SAND2019-9632PE

2019 Summer Internship Exit Seminar

1. Towards the Verification of a Generalized Schmid- and Taylor-factor Homogenization Scheme
2. Mesoscale Mesh Generation from Noisy Image Data

PRESENTED BY

Brian Phung, Coleman Alleman

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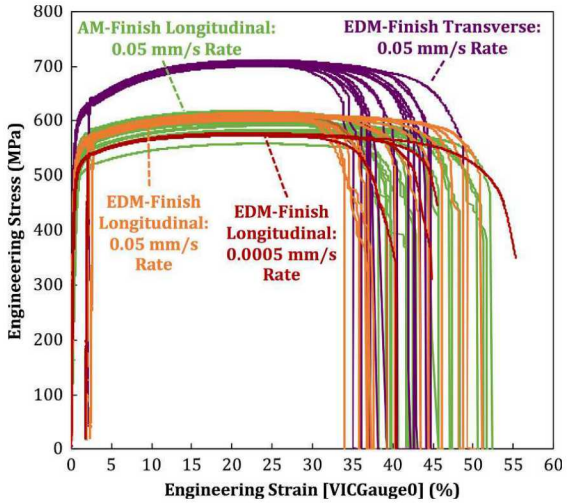
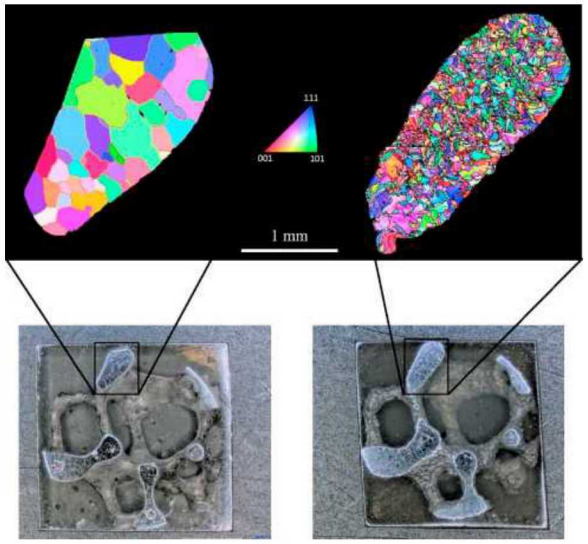
Towards the Verification of a Generalized Schmid- and Taylor-factor Homogenization Scheme

Motivation

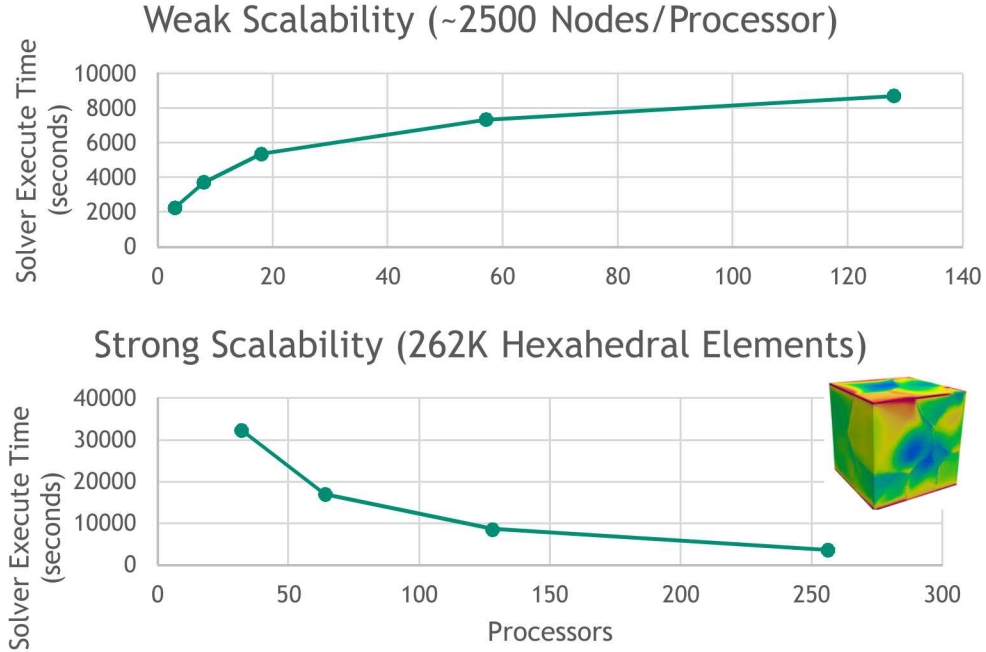
- Material performance can vary, even between two identical components
- Variability can stem from different sources (e.g. geometrical, microstructural)
- Performance variation stemming from microstructural variability can be investigated via a combination of:
  - Explicit material testing (e.g. tensile tests): potentially tedious and monotonous
  - Material science (e.g. grain orientation from EBSD): generally not used in a predictive manner
  - Computational models (e.g. crystal plasticity): computationally expensive at component scale



Calibration test data provided for the 3rd Sandia Fracture Challenge illustrates a level of variability in material performance for identical components [1]



Grain scale data of a traditionally and additively manufactured open-cell aluminum foam from Matheson, et al. [2]

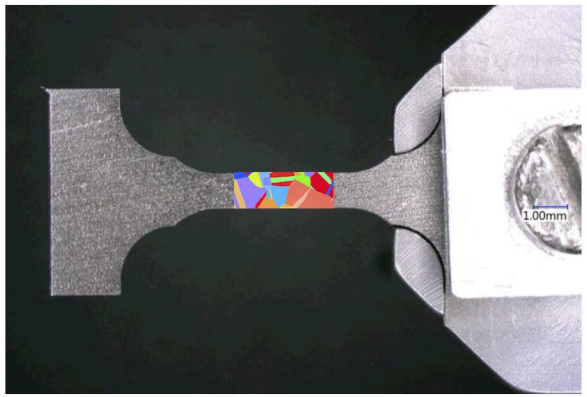


Scalability tests performed with a crystal plasticity constitutive model at 1% strain. Length scale of simulations in microns.

A simplified **microstructurally informed model** capable of **predicting variables of interest** may be useful in quantifying material variability **without explicit material testing or intractable simulations**

[1] S. Kramer, et al. *IJF* (2019). [2] K. Matheson, et al. *MSEA* (2017).

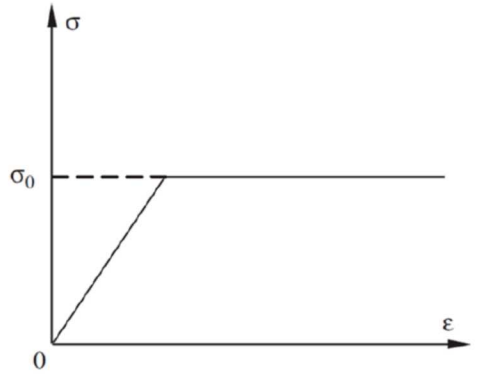
Example of a Proposed Simplified Model



Grain Orientation and Morphology Information

Simplified Model

E, σ_y



Constitutive Model With Relatively Lower Complexity Than Crystal Plasticity

Proposed generalized Schmid- and Taylor-factor homogenization scheme aims to provide a **yield stress approximation** given far-field loading conditions and local crystal properties **without performing a direct numerical simulation**

Generalized Schmid Factor (GSF) Theory

For a single grain, plastic dissipation due to slip is defined as:

$$d^p = \sum_\alpha \dot{\gamma}^\alpha \tau^\alpha$$

A fraction of the applied power dissipated is defined as a function of stress direction ($\underline{\underline{n}}$) and velocity gradient ($\underline{\underline{L}}$):

$$\boldsymbol{\mathcal{D}}^p = \phi_{cr}\underline{\underline{n}}:\underline{\underline{L}} \qquad \underline{\underline{n}} = \frac{1}{s}\underline{\underline{\sigma}}^{dev} \qquad s = \sqrt{\underline{\underline{\sigma}}^{dev}:\underline{\underline{\sigma}}^{dev}}$$

The yield criterion is when the dissipated power due to slip equals the available applied power dissipated:

$$d^p = \boldsymbol{\mathcal{D}}^p \Rightarrow \sum_\alpha \dot{\gamma}^\alpha \tau^\alpha = \phi_{cr}\underline{\underline{n}}:\underline{\underline{L}}$$

If the stress in each grain is approximated as equal to the macroscopic applied stress, τ^α can be found using the Schmid-factor:

$$f^\alpha = \frac{\tau^\alpha}{s} = \underline{\underline{n}}:\underline{\underline{P}}^\alpha \Rightarrow \tau^\alpha = f^\alpha s$$

And the plastic slip rate is commonly approximated via a power law:

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left|\frac{f^\alpha s}{g}\right|^k \operatorname{sgn}\tau^\alpha$$

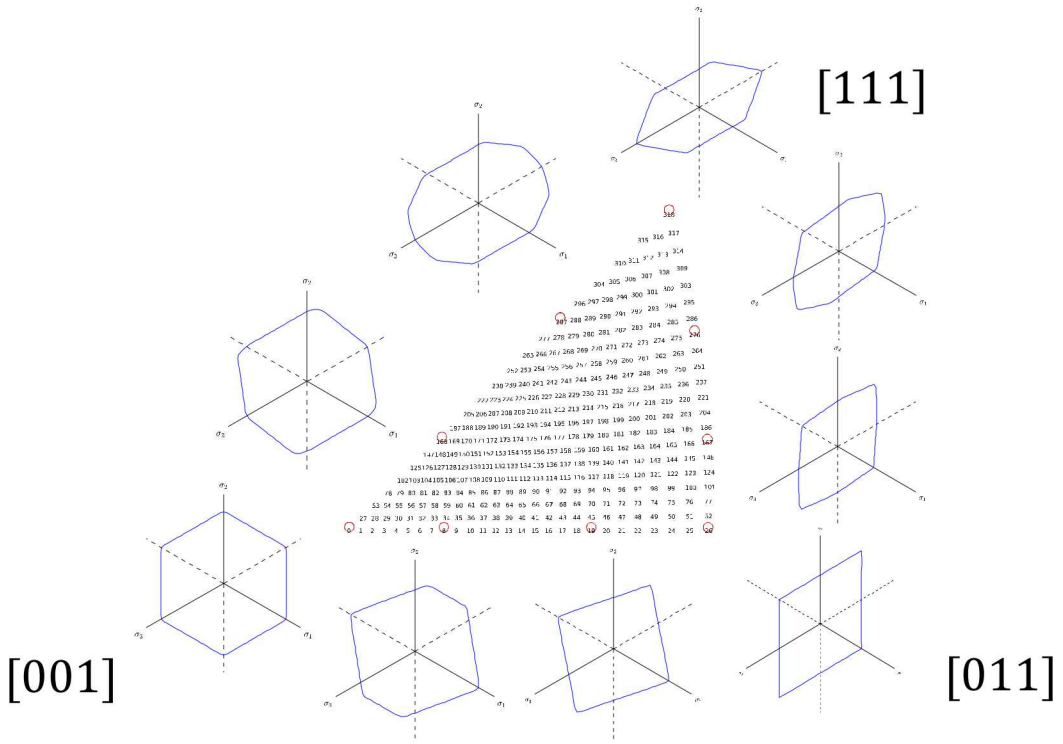
Substituting τ^α and $\dot{\gamma}^\alpha$ into the yield criterion, and solving for the yield stress, $s = S$:

$$S = g\left[\frac{\phi_{cr}\underline{\underline{n}}:\underline{\underline{L}}}{\dot{\gamma}_0 \sum_\alpha |f^\alpha|^{k+1}}\right]^{\frac{1}{k}} = \frac{\tau_{cr}}{\dot{\gamma}_0 \sum_\alpha |f^\alpha|^{1/k}}, \qquad \tau_{cr} = g\left[\frac{\phi_{cr}\underline{\underline{n}}:\underline{\underline{L}}}{\dot{\gamma}_0}\right]^{\frac{1}{k}}$$

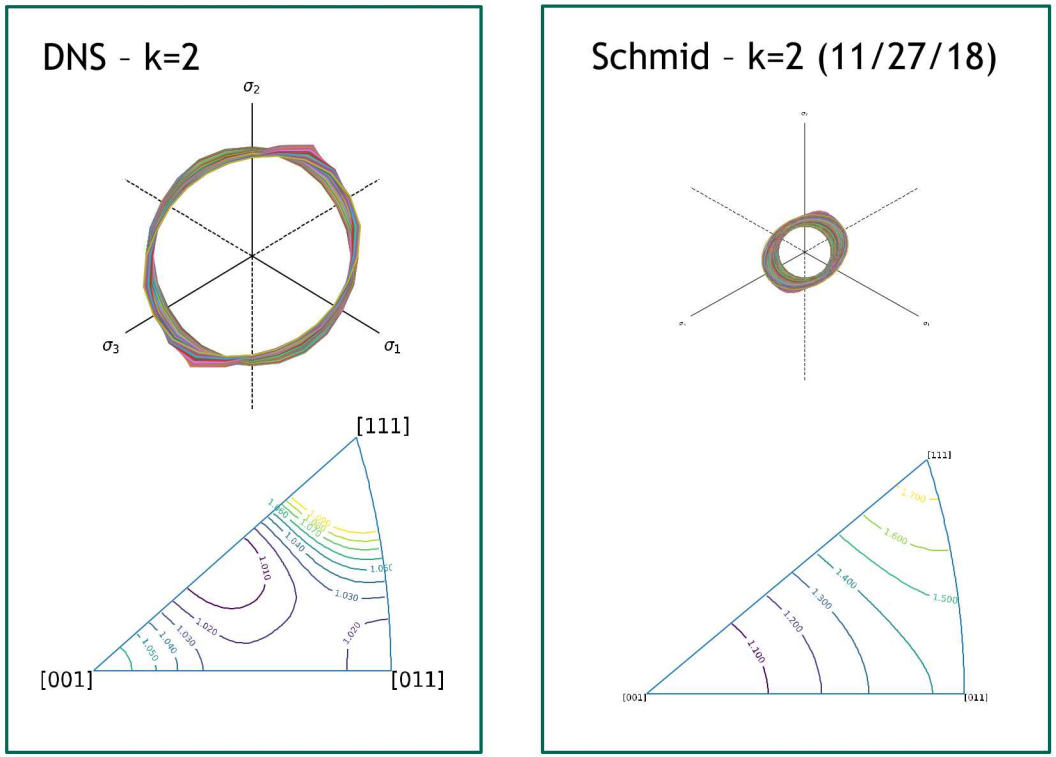
The stress at which the power dissipation due to slip equals the plastic fraction of power dissipated from loading is considered the yield stress.

GSF Single Crystal Verification Procedure

- For various measures of rate sensitivity k, run 319 simulations with orientations corresponding to discretized locations in the standard triangle
- Each orientation is subjected to 12 loading conditions with varying Lode angle, θ
- Yield surfaces are qualitatively compared between the direct numerical simulation (DNS) and GSF



The 319 discretized orientations of the standard triangle. Each yield surface is built from 12 loading conditions according to the Lode angle.



A comparison between the DNS and Modified Schmid Factor approximation for $k = 2$. The solution does not match.

GSF Discrepancy With High Rate Sensitivity

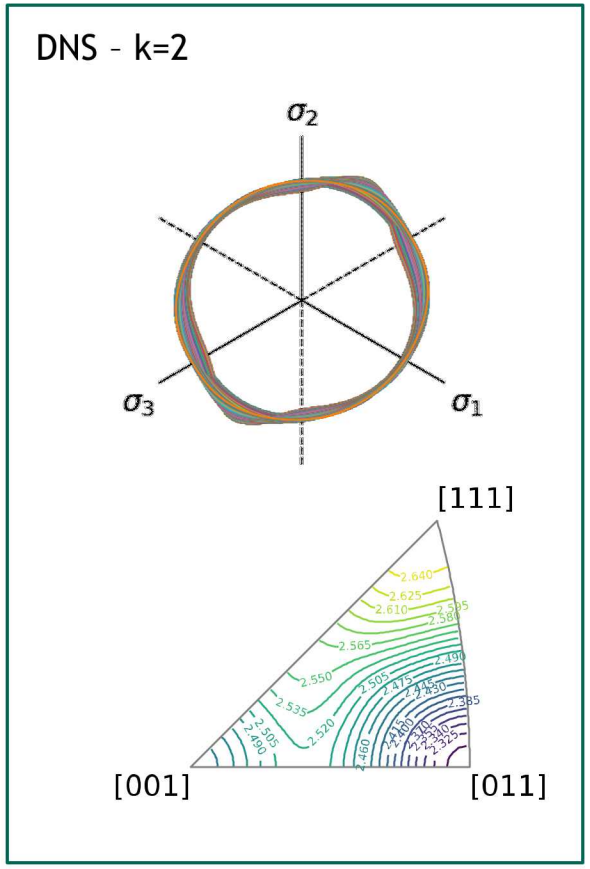
- Predictions with high rate sensitivity $(k < 20)$ did not show good qualitative agreement
- **Hypothesis**: simulations are loaded via stress boundary condition, therefore producing varied velocity gradients/strain rates. However, approximation assumed a constant velocity gradient.

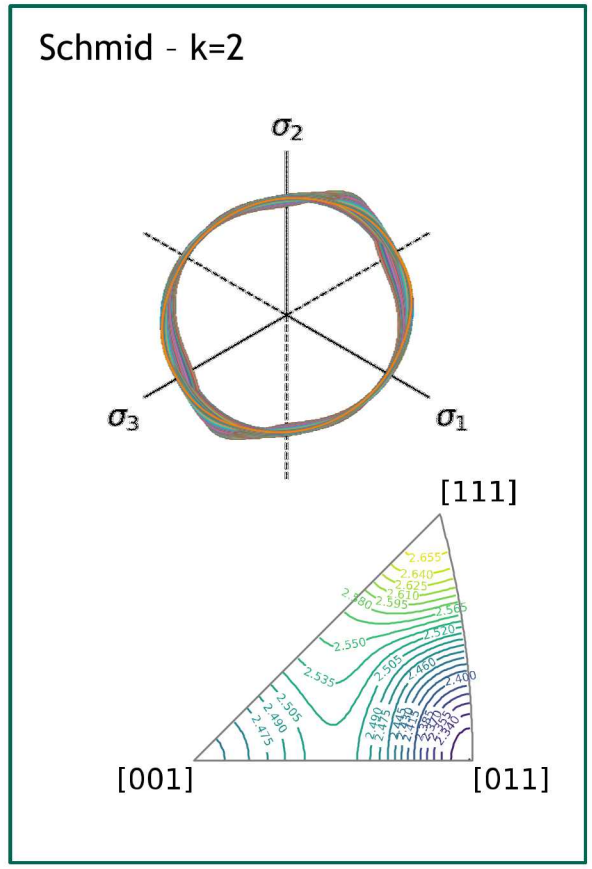
- This phenomenon is exacerbated with higher rate sensitivity

$$\tau_{cr} = g\left[\frac{\phi_{cr}\underline{\underline{n}}:\underline{\underline{L}}}{\dot{\gamma}_0}\right]^{\frac{1}{k}}$$
$$\tau_{cr} \approx g \qquad \forall\, k > 20$$

- **Proposed Solution**: explicitly approximate τ_{cr} from the loading conditions and compare DNS and GSF results

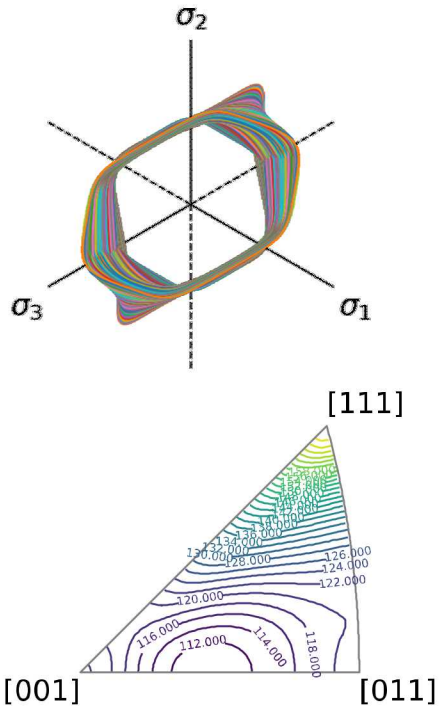
$$\tau_{cr} = g\left[\frac{\phi_{cr}\underline{\underline{n}}:\left(\mathbb{C}^{-1}:\underline{\underline{\dot{s}}}\right)}{\dot{\gamma}_0}\right]^{\frac{1}{k}}$$
$$\mathbb{C}_{ijkl} = R_{im}R_{jn}C_{mnop}R_{ko}R_{lp}$$



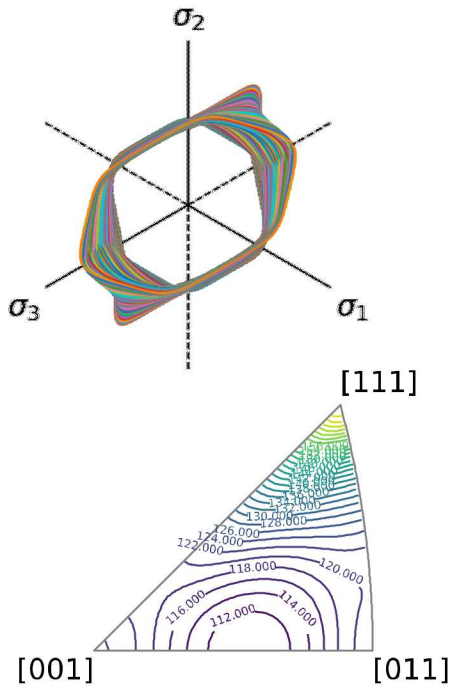


DNS and GSF Agreement

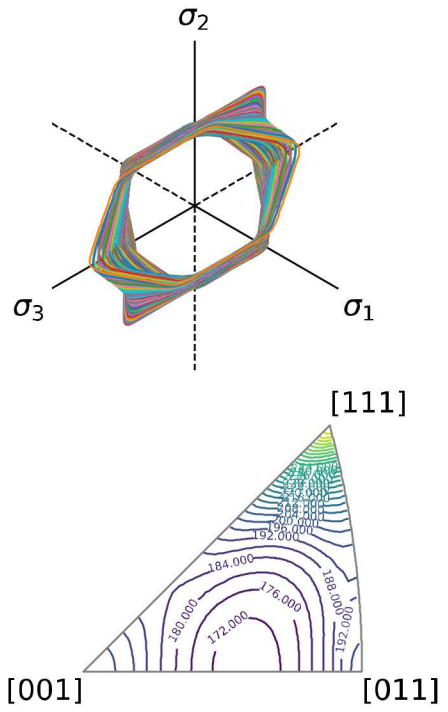
DNS – k=10



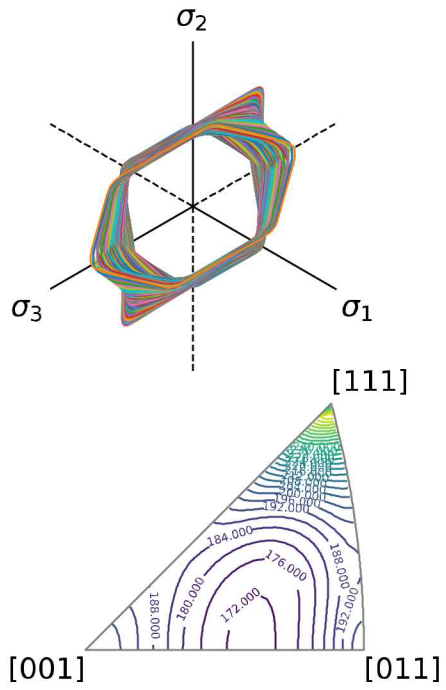
Schmid – k=10



DNS – k=20



Schmid – k=20



Comparisons of DNS and MSF. Fairly good qualitative agreement can be seen.

Generalized Taylor Factor Theory

Recall the yield criterion is when the dissipated power due to slip equals the available applied power dissipated:

$$d^p = \boldsymbol{\mathcal{D}}^p \Rightarrow \sum_\alpha \dot{\gamma}^\alpha \tau^\alpha = \phi_{cr} \underline{\underline{n}} : \underline{\underline{L}}$$

Making the simplifying assumption that the plastic velocity gradient is constant throughout the body, we define the strain-based equivalent to the Schmid factor, the Taylor Factor:

$$q^\alpha = \frac{\dot{\gamma}^\alpha}{\|\underline{\underline{L}}^p\|} = \frac{\dot{\gamma}^\alpha}{\dot{E}^p} \qquad \underline{\underline{L}}^p = \sum_\alpha \dot{\gamma}^\alpha \underline{\underline{P}}^\alpha$$

$$\dot{\gamma}^\alpha = q^\alpha \dot{E}^p$$

Inverting the power law and solving for the resolved shear stress:

$$\tau^\alpha = g \left(\frac{|q^\alpha| \dot{E}^p}{\dot{\gamma}_0} \right)^{\frac{1}{k}} \operatorname{sgn}(q^\alpha)$$

Substituting τ^α and $\dot{\gamma}^\alpha$ into the yield criterion will result in a highly non-linear equation for $\dot{E}_p$:

$$\dot{E}_p = \frac{\phi_{cr} \underline{\underline{n}} : \underline{\underline{L}}}{\sum_\alpha q^\alpha \tau^\alpha (q^\alpha \dot{E}^p)}$$

The plastic strain rate at which the power dissipation due to slip equals the plastic fraction of power dissipated from loading is considered the yield point

Optimizer Preconditioning

- Yield criterion expressed in terms of plastic strain rate is undesirable
- Equation recast in terms of stress results in constrained optimization problem:

$$\underline{\underline{\sigma}} = \text{argmax}_{\underline{\underline{\sigma}}} \sum_{\alpha} \dot{\gamma}^{\alpha} \tau^{\alpha}$$

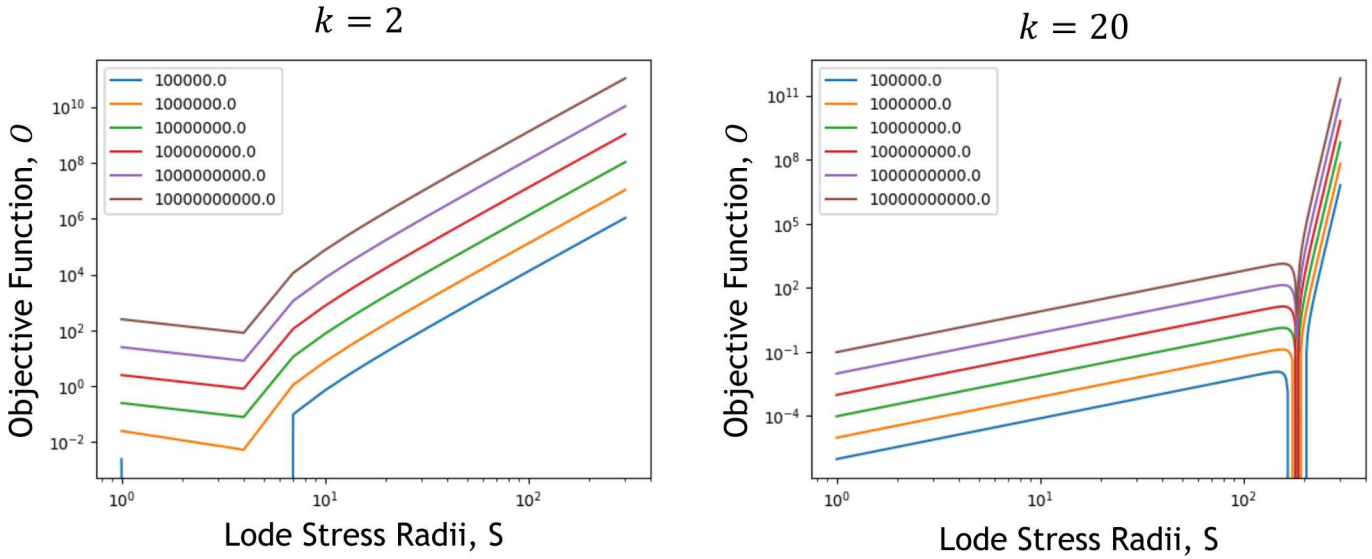
$$\sqrt{\underline{\underline{L}}^{p} : \underline{\underline{L}}^{p}} = \left[\frac{\phi_{cr} \underline{\underline{n}} : \underline{\underline{L}}}{g \sum_{\alpha} |q^{\alpha}|^{\frac{k+1}{k}} \dot{\gamma}_0^{\frac{-1}{k}}} \right]^{\frac{k}{k+1}}$$

Simplified for single crystal verification test, the objective function minimized is:

$$O = -\sum_{\alpha} \dot{\gamma}^{\alpha} \tau^{\alpha} + \mathcal{L}(LHS - RHS)^2$$

- Function is ill-mannered and generalized optimization packages (e.g. scipy) were unable to converge to the desired minimum
- Range of function values caused underflow errors

Typical Objective Functions



Solution: apply bounds to optimization problem:

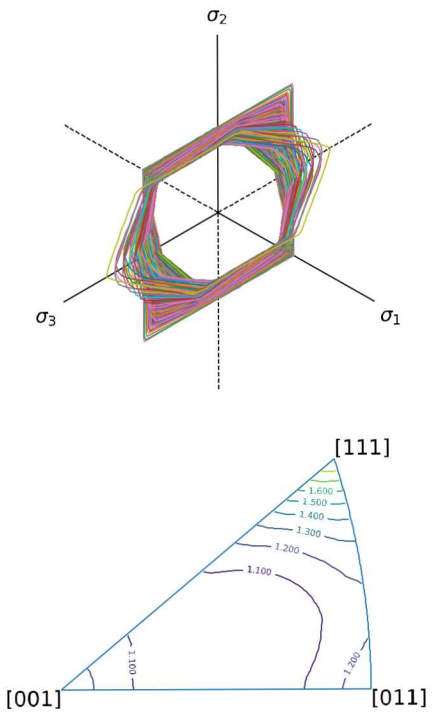
r_{min} is the minimum value of r where $^{dO}/_{dr} < 0$

r_{max} is the minimum value of $r > r_{min}$ where $^{dO}/_{dr} > 0$

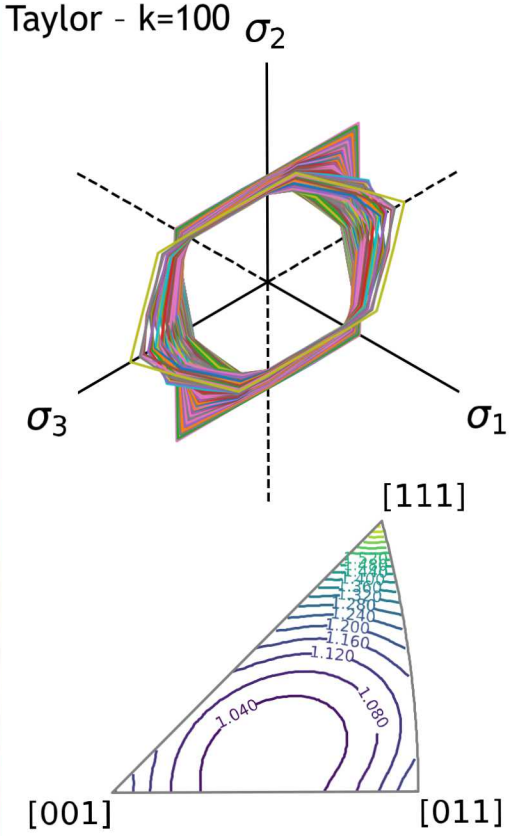
An initial large (10^6) Lagrange multiplier is used, and increased when underflow errors occurred

Comparison of DNS and GTF Yield Stress Predictions

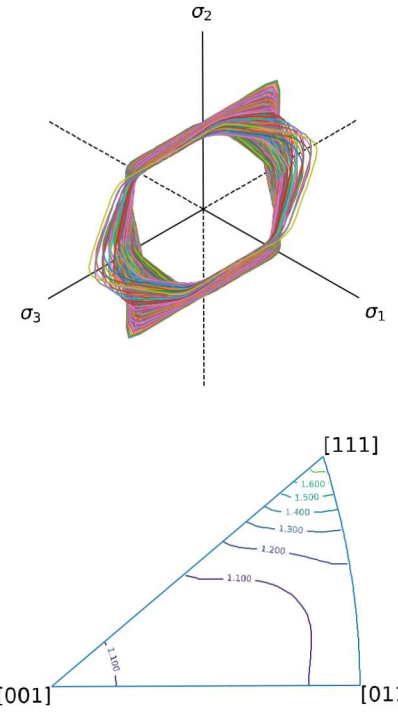
DNS - k=100



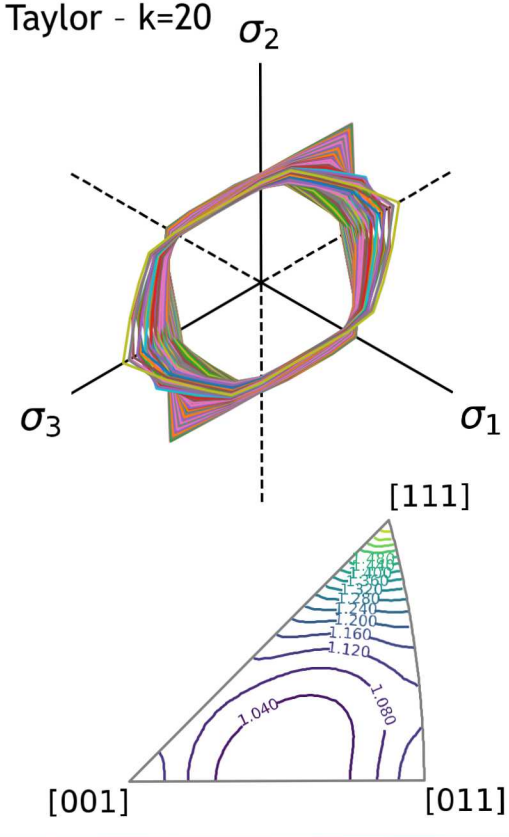
Taylor - k=100



DNS - k=20



Taylor - k=20



Ongoing Work: Polycrystalline Simulations

Recall the plastic dissipation due to slip:

$$d^p = \sum_{\alpha} \dot{\gamma}^{\alpha} \tau^{\alpha}$$

Hypothesis: the single grain case can be extended for the polycrystalline case via volume fractions

$$\sum_{i=1}^{N_{grains}} v_i d_i^p = \phi_{cr} \underline{\underline{n}} : \underline{\underline{D}}$$

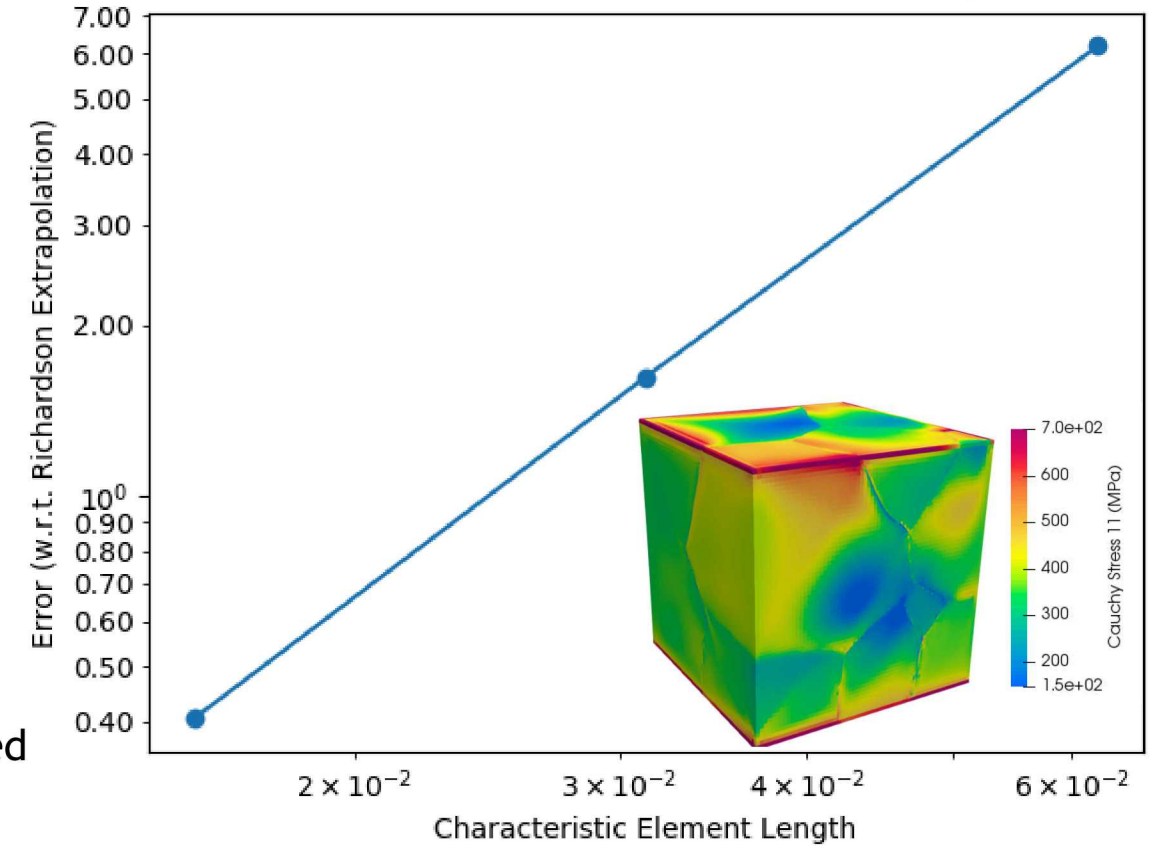
where v_i is a volume fraction

$$v_i = \frac{|\Omega_i|}{|\Omega|}$$

Procedure: simulate multiple ensembles of grain structures and compare yield stress values from the GSF/GTF to the DNF

- Multiple mesh convergence tests should be performed for each ensemble as a single polycrystal is unlikely to ensure convergence for a whole ensemble

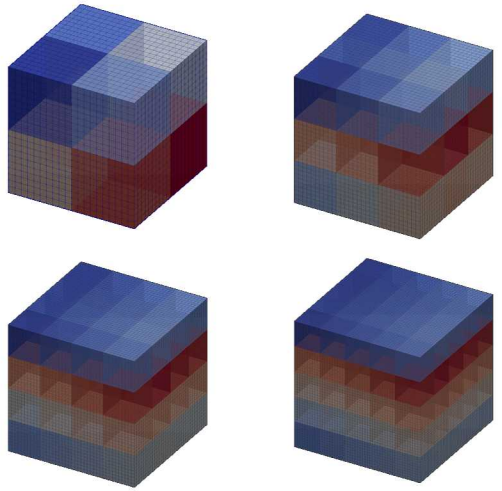
Mesh Convergence Study on σ_y



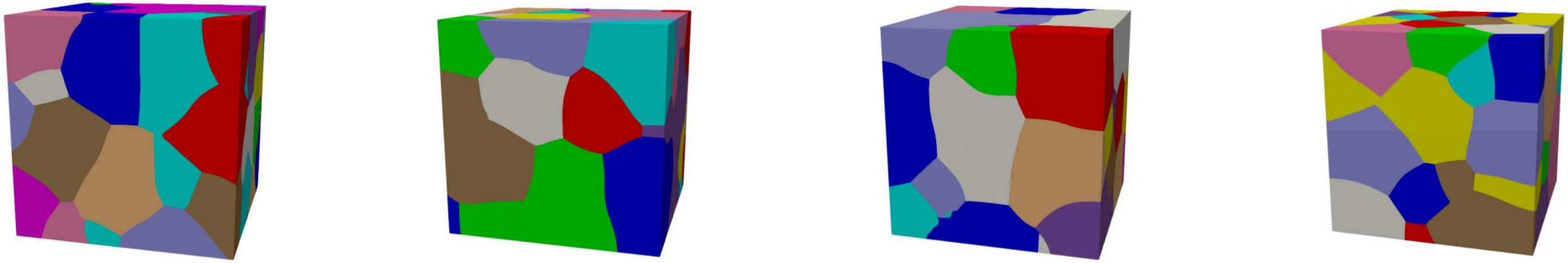
Preliminary mesh convergence tests performed for an ensemble averaging 40 grains, plotted as absolute error w.r.t. the Richardson extrapolation versus the characteristic element length. Errors are 0.12%, 0.44%, and 1.66% from most refined to least.

Summary and Future Work

- The generalized Schmid- (GSF) and Taylor-factor (GTF) homogenization scheme was verified for single crystals
- Initially poor qualitative agreement between the GSF and DNS for high rate sensitivity
  - Performed approximations using an estimated velocity gradient
  - Performed approximations using simulation velocity gradient
- GTF approximation requires solving a constrained optimization problem
  - Objective function is ill mannered, generalized solvers unable to converge to local minimum
  - Applied bounds to optimization problem based on the derivative of the objective function
  - Utilize a large initial Lagrange multiplier, and increased when numerical errors occurred
- Preliminary convergence testing of polycrystalline ensembles



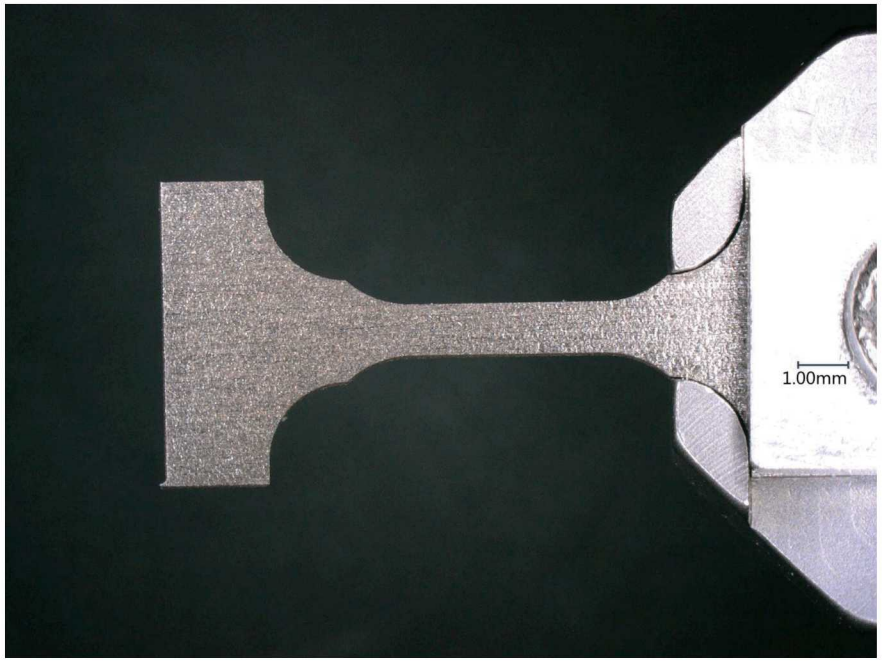
- **Future Work:**
  - Polycrystalline verification
    - Possibly initial attempt cases with idealized cubic microstructures
    - Verify with realistic synthetic microstructures
  - Quantitative measures of error
  - Investigate the effectiveness and limits of the GSF and GTF
  - Compare the accuracy of the MSF and MTF for various boundary conditions and microstructures

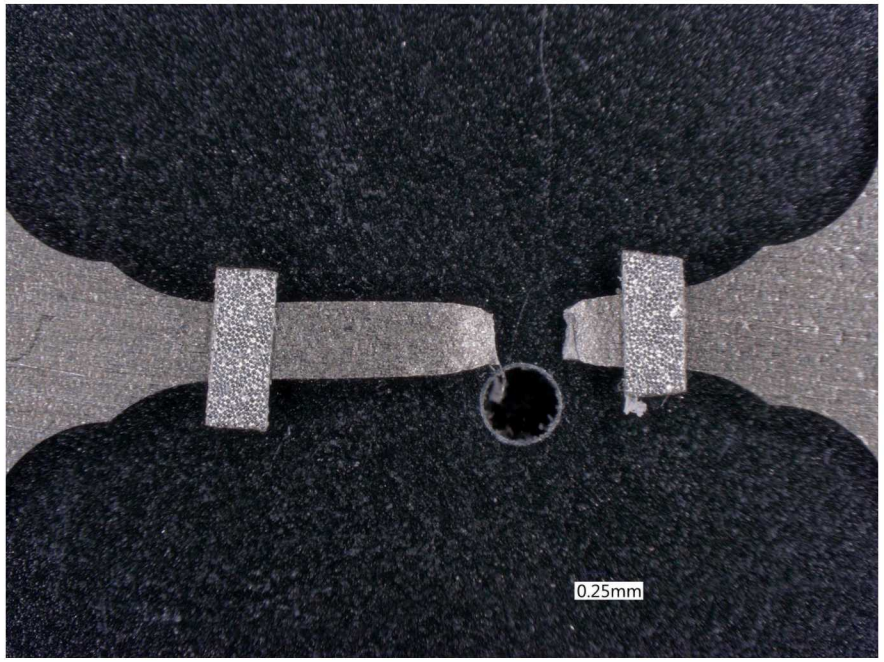


Mesoscale Mesh Generation from Noisy Image Data

Motivation

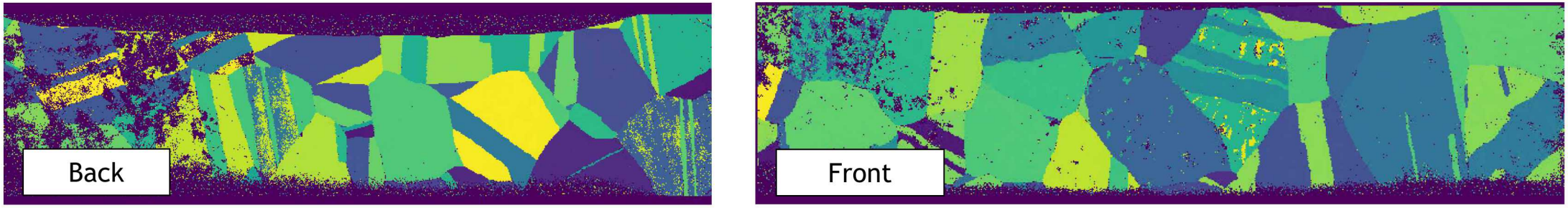
- Project from Hydrogen Materials Compatibility Consortium aims to improve reliability of materials in hydrogen storage applications
- Rather than perform alloy design (i.e. creating new alloys), investigate methods in designing the microstructure of existing alloys to improve performance of materials interaction with hydrogen (e.g. resistance to hydrogen embrittlement)
- 304 L Stainless Steel exhibits relatively good resistance to hydrogen embrittlement
- **Initial Computational Steps**: run a mesoscale simulation of a tensile sample of 304 L SS





Generation of Microstructure Meshes

- **Goal**: run a proof-of-concept mesoscale simulation from **electron-backscatter diffraction (EBSD)** images of a 304 L Stainless Steel sample, where **only noisy front and back surfaces are available**
- Microscope software can generally clean data automatically, but was insufficient



Front and back EBSD scans of 304 L Stainless Steel sample, where colors are the first Euler angle in the Bunge convention

- **Procedure:**

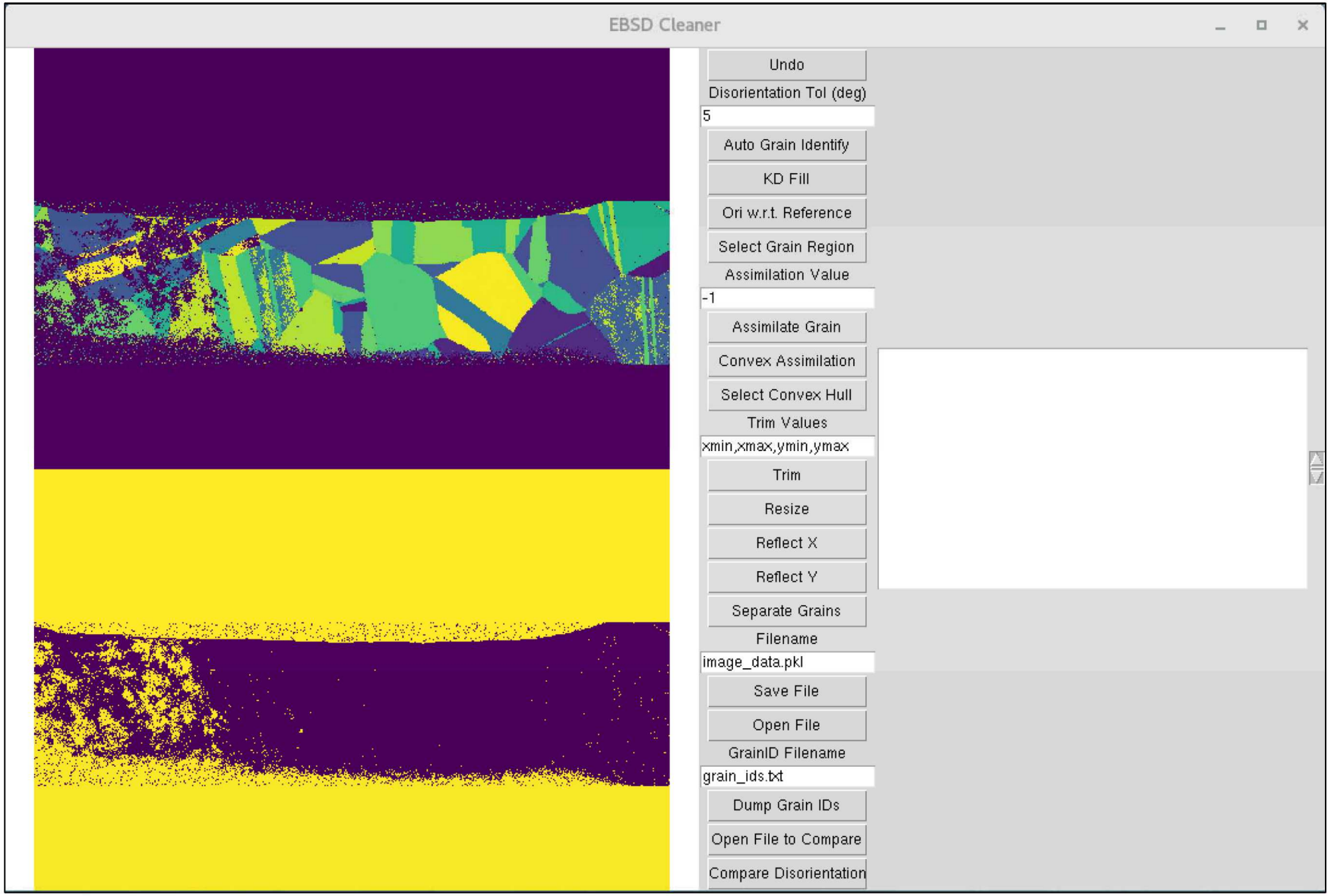
Obtain a voxelized description of the microstructure geometry → Utilize a meshing tool (e.g. Cubit, Sculpt) to generate a volume mesh from the voxelized description → Utilize mesh in a Finite Element simulation

Tasks:

1. Create a user-guided image cleaning tool
2. Run a grain growth simulation to “fill in” the interior volume
3. Generate a mesh and run a proof-of-concept crystal plasticity simulation

User-Guided Image Cleaning

- Minimal GUI built on tkinter python library
- Basic functionality:
  - Undo, Save, Load
  - Trim
  - Resize
  - Reflect
- Grain Identification
  - Disorientation-based identification
  - KD-tree based void fill
  - Grain separation
- Grain ID assimilation
  - Manual region selection
  - Grain convex hull
  - User-drawn convex hull

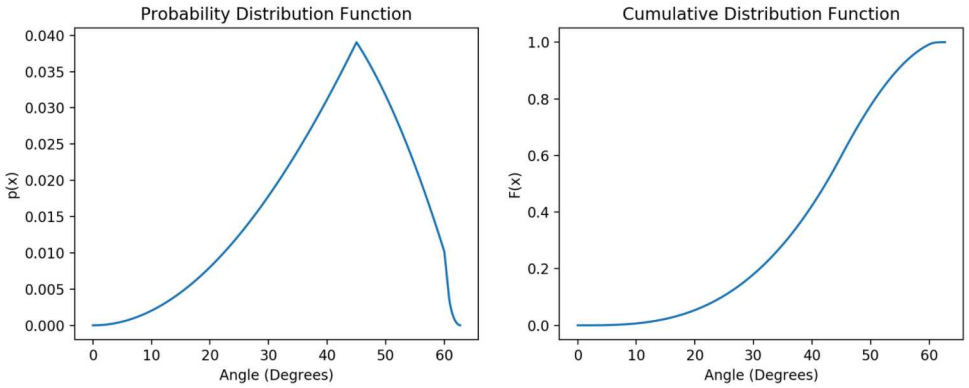


Grain Identification Using Disorientation Values

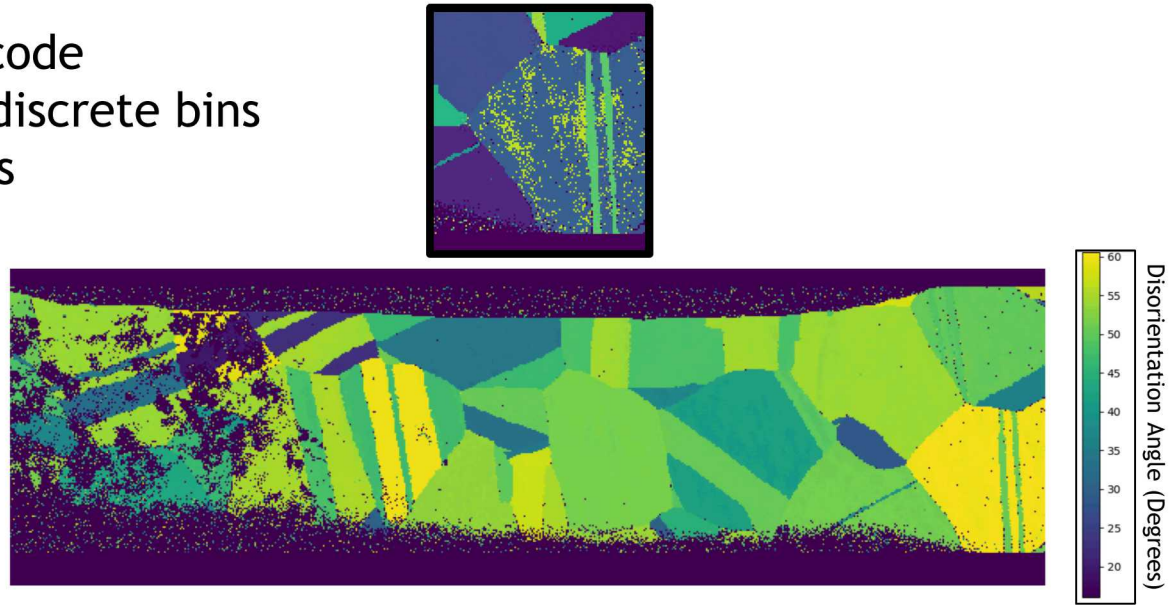
- Need to modify EBSD data format such that each location has a distinct grain ID

EBSD Data Format	Desired Format
1. Location (x,y) 2. Euler Angles	1. Location (x,y) 2. Grain ID

- Cannot compare Euler angle values, multiple set of Euler Angles that represent a single orientation
- **Solution**: assign points grain IDs based on disorientation of each point with respect to fixed coordinate system
  - Wrote and verified disorientation calculation code
  - Separated range of disorientation angles into discrete bins
  - Placed each (x,y) point into corresponding bins



Verification of the disorientation code. Uniformly random rotation matricies were generated using the Arvo Random Orientation Algorithm [1]. A distribution of disorientations was generated and verified against literature [2].

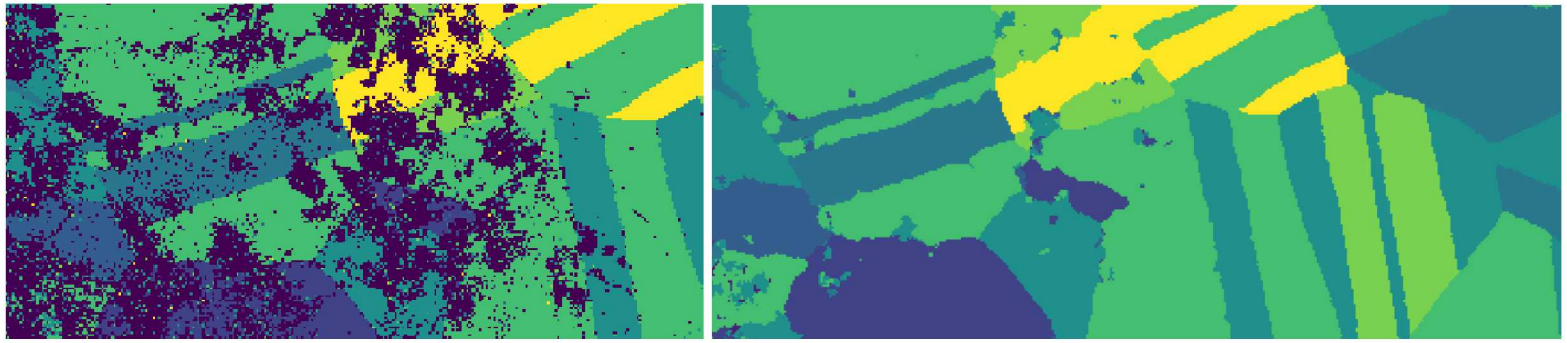


Disorientation of each point on the back image w.r.t. to a laboratory basis. Disorientation ranges from 0 degrees (coincident with the lab basis) to ~62 degrees (maximum disorientation angle for a cubic crystal structure [2]).

[1] R.M. Brannon. *Rotation, Reflection, and Frame Changes* (2018). [2] J.K. Mackenzie, *Biometrika* (1958).

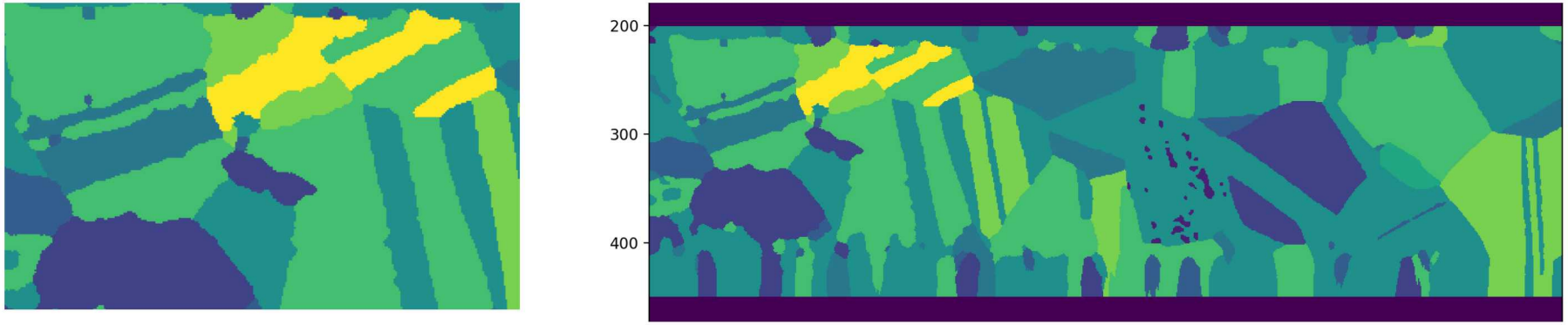
Data Cleaning Using a Weighted Nearest Neighbor Search

- Need to approximate grain ID of the void regions
- Used a KD-Tree to fill void regions using the 10 closest “good” points as defined by the EBSD microscope software



Voids regions filled using the closest 10 “good” points. Heavy noise is still prevalent due to erroneous “good” points.

- Running multiple iterations of this algorithm produces significantly cleaner results compared to the initial data
- Regions at the top and bottom are “stretched” due to lack of data (cropped in final mesh)

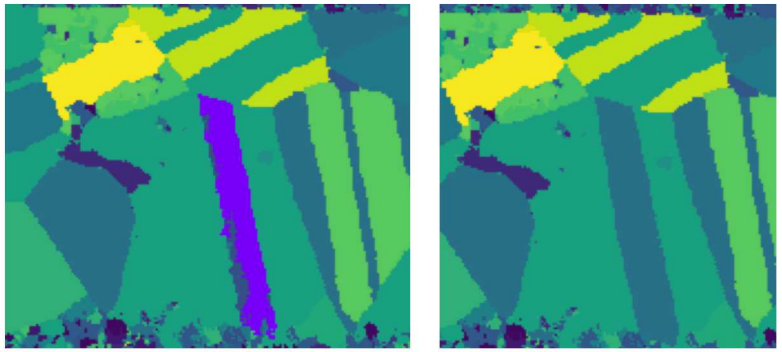


Grain Assimilation via Grain Selection

- After defining grain IDs, grain regions can be selected
  - Brute force algorithm probing surrounding points for matching Grain IDs
- Selected regions can be assimilated to the surrounding grain ID or to a user-specified ID

Left: example of an erroneous grain region selected
Right: the selected region is assimilated into the surrounding grain

- Alternatively, user can build a convex hull and assimilate all points inside the convex hull
  - Useful for large regions that need to be converted
  - Convex hull can be assembled from a selected grain region or from a set of clicks that define the convex hull

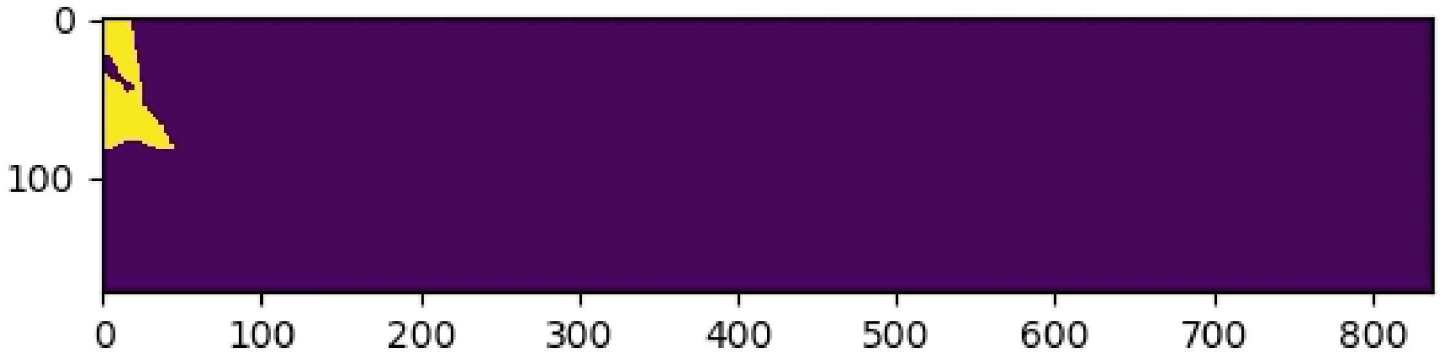


Left: example of a grain region selected
Right: a convex hull is constructed from the region, and all points in the hull are assimilated

Generating Unique Grain IDs

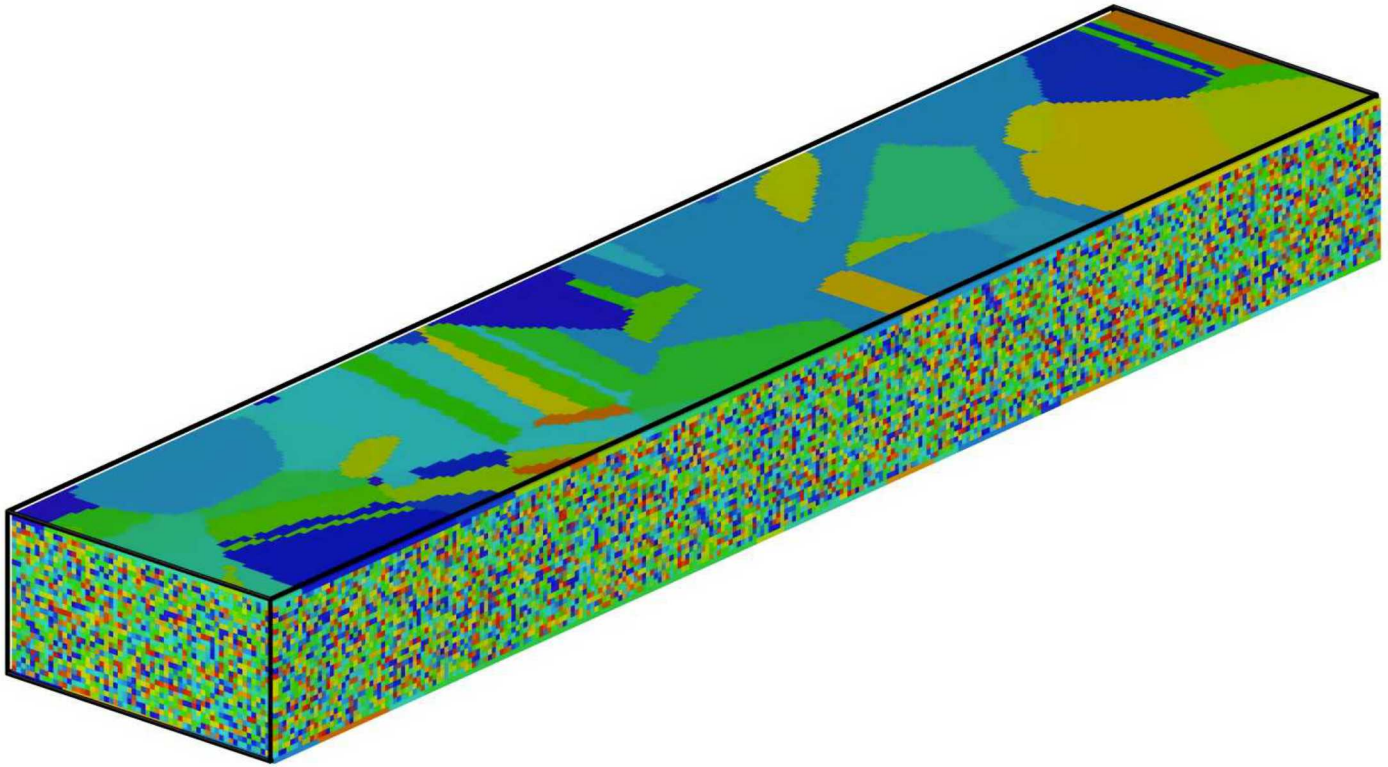
- Using the developed utility, “cleaned” images were generated

- Recall: grain IDs were generated from binning disorientation values
- Consequently, geometrically distinct grains in two locations may have the same grain ID identifier
- Extend previous algorithms to assign unique grain IDs to geometrically distinct grains



Grain Growth Simulation Using SPPARKS

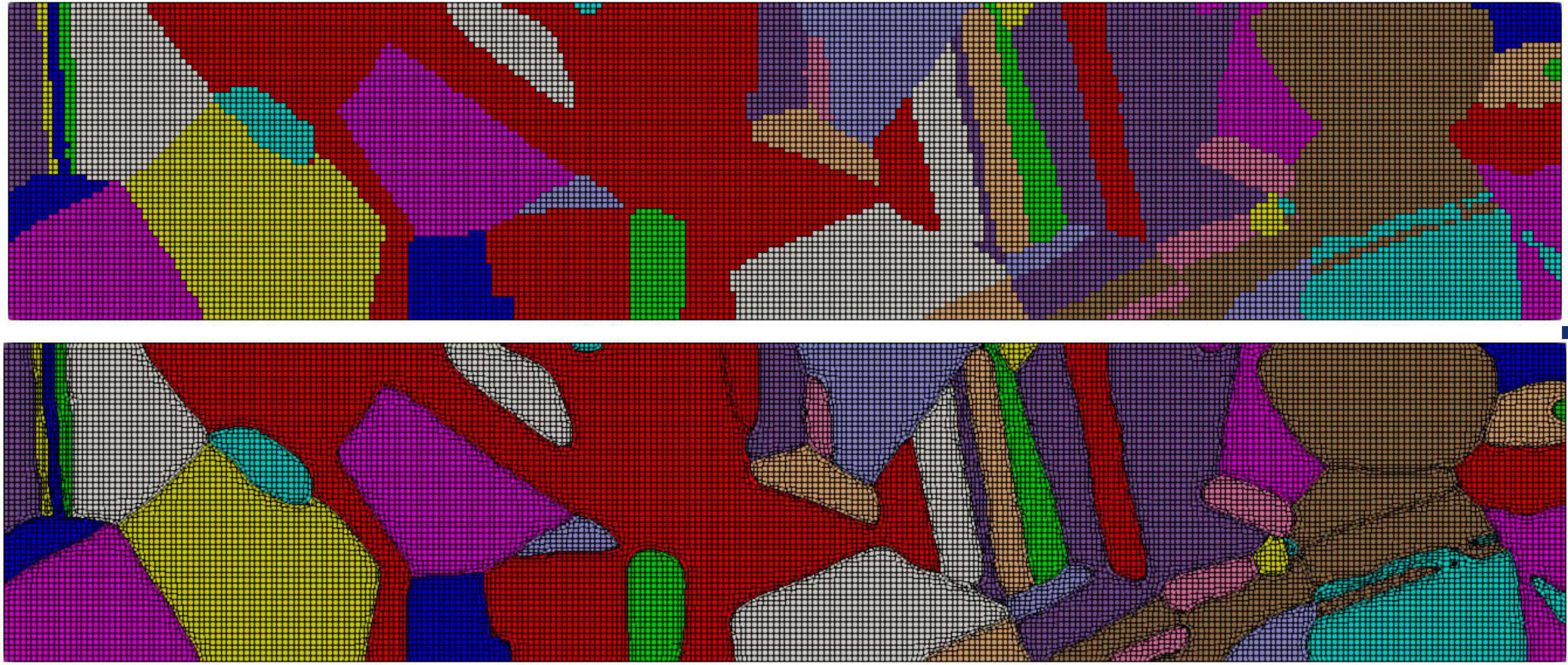
- Code was written to generate a 3D volume using the front and back images
- Undefined regions are given a random grain ID drawn from a uniform distribution
- A grain growth simulation is run using SPPARKS [1], holding the front and back faces fixed



[1] S. Plimpton, et al. *SAND2009-6226* (2009). http://spparks.sandia.gov/

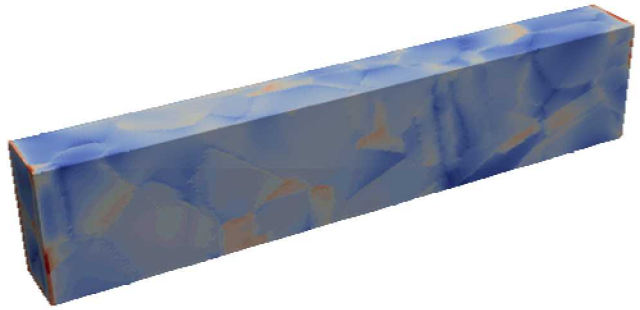
Structured and Unstructured Hex Meshes

- Using Sculpt, unstructured and conformal hex meshes were generated



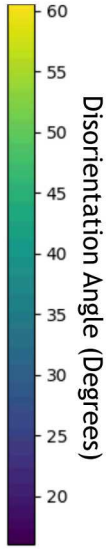
Ongoing and Future Work

- Due to time restrictions, the following issues are still present:
  - Conformal mesh: elements are generated with a negative/bad q
  - Structured mesh: simulation in progress



- **<u>Potential Future Work:</u>**
  - Resolving issues with conformal and structured meshes
    - Investigate convergence with an infinitesimal displacement/simple constitutive model (isolate if issue stems from mesh or model)
    - Further simplifying grain structure using developed tool
  - Explore a tetrahedral conformal mesh
  - Link grain IDs on the front/back face

Preliminary disorientation angles between the front and back faces. While no matching grains are immediately evident, a more thorough investigation should be performed



2019 Summer Internship Summary

- Work on two projects were peformed:
  1. Towards the Verification of a Generalized Schmid- and Taylor-factor Homogenization Scheme
  2. Mesoscale Mesh Generation from Noisy Image Data

GSF/GTF

1. The Generalized Schmid-Factor was qualitatively verified for single crystals under various loading conditions and rate sensitivities
2. The Generalized Taylor-Factor was implemented for single crystals by solving a pre-conditioned constrained optimization problem
3. The Generalized Taylor-Factor was qualitatively verified for single crystals under various loading conditions and rate sensitivities

Clean EBSD

1. A user-guided image tool was developed, capable of basic functionalities (undo, save, load, trim, resize, reflect), grain identification based on a verified disorientation code, and image cleaning.
2. Grains are given unique grain IDs and front and back faces are synthesized into a 3D volume format suitable for the grain growth simulator, sparks
3. Structured and conformal hexahedral meshes were generated