{\tau^{\alpha}}{g^{\alpha}} \right)^{1/m}$$

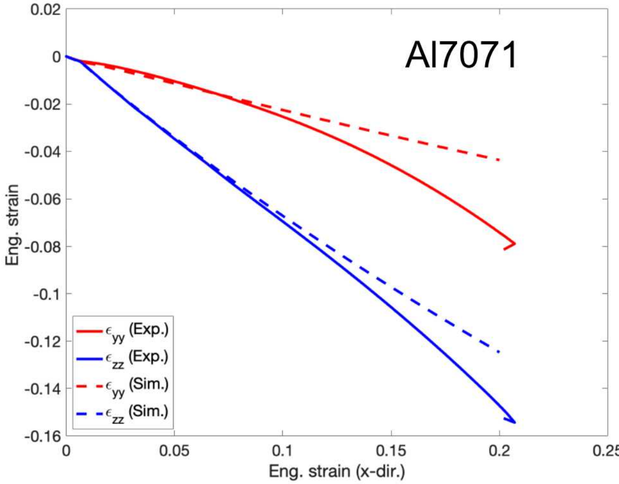


- **Grain-level approach** to materials modeling using multiscale strategies – realistic length and time scales
- Explicitly model discrete **grains** and **slip systems** based on dislocation slip
- Predicts **material's heterogeneous local responses** resulting from microstructure.
- **More predictive** than macroscopic plasticity models
    - Texture evolution & plastic anisotropy
    - Damage and Fracture, fatigue, void growth
    - Deformation twinning, martensitic transformation, recrystallization
    - Nonlocal formulations, grain boundary mechanics & grain size effects
    - Metal forming

CP-FEM predictions

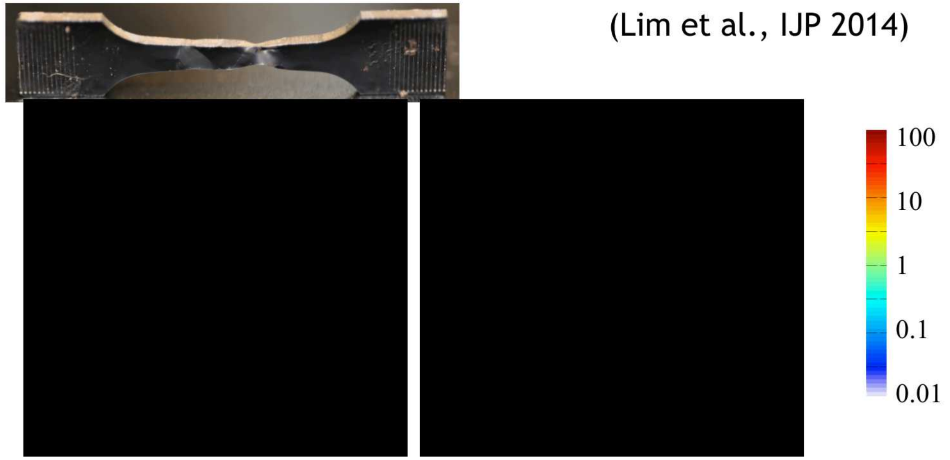
Plastic anisotropy



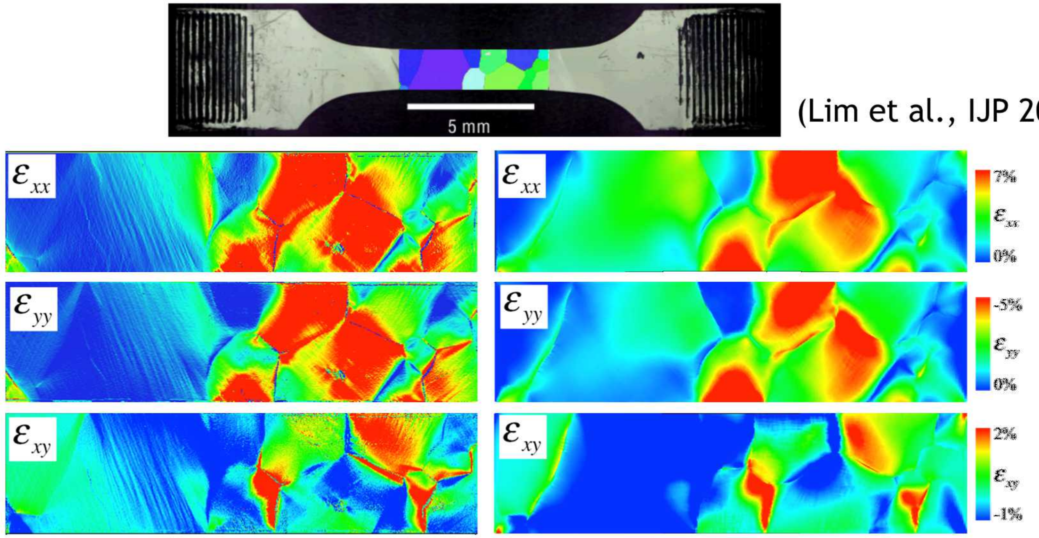


Texture evolution

(Lim et al., IJP 2014)



Local strain fields



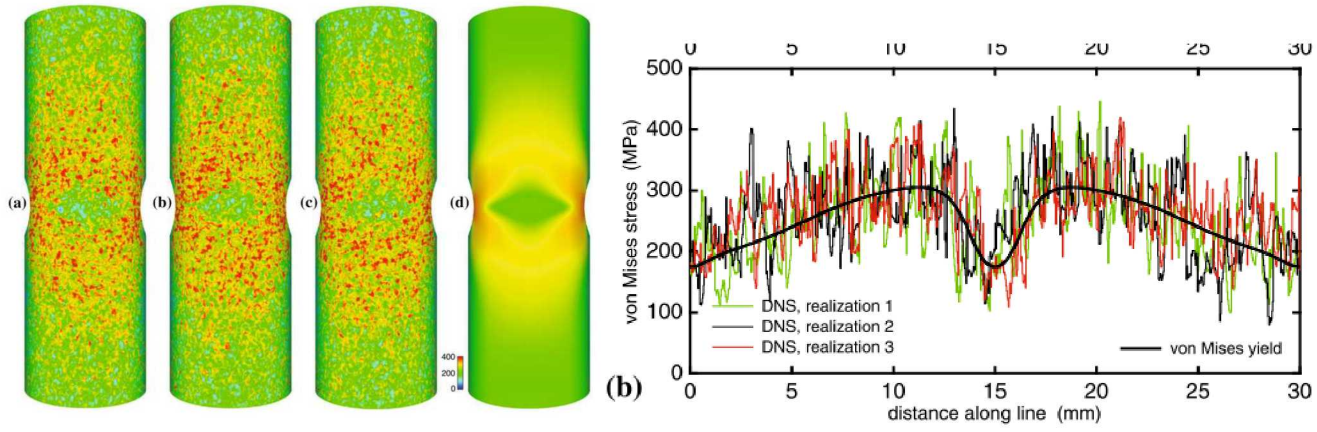
(Lim et al., IJP 2014)

(a) HR-DIC measurements

(b) CP-FEM predictions

Materials variability

(Bishop et al., JOM, 2016)



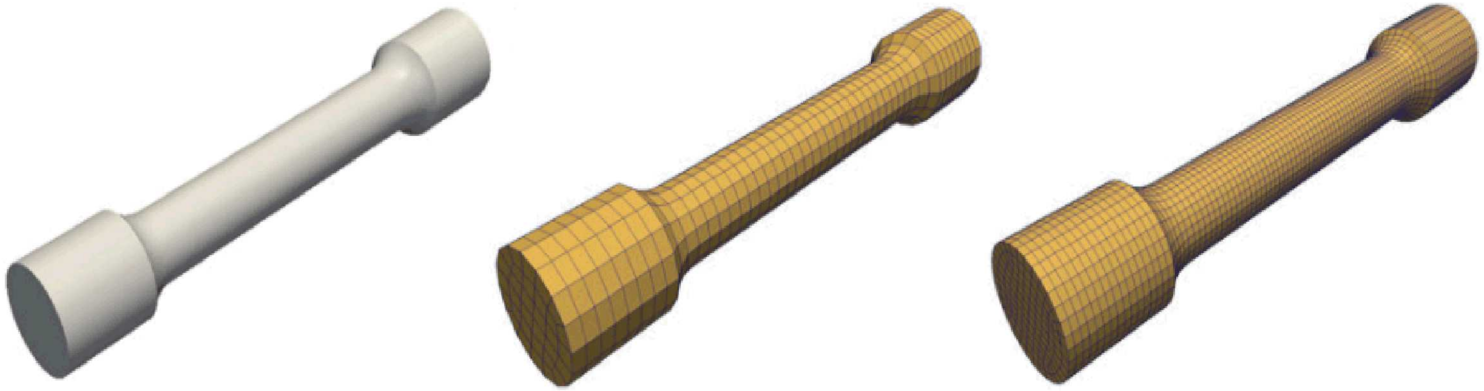
Outline

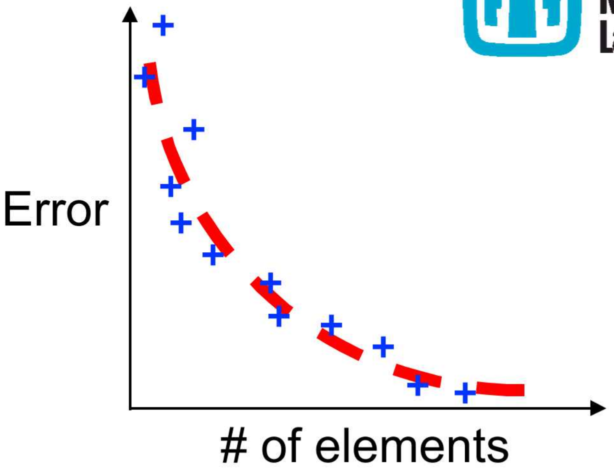
- ***Mesh sensitivity*** **in single crystal / polycrystalline CP-FEM simulations**
- ***Polycrystalline RVEs*** **in CP-FEM simulations**
- **Conclusions**

Lim et al., *International Journal of Plasticity* 121 (2019) 101-115.
Bishop et al., *JOM* 68 (2016) 1427-1445.
Bishop et al., *Comput. Methods Appl. Mech. Engrg.* 287 (2015) 262-289.

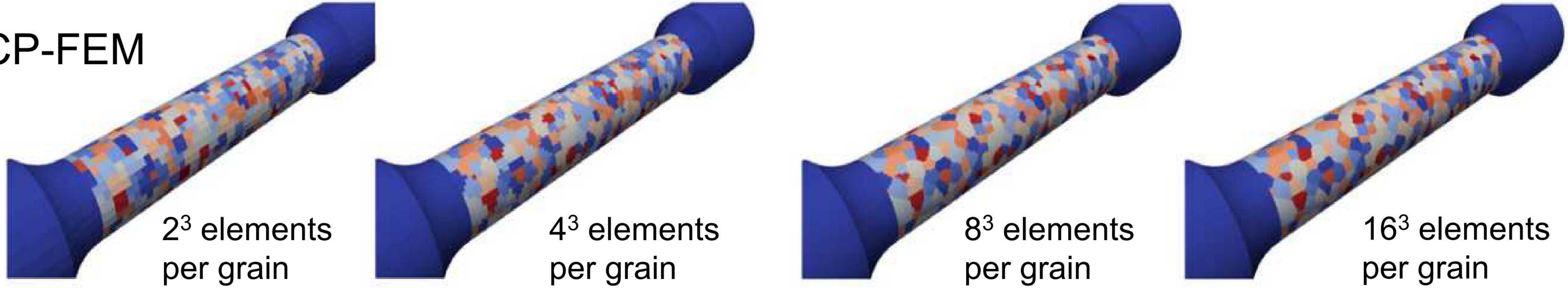
Mesh sensitivity in CP-FEM simulations

FEM





CP-FEM



Mesh sensitivity in CP-FEM:

Computationally expensive

Need to consider microstructural effects

CP-FEM simulation procedures

- ***Slip rate:*** $$\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha} \left(\frac{\tau^{\alpha}}{g^{\alpha}} \right)^{1/m}$$

- ***Perfect hexahedral finite element mesh***
- ***Single integration point at the center of FE***

Slip resistance:

$$g^{\alpha} = A\mu b \sqrt{\sum_{\beta=1}^{12} \rho^{\beta}} \qquad \dot{\rho}^{\alpha} = \left(\kappa_1 \sqrt{\sum_{\beta=1}^{12} \rho^{\beta}} - \kappa_2 \rho^{\alpha} \right) |\dot{\gamma}^{\alpha}|$$ (Dislocation density based hardening)

$$\dot{g}^{\alpha} = \sum_{\beta}^{12} h^{\alpha\beta} |\dot{\gamma}^{\beta}|. \qquad h^{\alpha\beta} = q^{\alpha\beta} h_0 \left(1 - \frac{g^{\beta}}{g_s} \right)^{a}$$ (Slip based hardening)

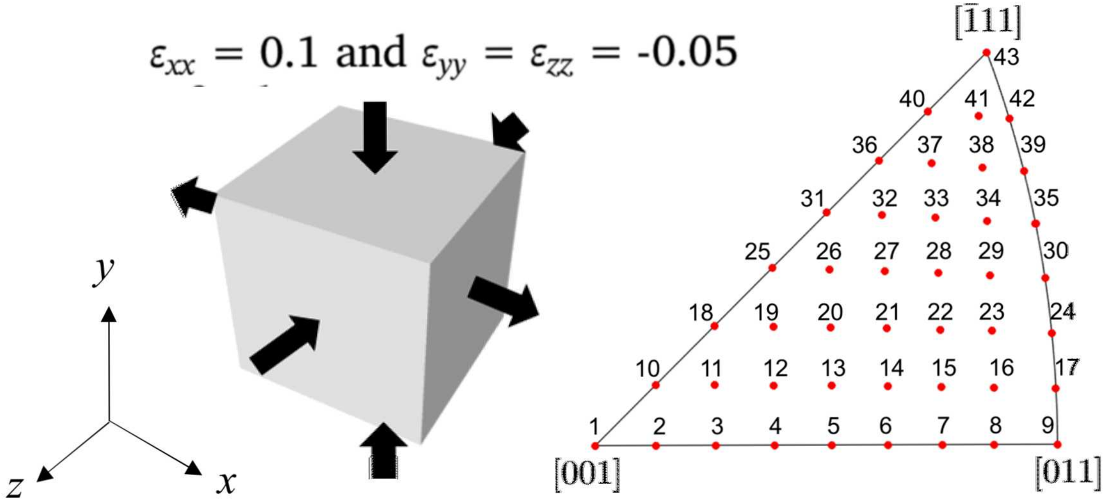
$$g^{\alpha} = a_1 + a_2 (\bar{\varepsilon}_p)^n$$ (Isotropic power-law hardening)

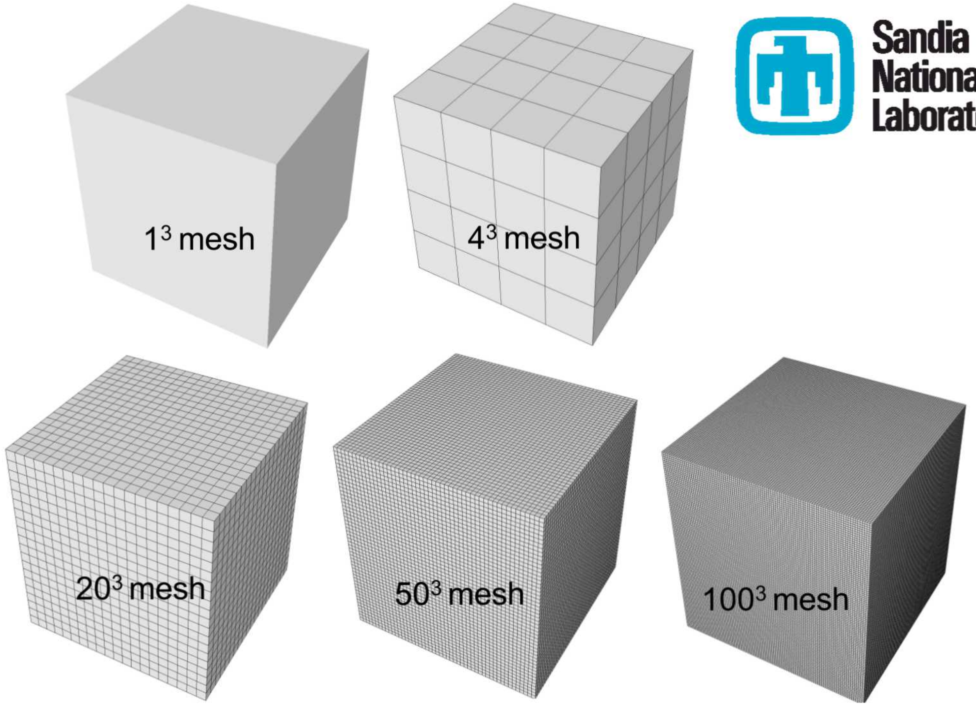
- ***Material parameters for SS304L***

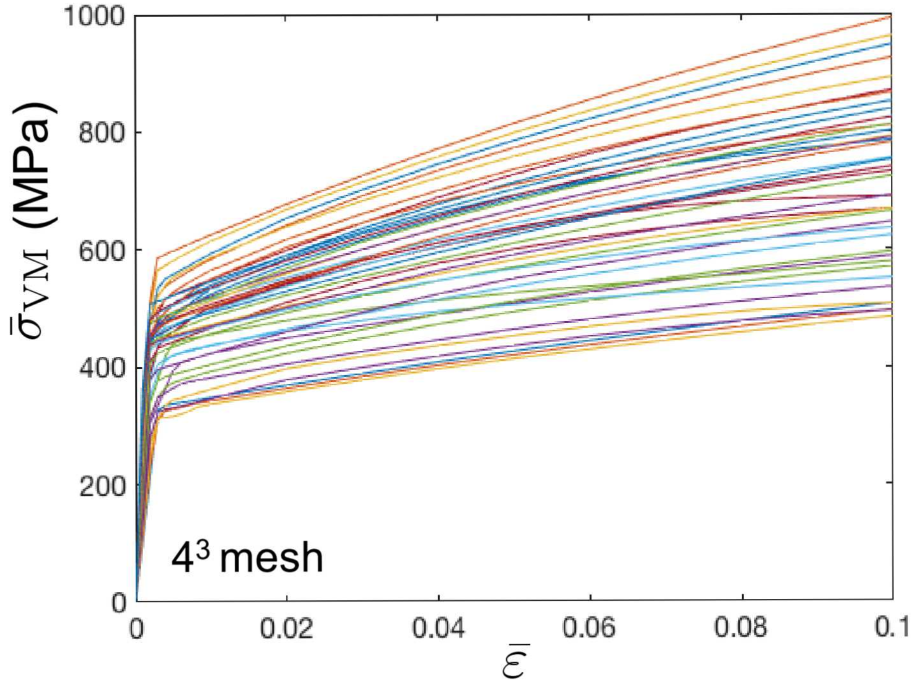
Hardening constants			
$C_{11} = 197.5$ GPa	$C_{12} = 125.0$ GPa	$C_{44} = 122.0$ GPa	$\mu = 55.9$ GPa
$\dot{\gamma}_0 = 1\ s^{-1}$	$m = 0.012$		
$A = 0.4$	$\rho_0 = 5.46 \times 10^{12}\ m^{-2}$	$\kappa_1 = 2\times 10^6\ m^{-1}$	$\kappa_2 = 20$
$g_0 = 150$ MPa	$g_s = 1100$ MPa	$h_0 = 300$ MPa	$a = 3.0$
$a_1 = 150$ MPa	$a_2 = 500$ MPa	$n = 0.8$	

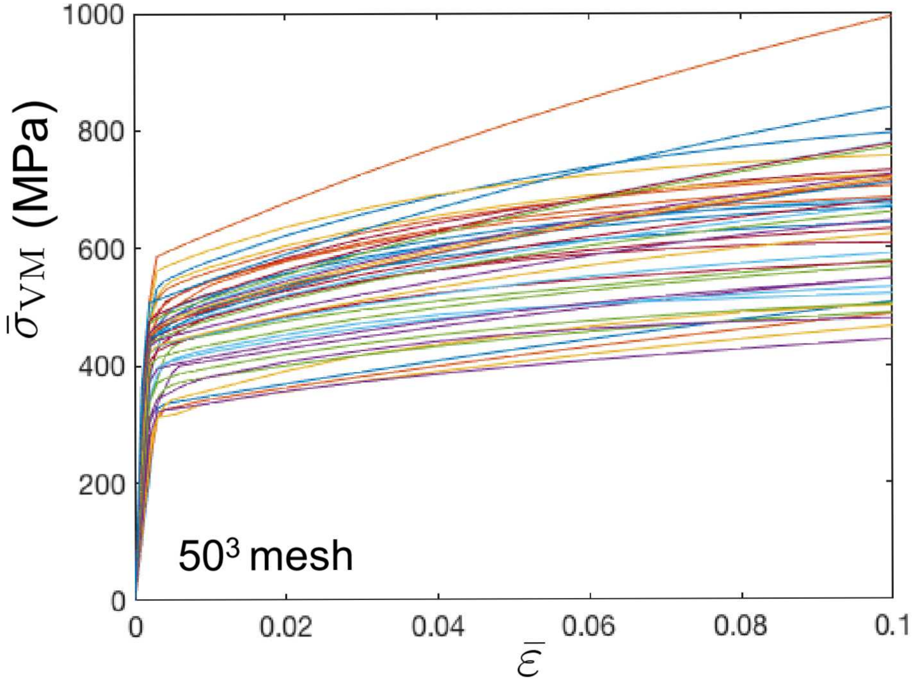
Simulations of single crystals

$\varepsilon_{xx} = 0.1$ and $\varepsilon_{yy} = \varepsilon_{zz} = -0.05$



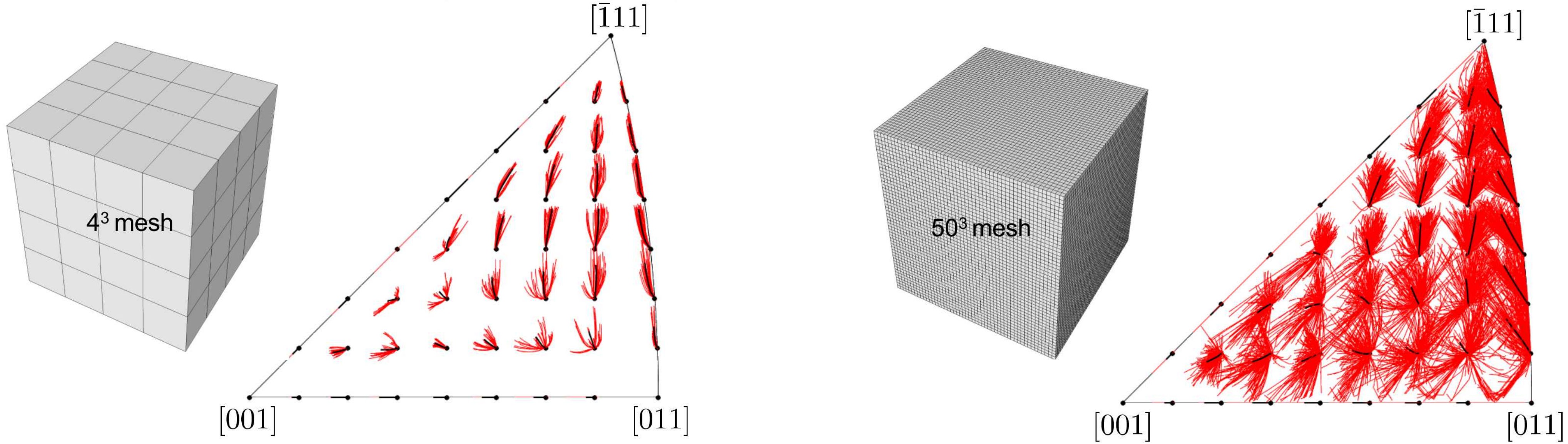




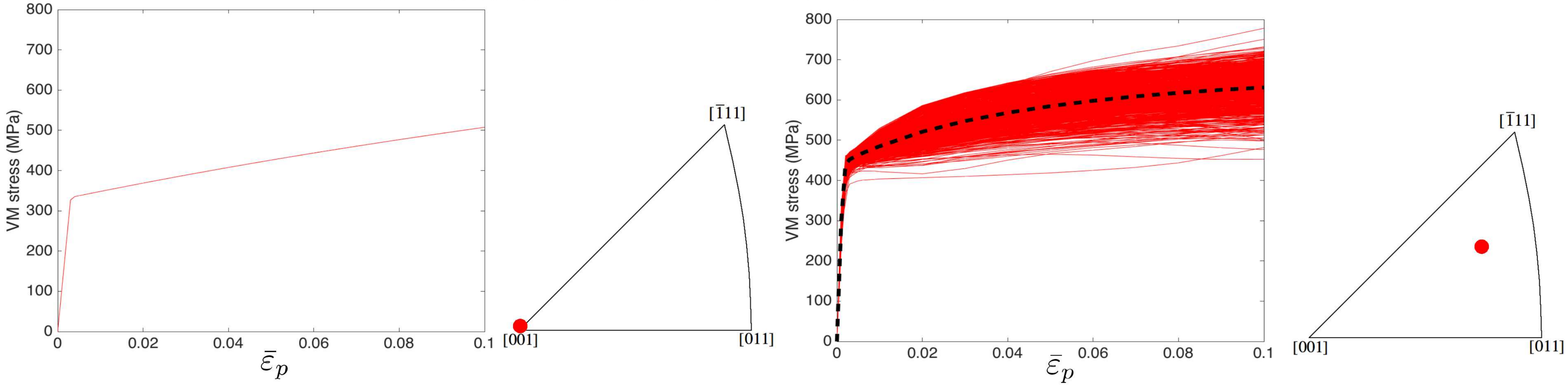


Effects of crystal orientations

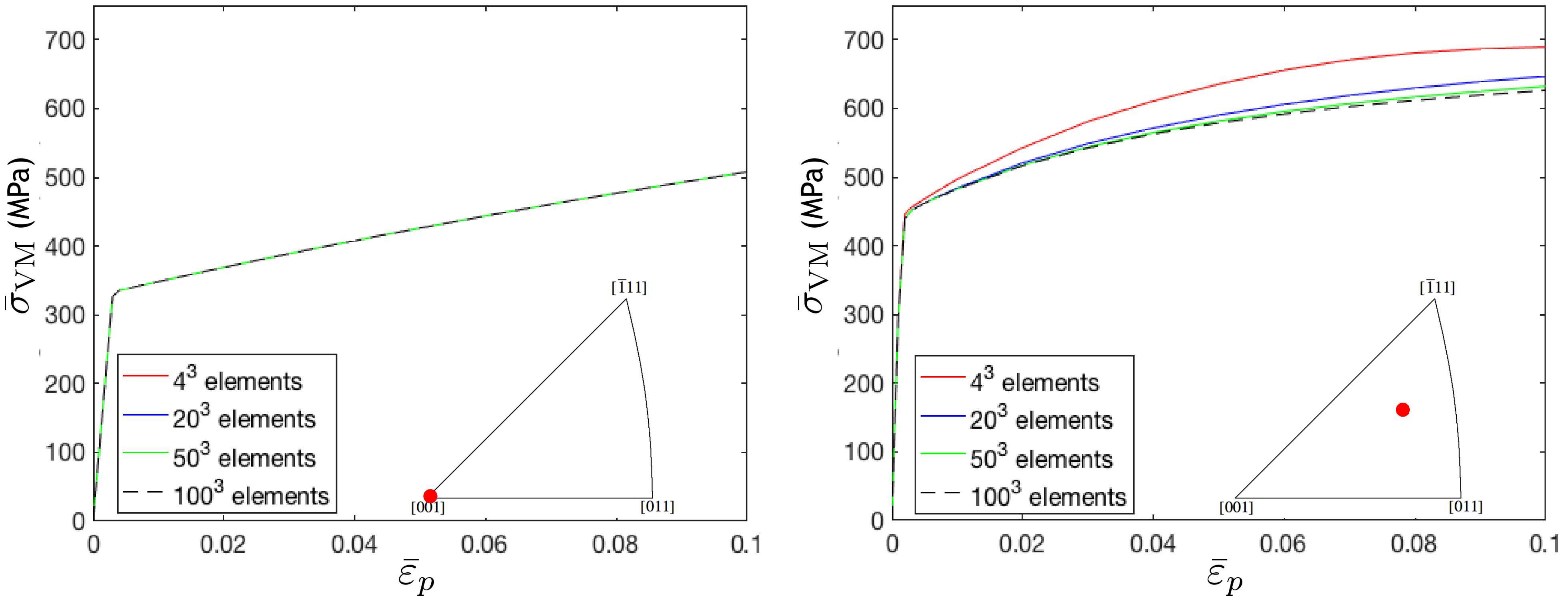
Crystal rotation along x directions after 10% isochoric deformation



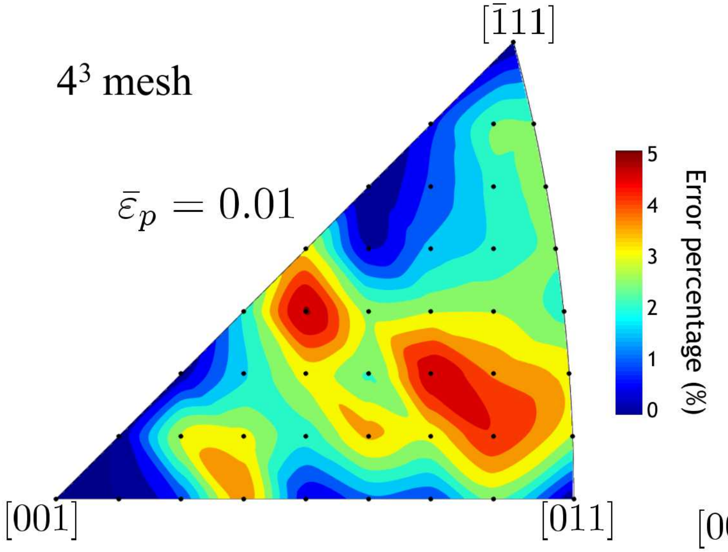
Von Mises stress vs. EQPS from all FE within 50^3 mesh

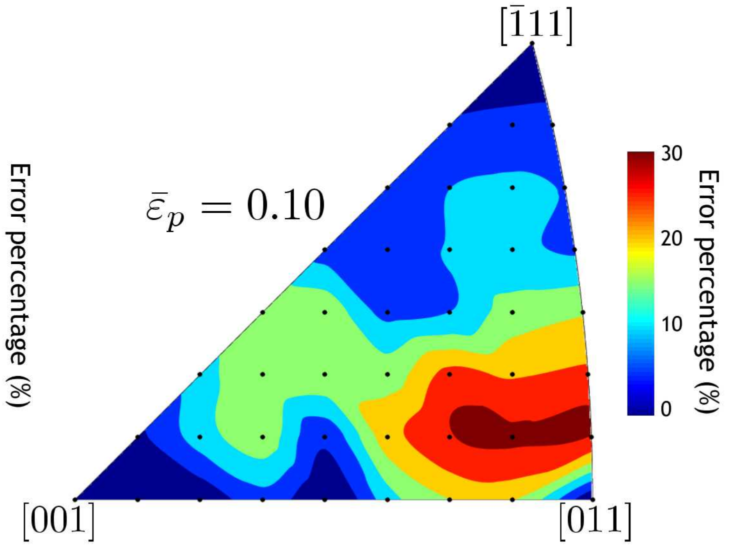


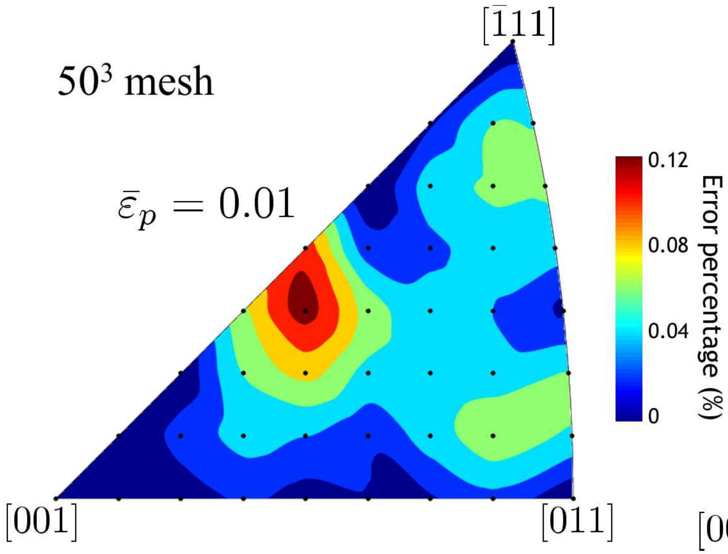
Mesh sensitivity – crystal orientation effect

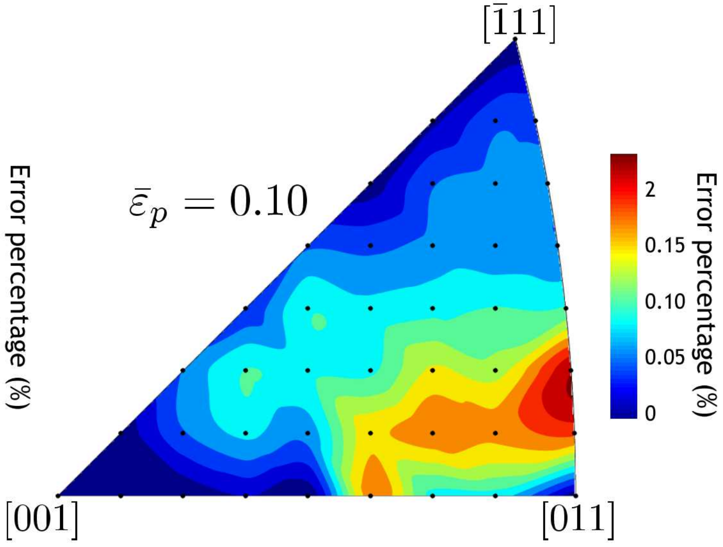


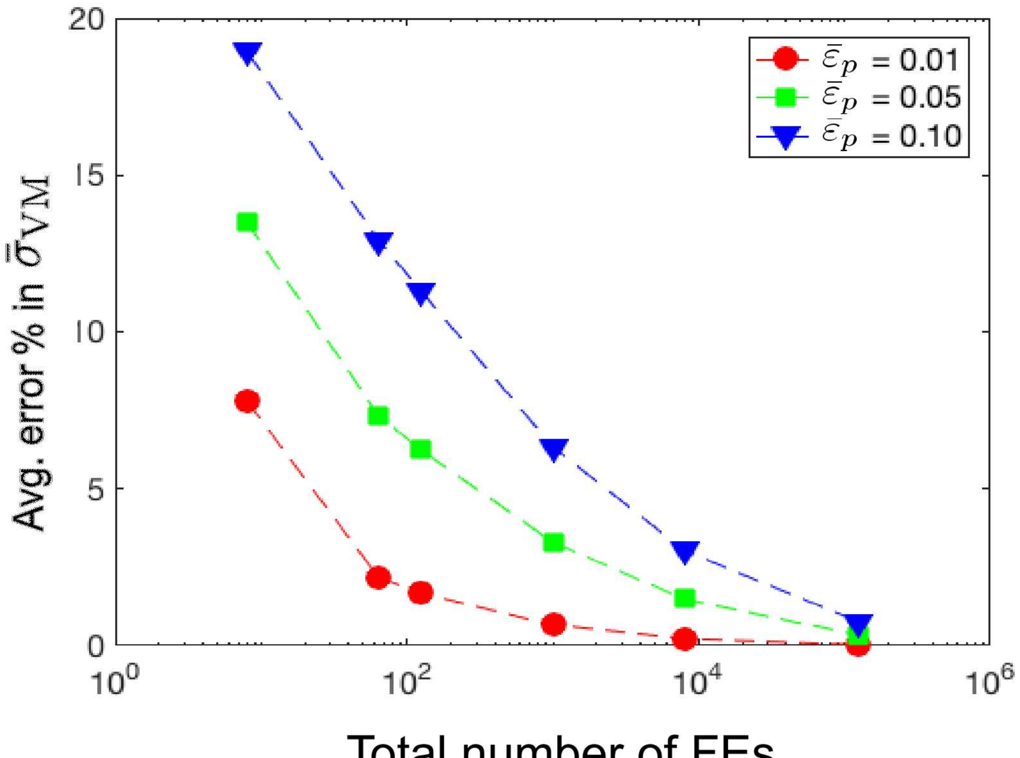
Error percentages



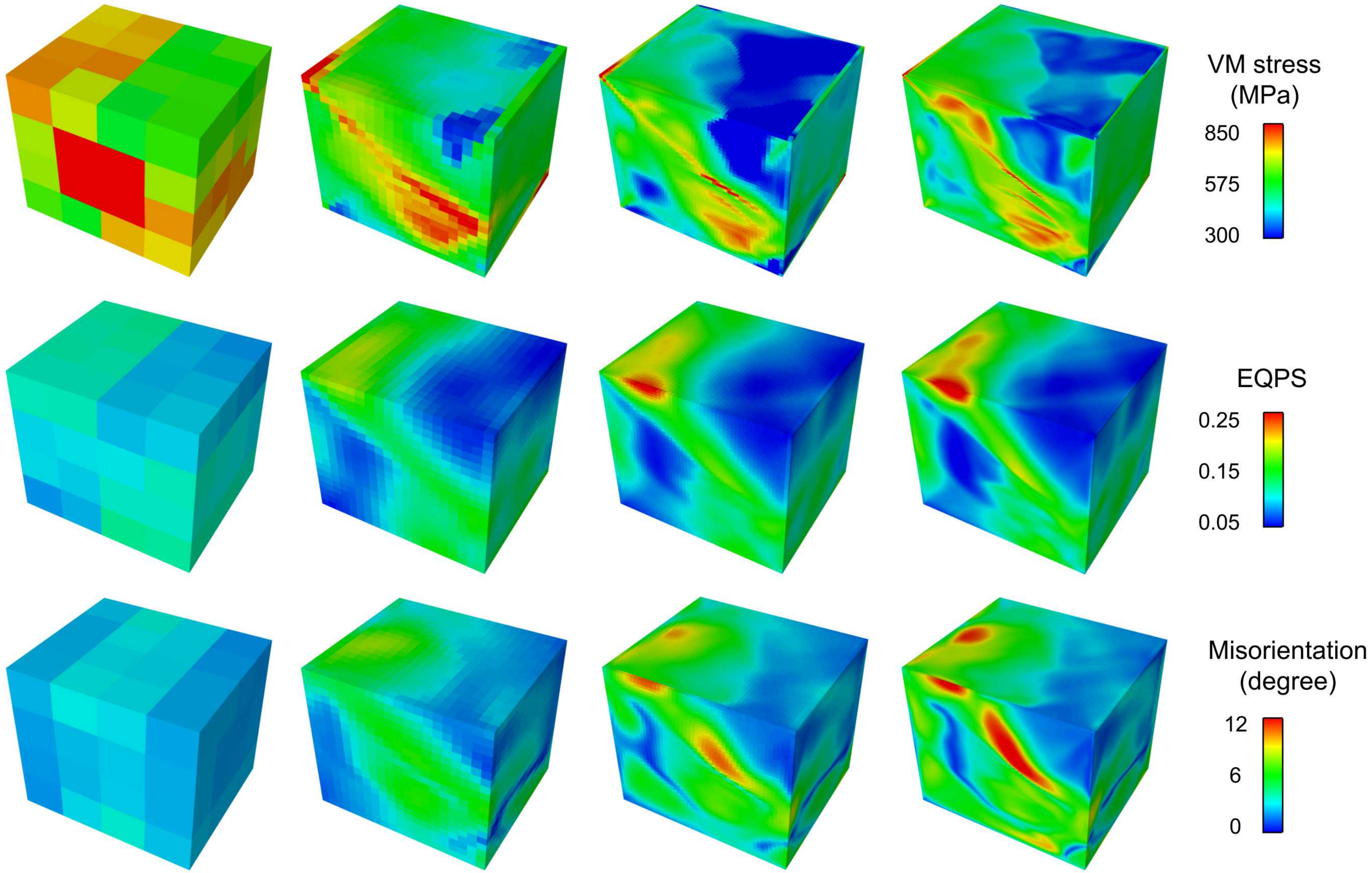








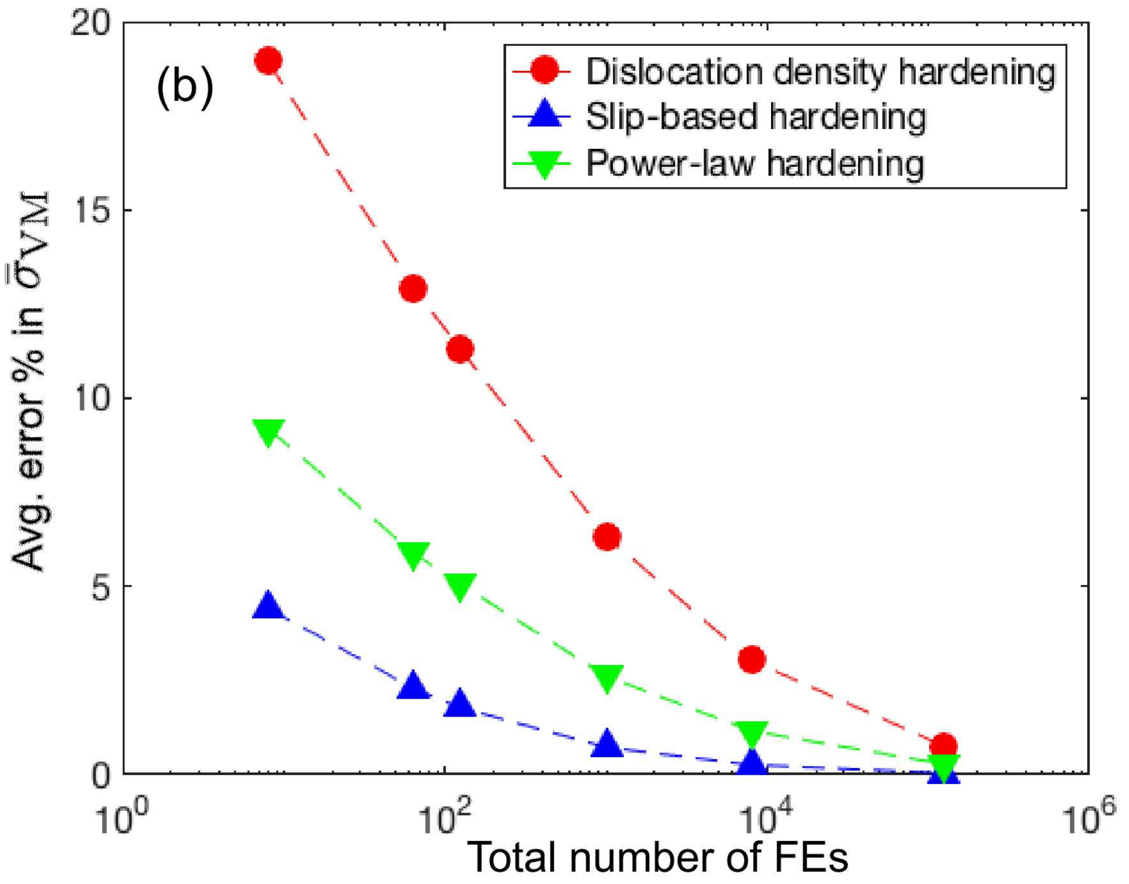
Mesh sensitivity in local variables



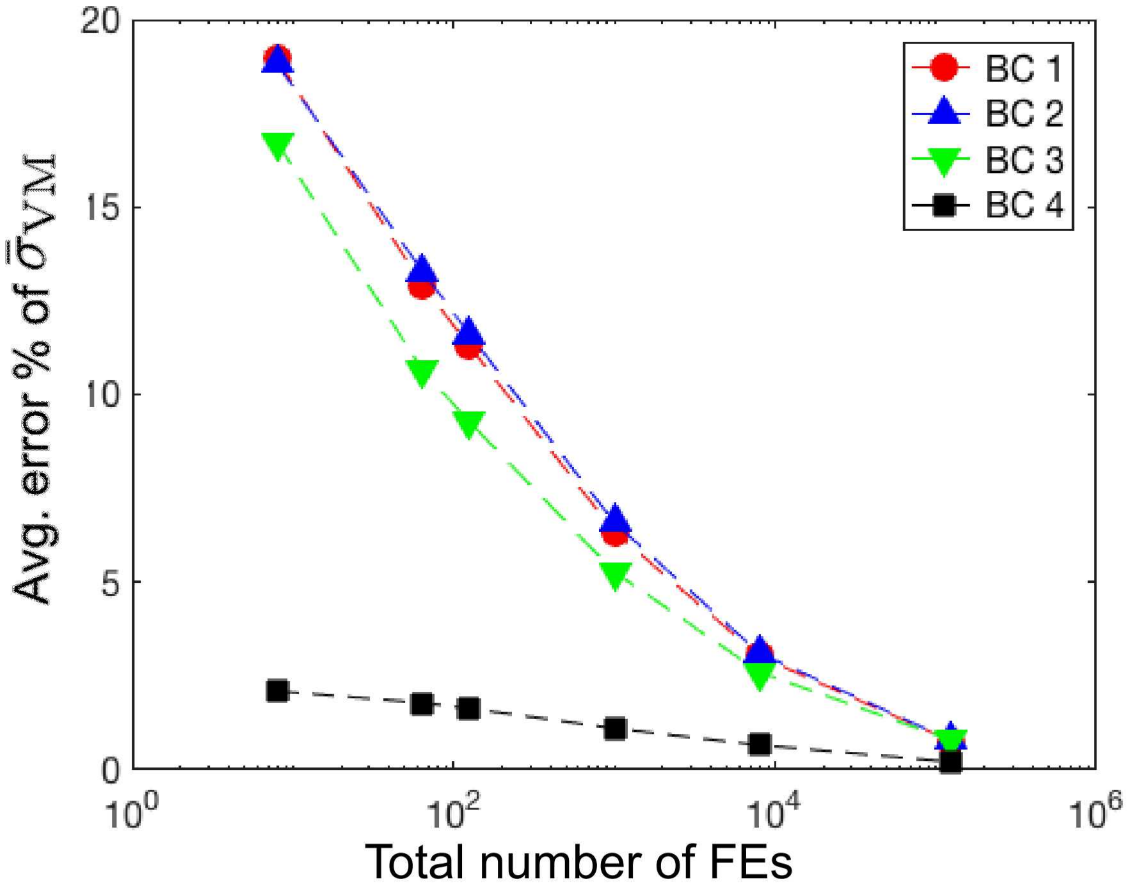
(a) 4^3 mesh (b) 20^3 mesh (c) 50^3 mesh (d) 100^3 mesh

Other effects

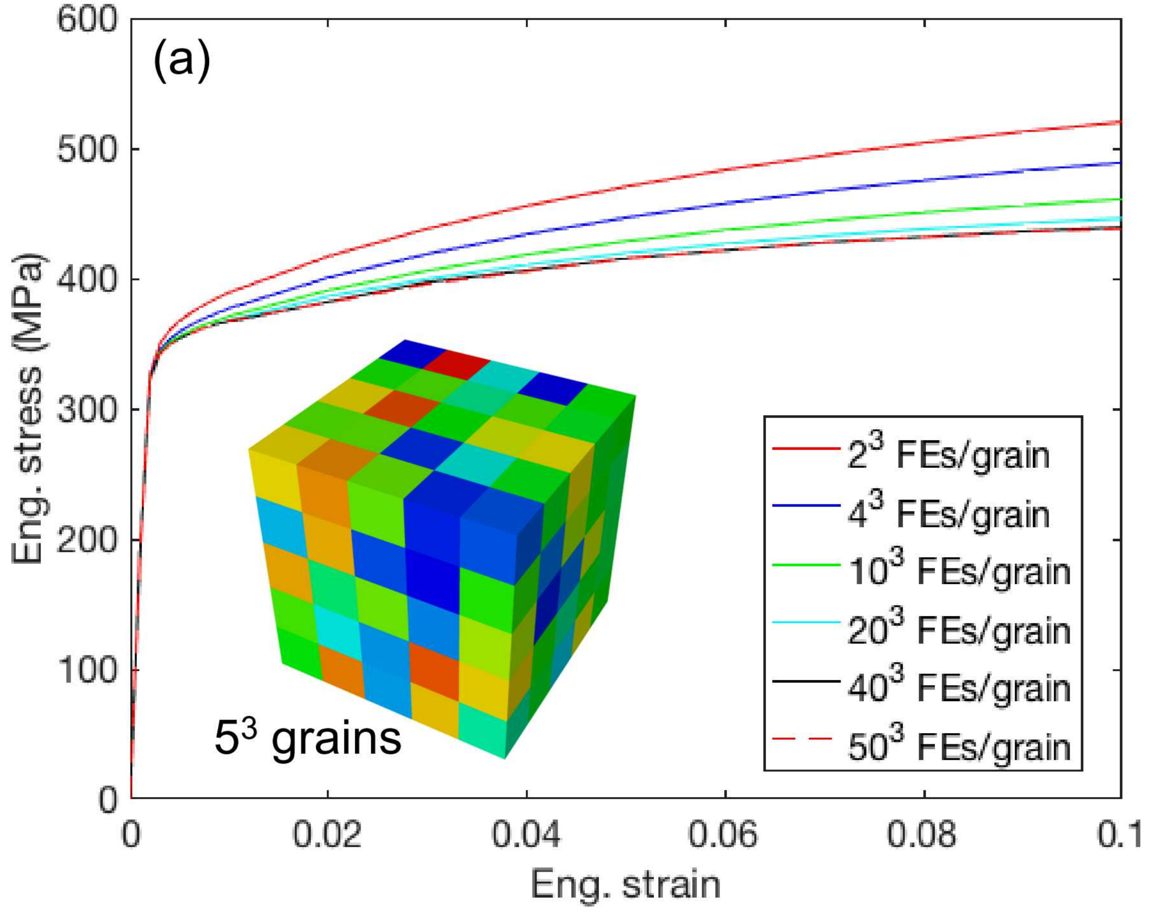
- Dislocation density based hardening: $g^{\alpha} = A\mu b\sqrt{\sum_{\beta=1}^{12} \rho^{\beta}}$
- Slip based hardening: $\dot{g}^{\alpha} = \sum_{\beta}^{12} h^{\alpha\beta}|\dot{\gamma}^{\beta}|.$
- Isotropic power-law hardening: $g^{\alpha} = a_1 + a_2(\bar{\varepsilon}_p)^n$

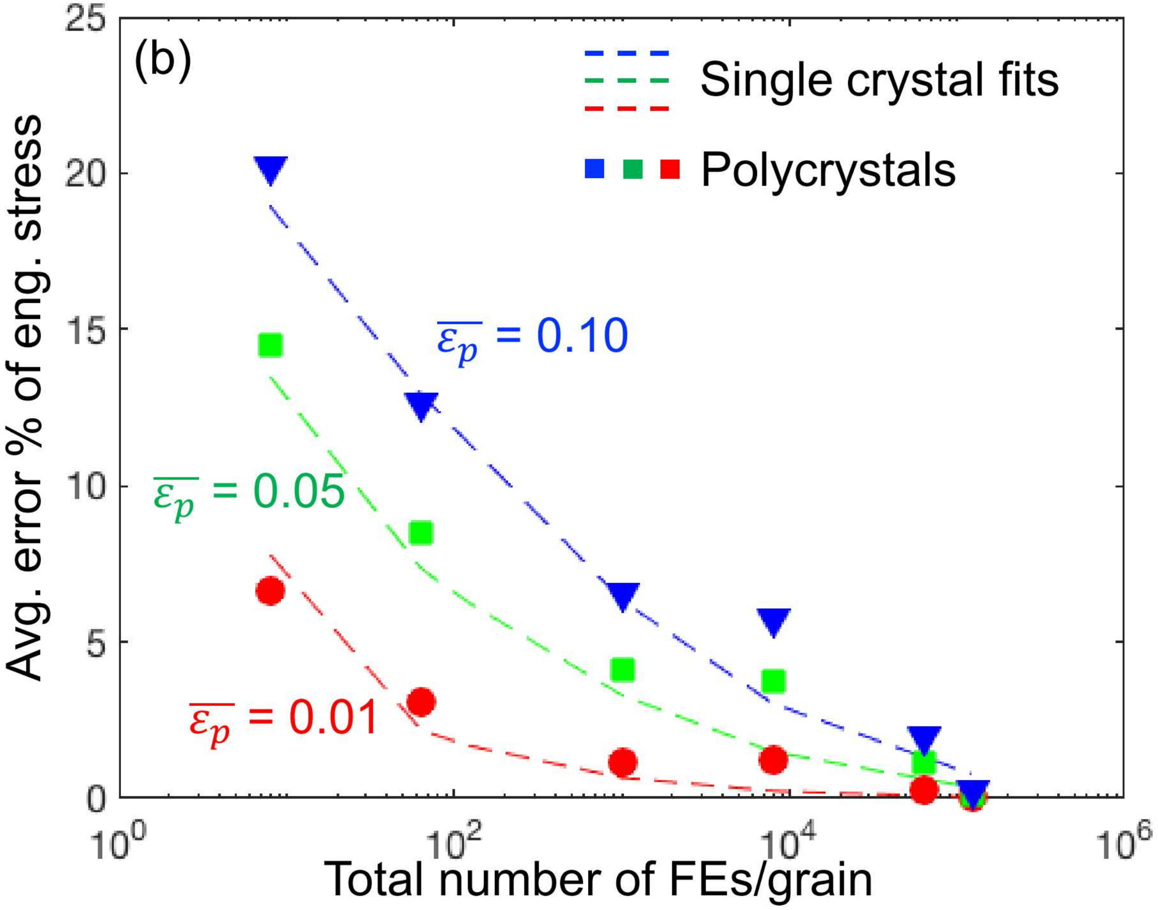


- BC1: $\varepsilon_{xx} = 0.1$ and $\varepsilon_{yy} = \varepsilon_{zz} = -0.05$
- BC2: $\varepsilon_{yy} = 0.1$ and $\varepsilon_{xx} = \varepsilon_{zz} = -0.05$
- BC3: $\varepsilon_{xx} = 0.122$ and $\varepsilon_{yy} = \varepsilon_{zz} = 0$
- BC4: $\varepsilon_{xx} = 0.122$

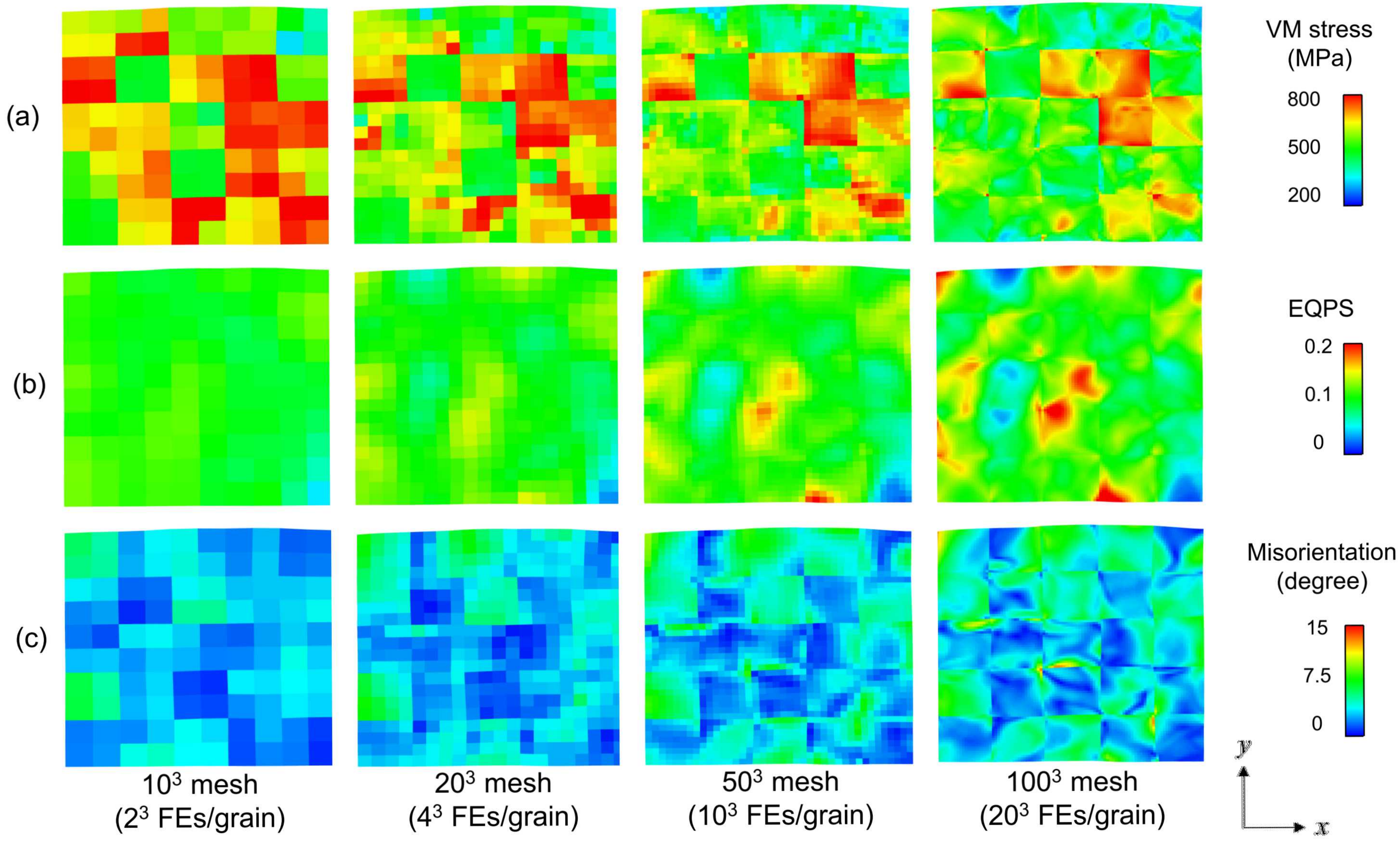


Mesh sensitivity in polycrystalline CP-FEM simulations

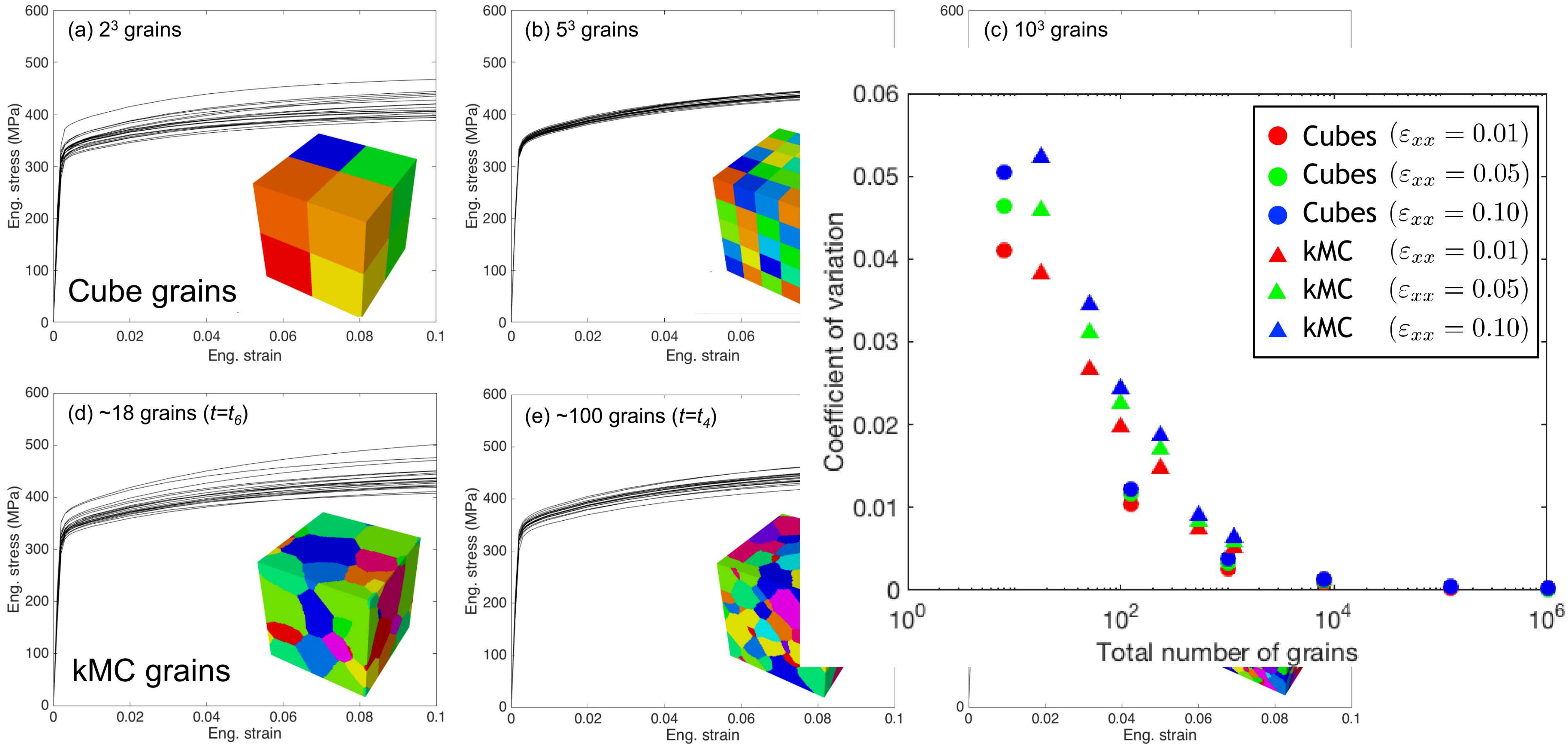




Mesh sensitivity in polycrystalline CP-FEM simulations



RVE size in CP-FEM simulations



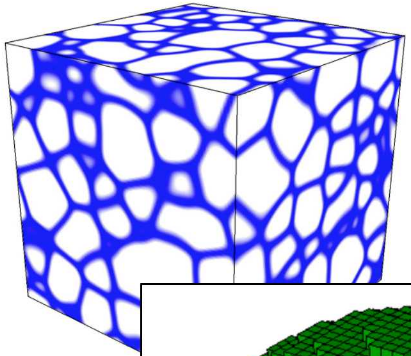
Constructing interface-conformal polycrystal FE mesh

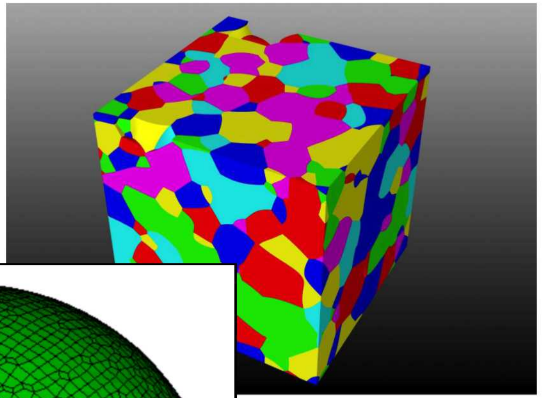
Computational/Experimental Voxelated 3D microstructure

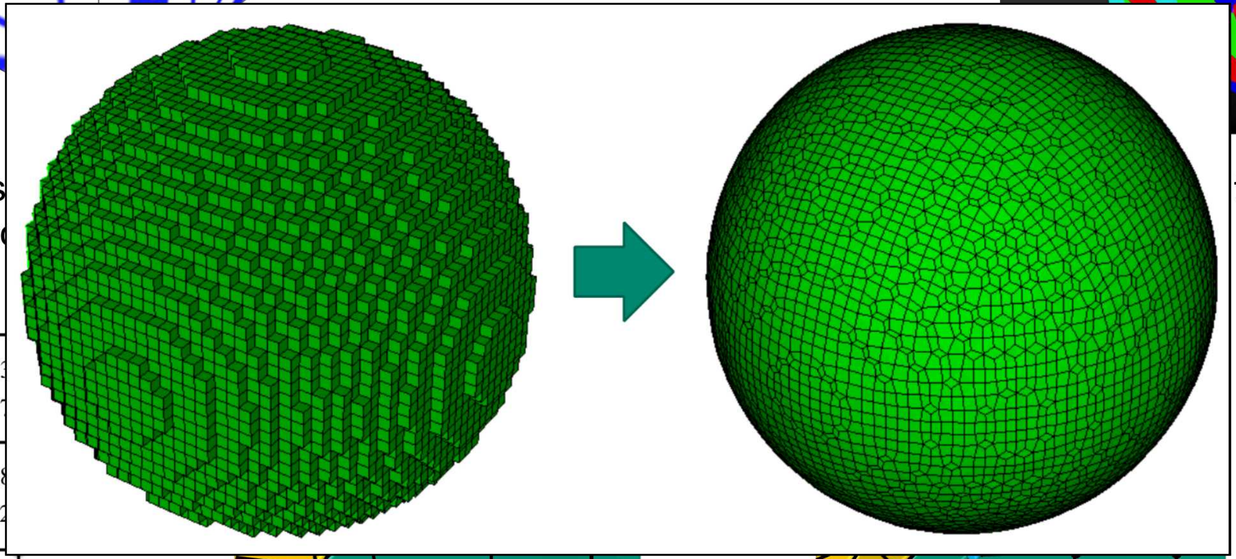
Interface-conformal hexahedral FE mesh

Cubit 'Sculpt'

www.cubit.sandia.gov



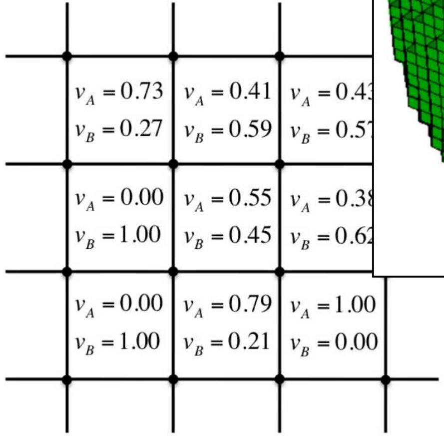


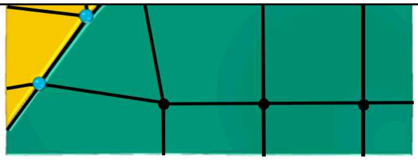


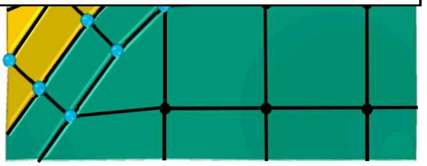
Volume fractions repres
percent of grains for ea

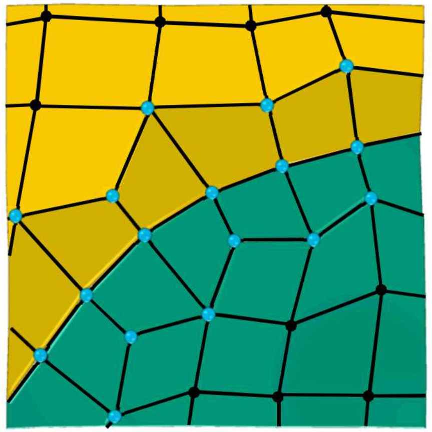
ts

Perform smoothing and pillowing to improve the mesh quality.





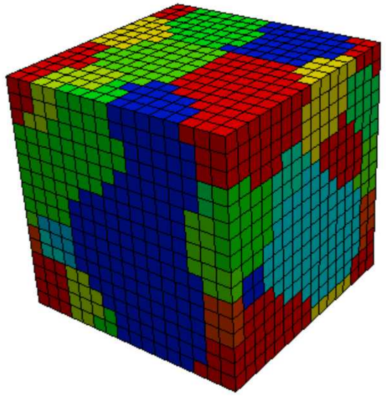


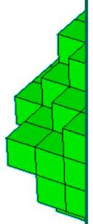


Lim et al., MSMSE (2016)

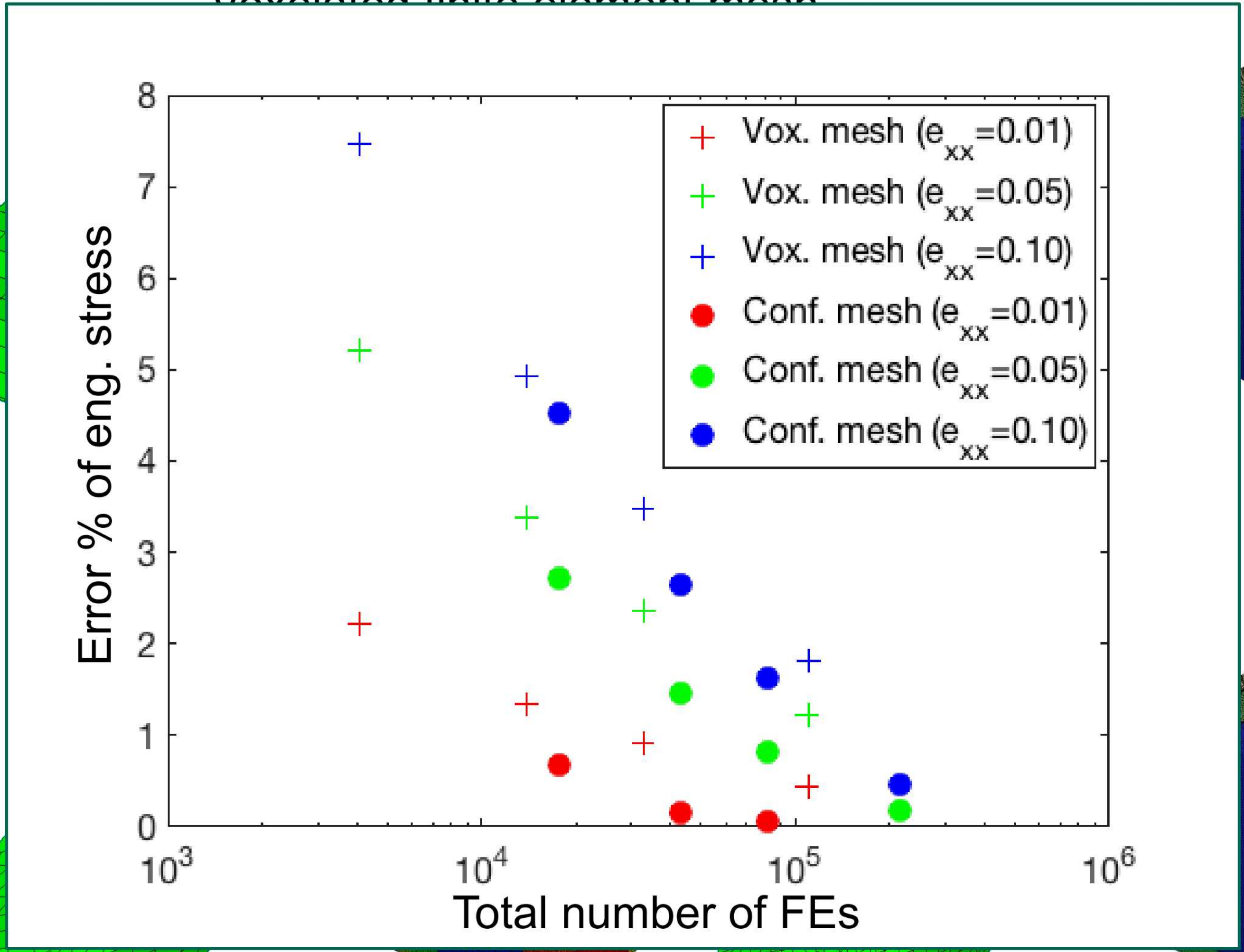
Interface conformal mesh

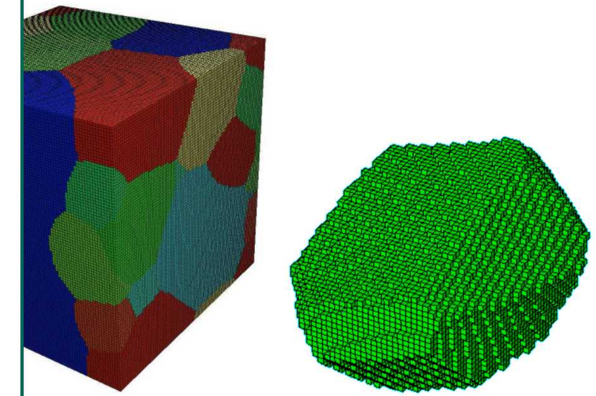
Voxelated finite element mesh



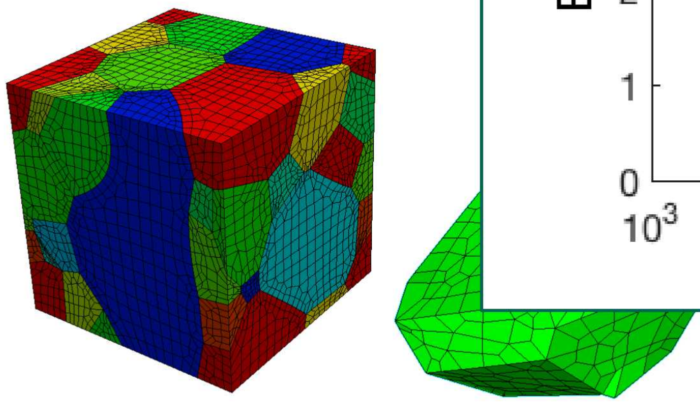


Mesh 1

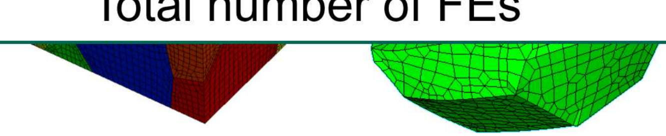




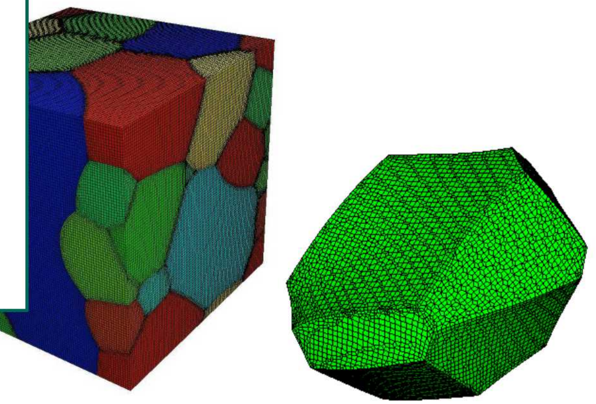
Mesh 5



Mesh 1



Mesh 3



Mesh 5

Conclusions

- Mesh convergence in CP-FEM is very sensitive to the crystal orientation, hardening model and applied boundary conditions.
- Approximately 10^4 finite elements per grain are required to reasonably achieve mesh convergence in CP-FEM simulations.
- Approximately 10^3 grains are required to adequately reproduce polycrystalline RVEs.
- Interface conformal mesh reduces error compared to voxelated mesh.

THANK YOU !

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