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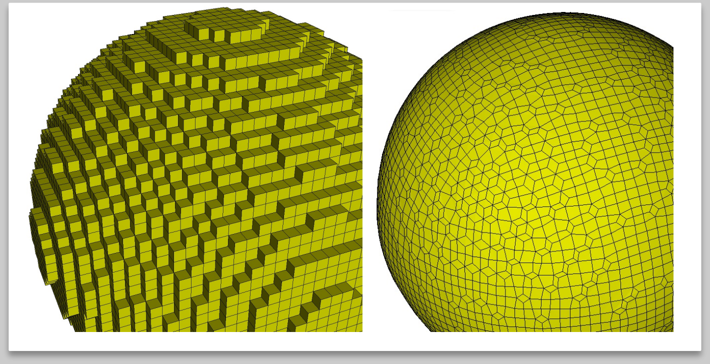

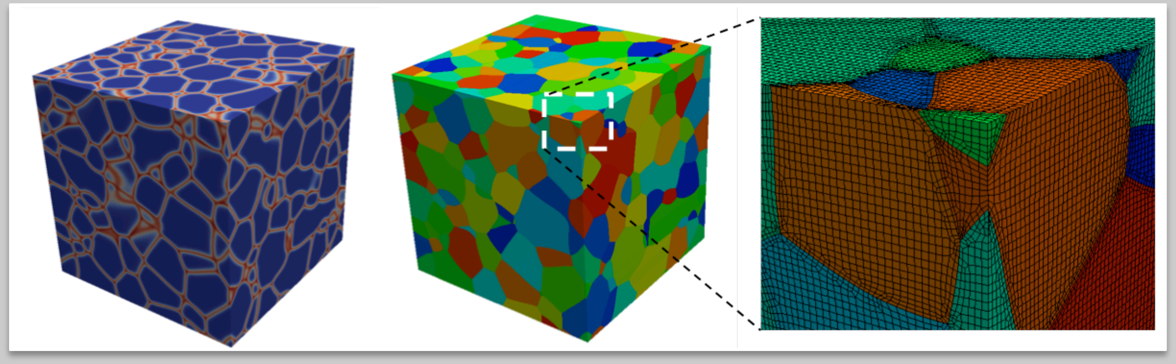

Developing Physically-based Three Dimensional Microstructures:

Bridging Phase Field and Crystal Plasticity Models

Hojun Lim[1], Fadi Abdeljawad[1], Steve Owen[2] and Corbett Battaile[1]

[1]Computational Materials & Data Science, [2]Simulation Modeling Science,
Sandia National Laboratories

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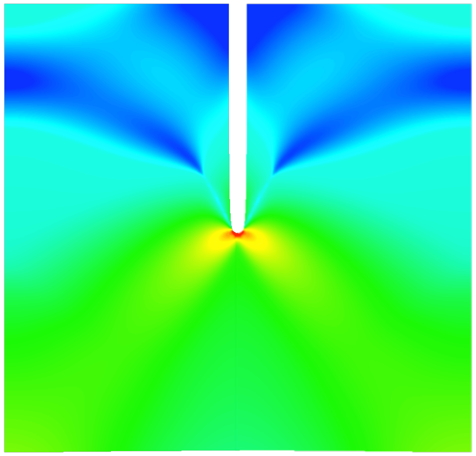
Outline

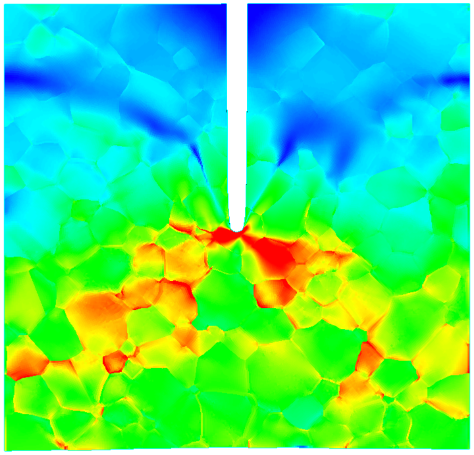
- Background
- 3D Interface-conformal Hex Meshing Technology (Sculpt)
- Crystal Plasticity – Finite Element (CP-FE) Simulations
- Applications
- Summary

Grain-scale variability in metals

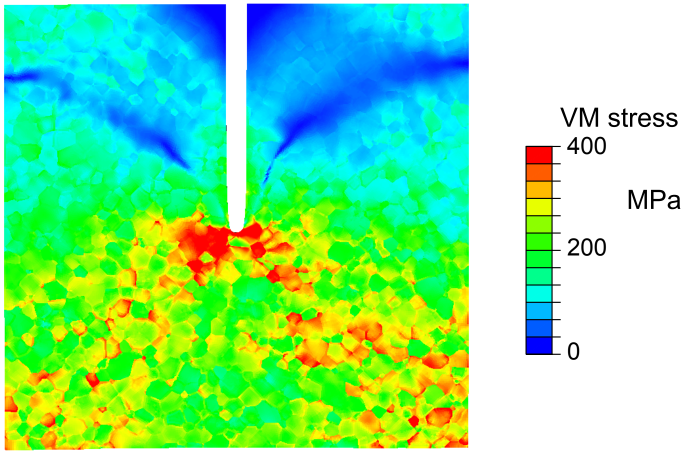
High fidelity modeling requires sophisticated material model & ***accurate representation of microstructure***.



Continuum simulation (J2)

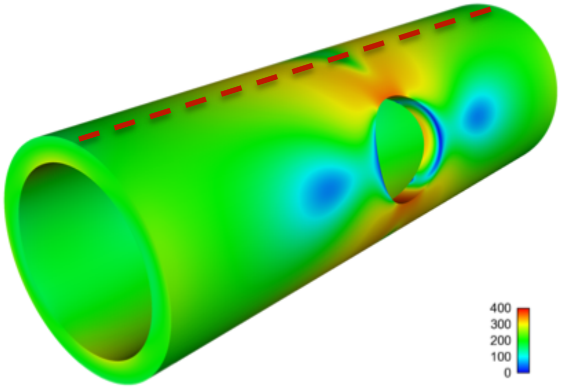


CP-FEM simulation (~200 grains)

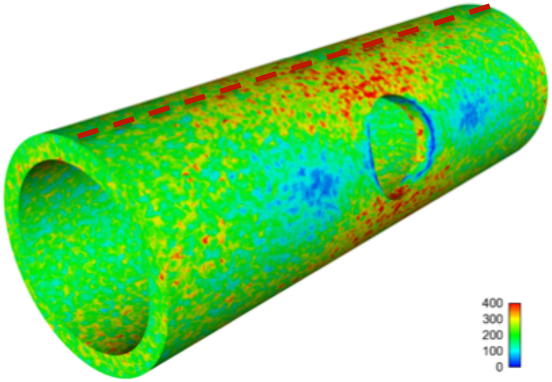


CP-FEM simulation (~1000 grains)

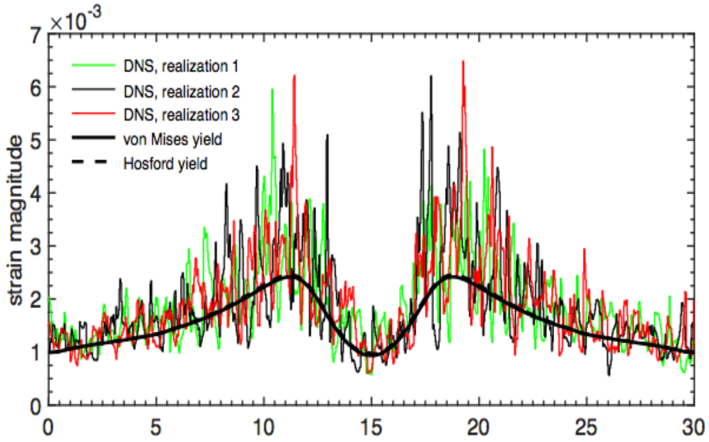
(Lim et al., 2016)



Continuum simulation (J2)



CP-FEM simulation (~50,000 grains)

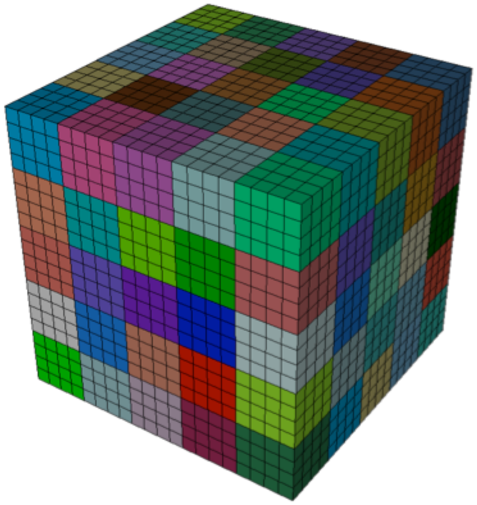


(Bishop et al., 2016)

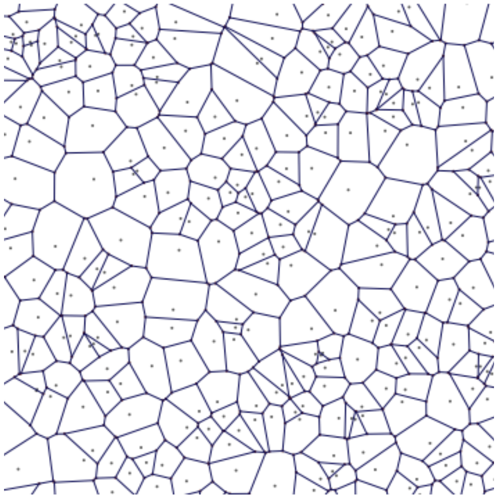
Motivation

However, fidelity of large-scale polycrystalline simulations are hindered by limited capabilities to model realistic 3D microstructures.

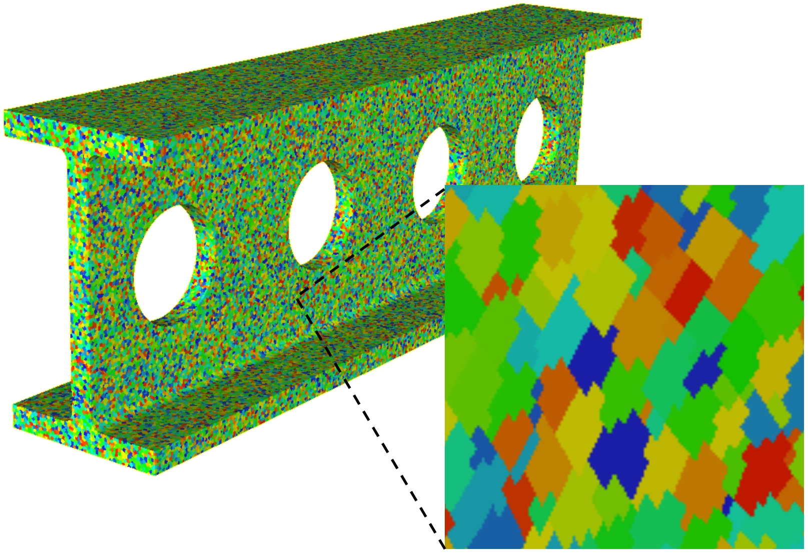
- Most finite element based polycrystalline models use idealized grain shapes or Voronoi tessellations.
- 3D microstructures digitized from experiments conform to a uniform grid.
- Reduce discretization error in FE based simulations.



Idealized grain representation
(Lim et al., 2014)



Voronoi Tessellation[1]



Voxelated grain representation
(Bishop et al., 2014)

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

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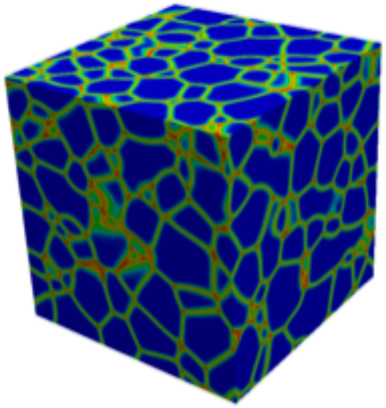
[1] http://philogb.github.io/blog/2010/02/12/voronoi-tessellation/

Constructing interface-conformal FE mesh

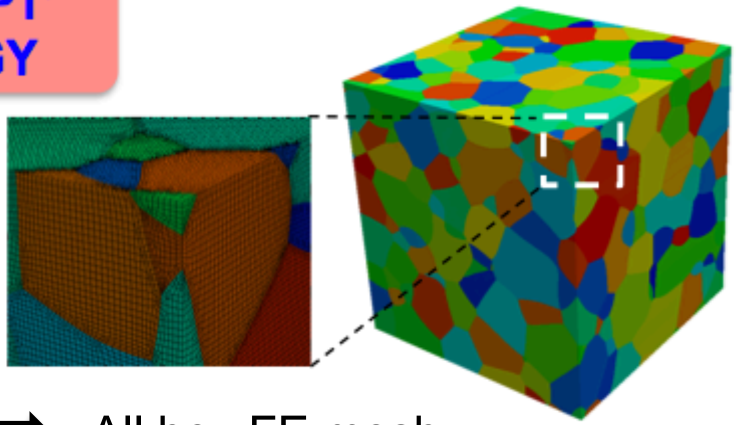
PHASE FIELD GRAIN GROWTH SIMULATIONS

CRYSTAL PLASTICITY FINITE ELEMENT SIMULATIONS

CUBIT ‘SCULPT’ TECHNOLOGY



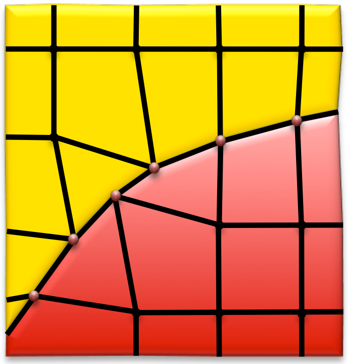
Realistic 3D microstructure
Conformal grain boundary mesh
Generates hexahedral elements



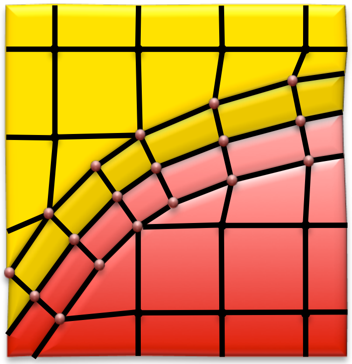
Volume fraction data → All hex FE mesh

$v_A = 0.73$ $v_B = 0.27$	$v_A = 0.41$ $v_B = 0.59$	$v_A = 0.43$ $v_B = 0.57$
$v_A = 0.00$ $v_B = 1.00$	$v_A = 0.55$ $v_B = 0.45$	$v_A = 0.38$ $v_B = 0.62$
$v_A = 0.00$ $v_B = 1.00$	$v_A = 0.79$ $v_B = 0.21$	$v_A = 1.00$ $v_B = 0.00$

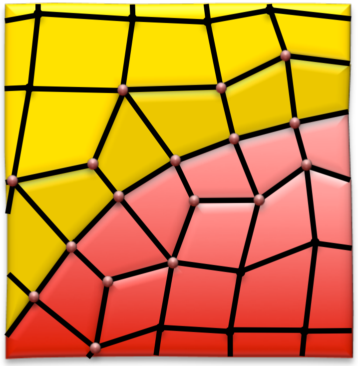
Volume fractions representing percent of grains for each cell



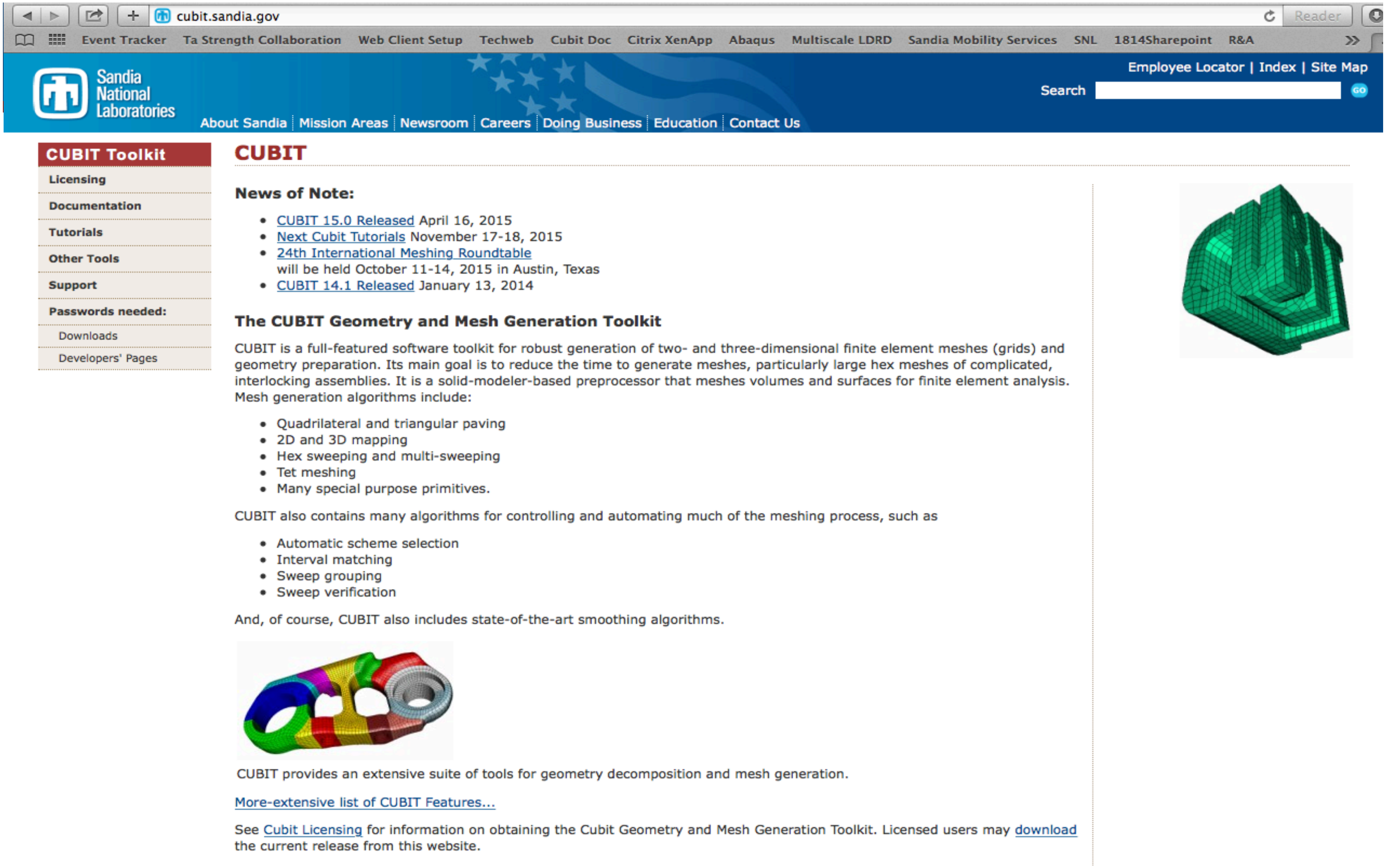
Resolve grain interfaces and project nodes to surfaces



Insert layer of hex elements at interfaces



Perform smoothing



CUBIT

News of Note:

- CUBIT 15.0 Released April 16, 2015
- Next Cubit Tutorials November 17-18, 2015
- 24th International Meshing Roundtable
  will be held October 11-14, 2015 in Austin, Texas
- CUBIT 14.1 Released January 13, 2014

The CUBIT Geometry and Mesh Generation Toolkit

CUBIT is a full-featured software toolkit for robust generation of two- and three-dimensional finite element meshes (grids) and geometry preparation. Its main goal is to reduce the time to generate meshes, particularly large hex meshes of complicated, interlocking assemblies. It is a solid-modeler-based preprocessor that meshes volumes and surfaces for finite element analysis. Mesh generation algorithms include:

- Quadrilateral and triangular paving
- 2D and 3D mapping
- Hex sweeping and multi-sweeping
- Tet meshing
- Many special purpose primitives.

CUBIT also contains many algorithms for controlling and automating much of the meshing process, such as

- Automatic scheme selection
- Interval matching
- Sweep grouping
- Sweep verification

And, of course, CUBIT also includes state-of-the-art smoothing algorithms.

CUBIT provides an extensive suite of tools for geometry decomposition and mesh generation.

More-extensive list of CUBIT Features...

See Cubit Licensing for information on obtaining the Cubit Geometry and Mesh Generation Toolkit. Licensed users may download the current release from this website.

- No charge for U.S. government-use licenses of CUBIT
- For academic and commercial licensing terms and pricing, visit http://www.csimsoft.com

Phase field grain growth model

❖ Total free energy

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

$\mathcal{F}_{tot}$: total free energy

$\phi_i(\mathbf{r}, t)$: order parameters

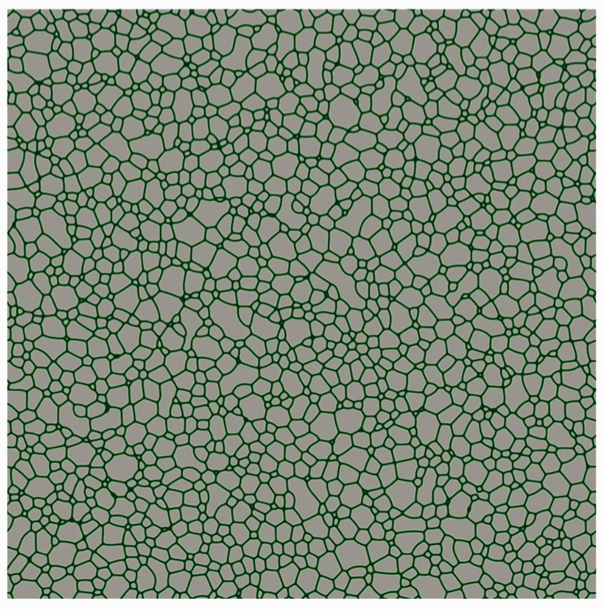
ϵ_i : GB parameter

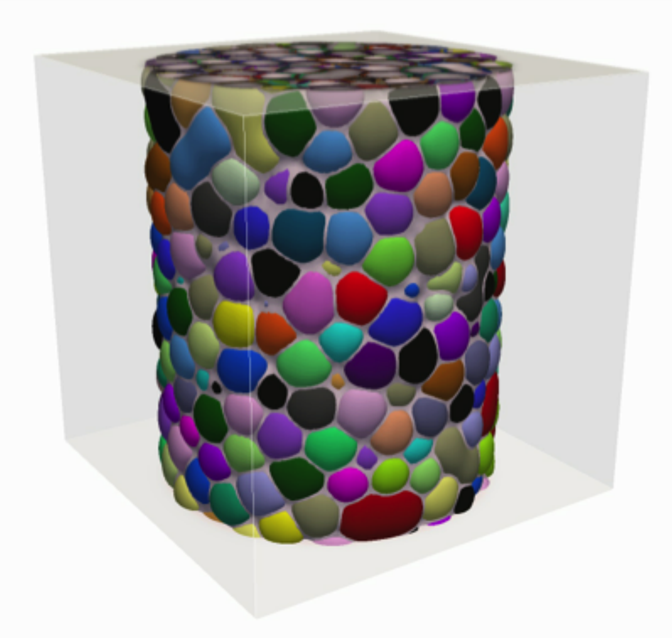
L_i : GB mobility parameter

❖ Dynamics

$$\frac{\partial \phi_i}{\partial t} = -L_i \left(\frac{\delta \mathcal{F}_{tot}}{\delta \phi_i} \right)$$

Allen-Cahn Eq. (Gradient flow of $\mathcal{F}_{tot}$)





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

Crystal plasticity finite element model

- Crystal Plasticity - Finite Element Method (CP-FEM) model
  - Realistic length/ time scales
  - Considers microstructural variability, i.e. grain morphology
  - Predicts macroscopic stress-strain response, local stress/ strain fields, texture evolution

- Solid mechanics code developed at Sandia National Laboratories (JAS-3D)
- 24 {110}<111> slip systems for BCC Ta
- Slip rate: $\dot{\gamma}^{\alpha} = \dot{\gamma}^{0} \left(\frac{\tau^{\alpha}}{g^{\alpha}} \right)^{1/m}$
- Slip resistance: $g^{\alpha} = \min\left(\tau_{EI}^{*\alpha}, \tau_{LT}^{*\alpha} \right) + \tau_{obs}^{\alpha}$

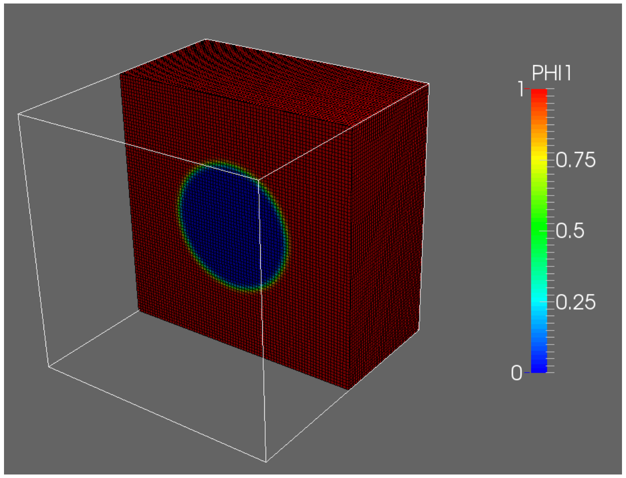
  Obstacle stress

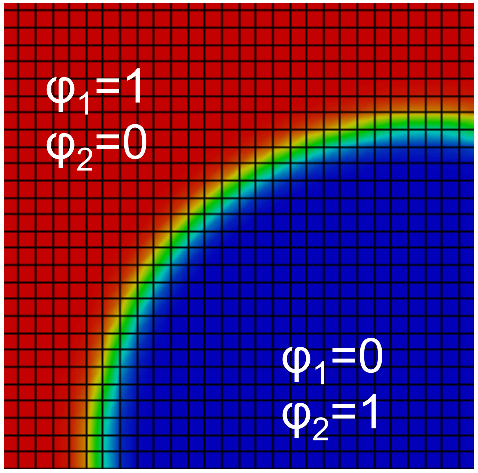
  Lattice friction

- Obstacle stress: $\tau_{obs}^{\alpha} = A\mu b \sqrt{\sum_{\beta=1}^{24} \rho^{\beta}}$ $\qquad$ $\dot{\rho}^{\alpha} = \left(\kappa_1 \sqrt{\sum_{\beta=1}^{\mathrm{NS}} \rho^{\beta}} - \kappa_2 \rho^{\alpha} \right) \cdot |\dot{\gamma}^{\alpha}|$

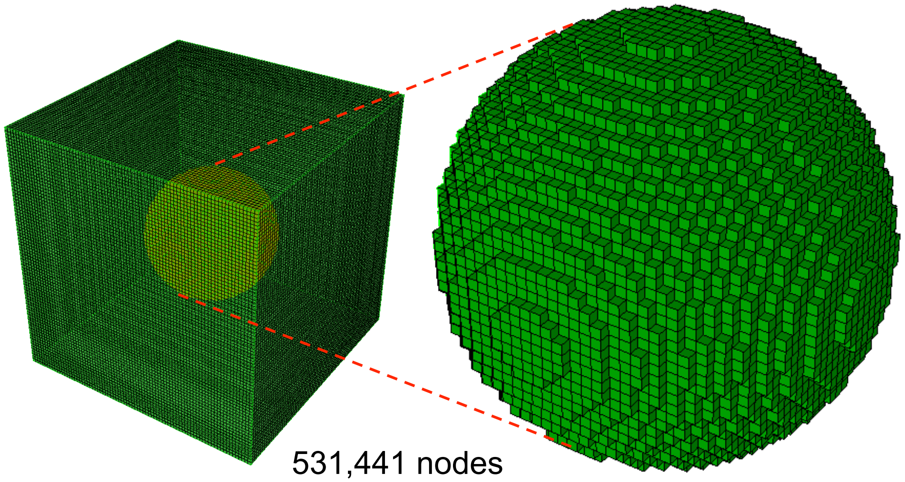
Spherical grain within a cubic matrix

Phase field



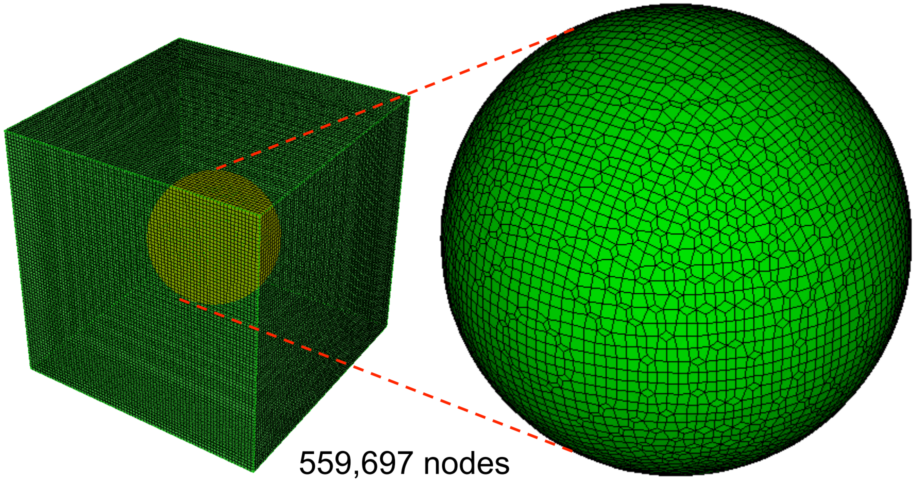


Voxelated FE mesh



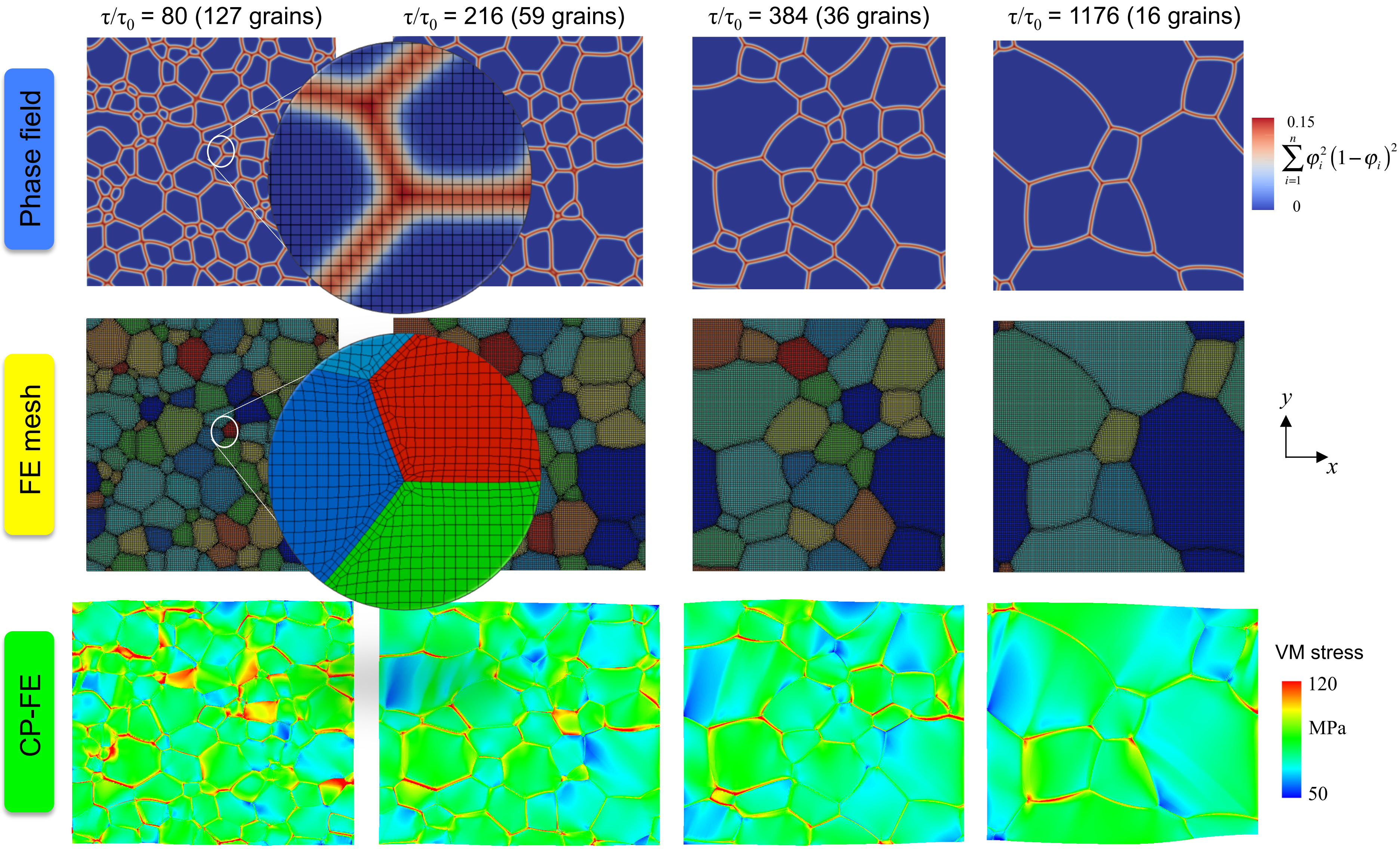
531,441 nodes
512,000 elements

Conformal FE mesh



559,697 nodes
540,248 elements

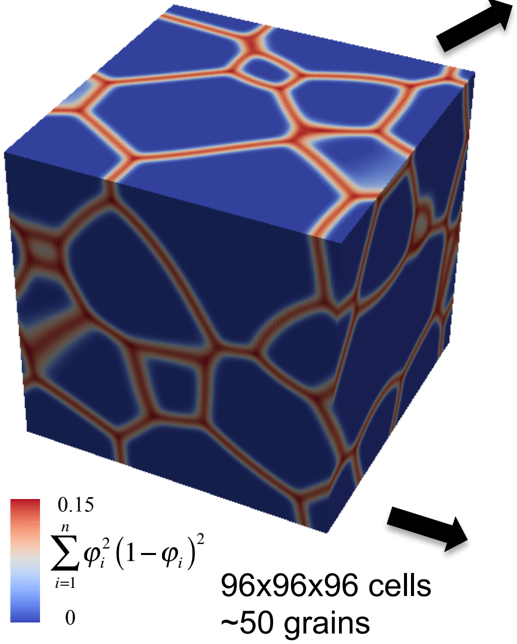
Simulations of 2D polycrystals



10% Uniaxial tension along x direction

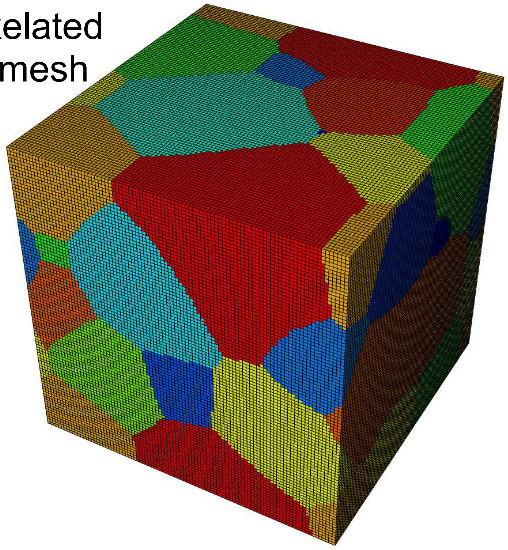
Simulations of 3D polycrystals

Phase Field Simulation

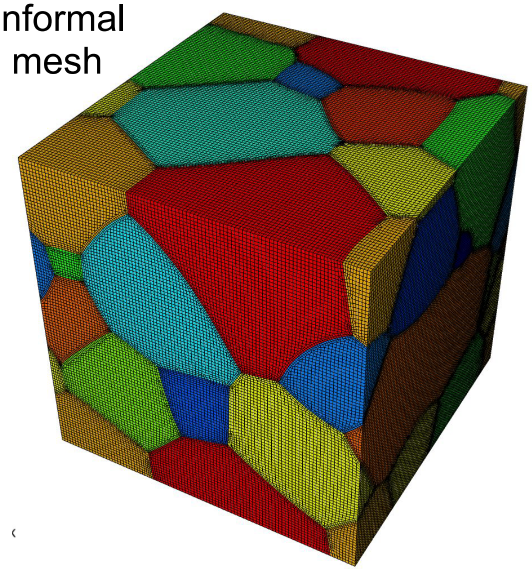


96x96x96 cells
~50 grains

Voxelated
FE mesh

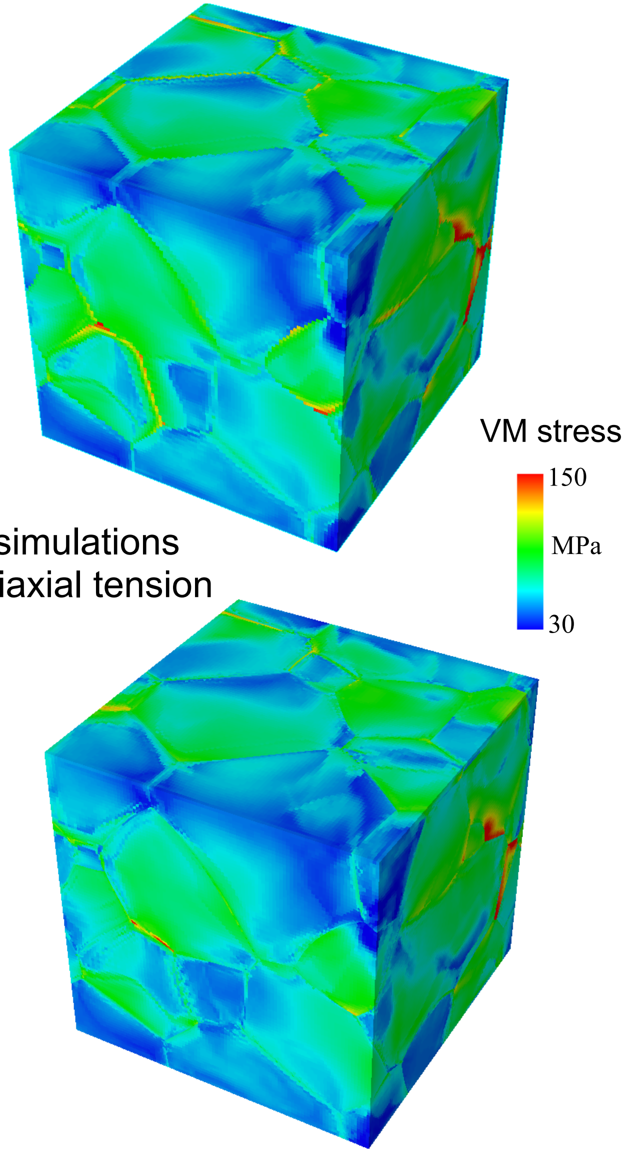


Conformal
FE mesh

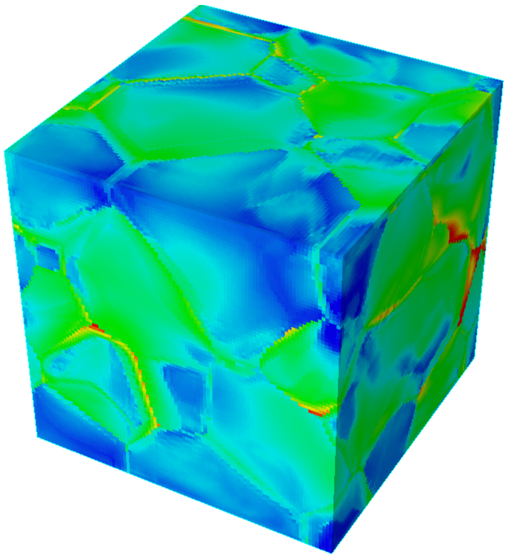


CP-FE simulations
10% uniaxial tension

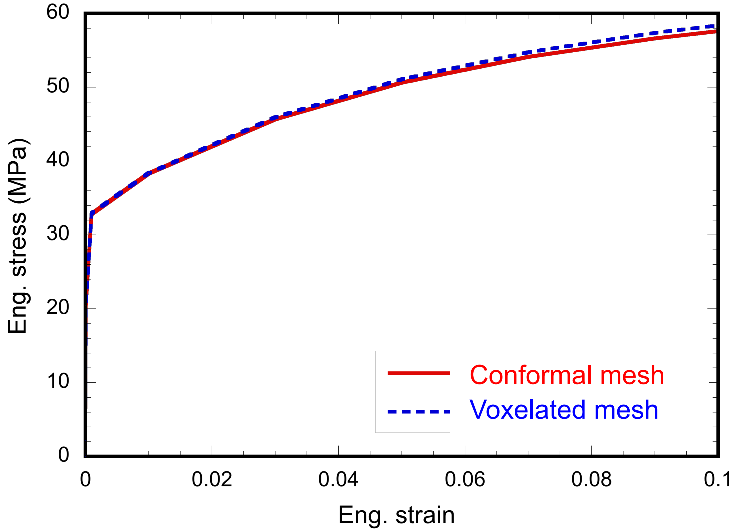
VM stress

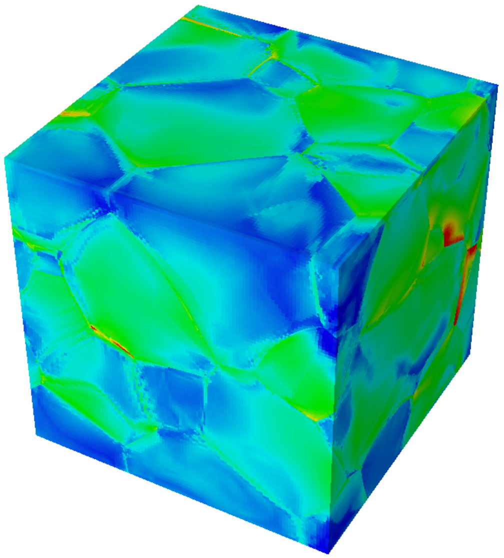


Macroscopic responses (10% deformation)



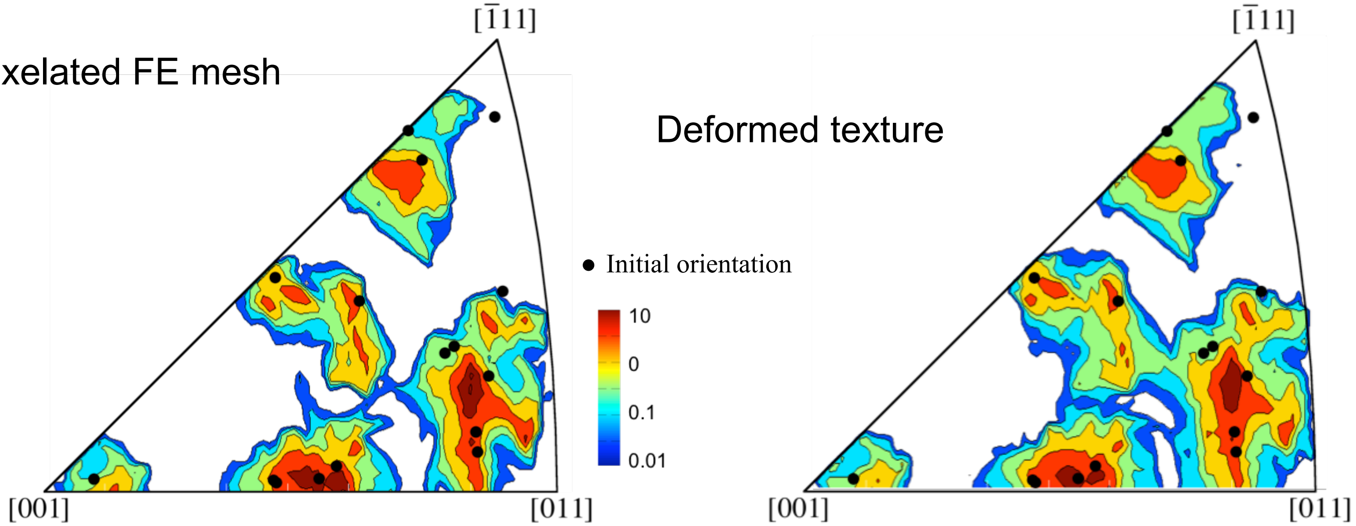
Macroscopic stress-strain response





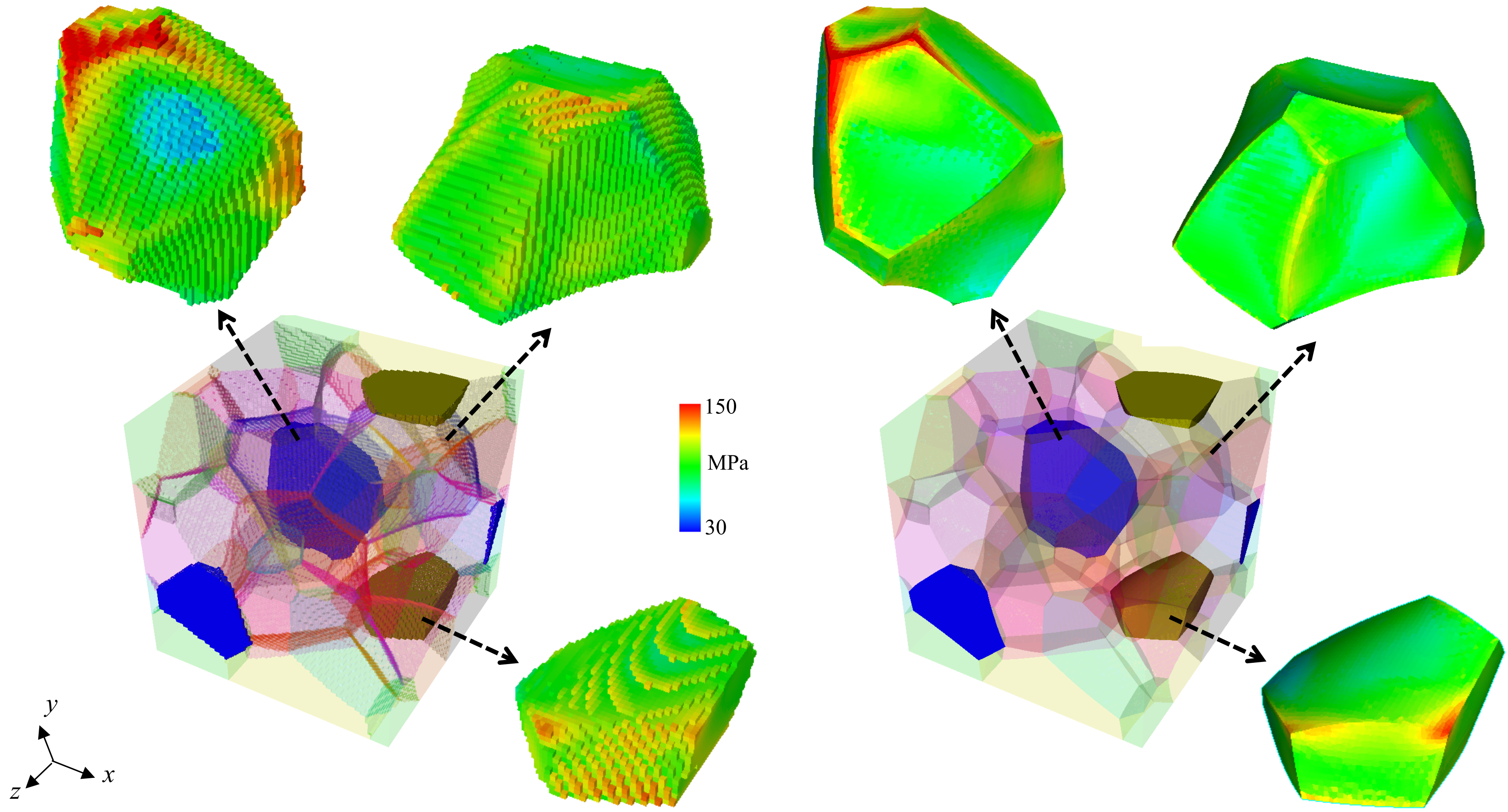
Voxelated FE mesh

Deformed texture



Conformal FE mesh

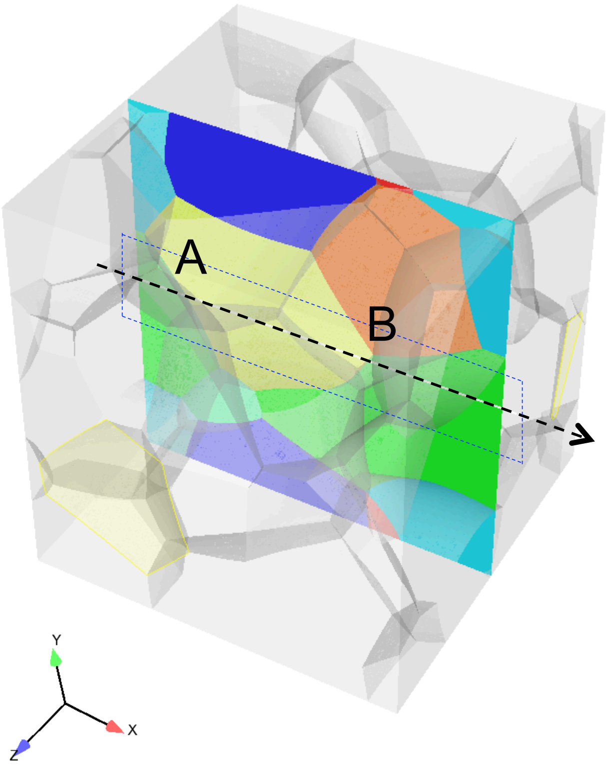
Local stress fields (10% deformation)

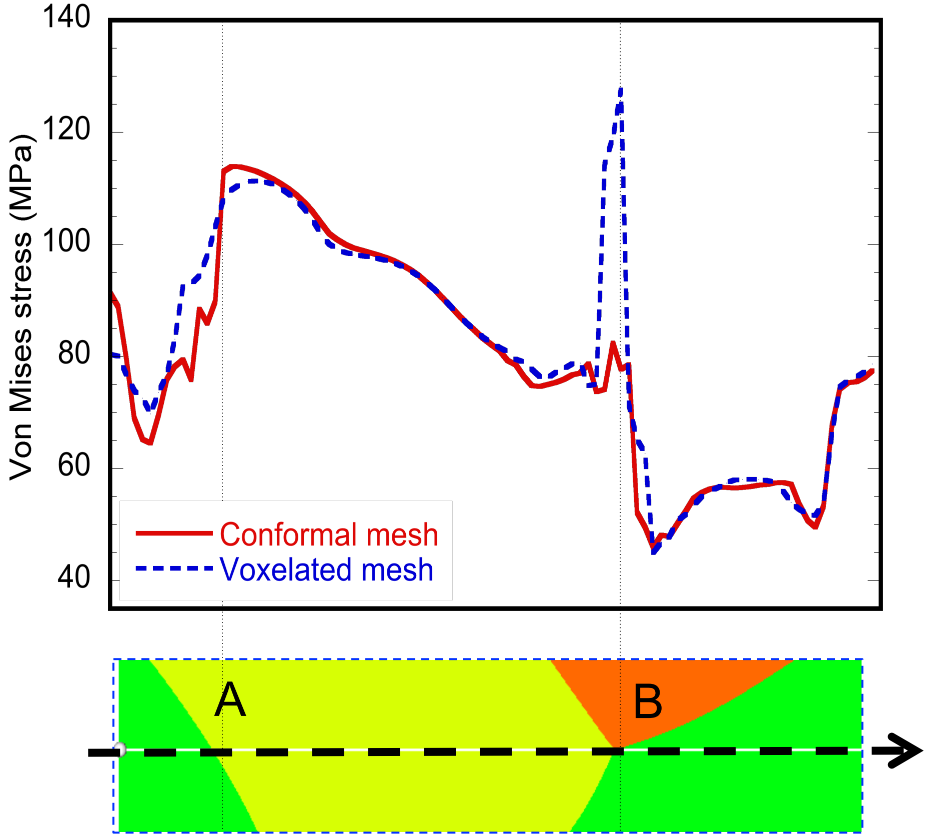


Voxelated FE mesh

Conformal FE mesh

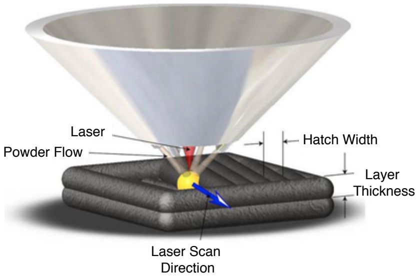
Local stress fields (10% deformation)

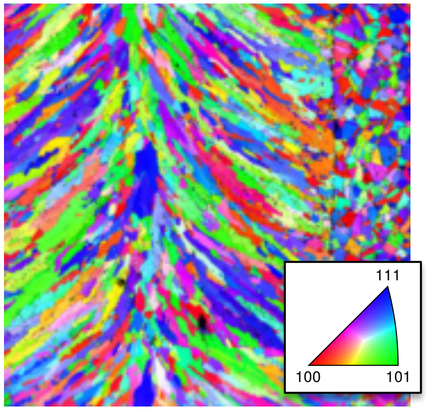




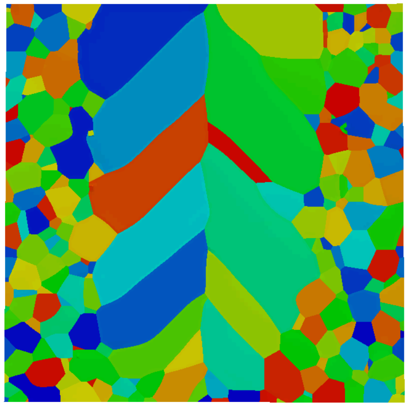
Applications of SCULPT technology

Laser Engineered Net Shaping (LENS®), Additively manufactured 304L SS

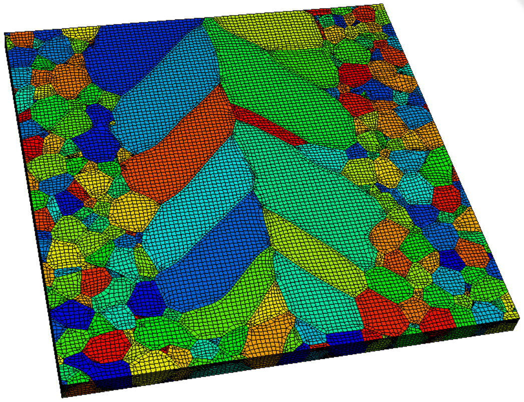




EBSD
(Adams et al., 2016)

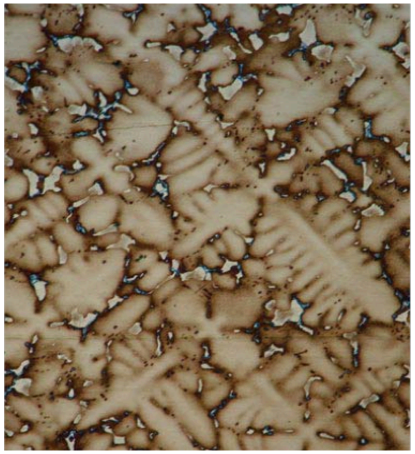


SPPARKS
(Rodgers et al., 2016)

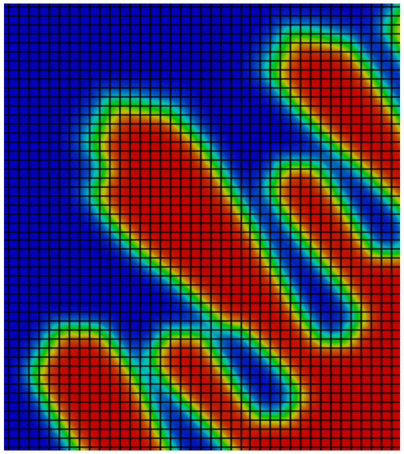


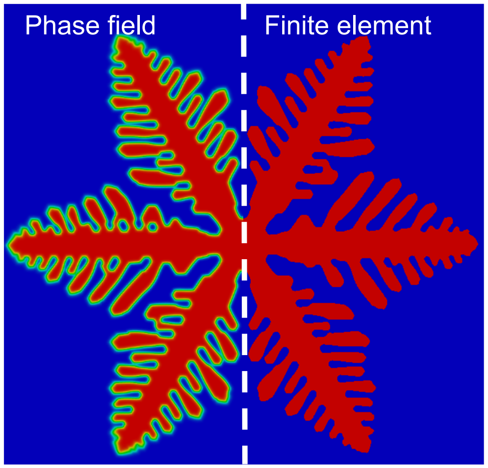
Conformal FE mesh

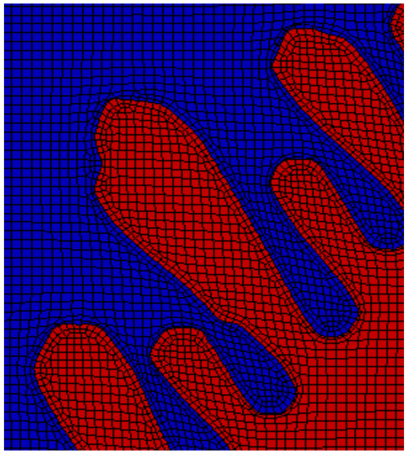
Dendritic microstructure



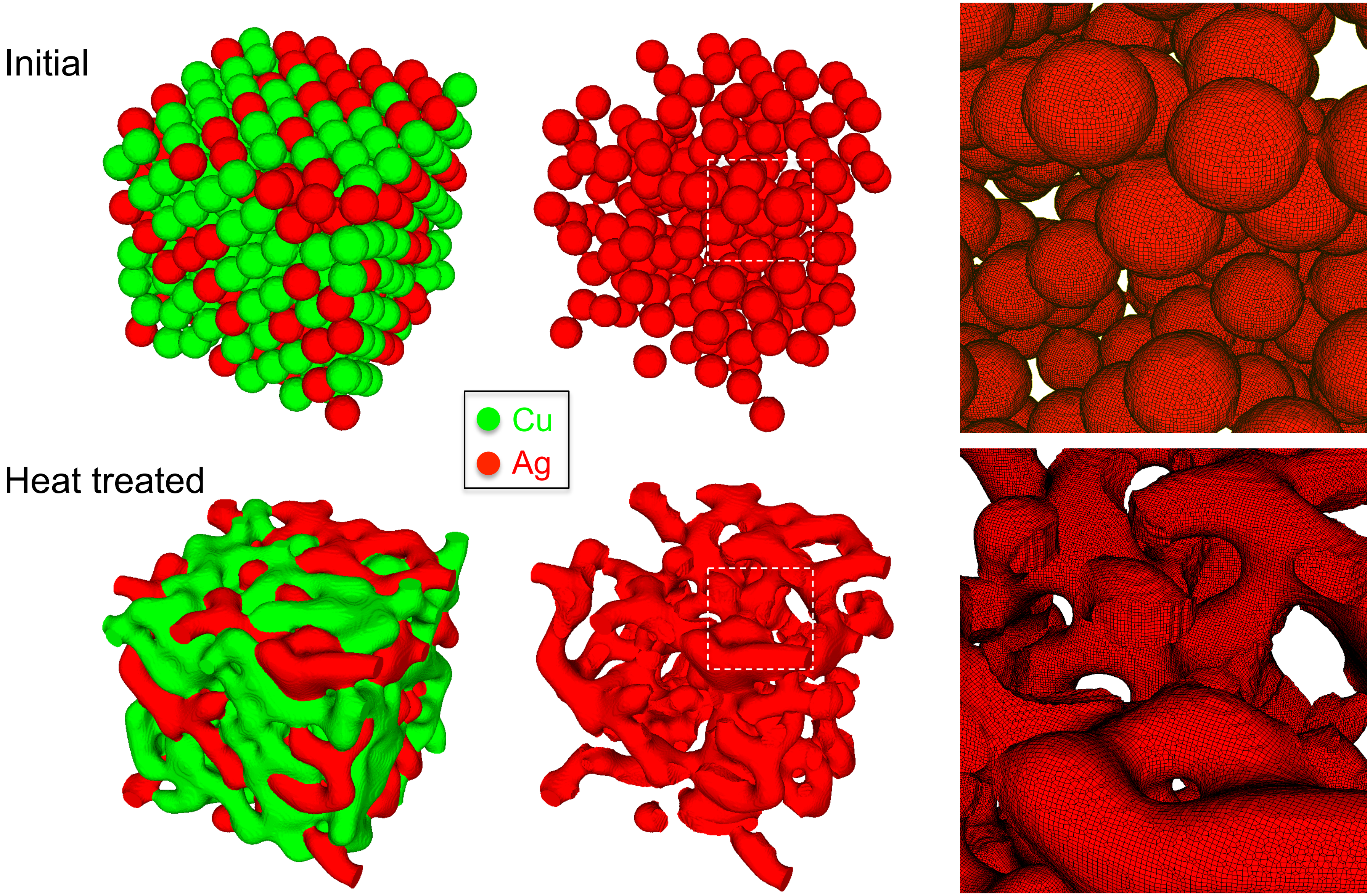
(Madison et al., 2008)







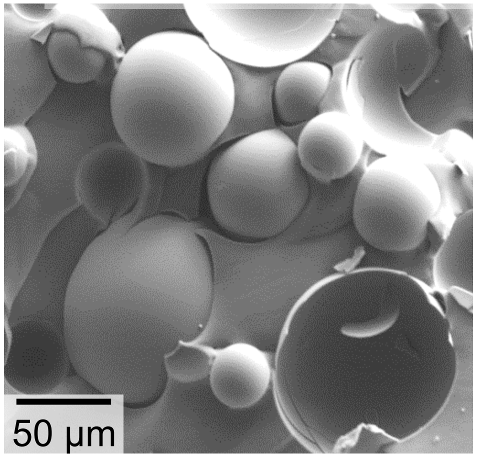
Multi-phase microstructure



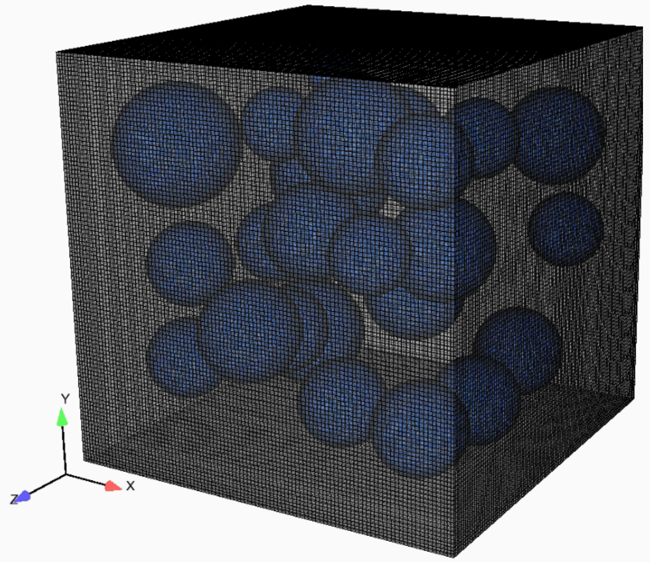
Sylgard® with A-16 Glass Microballoon Fillers

Investigating failure mechanisms of 'syntactic foam' using microstructure aware model

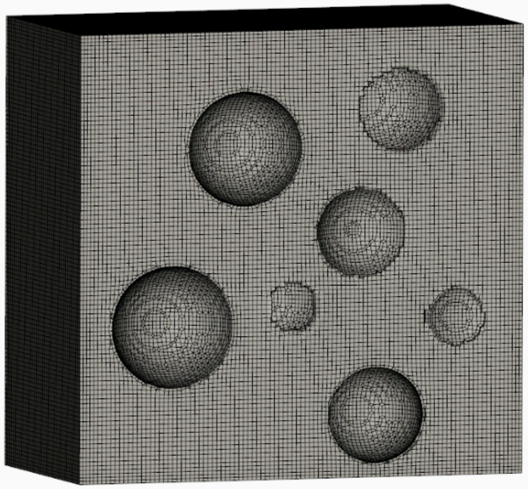
Ahmadi et al., 2014



Representative volume element meshed with Sculpt

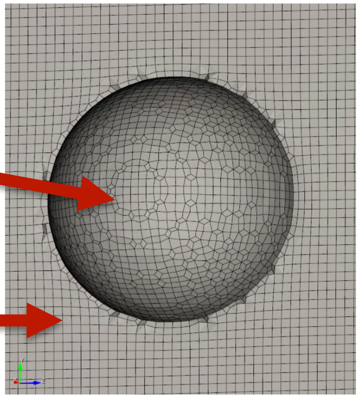


Cross section of Sculpt mesh



Microballoons meshed with quad 4 shell elements

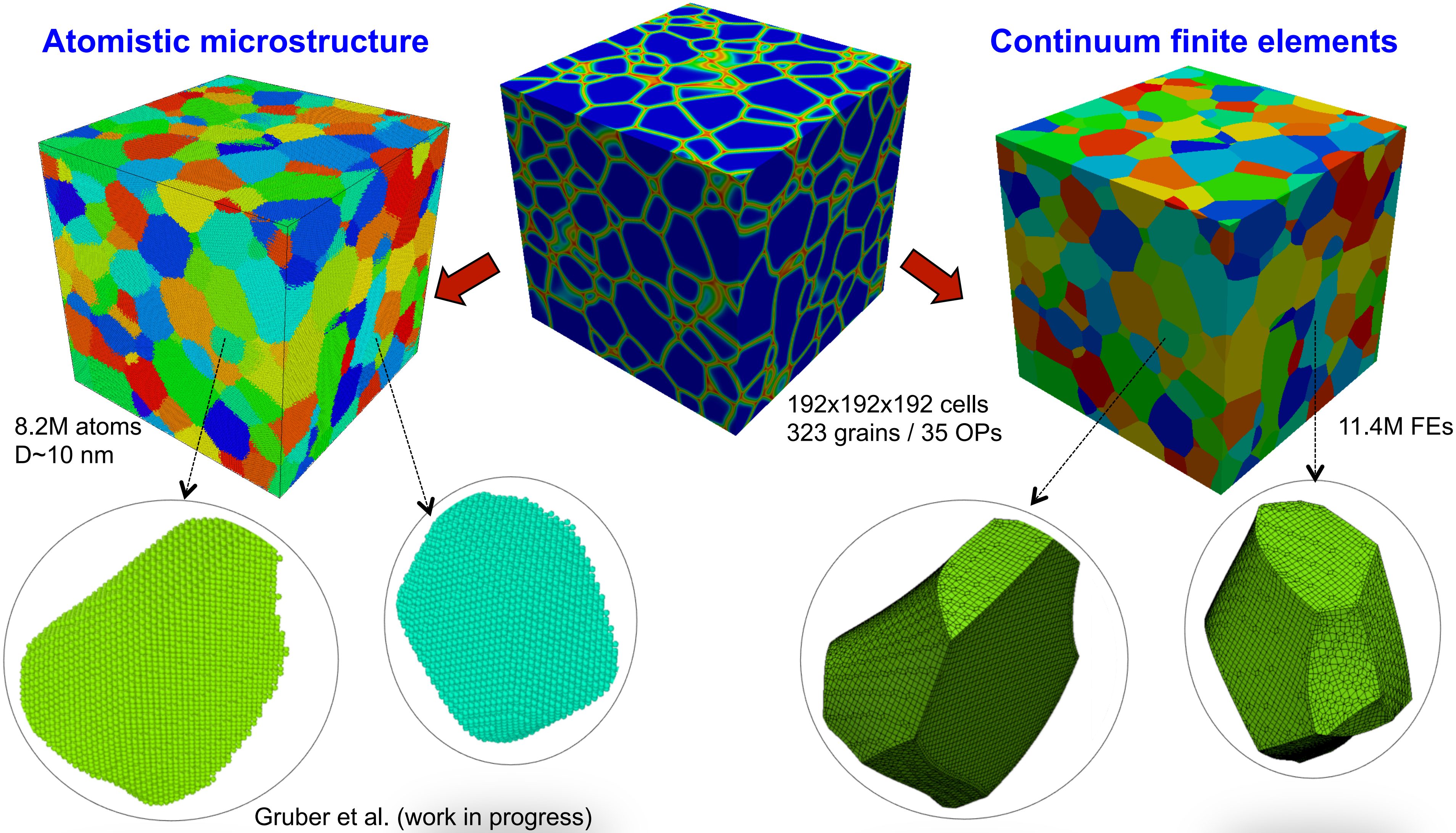
Sylgard matrix meshed with hex 8 solid elements



J. Brown & K. Long, work in progress

Current work/ future directions

Phase field grain growth model



Atomistic microstructure

Continuum finite elements

8.2M atoms
D~10 nm

192x192x192 cells
323 grains / 35 OPs

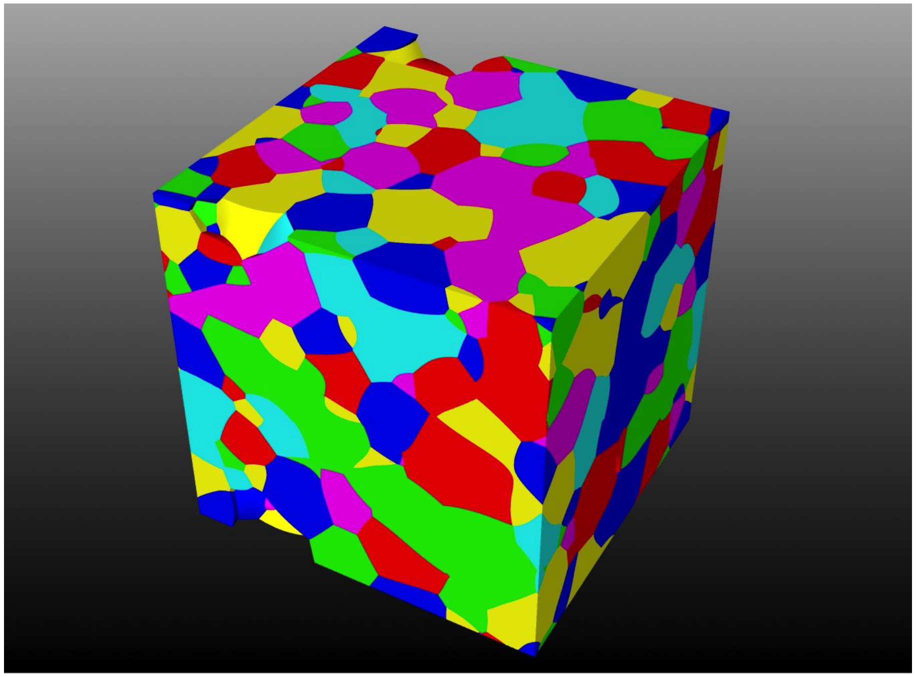
11.4M FEs

Gruber et al. (work in progress)

Summary

- Developed conformal, hexahedral finite element meshing technology for three-dimensional polycrystalline microstructures.
- Interface-conformal FE discretization technique reduces local discretization errors.

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



Thank you!

Hojun Lim
hnlim@sandia.gov
505-284-3177