SAND2015-7400PE

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3D microstructure modeling using phase field grain growth model

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Sandia National Laboratories

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U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

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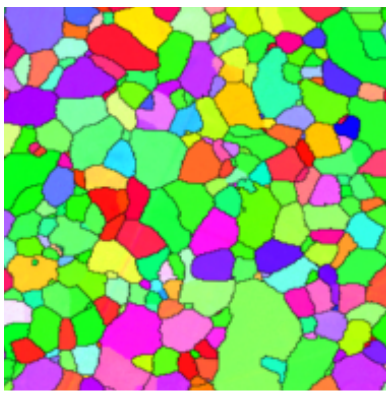
Motivation

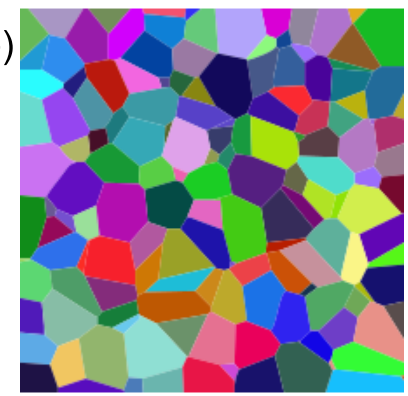
Large-scale continuum simulations with microstructure fidelity are hindered by limited capabilities to model realistic 3D microstructures (Fig (a)).

- Most finite element based polycrystalline models use idealized grain shapes or Voronoi tesselations (Fig. (b)).
- 3D microstructures digitized from experiments conform to a uniform grid. (Fig. (c))

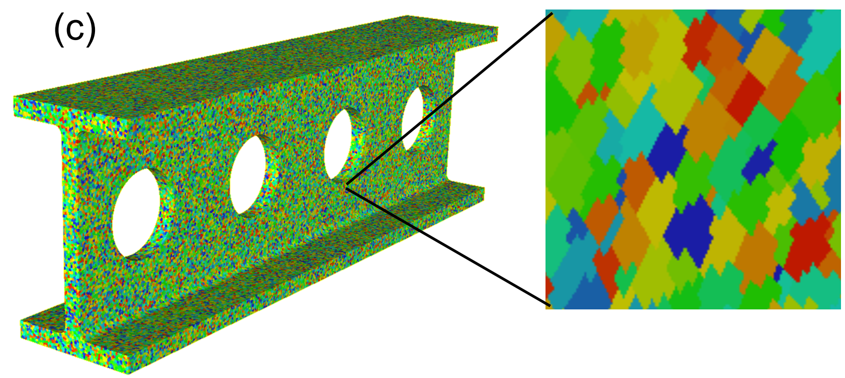
(a)



(b)



(c)



Microstructures from (a) electron back scatter diffraction, (b) Voronoi tesselation and (c) voxelated 3D structure of I-beam [Bishop et al., 2014].

Need a technique to create physically-based three-dimensional microstructures!

Phase field grain growth model

- **Total free energy**

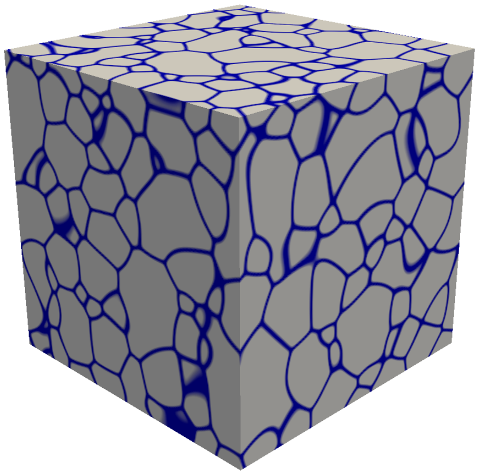
$$\mathcal{F}_{tot} = \int d\mathbf{r} \left\{ \underbrace{\frac{4}{3}\left[1 - 4\sum_{i=1}^{n_\phi} \phi_i^3 + 3\left(\sum_{i=1}^{n_\phi} \phi_i^2\right)^2\right]}_{\text{Bulk thermodynamics: chemical, elastic, etc…}} + \underbrace{\sum_i^{n_\phi} \frac{\epsilon_i^2}{2} |\nabla \phi_i|^2}_{\text{Interfacial energy: GBs}} \right\}$$

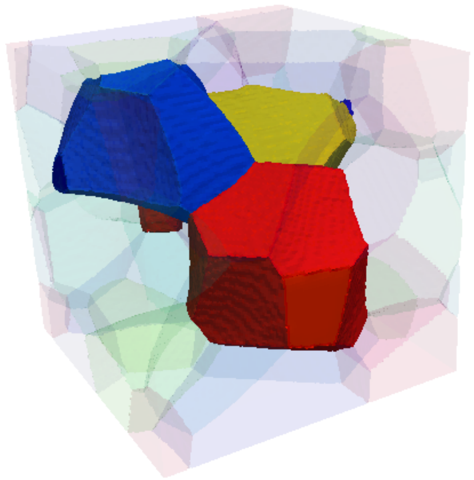
- **Dynamics**

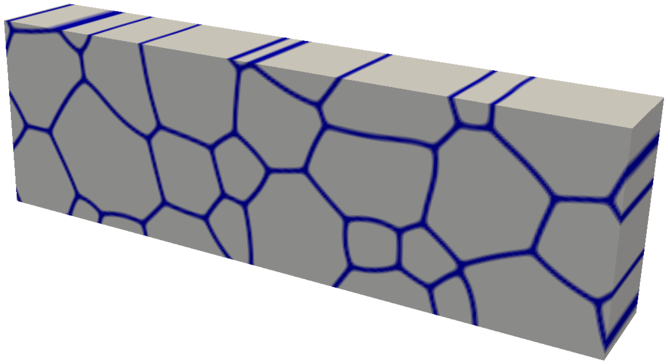
Abdeljawad et al. J. Power Sources **250** (2014)

Non-conserved quantities (grain orientation, solidification, phase transitions)

- Model A: $\dfrac{\partial \phi_i}{\partial t} = -L_i \left(\dfrac{\delta \mathcal{F}_{tot}}{\delta \phi_i} \right)$ Allen-Cahn Eq. (Gradient flow of $\mathcal{F}_{tot}$)







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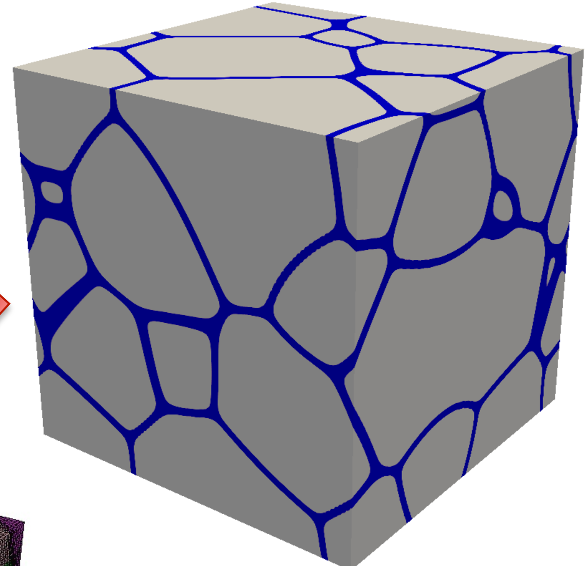
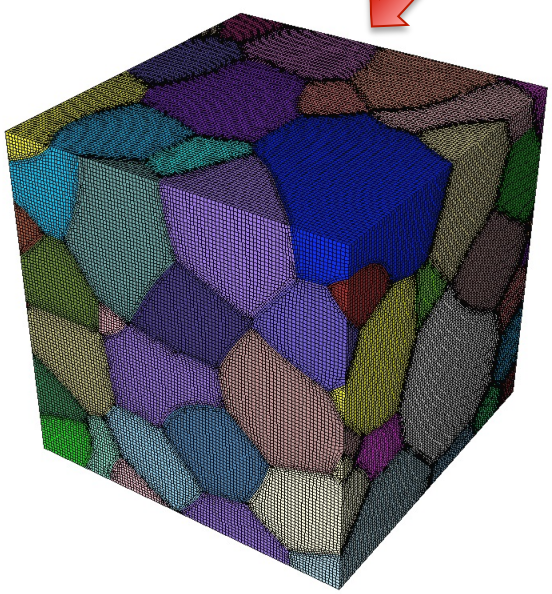
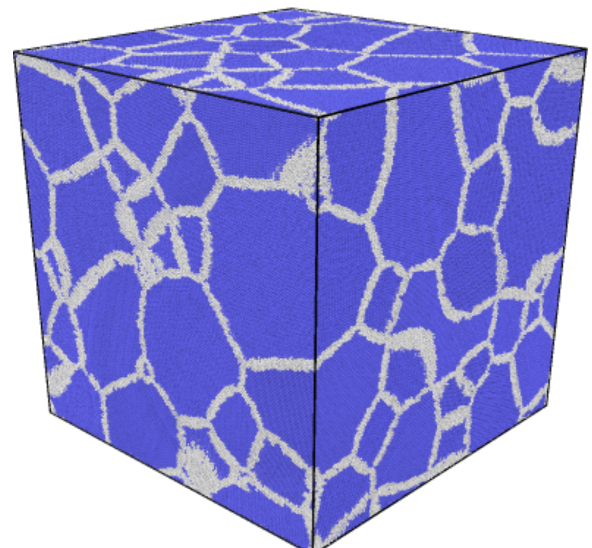
Microstructure modeling using PF

Phase field grain growth model





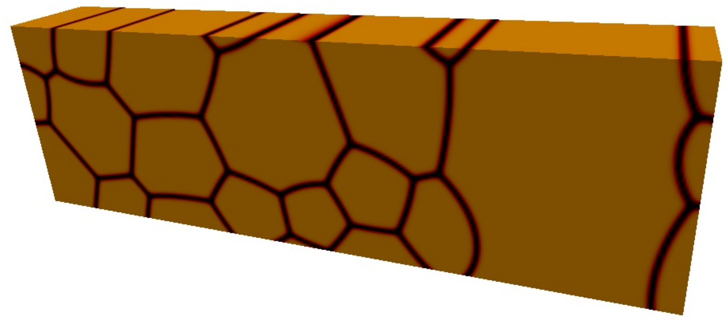
Finite element mesh



Atomistic microstructure

Approach: Phase field to CP-FEM

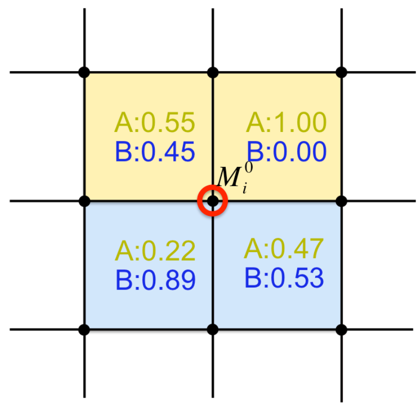
PHASE FIELD GRAIN GROWTH SIMULATIONS

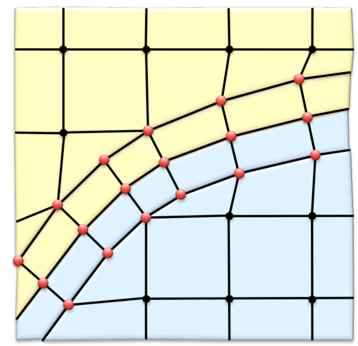


INPUT: (x, y, z, Φ(i))

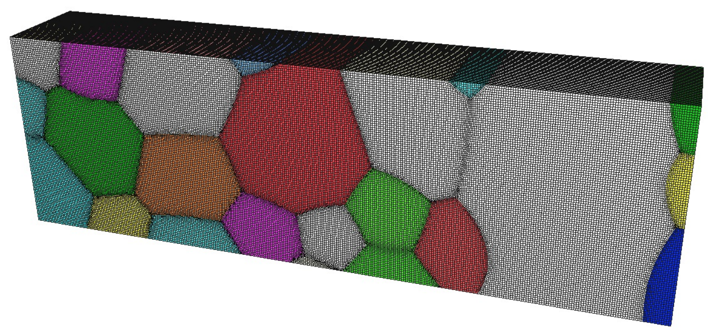
CUBIT 'SCULPT' TECHNOLOGY

OUTPUT: Exodus mesh

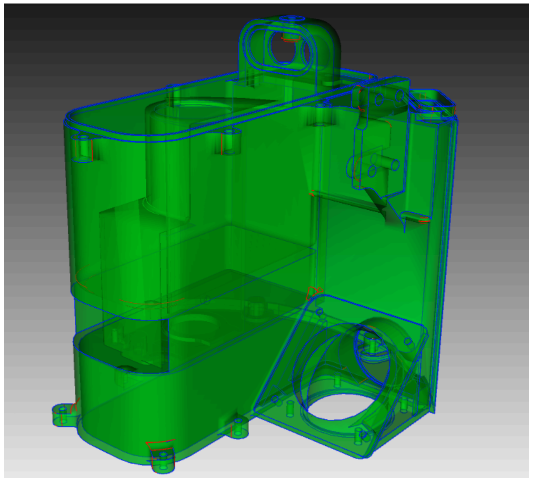




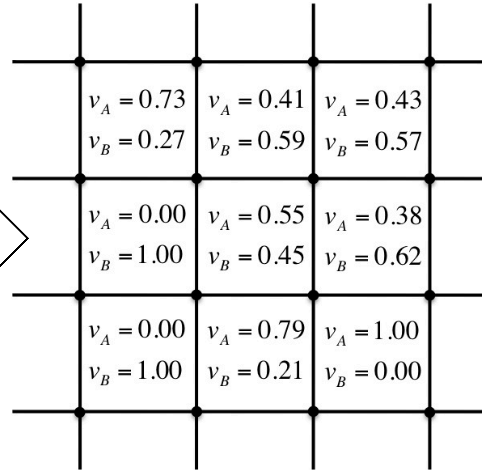
CRYSTAL PLASTICITY FINITE ELEMENT SIMULATIONS



Sculpt technology

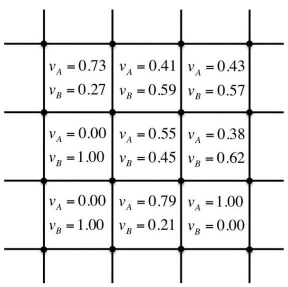


STL File

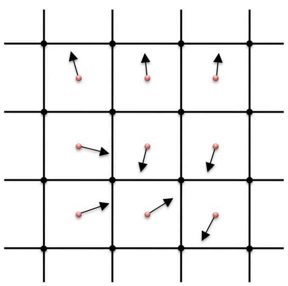


Volume Fraction Data

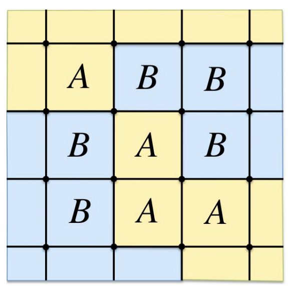
All-hex mesh



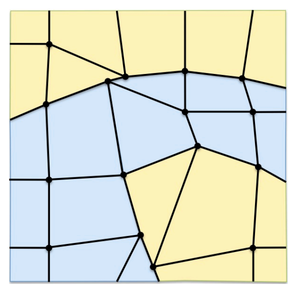
Establish parallel Cartesian grid



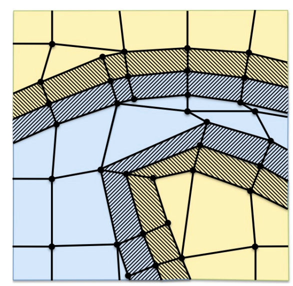
Estimate gradients at cell centers



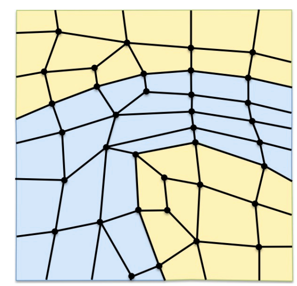
Assign materials to cell. Resolve non-Manifold cases



Compute virtual edge crossings and move grid points to iso-surface.

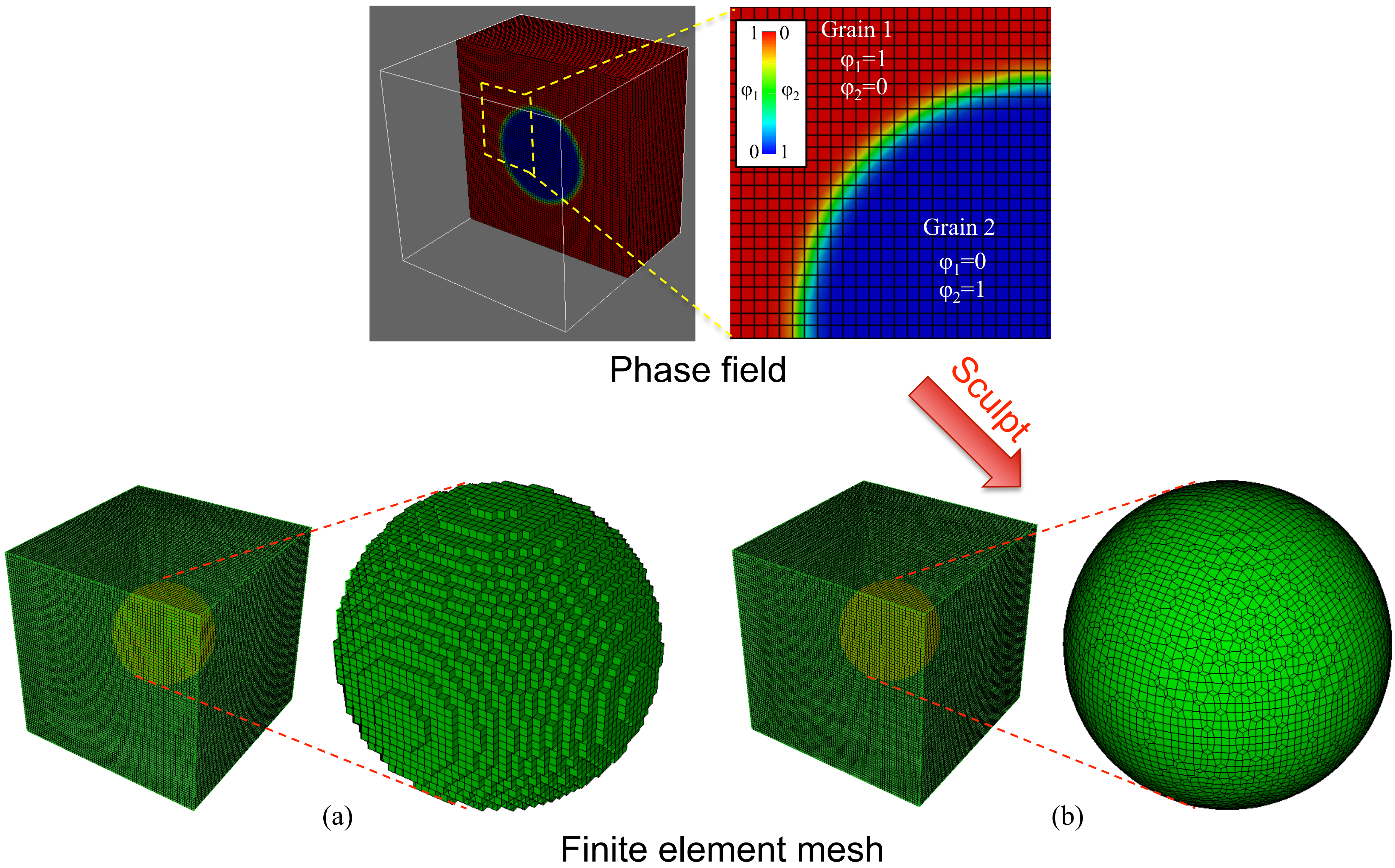


Insert hex buffer layer



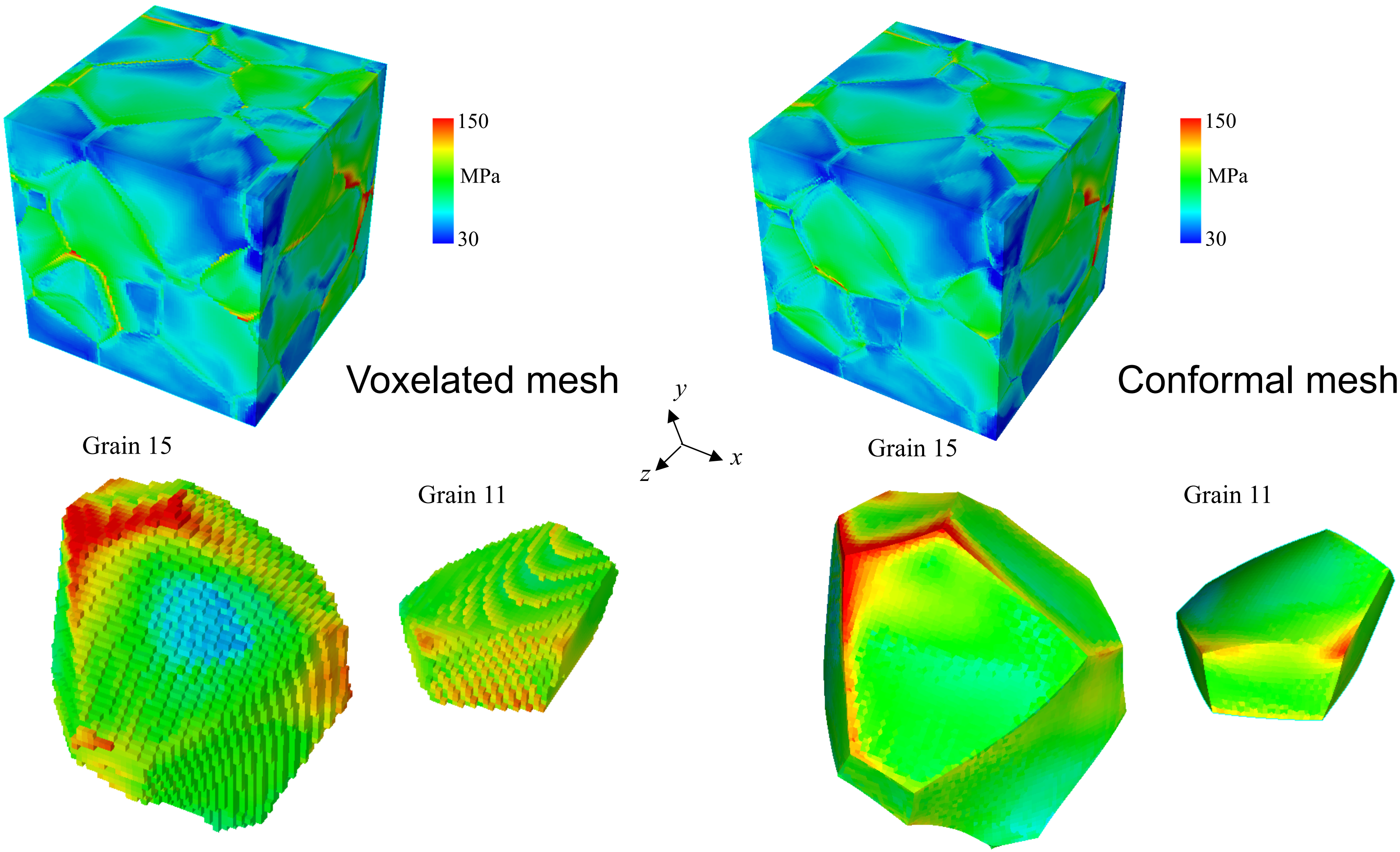
Smooth

Case 1: sphere in a cube

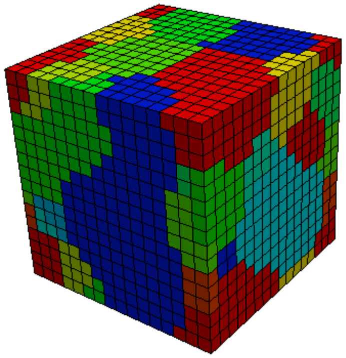


3D polycrystal: 10% deformation

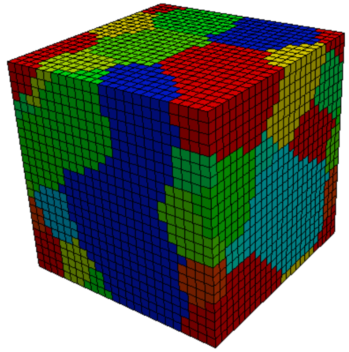
Stress distributions at 10% deformation



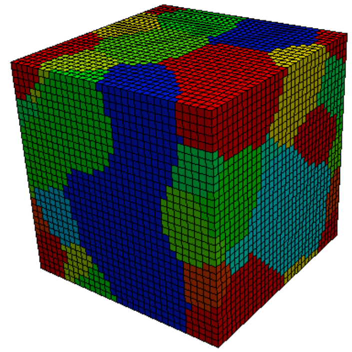
Mesh convergence test: Initial mesh



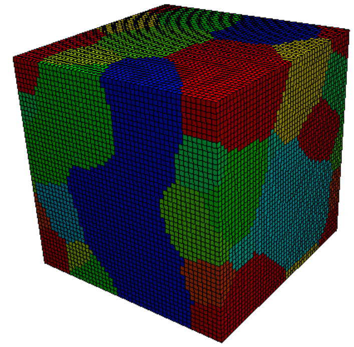
4,096 elements



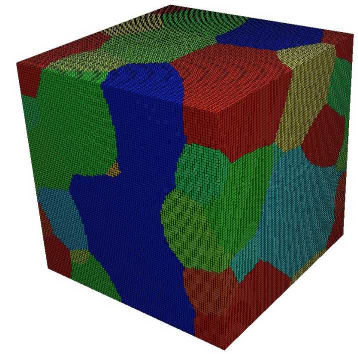
13,824 elements



32,768 elements

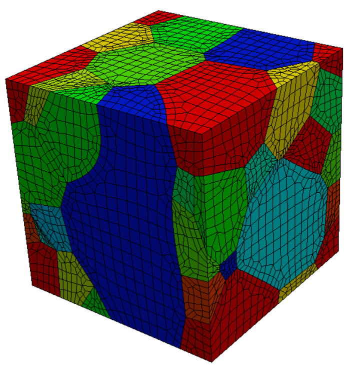


110,592 elements

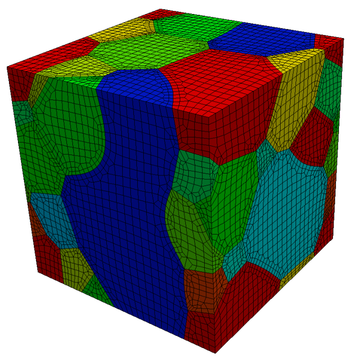


884,736 elements

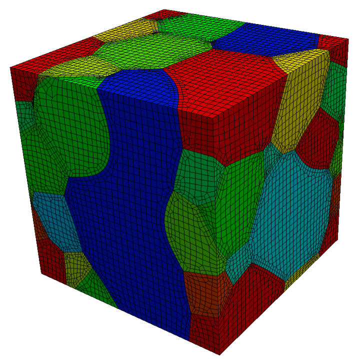
Voxelated mesh



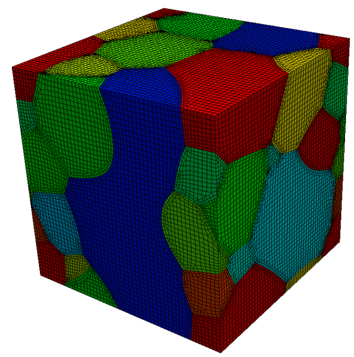
17,730 elements



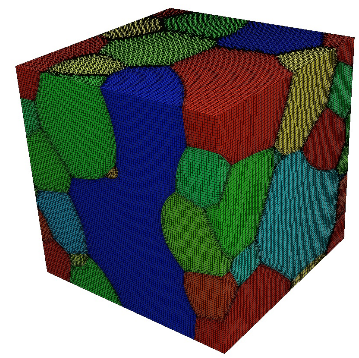
42,922 elements



81,838 elements



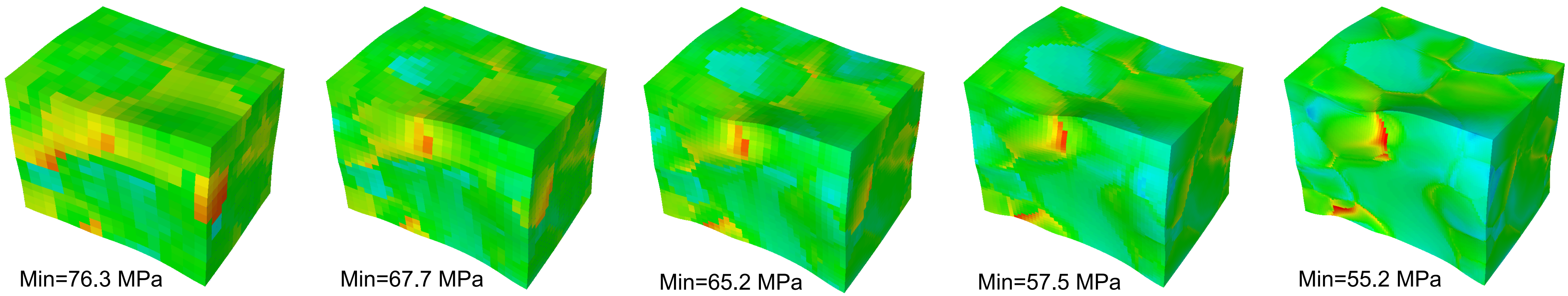
215,714 elements



1,281,856 elements

Conformal mesh

Von Mises Stress (20% deformation)



Min=76.3 MPa
Max=264.2 MPa
4,096 elements

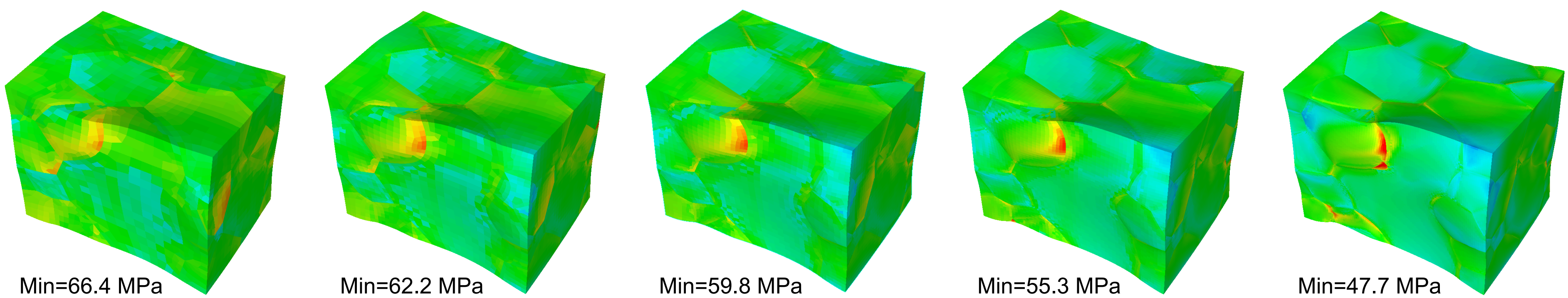
Min=67.7 MPa
Max=292 MPa
13,824 elements

Min=65.2 MPa
Max=258.4 MPa
32,768 elements

Min=57.5 MPa
Max=266.3 MPa
110,592 elements

Min=55.2 MPa
Max=287.3 MPa
884,736 elements

Voxelated mesh



Min=66.4 MPa
Max=247.7 MPa
17,730 elements

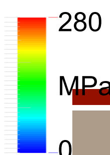
Min=62.2 MPa
Max=257.6 MPa
42,922 elements

Min=59.8 MPa
Max=261.1 MPa
81,838 elements

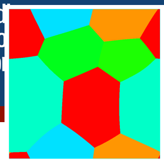
Min=55.3 MPa
Max=271.9 MPa
215,714 elements

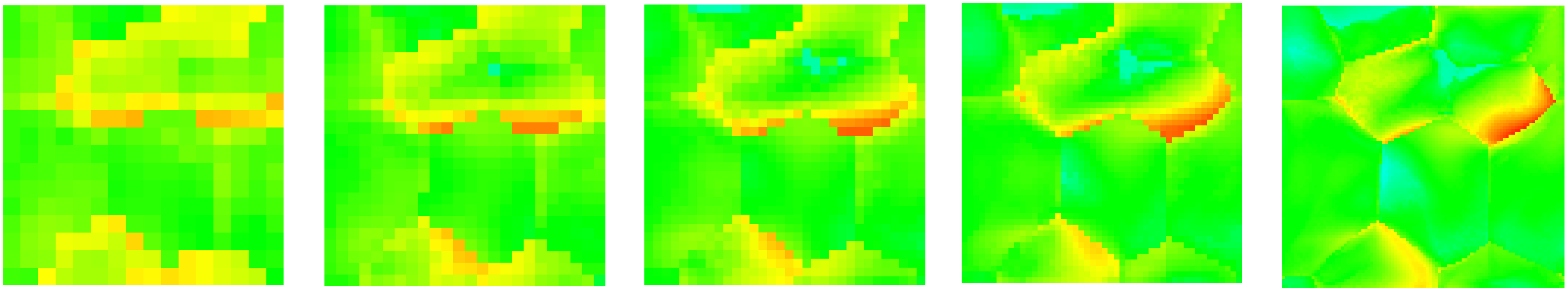
Min=47.7 MPa
Max=328.1 MPa
1,281,856 elements

Conformal mesh



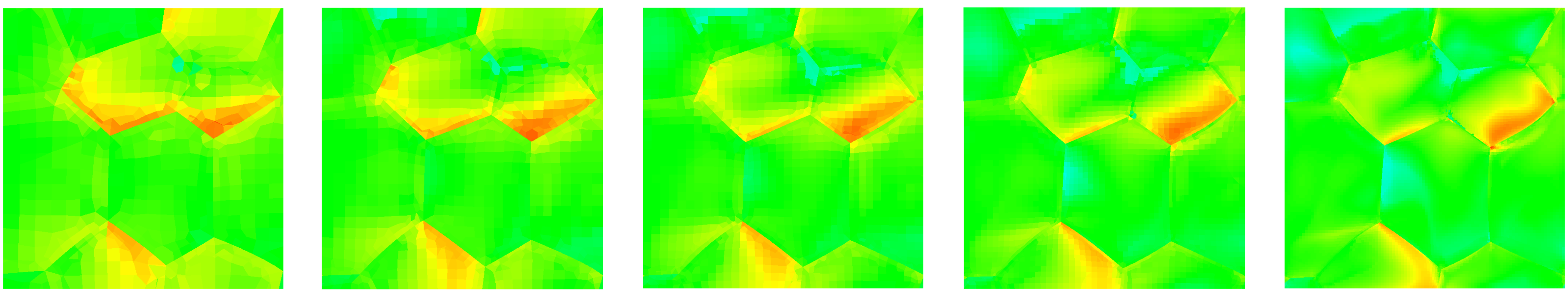
Von Mises Stress (mid z surface)





4,096 elements | 13,824 elements | 32,768 elements | 110,592 elements | 884,736 elements

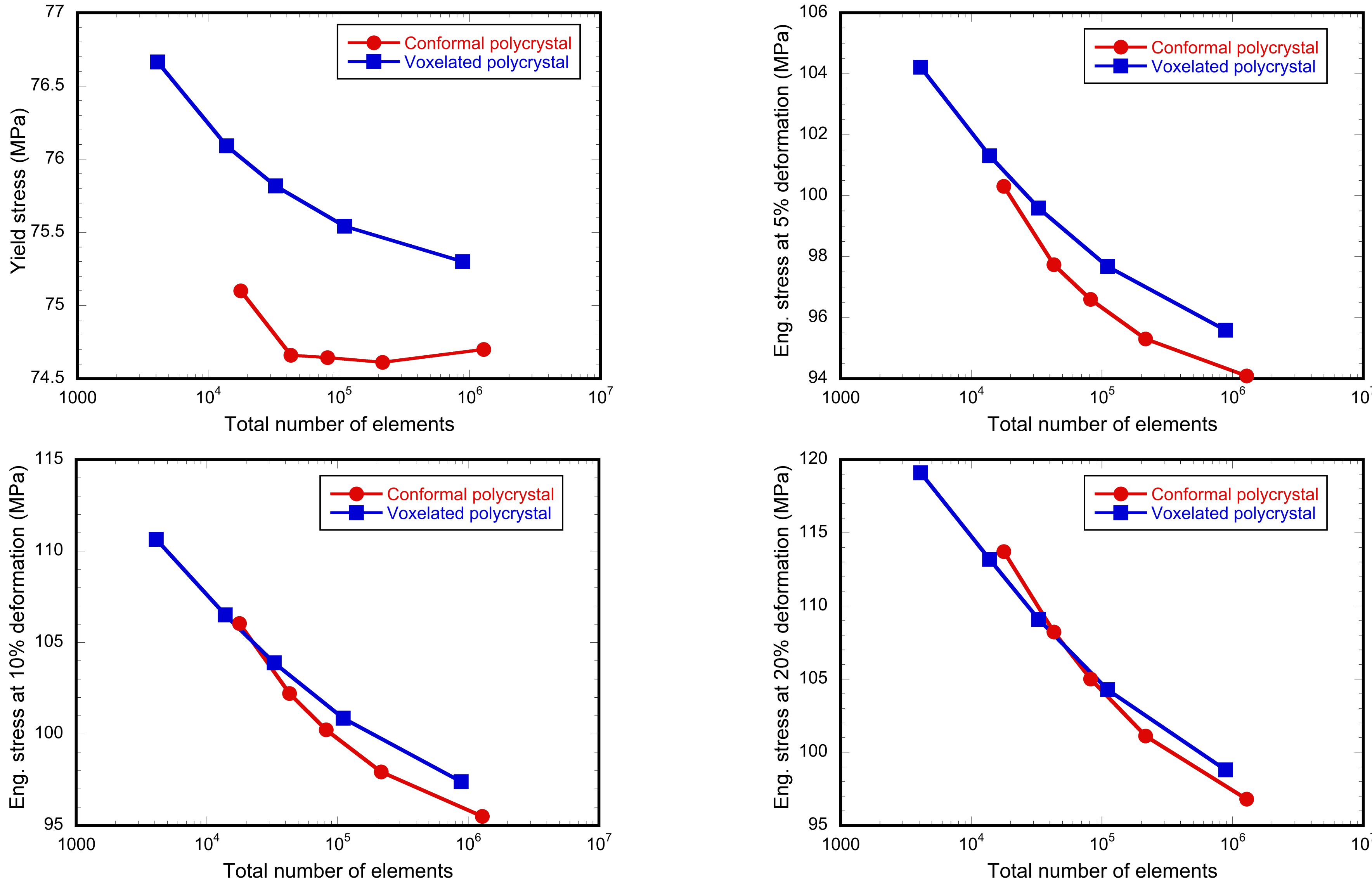
Voxelated mesh



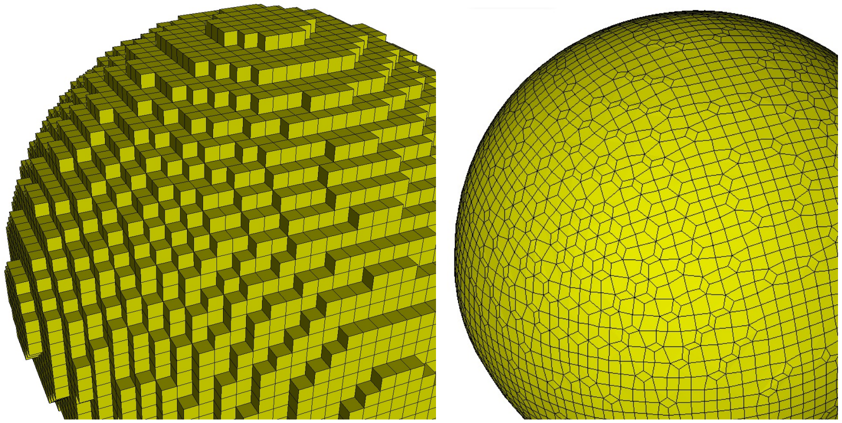
17,730 elements | 42,922 elements | 81,838 elements | 215,714 elements | 1,281,856 elements

Conformal mesh

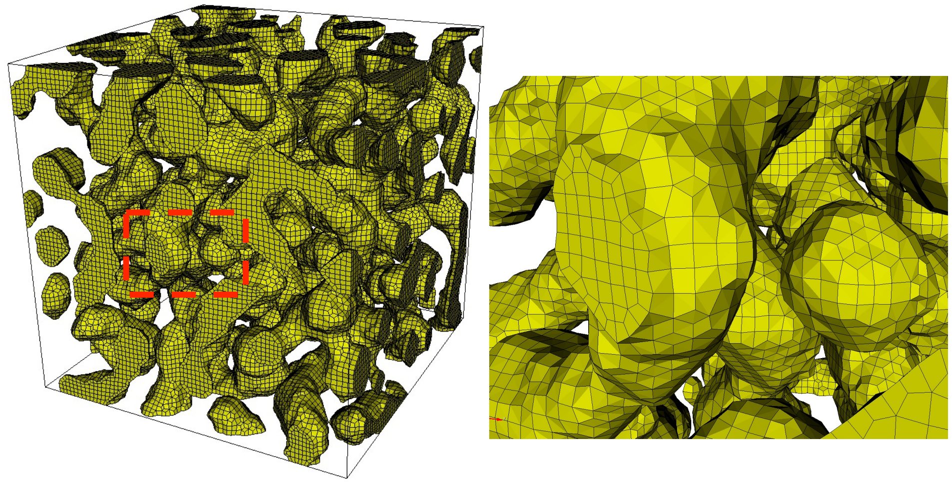
Mesh convergence



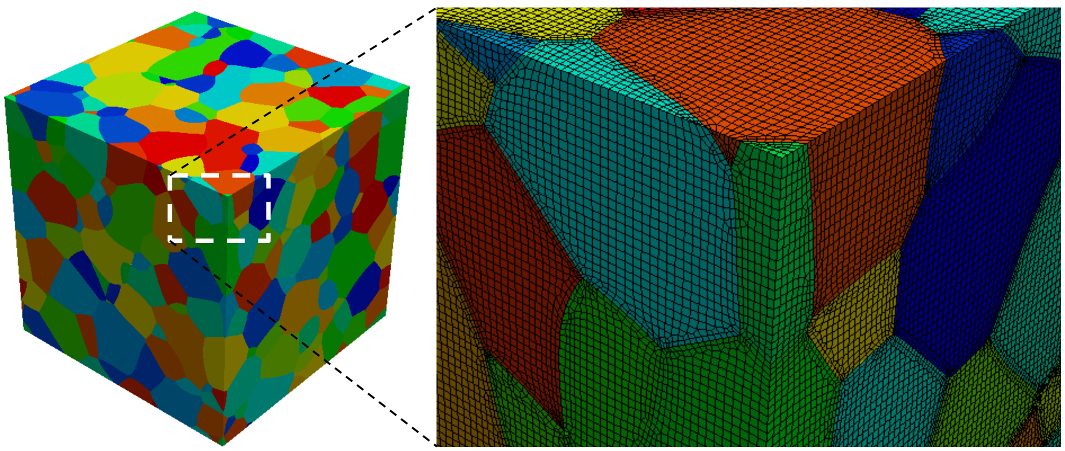
Enhanced capabilities in CUBIT



Voxelated mesh ➔ conformal mesh

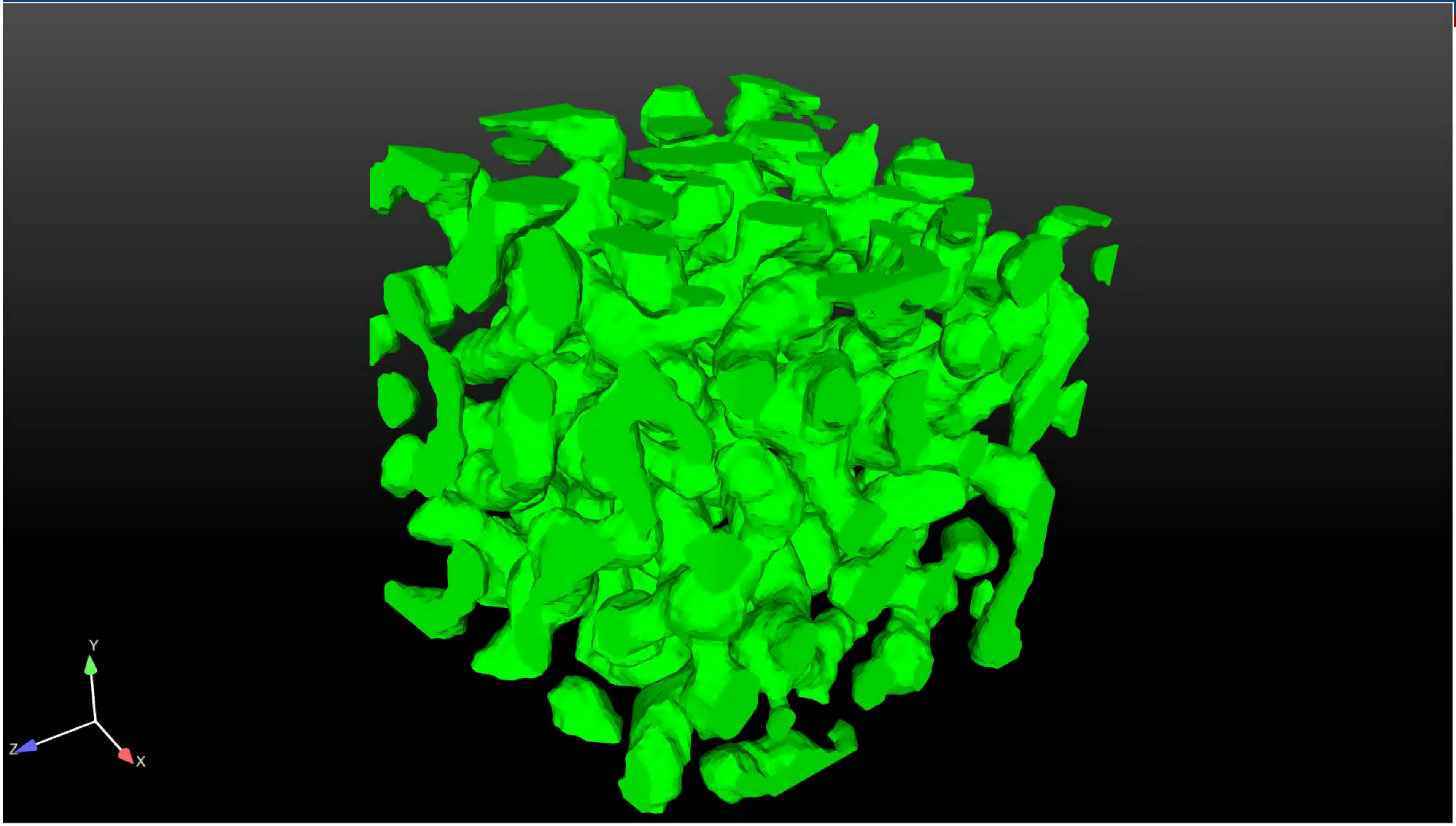


Monte Carlo grain growth➔ conformal mesh



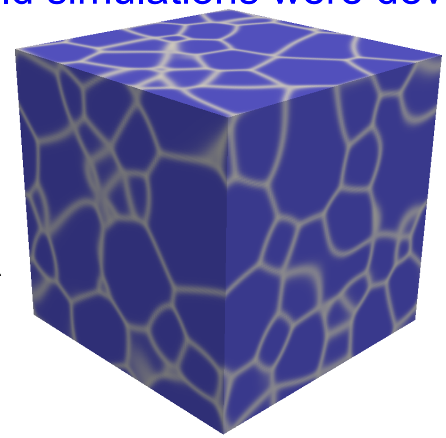
Robustness:52 grains using 1.2 million hex elements

FE mesh from two-phase Monte Carlo simulation

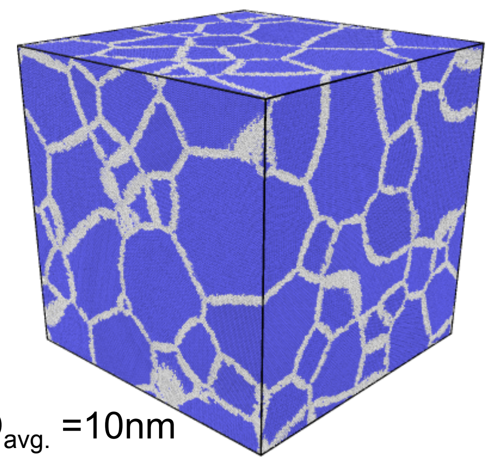


Creating physically-based multi-scale 3D microstructure

A new technique to produce ***physically-based multi-scale 3D microstructures*** using results from grain growth phase field simulations were developed.

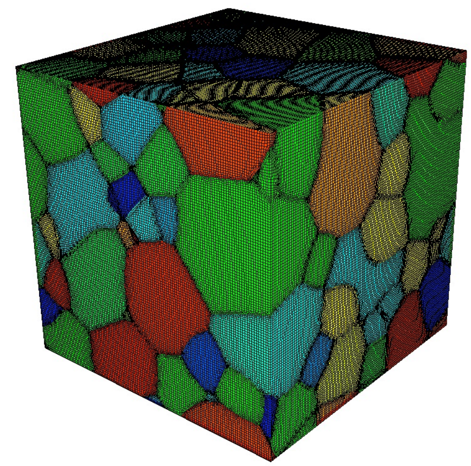


Phase field grain growth model



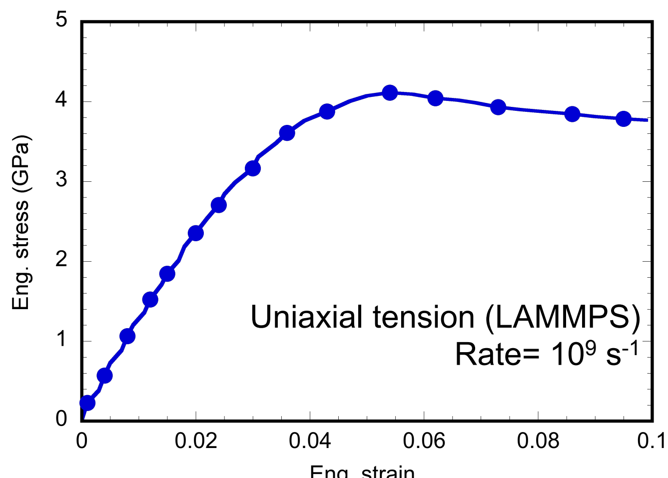
$D_{avg.}$ =10nm

Atomistic microstructure

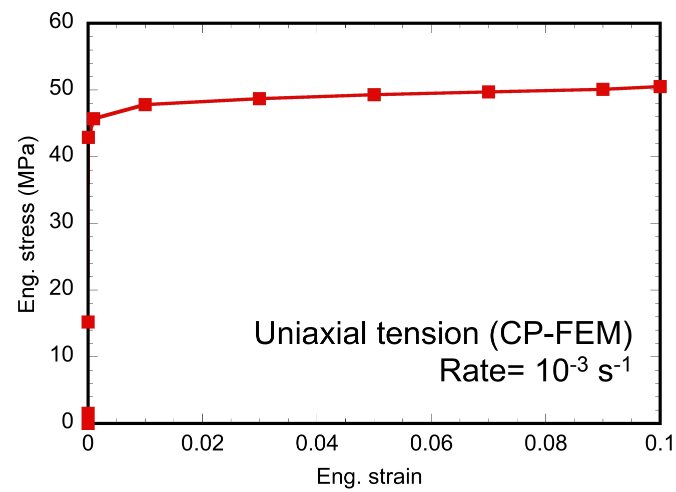


Finite element mesh

Microstructure



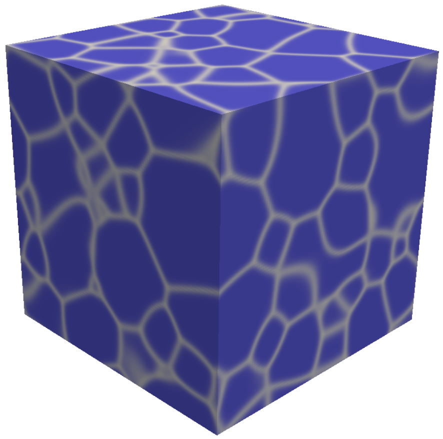
Mechanical properties at different length scales



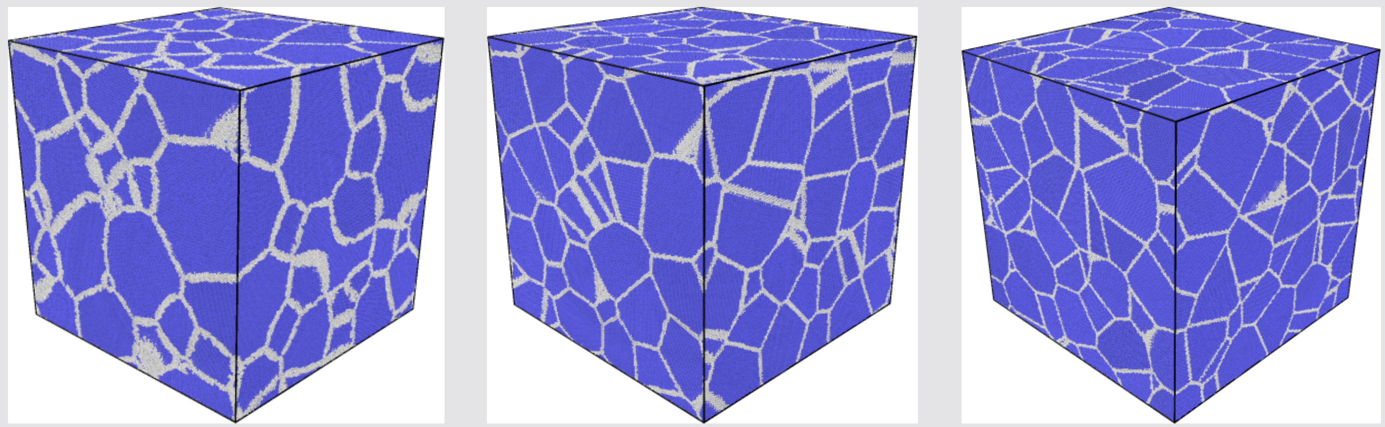
Phase field to atomistics

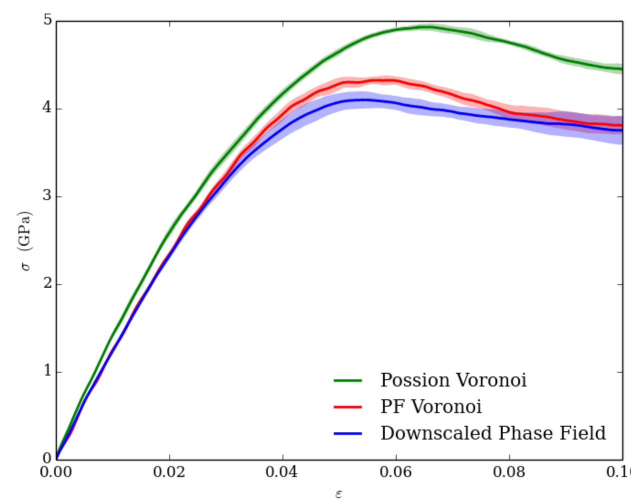
Effects of initial microstructure on mechanics of nanocrystalline materials

Phase Field



Downscaled Phase Field | Phase Field Voronoi | Poisson Voronoi





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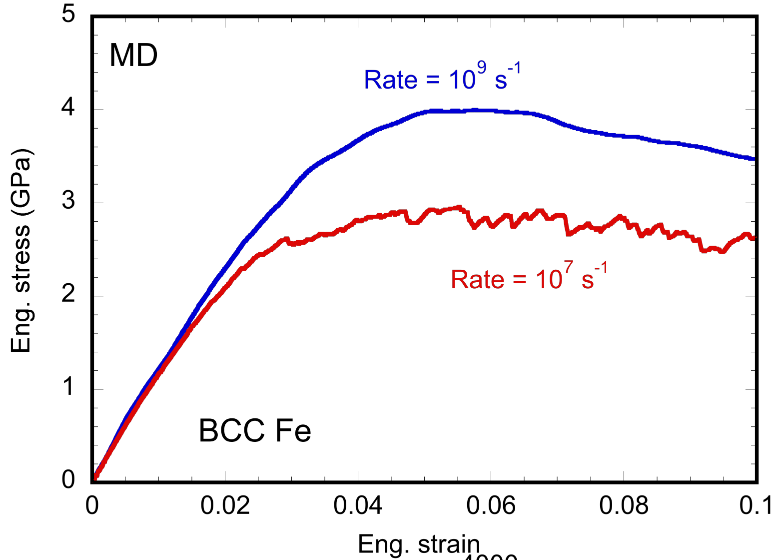

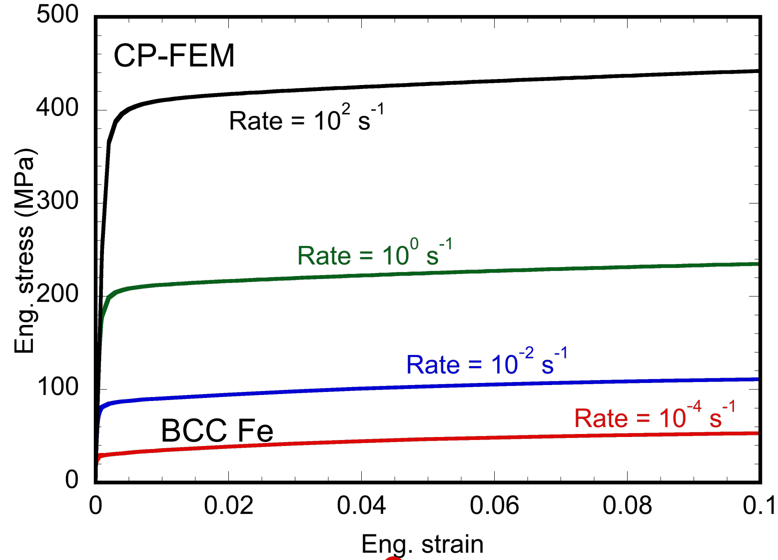

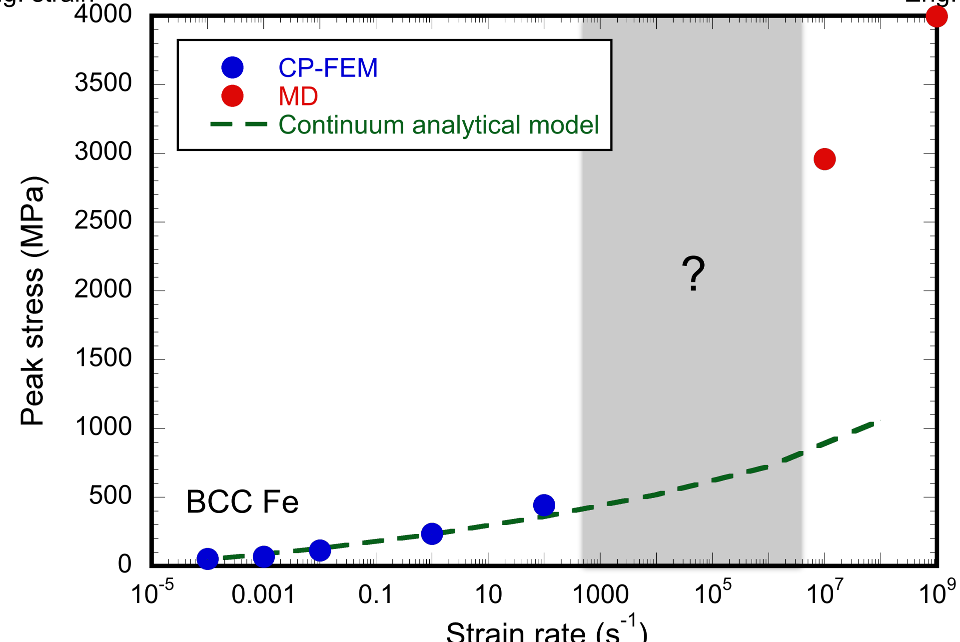

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THANK YOU !

Email: hnlim@sandia.gov