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MECHANICAL PROPERTY PREDICTIONS OF ADDITIVELY MANUFACTURED MICROSTRUCTURES VIA SURROGATE MODELING

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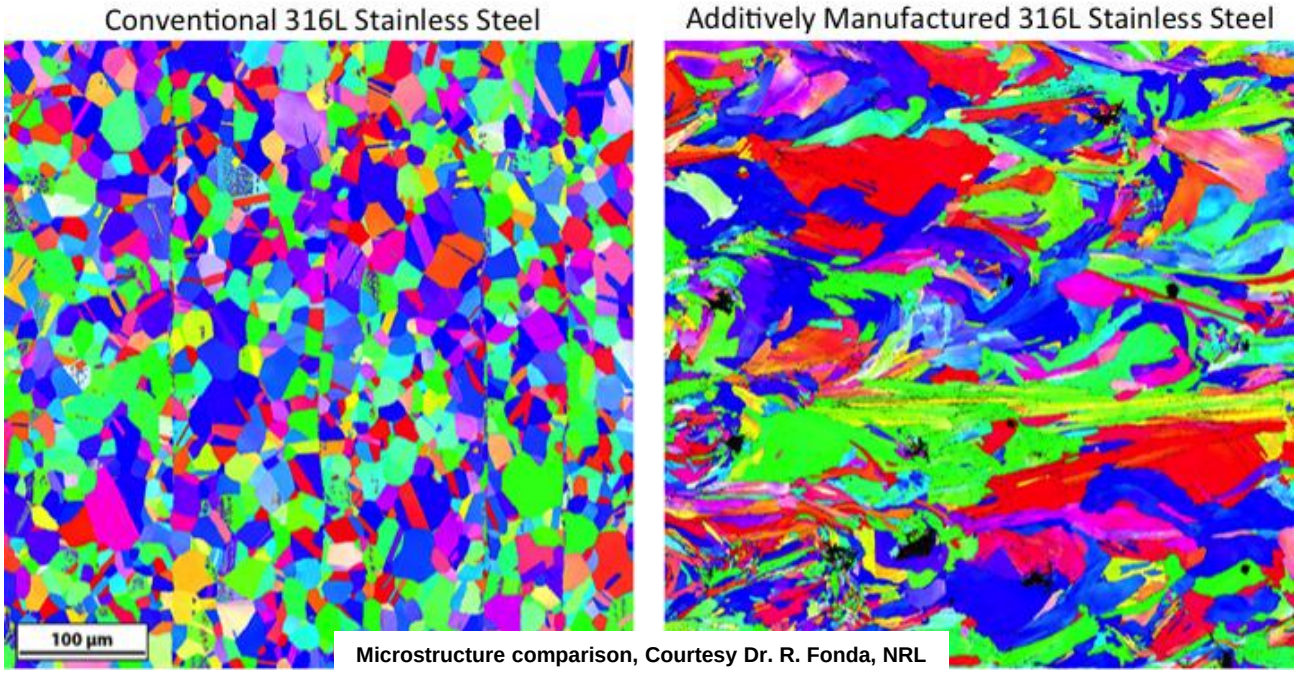
Motivation & Needs

Powder-based AM produces non-uniform microstructures

- Process parameters define the evolution of the microstructure
  - Significantly different from conventional manufacturing
- Columnar grains are widely reported
  - Grain size and shape variations
  - Conventional crystal plasticity constitutive models are not feature size dependent



Microstructure comparison, Courtesy Dr. R. Fonda, NRL

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Motivation & Needs

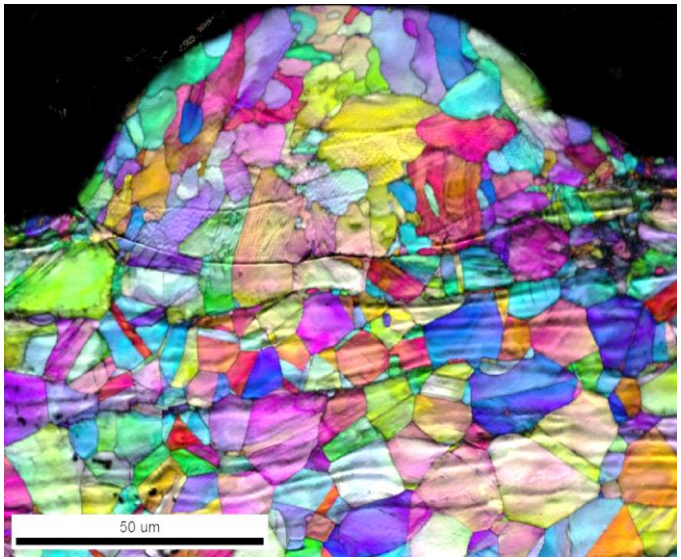
Develop a data-driven statistical surrogate to capture the mechanical behavior

- Utilize synthetic microstructures and image segmentation techniques

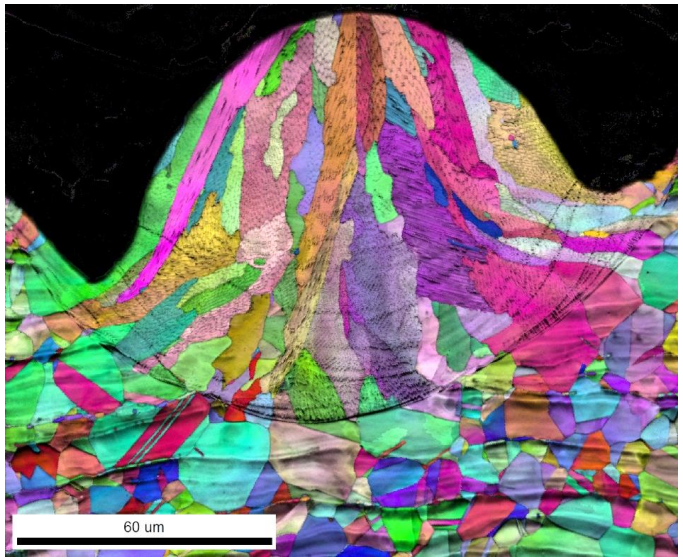
Determine process-property correlations

- Generate data relating synthetic microstructure features to constitutive behavior
- Relate process parameters to microstructure features

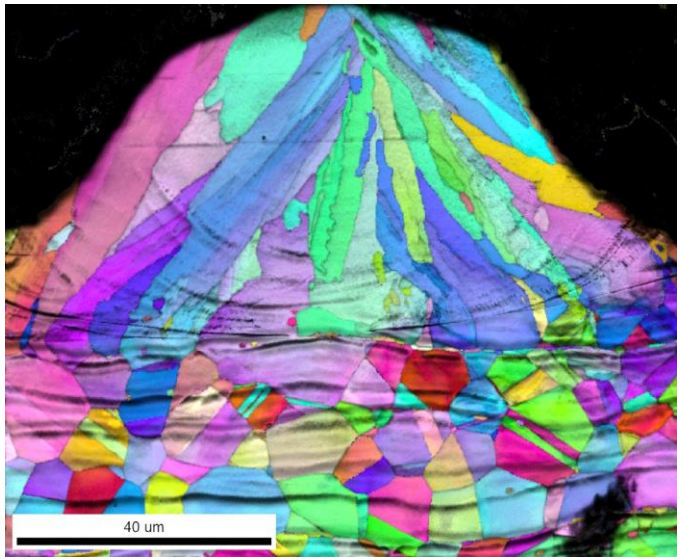
P = 40 W, v = 100 mm/s



P = 370 W, v = 900 mm/s



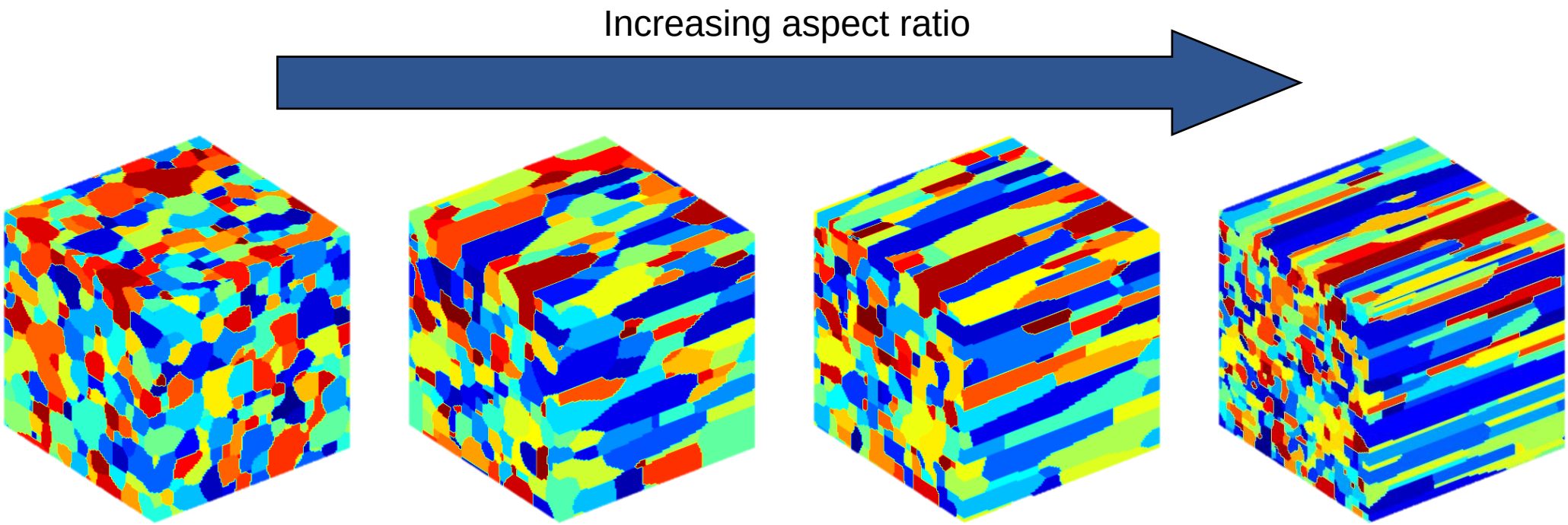
P = 400 W, v = 2,000 mm/s



Microstructure Synthesis

Continuum diffuse interface model for simulating grain evolution

- Generative capability between fidelity of statistical methods (Monte Carlo) and cellular automaton
- Extended to 3D with aspect ratio controls
  - Ability to generate realistic **single track** AM microstructures with columnar grains
- Randomly placed seed points grow based on physics based evolution
- Result is a matrix with each (*i, j, k*) location containing a grain label from 1 to N

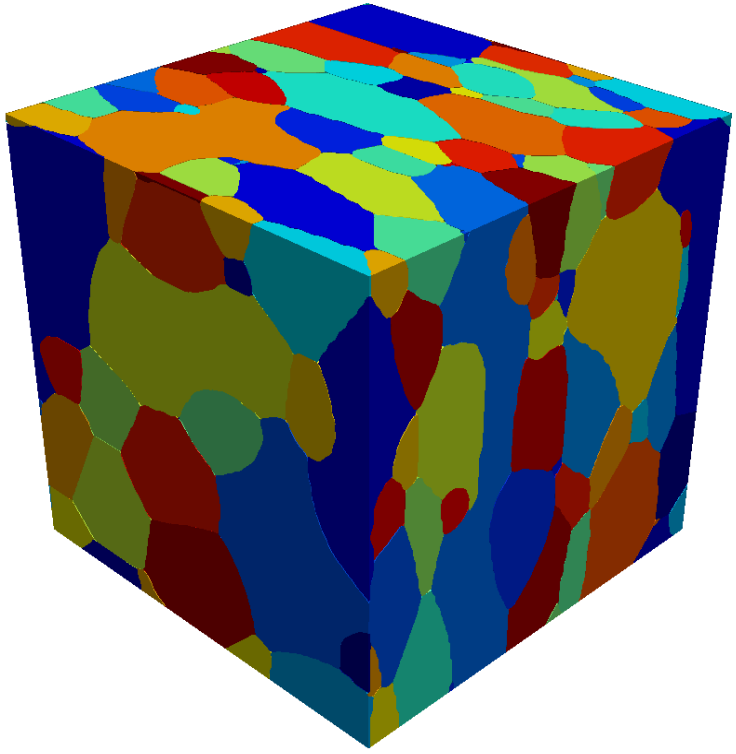


Microstructure Segmentation

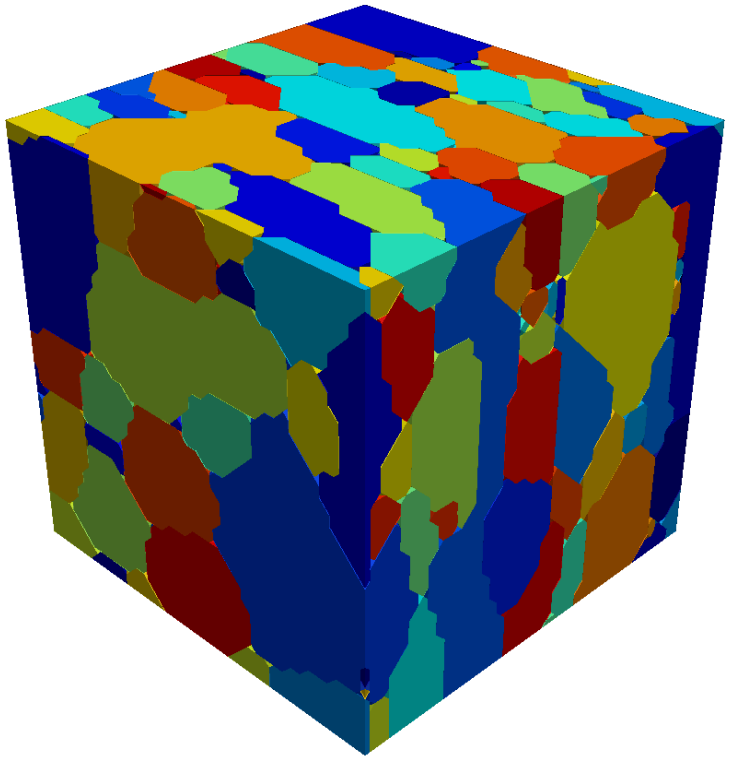
Matrix data is converted into a bitmapped voxel image

- Automatically imported into Simpleware ScanIP using Simpleware Scripting interface
  - Each grain is segmented based on assigned grain labels using a single multi-label mask
  - Generation of a surface representation of each grain in the RVE
- Surface representations can be used for structured or unstructured FE mesh generation
  - Structure representation uses **hexahedral** elements but has a “stair-stepping” effect
  - Unstructured representation uses **tetrahedral** elements but is smooth and can capture much finer details

Unstructured Grain Surfaces



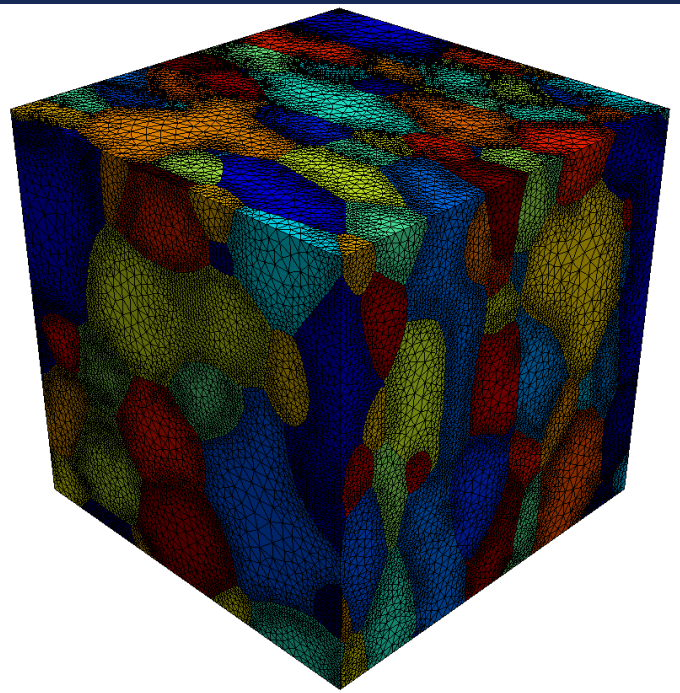
Structured Grain Surfaces



Finite Element Discretization

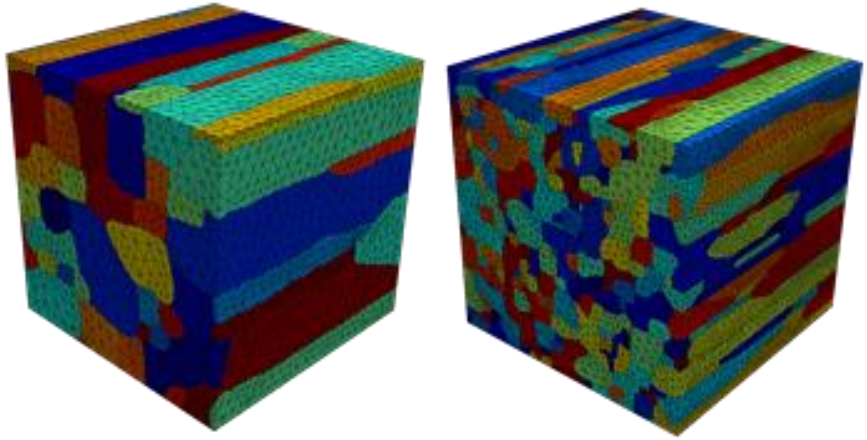
Microstructure grain surfaces converted to FE mesh

- Curved quadratic tetrahedral elements generated with Simpleware's +FE Free algorithm
  - Varied element density based on geometry
  - Decimation used to reduce size of the mesh
- Exported to Abaqus/Standard *inp file
  - Abaqus 10 noded tetrahedral elements (C3D10)
- FE model parameters
  - Crystal plasticity model implemented via user subroutine (UMAT)
  - Parameters of 316L stainless steel
  - Periodic boundary conditions on all external faces
  - Displacement driven to obtain ~10% nominal strain



What is the optimal mesh resolution and number of grains to minimize simulation time?

- Unstructured mesh
  - Too few – inaccurate results
  - Too many – long simulation times
- Number of grains
  - Too many – difficult to mesh and simulation
  - Too few – statistics are not representative



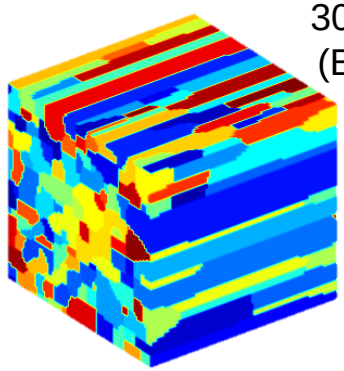
Mesh and Grain Variations

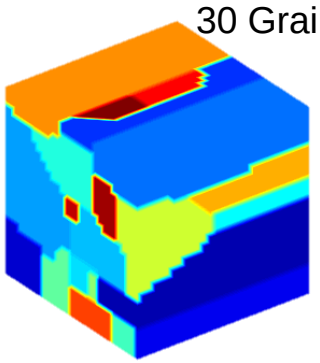
Vary mesh and number of grain simultaneously

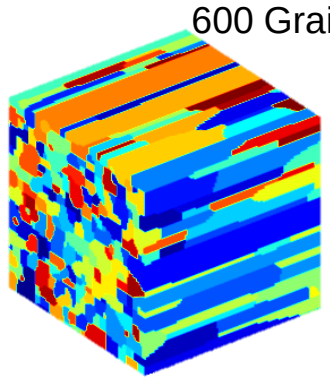
- Start from a converged baseline
  - ~300 grains, ~300k nodes, ~250k elements
  - Simulation time of ~80 hours on DOD HPC system
- Vary grains from 30 to 600
  - Scale RVE so that mean/median grain size is constant
- Vary mesh from 75k – 1.5M nodes and 50k – 1M elements

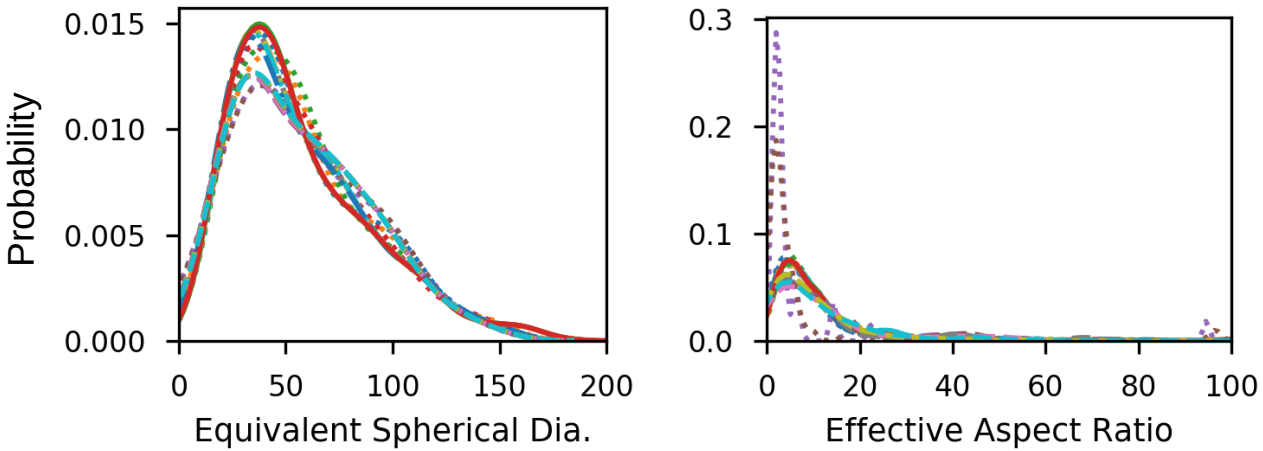
Use ESD and effective aspect ratio to determine equivalence

- ESD shows no significant differences
- Aspect ratio shows only 30 grain cases differ in distribution





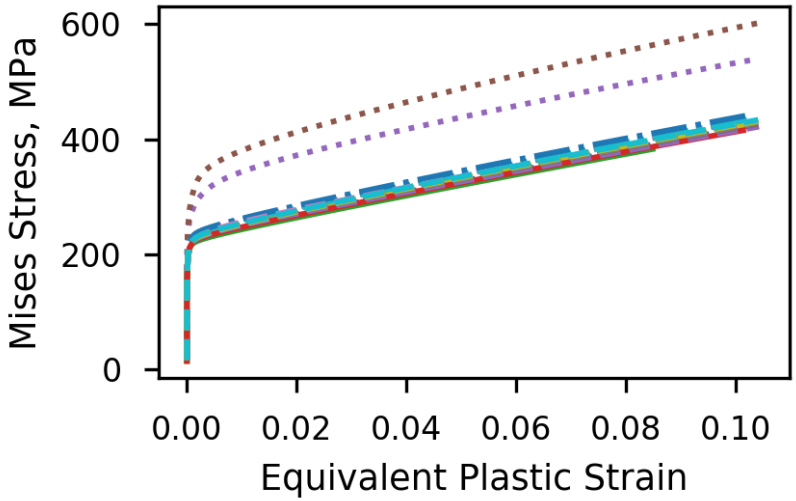


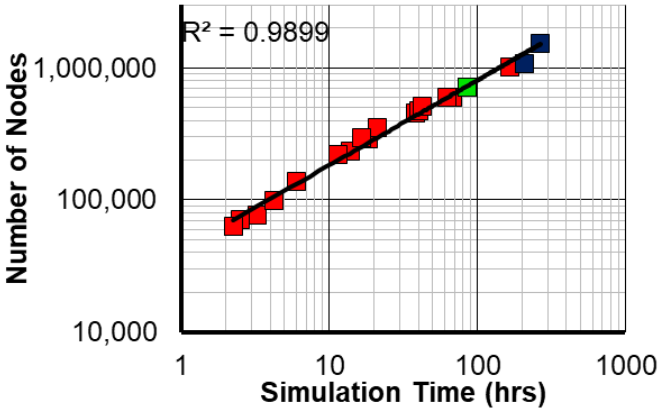


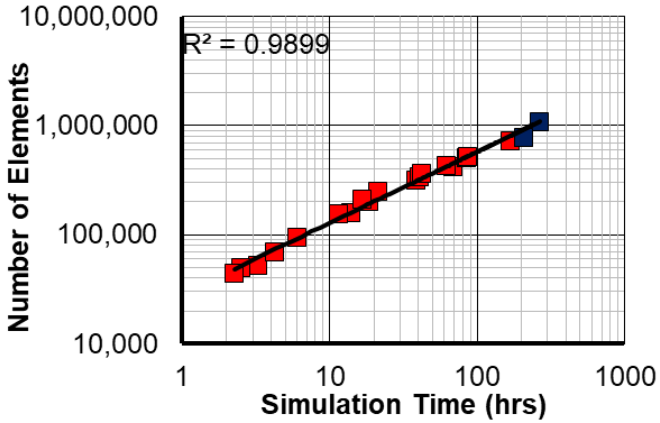
Mesh and Grain Variations

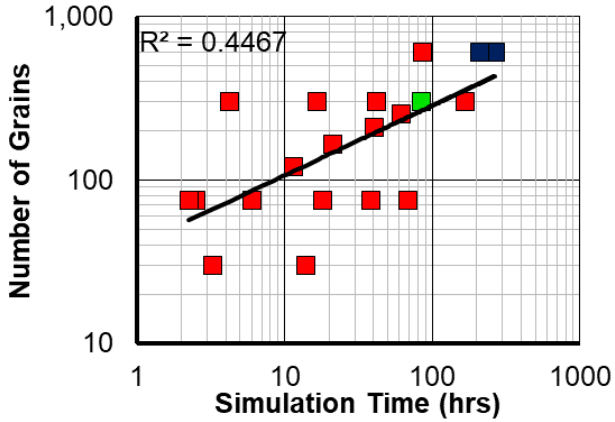
Stress-Strain used to determine RVE equivalence

- 30 grain case shows significant differences
- All other cases show no statistically significant differences
  - Max discrepancy of 15 MPa
- Simulation time increased exponentially as node/elements increased
  - Number of grains has a small effect on simulation time but not significant
- New baseline case for data driven modeling
  - **100 grains, 200-250k nodes, and 150-200k elements**
  - 10-15hr simulation time – reduced to 1/8th original time
  - Not significant difference in mechanical results









Data Driven Surrogate Modeling

Typically 1 RVE → 1 stress-strain plot

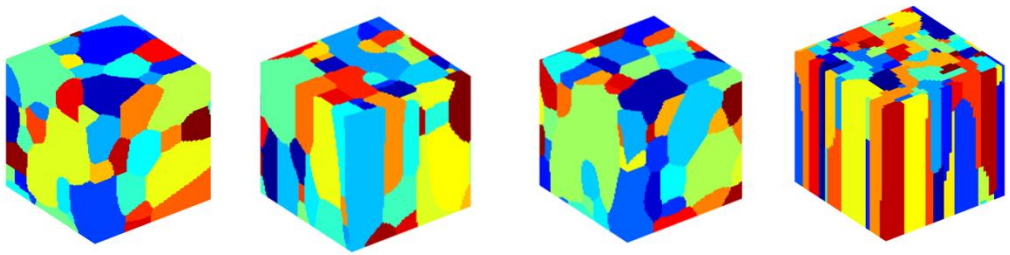
- 10+ hour simulation time is still relatively long
  - Data driven models need 100's or 1000's of points

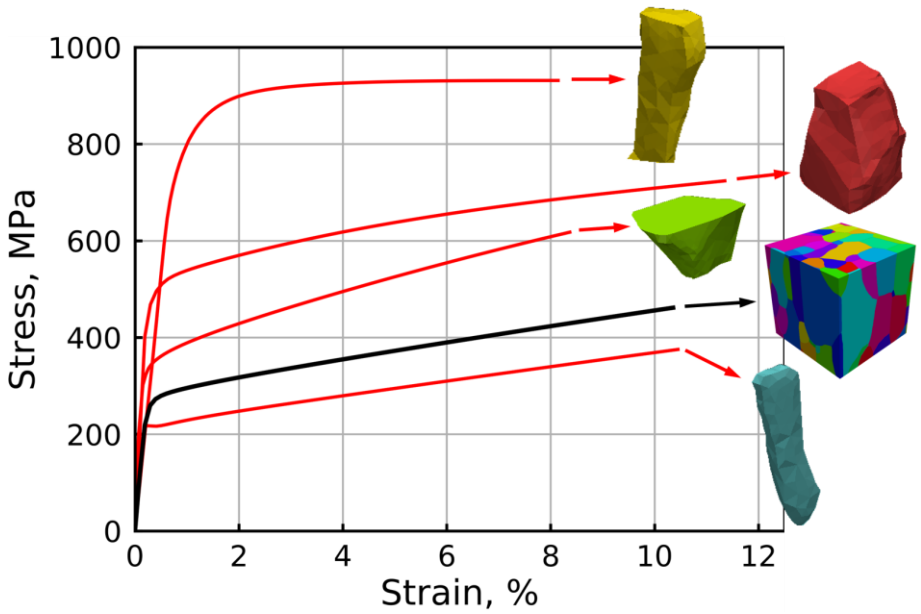
To increase data, each grain produces 1 stress-strain plot

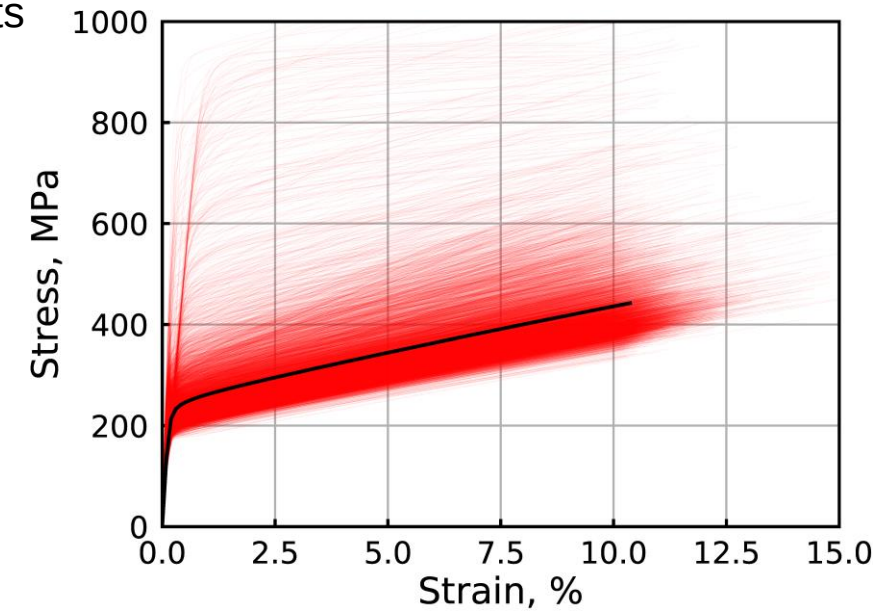
- Increase data 100x
- Assume boundary and grain interaction effects small

Data Generation

- Use Latin Hypercube based design of experiments
- Vary grain shape/aspect ratio and size
  - 50 RVEs generated (CDIM) and meshed (ScanIP)
    - 1 case with a = b = c
    - 22 cases with a = b < c
    - 27 cases with a < b < c
  - Size varied by linear scaling of RVEs



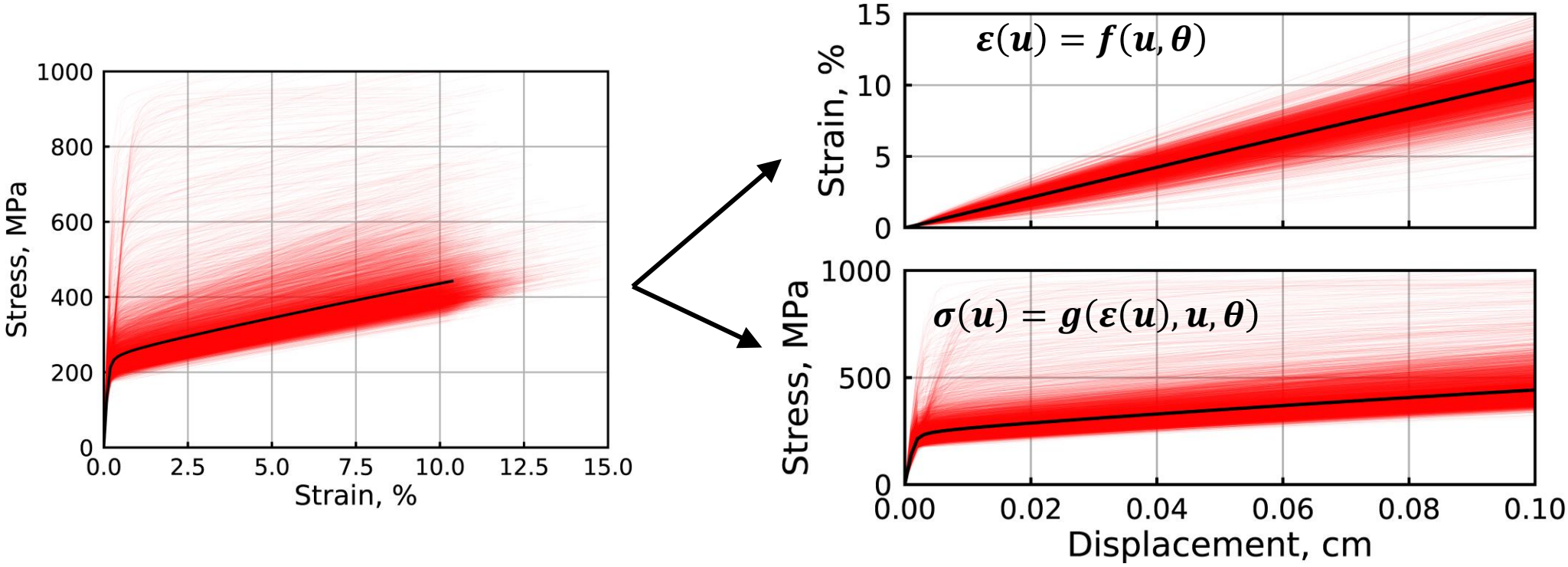




Data Driven Surrogate Modeling

Recognize that the FE method is displacement driven

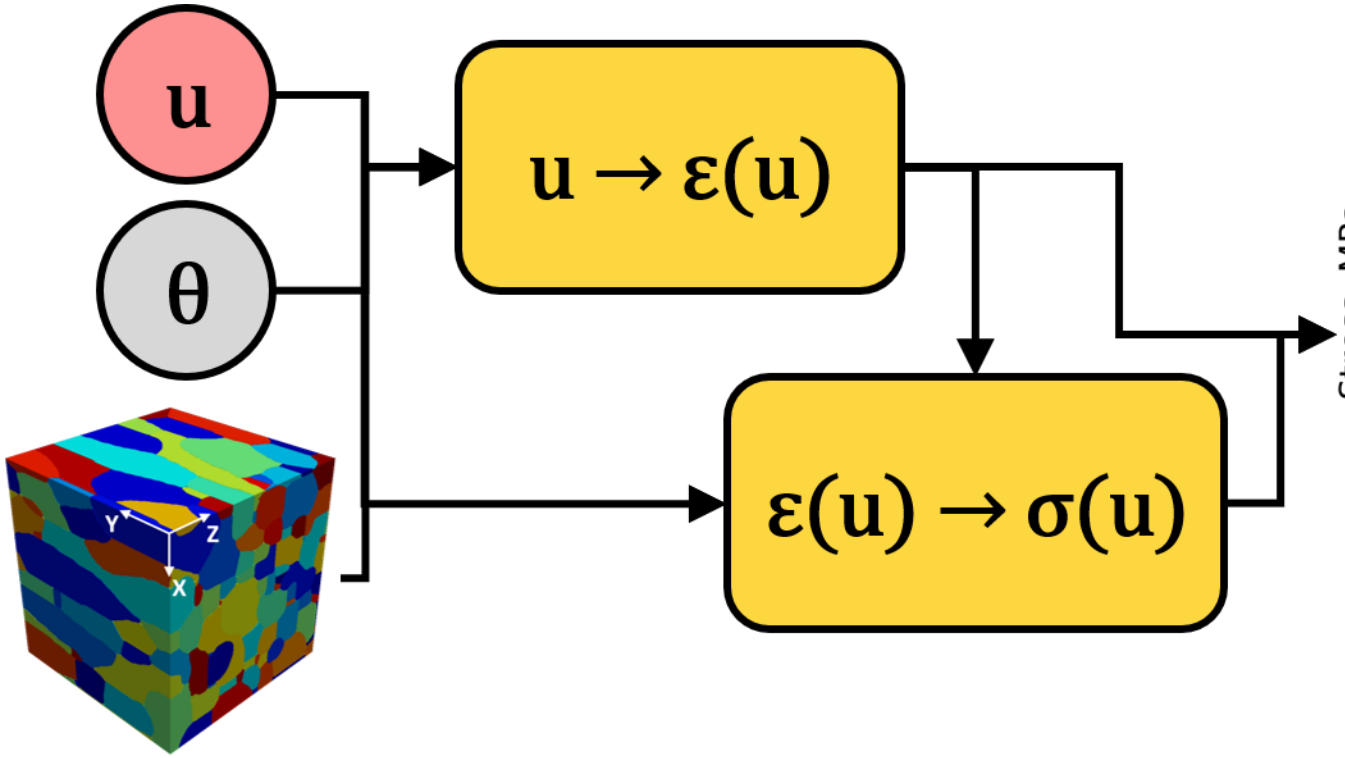
- Strain and stress are uniform when plotted against the commanded displacement
- Strain can be represented by a function of displacement and fixed parameters
- Stress depends on the displacement, fixed parameters, as well as strain
- Need to determine two functional outputs
  - Both can be observed
  - One depends on the other

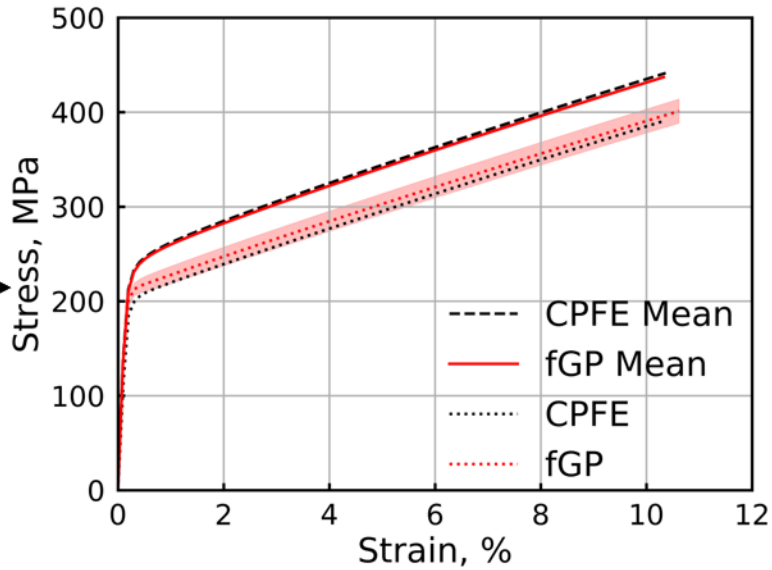


Data Driven Surrogate Modeling

Methodology

- Input: Known grain morphology (experiments, phase field, CA, etc.), constitutive model parameters, displacement
- Output 1: Predict strain from inputs
- Output 2: Predict stress from inputs and predicted strain
- Final: Combine outputs to predict stress-strain behavior

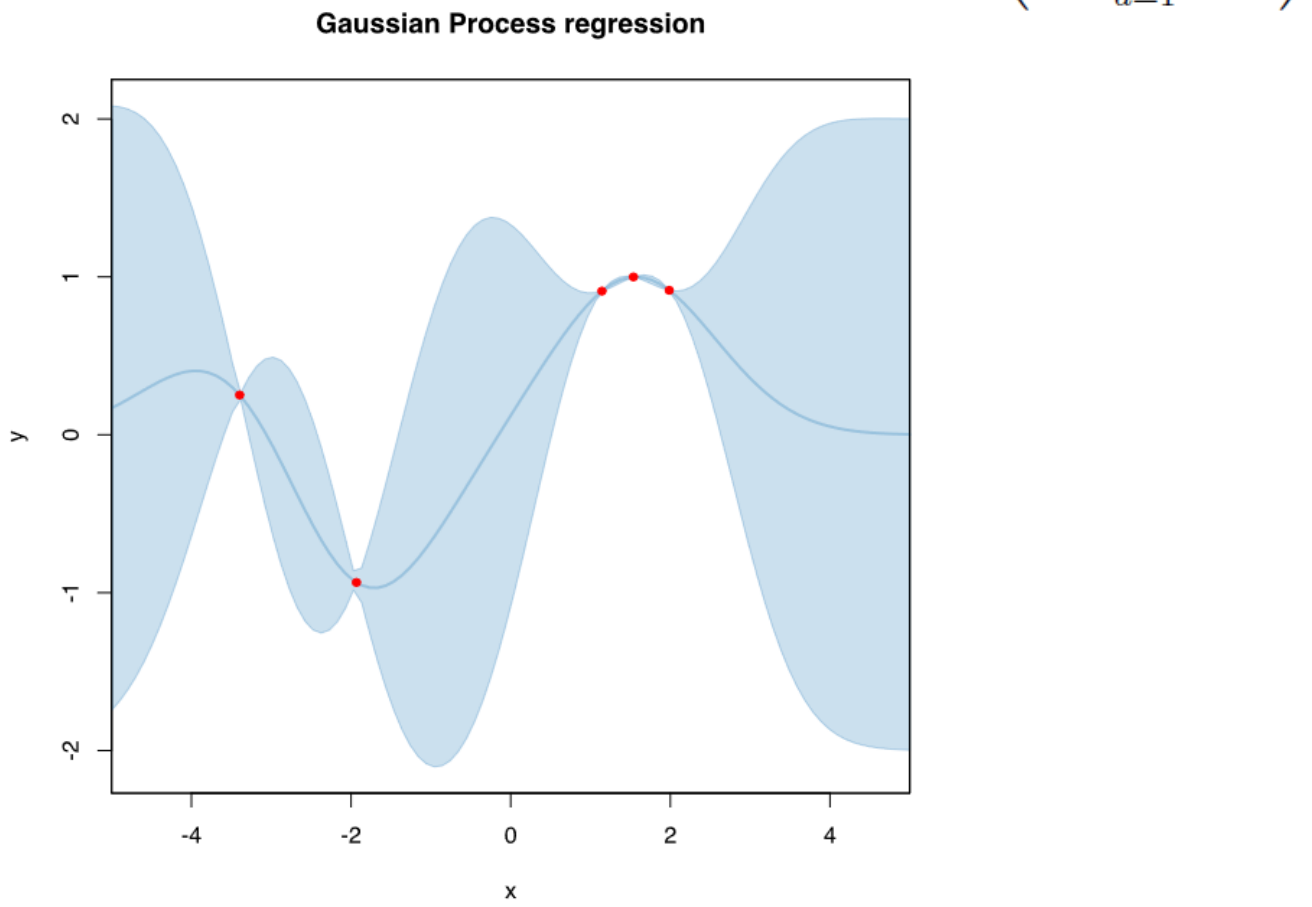




Functional Gaussian Process Regression

Gaussian Process Regression

- Want to solve the problem of $y_i = f(x_i) + \epsilon_i$
- By assuming the function follows $p(\mathbf{f}|\mathbf{X}) = \mathcal{N}(\boldsymbol{\mu}, \mathbf{K})$
  - With mean, μ, and covariance, K
  - Squared exponential or Gaussian kernel for covariance $k(\cdot,\cdot) = \sigma_f^2 \exp\left(-\frac{1}{2}\sum_{d=1}^{q}\theta_d h_d^2\right)$



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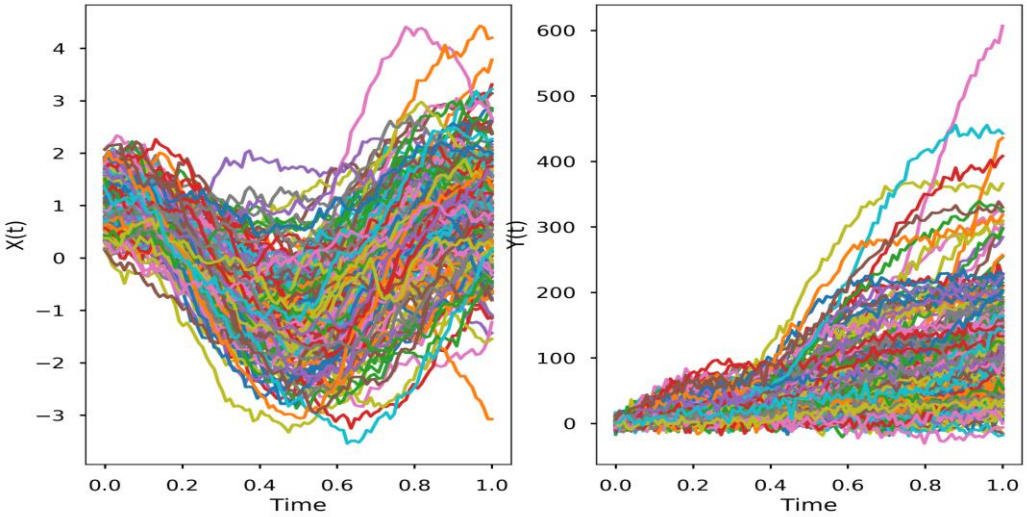
Functional Gaussian Process Regression

- Want to solve the problem of $Y = f(X, z_i) + \epsilon_i(t_j)$
  - Both Y and X are functions of another variable (time, displacement, etc.)
- The kernel is now a product of two kernels
  - Gaussian kernel for scalar parameters
  - Non-parametric functional data analysis is used to define a distance in functional space (semi-metric distance)
  - Squared exponential or Gaussian kernel for covariance

$$\sigma_f^2 \exp\left(-\frac{1}{2}\sum_{d=1}^{p}\theta_d ||z_{id} - z_{jd}||^2 - \frac{1}{2}\sum_{d=1}^{q}\phi_d ||X_{id} - X_{jd}||_d^2\right)$$



$$Y_i(t_j) = f(X_i)(t_j) + \varepsilon_i(t_j)$$

$$f(X_i)(t_j) = \int_0^{t_j} X_i^2(u)du$$

Wang, Bo, and Aiping Xu. "Gaussian process methods for nonparametric functional regression with mixed predictors." *Computational Statistics & Data Analysis* 131 (2019): 80-90.

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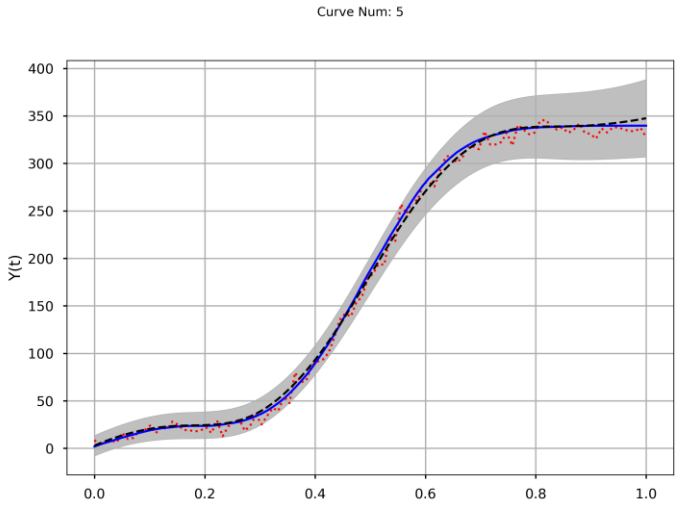
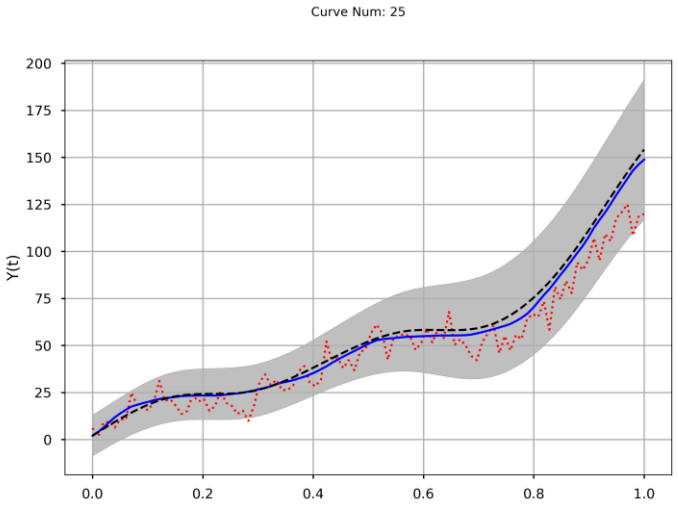
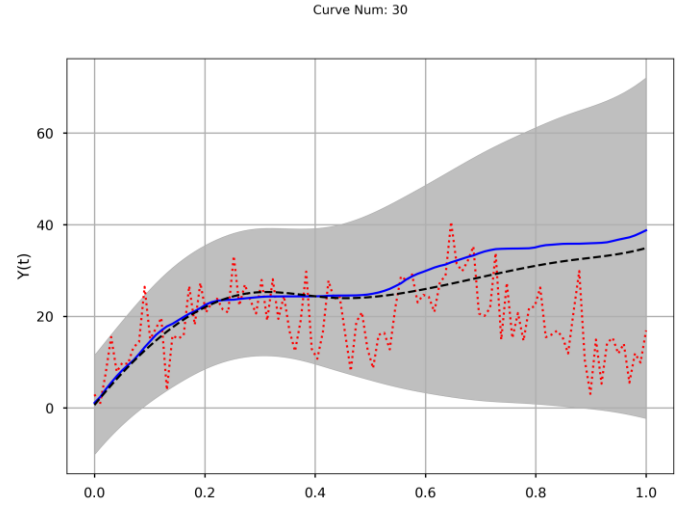
Functional GP – Demonstration

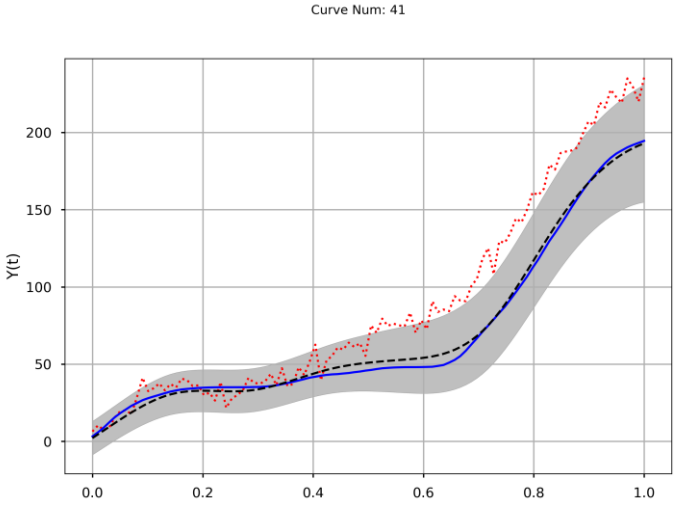
Demonstration

- Predicted (black) matches true response (blue)
- Larger error bounds for input values (red) that have a lot of noise







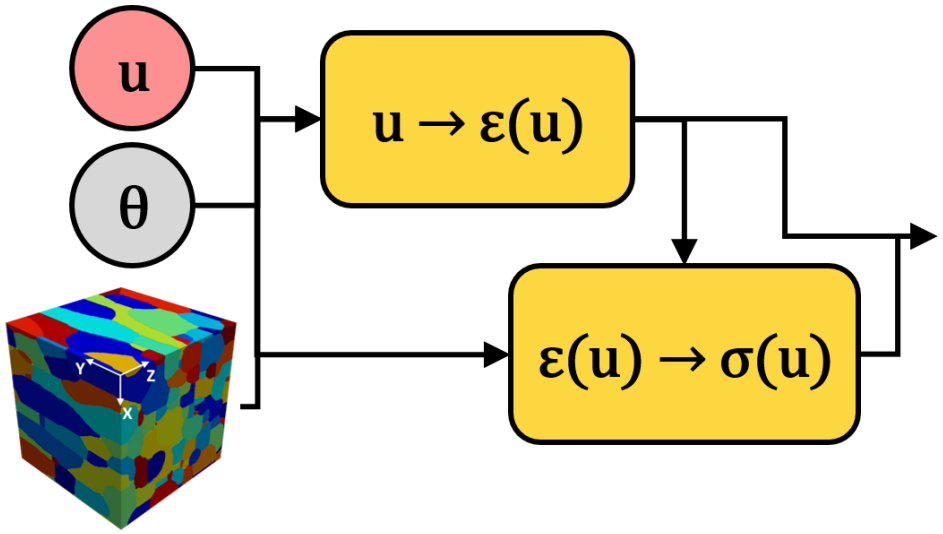


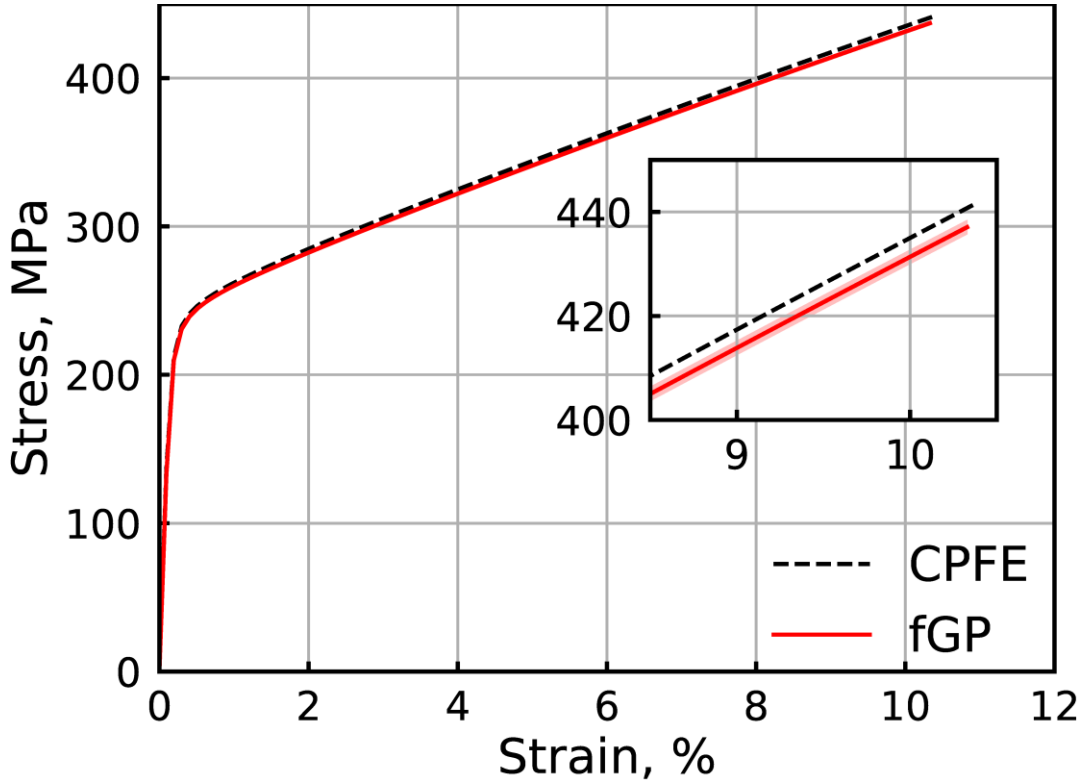
fGP Network Predictions

Performance

- Network is trained on the 50 RVE data sets
  - 70% used for training, 30% withheld
- Performance on withheld data is under 10% error
- Mean behavior is almost indistinguishable between CPFE and fGP

	MSE	MAPE	MAE
Strain	4.388e-5	9.13%	4.203e-3
Stress	1756.9	5.68%	21.51





fGP Network Predictions

Performance

- Network is trained on the 50 RVE data sets
  - 70% used for training, 30% withheld
- Performance on withheld data is under 10% error
- Mean behavior is almost indistinguishable between CPFE and fGP
- Many individual grains are predicted well
  - Grains with strains far above/below 10% strain are generally not predicted well

	MSE	MAPE	MAE
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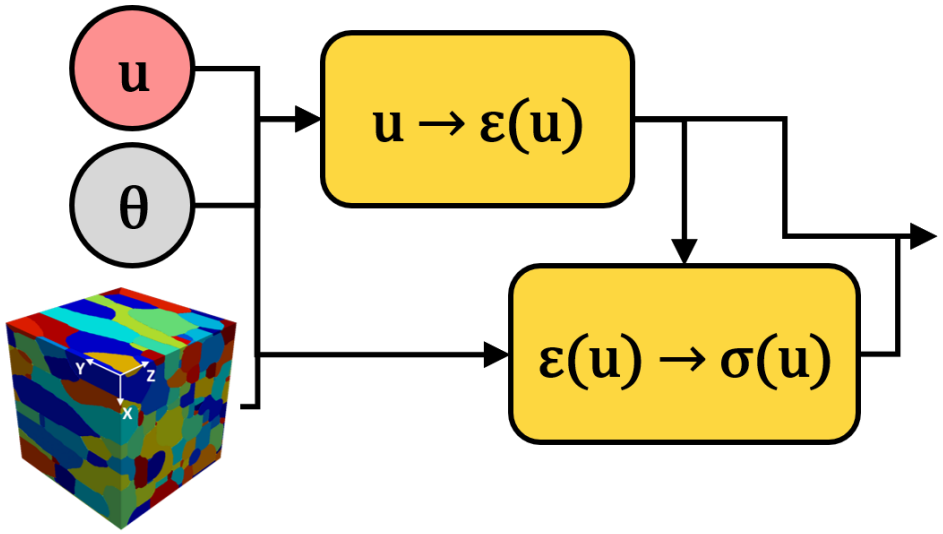
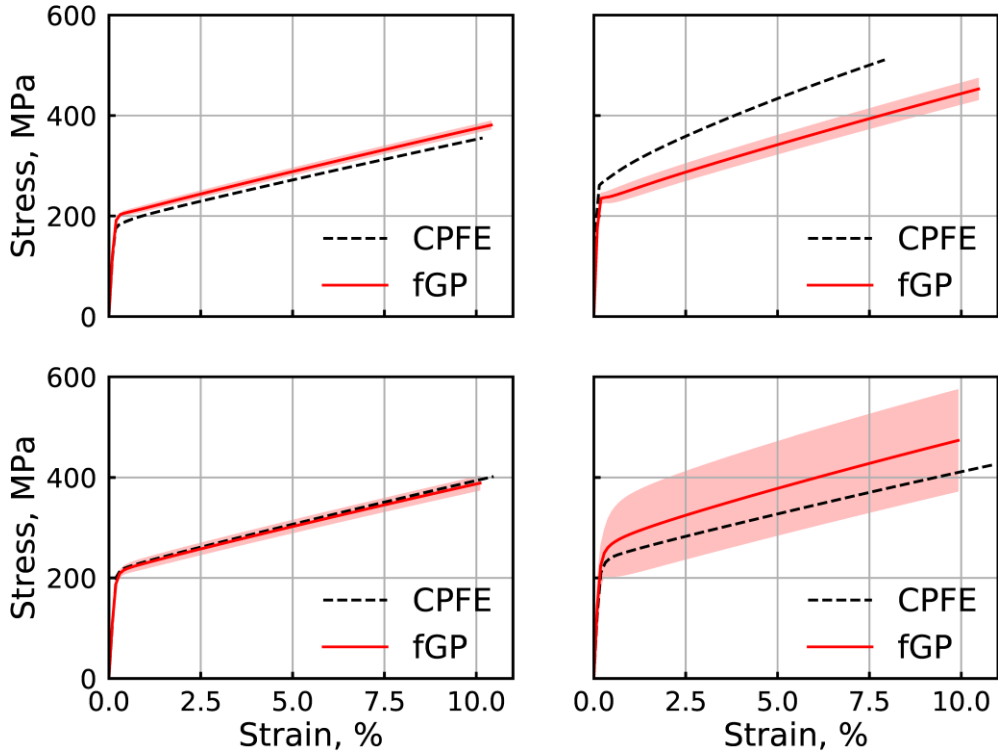




Prediction On New Data

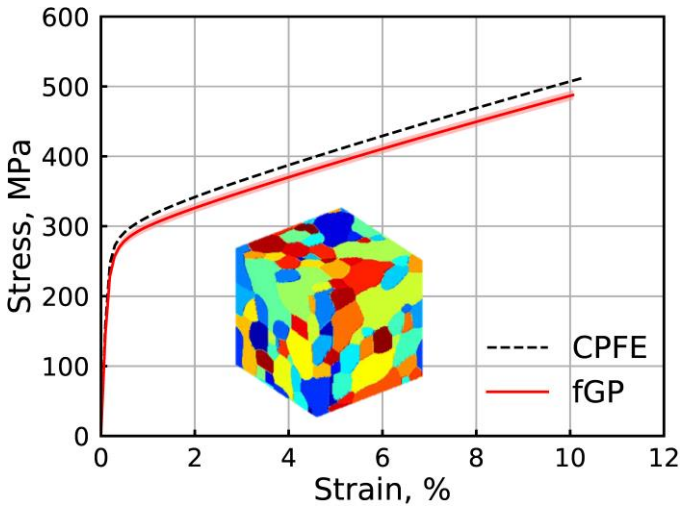
New 300 Grain RVEs

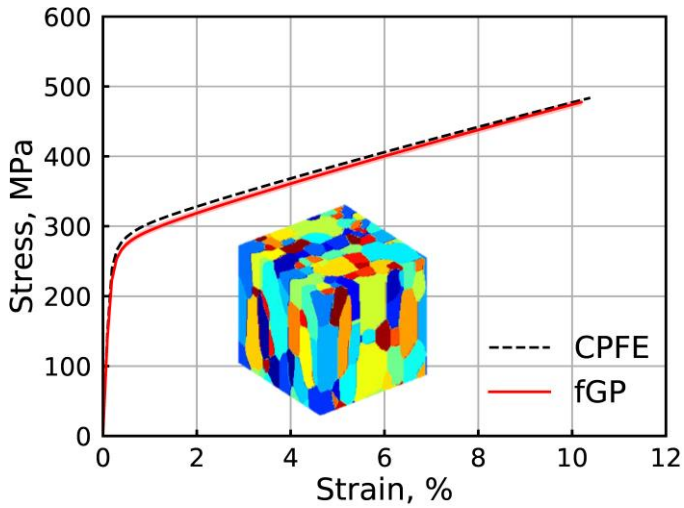
- Previous RVEs contain 100 grains
- Generate new RVEs in the same manner with 300 grains
  - Closer to what is normally done in CPFE
  - Test how the fGP network scales up

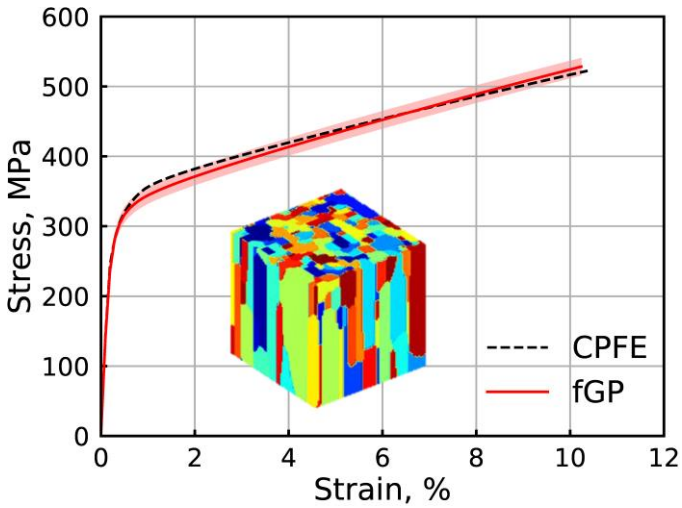
	MSE	MAPE	MAE
Strain	6.41e-5	11.2%	0.0052
Stress	7076.6	8.44%	41.2

Performance

- Without retraining, the fGP network performs similar to the previous performance
- Highest errors in equiaxial case
- Demonstrates ability to scale up to much larger microstructures than those used in training
  - EBSD or physical simulations can yield microstructures with 1000s of grains
  - To costly to simulate with CPFE, easily approximated with fGP network







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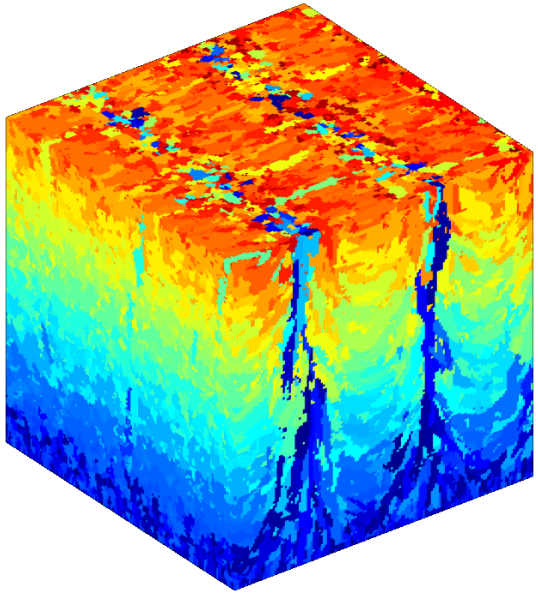
Cellular Automaton Data

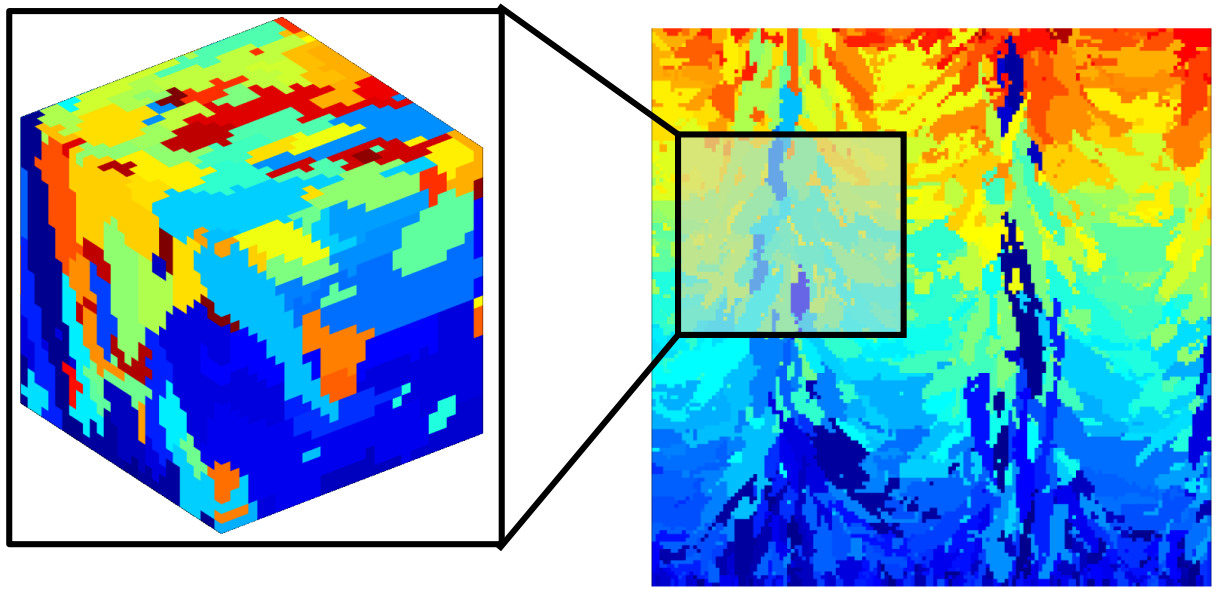
Cellular Automaton Finite Element (CAFE) Model

- High fidelity than CDIM
  - Still less expensive than phase field models
- Further modified for computational efficiency with AM microstructures
  - Solidification time scale is independent of temperature time steps
  - Predictions used in neighbors of current voxel
  - Determination of active regions for improved CPU utilization
- Simulation of epitaxial growth from the base plate
  - 3 tracks with many layers



Finite Element Model

- Extracted randomly from full CA model
  - Contains ~300 grains again
- Segmented and meshed using ScanIP as before
- CPFE model setup as before

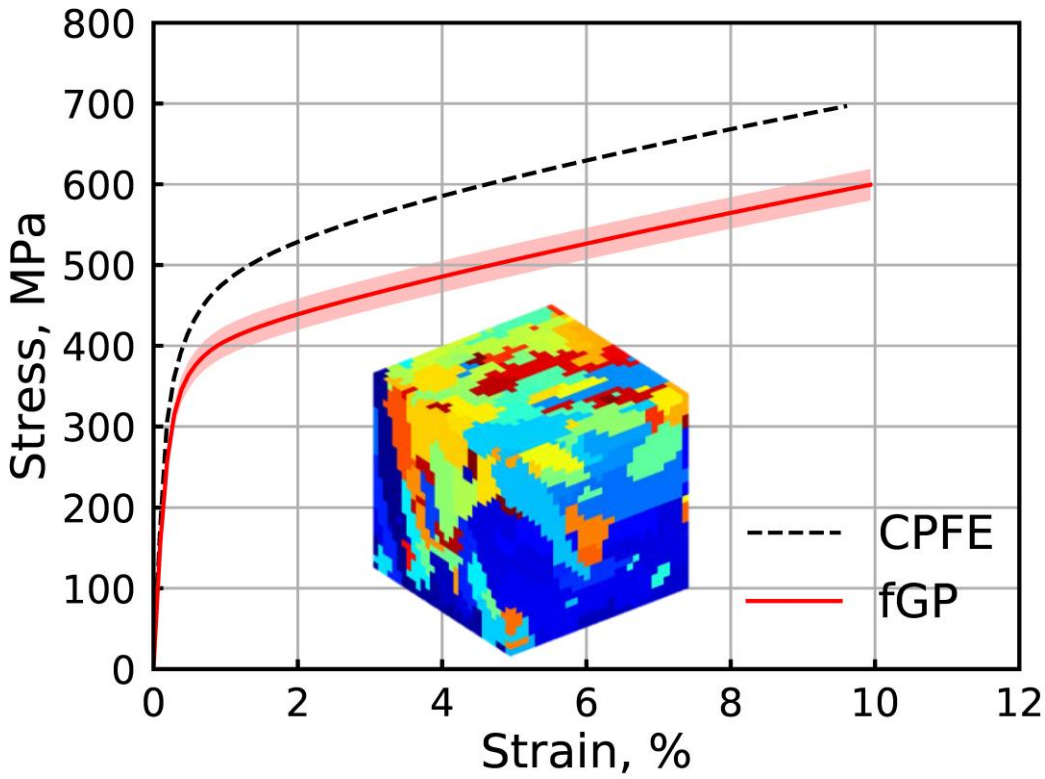


Cellular Automaton Data

Performance

- Without retraining, the fGP network does not perform well
- Diagnosis:
  - The features used to train the CDIM model are always aligned with an axis
  - The CDIM produces microstructures that resemble single track builds
  - In AM, the grains generally exhibit a much richer feature set especially with multiple tracks
  - Data-driven models cannot be expected to capture behavior they have not seen before
- Solution:
  - Modify CDIM model to include more features mimicking multi-track AM builds
  - Use multiple (~10s) CAFE model simulations and extract many small RVEs (~50s)
  - Retrain fGP with new data set

	MSE	MAPE	MAE
Strain	2.28e-4	31.2%	0.0105
Stress	46622.6	19.5%	135.74



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Summary & Future Work

A functional Gaussian Process network has been developed

- Use continuum diffuse interface model to generate RVEs
- ScanIP to segment and mesh RVEs automatically
- Grain size and shape dependent crystal plasticity model to simulate RVE mechanical behavior
- Train a network of fGPs to predict mechanical behavior

fGP network accurately predicts mechanical behavior from microstructure

- Given a set of microstructural features the fGP can achieve sub-10% error rates
- The network can scale up to large microstructures that may be too costly for CPFE models

Continuing and future work

- Generate new training data from CAFE model and retrain model
- Test prediction on new RVEs
  - Synthetically generated and physically generated (phase field, CA, EBSD, etc.)
- Utilize Bayesian methods
  - Propagate uncertainty through the fGP network
  - Sample the model to determine desirable and undesirable features
- Link fGP network to process-structure models for full PSP linkages in realtime

U.S. NAVAL RESEARCH LABORATORY

Questions?

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Classical Crystal Plasticity

Dislocation nucleation and motion produce plasticity

- Shear strength of a slip system

$$g^{(\alpha)}(r,t) = \tau_{0\infty} + \int_0^t \dot{g}^{(\alpha)}(r,t')\,dt'$$

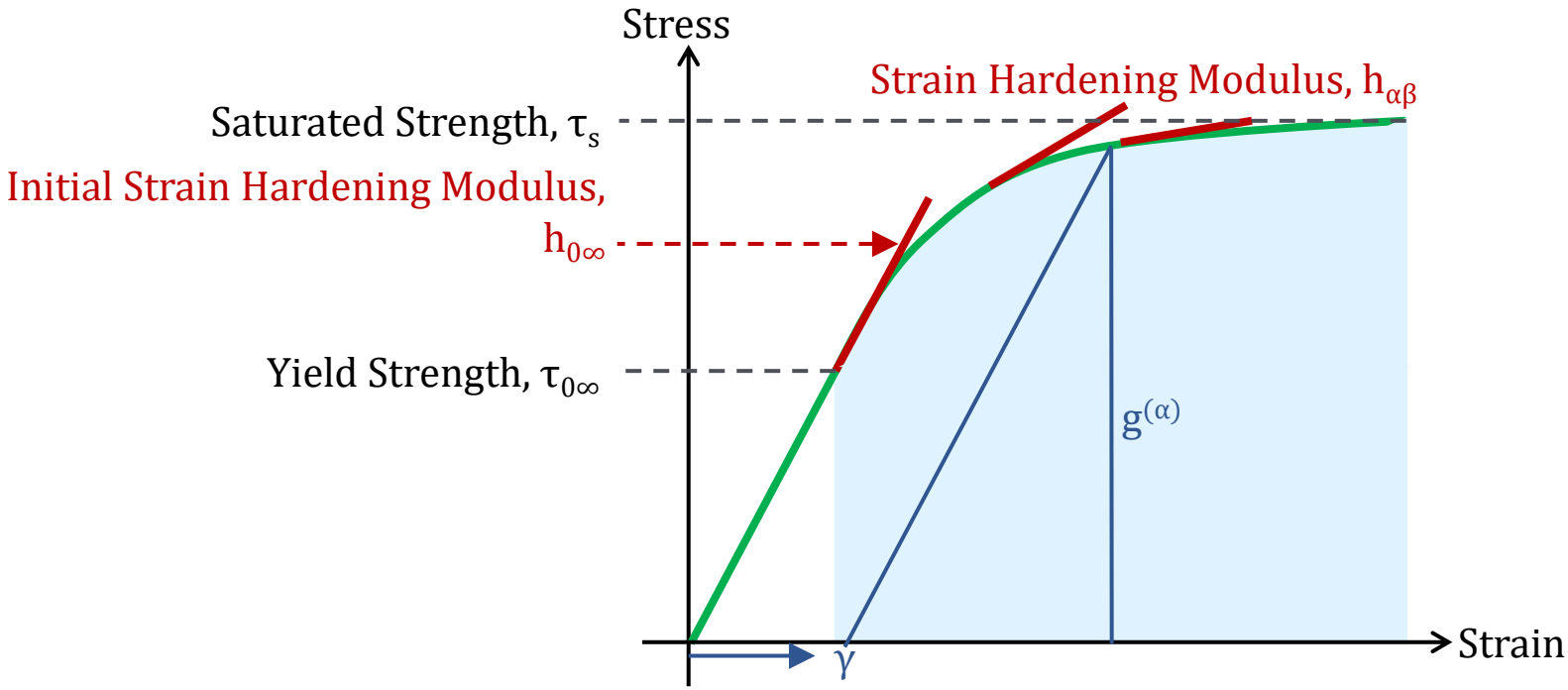
- Strain hardening rule

$$\dot{g}^{(\alpha)}(r,t) = \sum_{(\beta)} h_{\alpha\beta}(\gamma)\left|\dot{\gamma}^{(\beta)}\right|$$

- Flow rule and cumulative shear flow strain

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}^{(\alpha)}\left(\tau^{(\alpha)}, g^{(\alpha)}\right)$$

$$\gamma = \sum_{(\alpha)} \int_0^t \left|\dot{\gamma}^{(\alpha)}\right| dt$$



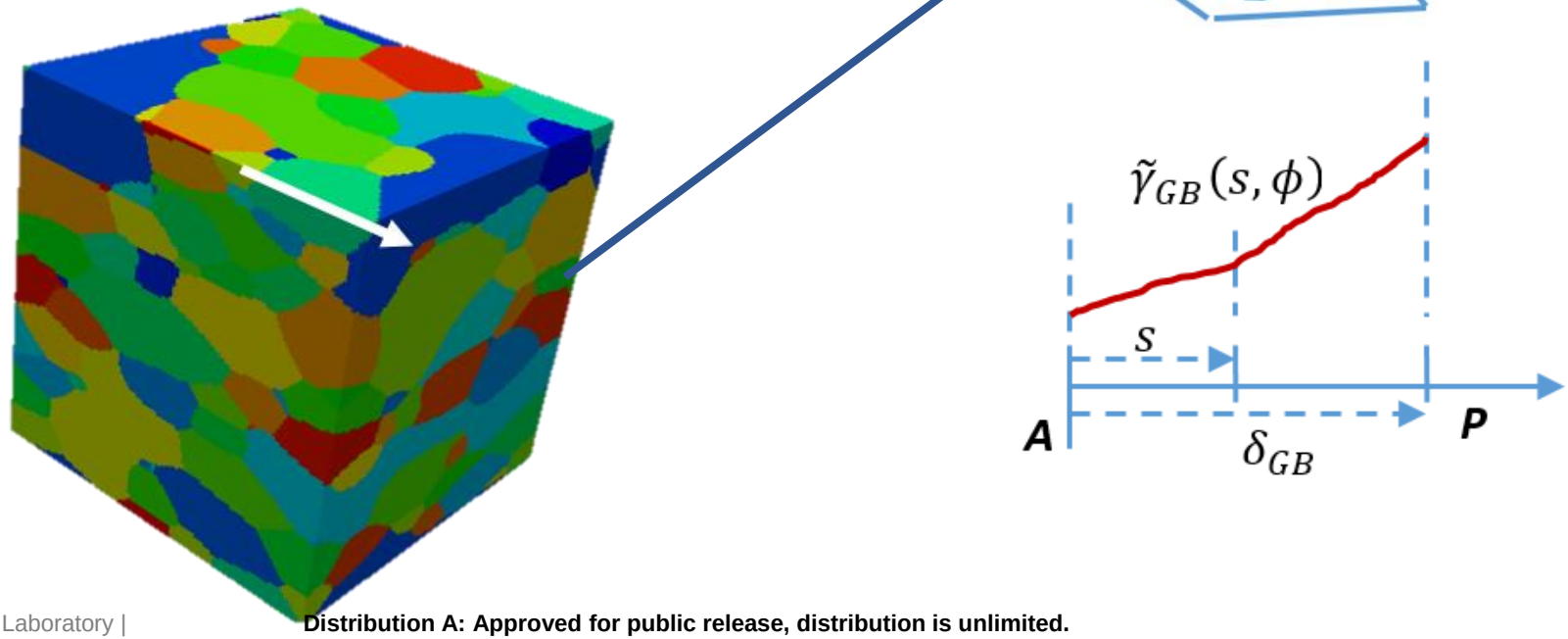
Size-Dependent Crystal Plasticity

Higher resistance to dislocation nucleation and motion near the grain boundary

- Extending the crystal plasticity framework to capture the resistance to dislocation in the grain boundary mantle
- Strength and hardening modulus in the grain boundary region related through shear flow strain
- Introduce an equivalent shear strain flow ($\tilde{\gamma}_{GB}$) for the grain boundary

$$g^{(\alpha)}(r,t) = \tau_{0\infty} + {g_{GB}}^{(\alpha)}(r) + \sum_{(\beta)} \int_0^t h_{\alpha\beta}(\gamma)\left|\dot{\gamma}^{(\beta)}\right| dt'$$

$${g_{GB}}^{(\alpha)}(r) = \sum_{(\beta)} \int_0^{\tilde{\gamma}_{GB}(r)} h_{\alpha\beta}(\gamma) d\gamma$$



Grain Homogenization

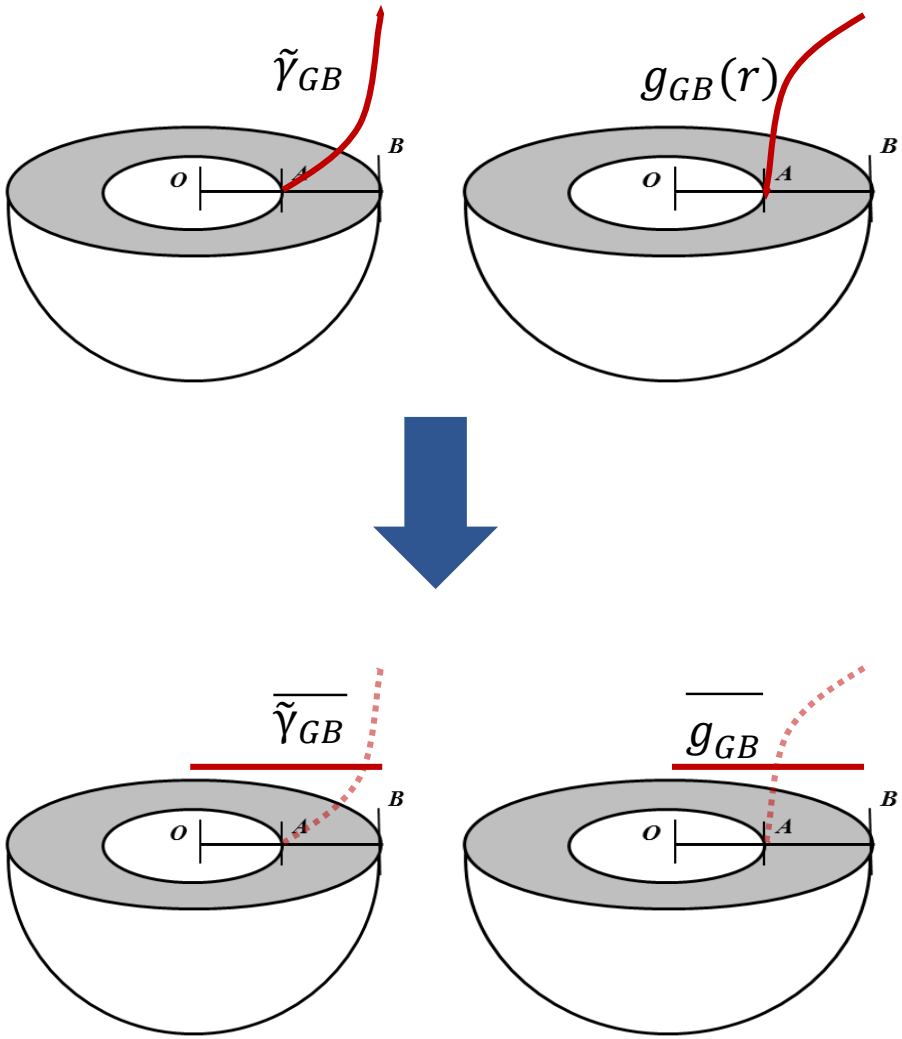
- Material point implementation is computationally challenging and requires a precise spatial description
- Homogenize the boundary for each grain to achieve an equivalent grain volume average effect

$$\overline{\tilde{\gamma}_{GB}} = \frac{\int_{V_{GB}} \tilde{\gamma}_{GB}(r)\mathrm{dV}}{V}$$

$$\dot{\mathrm{g}}^{(\alpha)}\left(\gamma, \dot{\gamma}^{(\alpha)}\right) \longrightarrow \dot{\mathrm{g}}^{(\alpha)}\left(\gamma + \overline{\tilde{\gamma}_{GB}}, \dot{\gamma}^{(\alpha)}\right)$$

$$\mathrm{g}^{(\alpha)} = \tau_{0\infty} + \overline{g_{GB}} + \int_0^t \dot{\mathrm{g}}^{(\alpha)}\mathrm{dt}$$

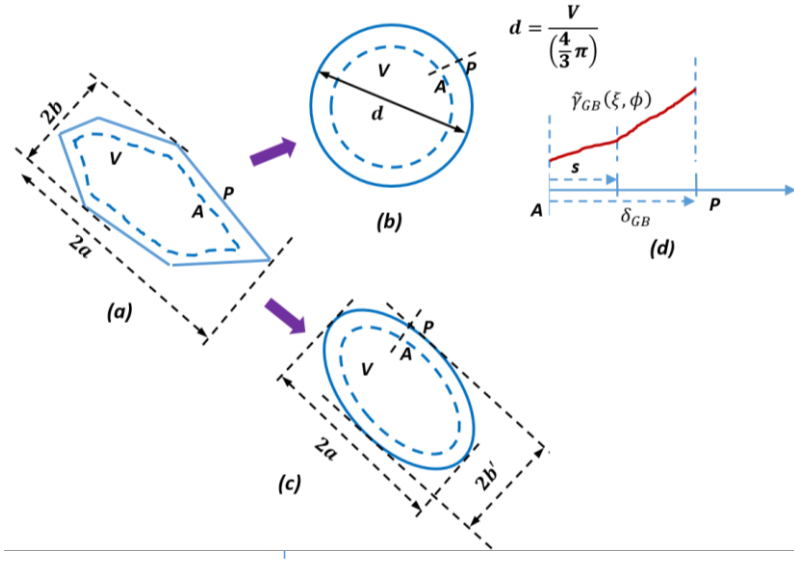
$$\overline{g_{GB}} = \frac{h_{0\infty}\dfrac{(N_{SS}-1)q+1}{N_{SS}}(\tau_s - \tau_{0\infty})}{h_{0\infty}} \tanh\left|\frac{h_{0\infty}\overline{\tilde{\gamma}_{GB}}}{\tau_s - \tau_{0\infty}}\right|$$



Grain Constitutive Shape Representation

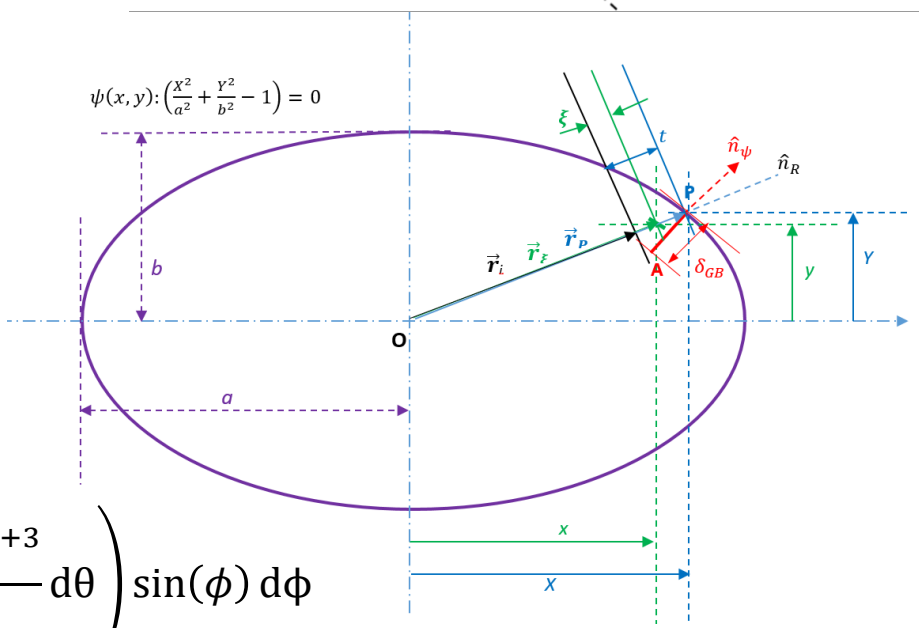
Map each grain to a simple equivalent domain for homogenization

- Simple spherical representation is sufficient to capture size effects
- Ellipsoidal representation is used to capture columnar nature of grains
  - Fit a general quadric surface to the nodes on the exterior of each grain
  - LLSQ minimization gives the 10 term polynomial coefficients



Homogenized grain boundary mapping

- Arbitrary grain mapped to an ellipsoid with constant grain boundary influence region thickness
- Parameterize the grain boundary influence region along r
  - Allows for integration to be accomplished using numerical quadrature techniques

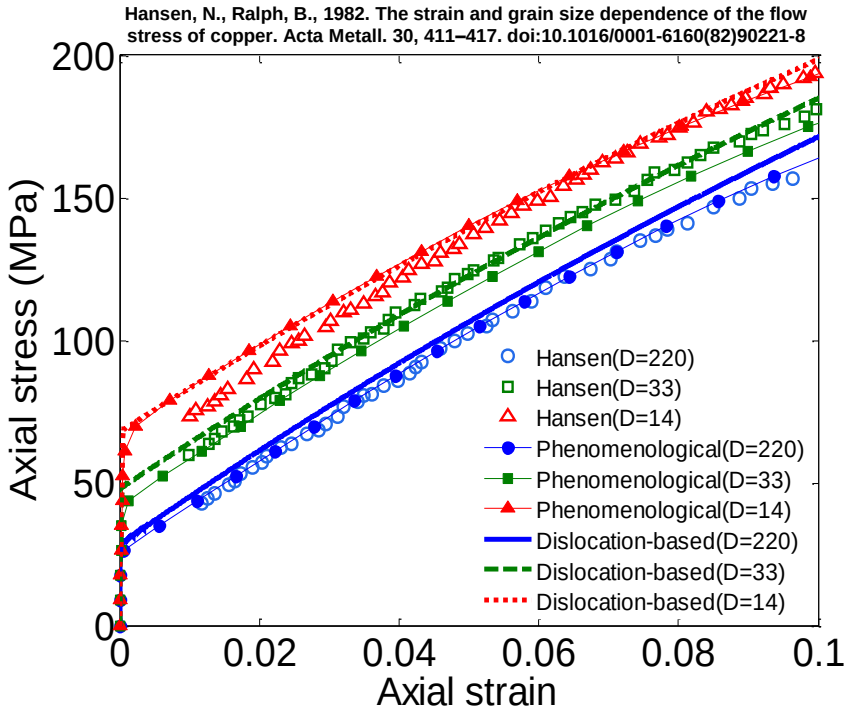


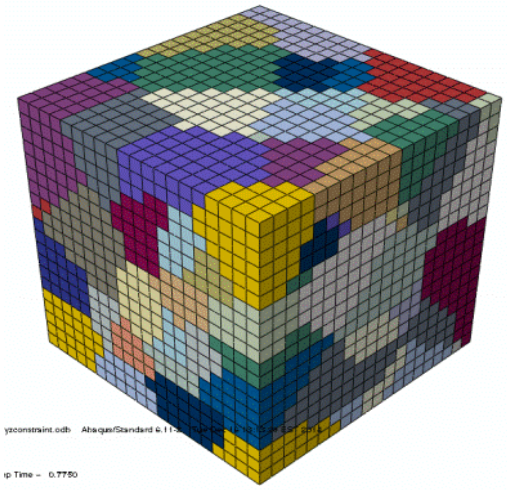
$$\overline{\tilde{\gamma}_{GB}} = \frac{\int_{V_{GB}} \tilde{\gamma}_{GB}(r)\mathrm{dV}}{V} = \frac{8}{V}\sum_{i=0}^{\infty}\int_{0}^{\pi/2}\left(\int_{0}^{\pi/2}\tilde{\gamma}_i(\theta,\phi)\frac{\|R_p\|^{i+3}-\|R_i\|^{i+3}}{i+3}\mathrm{d}\theta\right)\sin(\phi)\,\mathrm{d}\phi$$

Grain Size Effect Validation

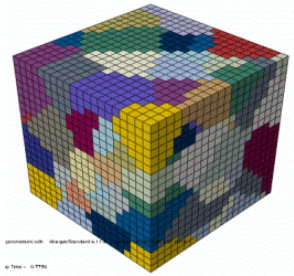
Compare with Hansen *et al.* experiments

- Copper with 125 randomly sized grains
  - Grains have a specified average diameter
- Size effect only
  - Grains represented as simple spheres
  - Linear $\tilde{\gamma}_{GB}$ profile
  - $\delta_{GB} = 0.33\mu m$
- Uniaxial loading rate of 350 MPa/s
- Periodic boundary conditions

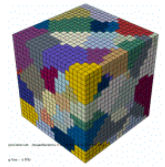




D_{ave} =220 μm



D_{ave} =33 μm



D_{ave} =14 μm