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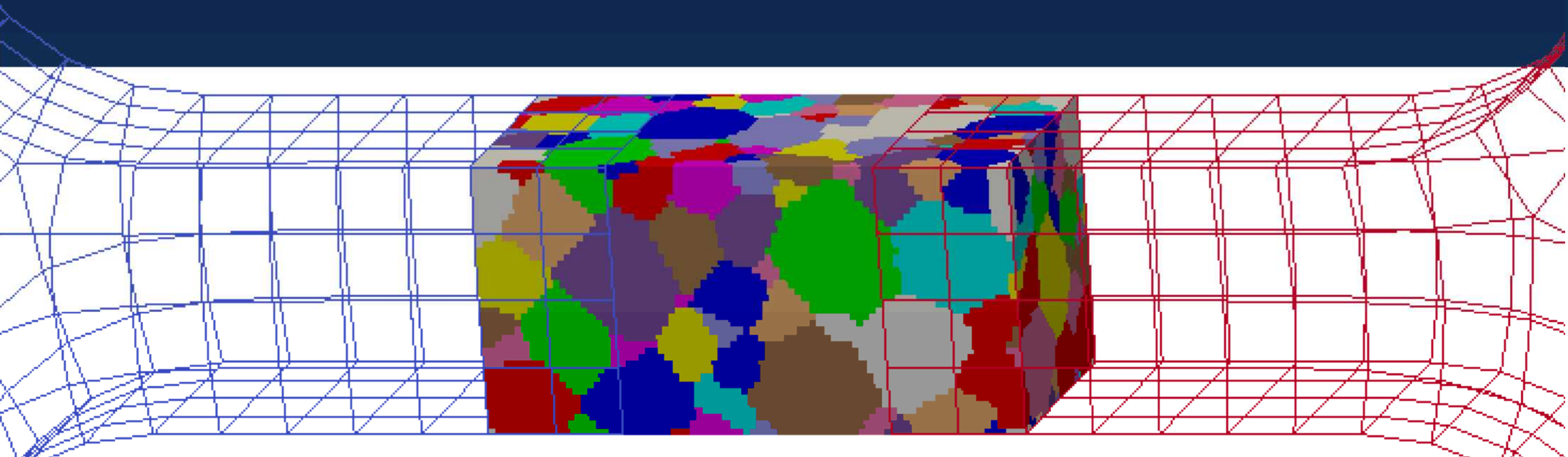

Concurrent Multiscale Modeling of Microstructural Effects on Localization Behavior in Finite Deformation Solid Mechanics

Coleman Alleman, Corbett Battaile, James Foulk, Hojun Lim, David Littlewood, Alejandro Mota, Jake Ostien, Irina Tezaur

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Multiscale modeling of localization

Connect physical length scales to engineering scale models

Investigate importance of microstructural detail

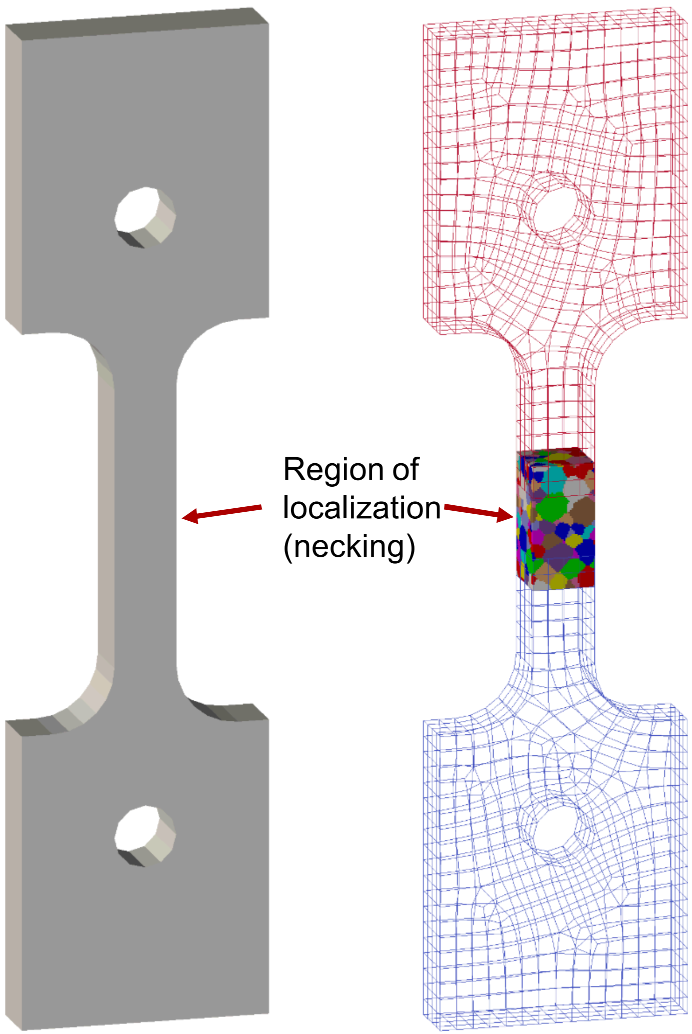
Develop scale bridging technologies for spatial multiscale/multiphysics

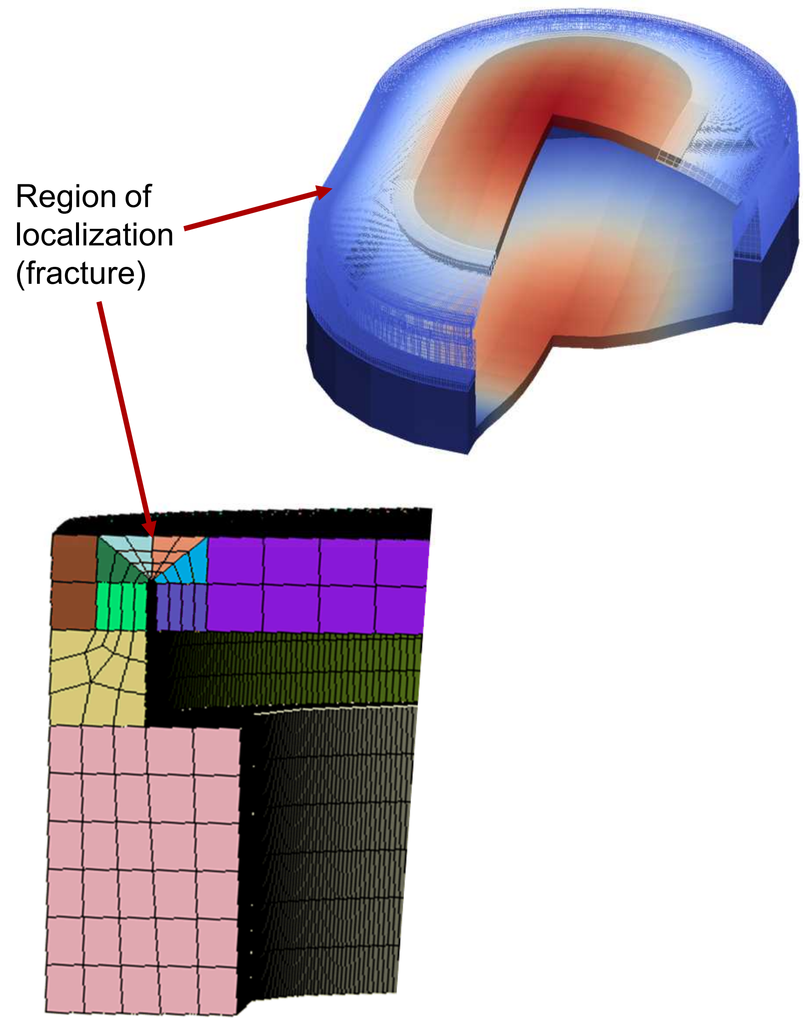
Developing strong, concurrent, multiphysics, multiscale coupling to understand the impact of microstructural mechanisms on the structural scale

- Applications invoke microstructure
- Explicitly connecting scales
- Resolving strong multiphysics
- Developing discrete microstructural models
- Resolution through manycore/GPUs

Goal: Predict void nucleation at the microscale

Problems Involving Localization

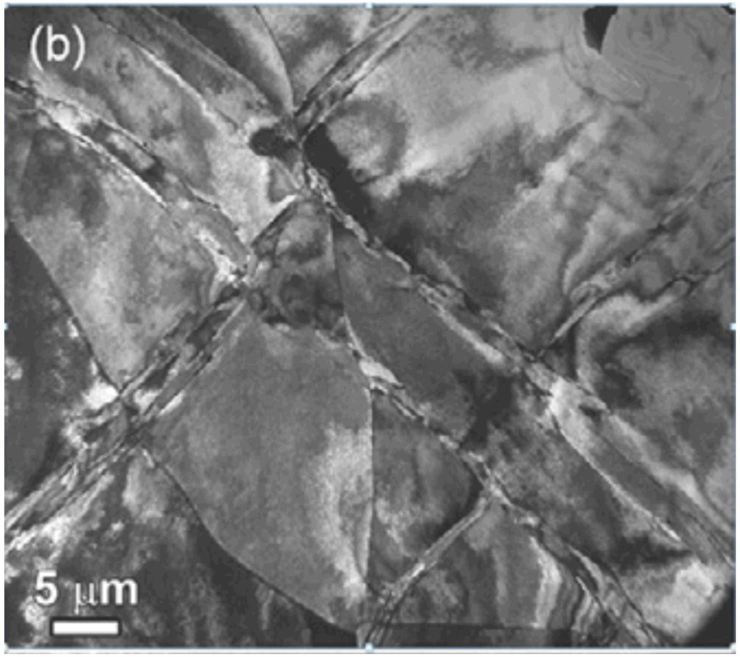




Project scope

- *Strong multiphysics*
  - Implement/verify multiphysics surface elements
  - Develop/implement block preconditioners for multiphysics
- *Concurrent multiscale*
  - Couple the microstructural and structural scales w/multiphysics
- *Microscale physics*
  - Develop/implement models for twinning in FCC and BCC systems
  - Develop/Implement thermal & transport models for boundaries and twins
  - Model discrete twins in grains
- *New architectures*
  - Prototype Kokkos implementation for manycore simulations
- *Applications*
  - Develop ensembles of microstructure for FCC austenitic stainless steel
  - Develop ensembles of microstructures for BCC tantalum (Ta)
  - Simulate hydrogen embrittlement of SS microstructures

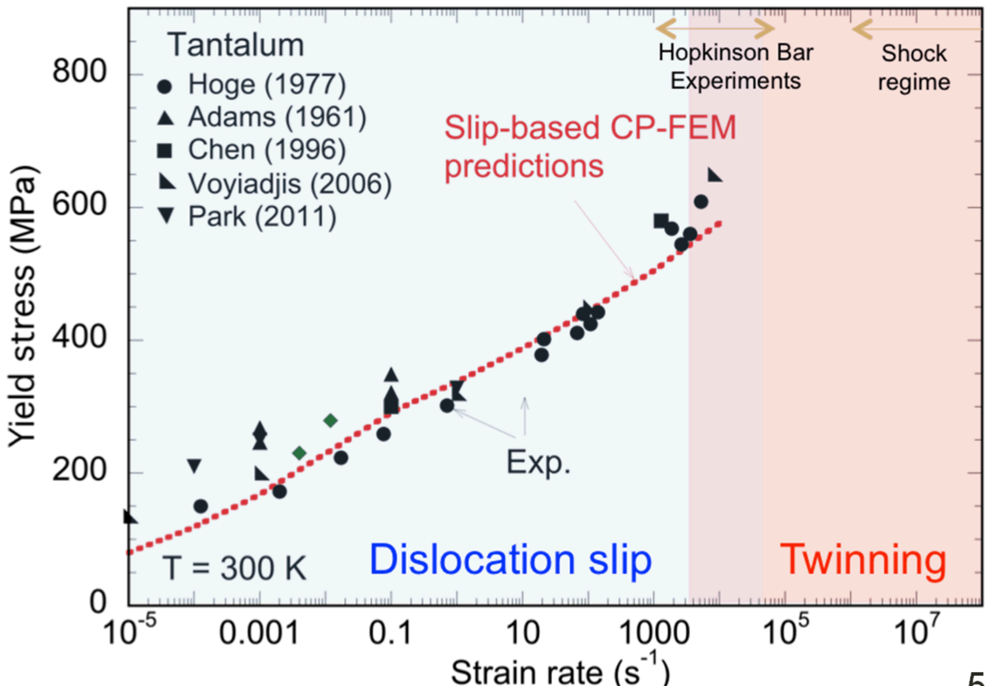
Temperature/strain-rate activates microstructure (Ta)



TEM micrograph of deformation twins in Ta[1]
(T=77 K and $\dot{\varepsilon}$ =2.2x10^4 s^{-1}).

Strain rate & temperature *activates* microstructure and *localizes* deformation

- Increased strain rate (10^3, 10^4) and decreased temperature aids twinning (*nm*)
- Accentuates grain boundary interactions (*nm*)

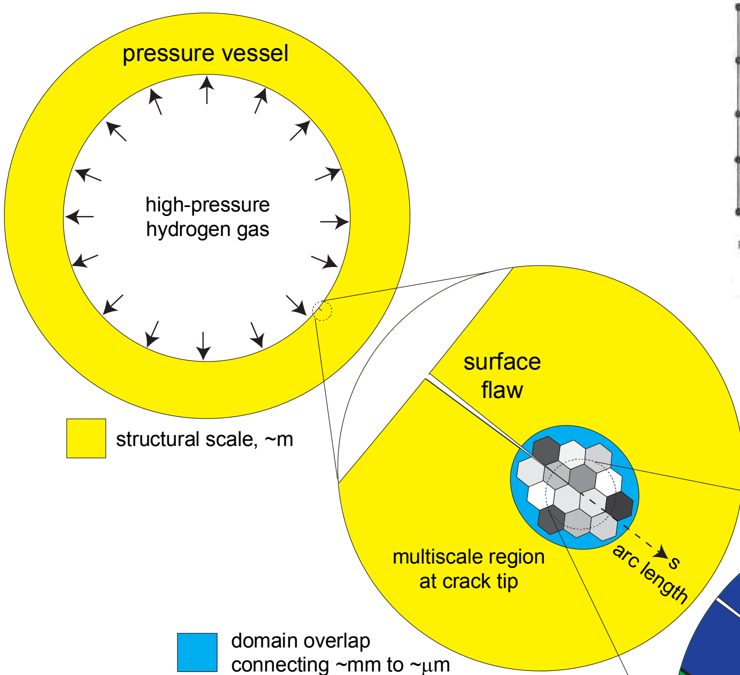


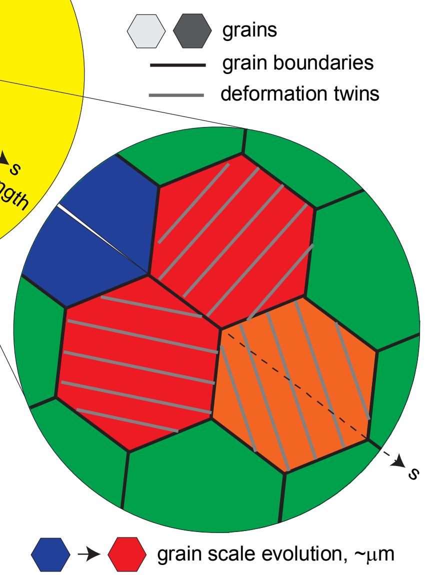
Length scales span 10*μm* – 1*mm*

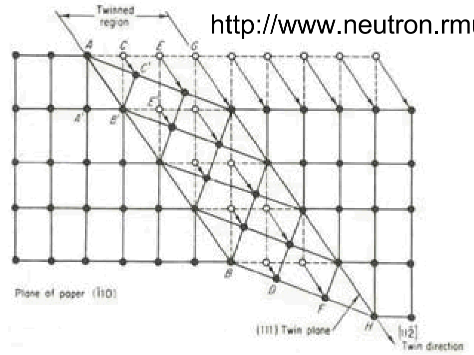
- Extensive slip within grains
- Twins evolve within steep gradients

[1]Chen, et. al., *Scripta Mater.* 69 (2013) 709 – 712.

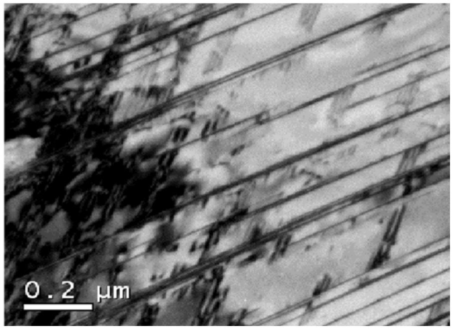
Hydrogen activates microstructure (stainless steel)



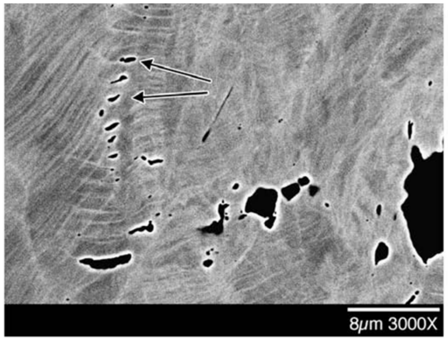




http://www.neutron.rmutphysics.com



extensive slip and deformation twinning

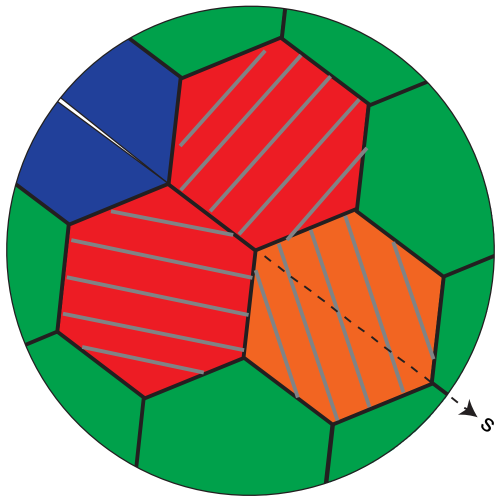


premature void nucleation*

- Localizes deformation (μm)
- Aids deformation bands/twinning (*nm*)
- Accentuates boundary interactions (*nm*)

*Nibur, et. al., Acta Mater., 2009.

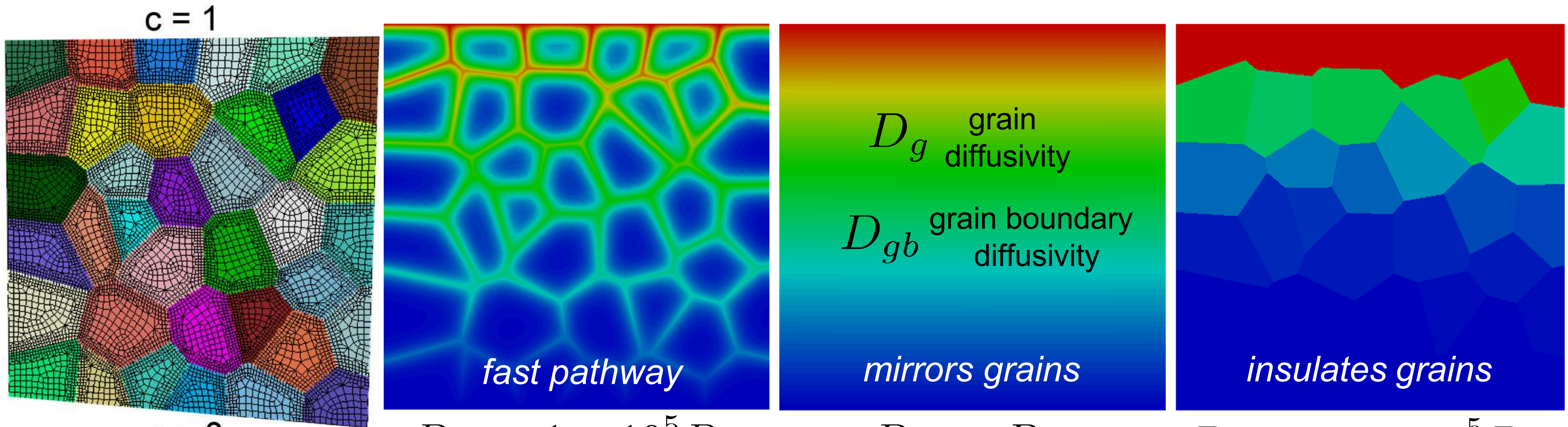
Multiphysics: Mechanics and Diffusion



Microstructure impacts deformation and diffusion

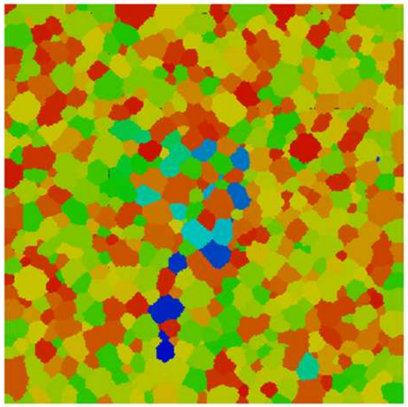
Deformation alters effective diffusion constant

Diffused species affect fracture behavior

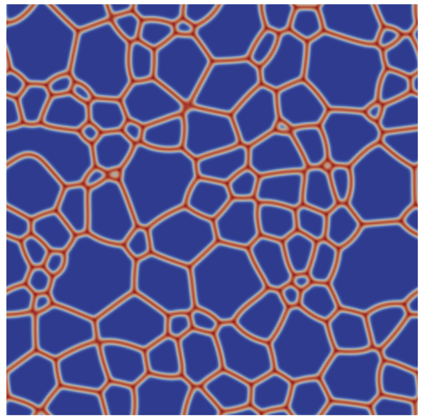


$D_{gb} = 1 \times 10^5 D_g$ $\quad$ $D_{gb} = D_g$ $\quad$ $D_{gb} = 1 \times 10^{-5} D_g$

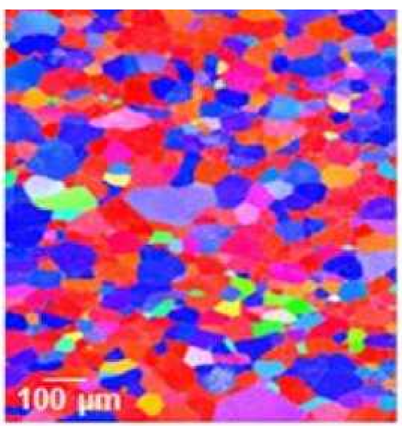
Create and Characterize Microstructure



Kinetic Monte Carlo grain growth model



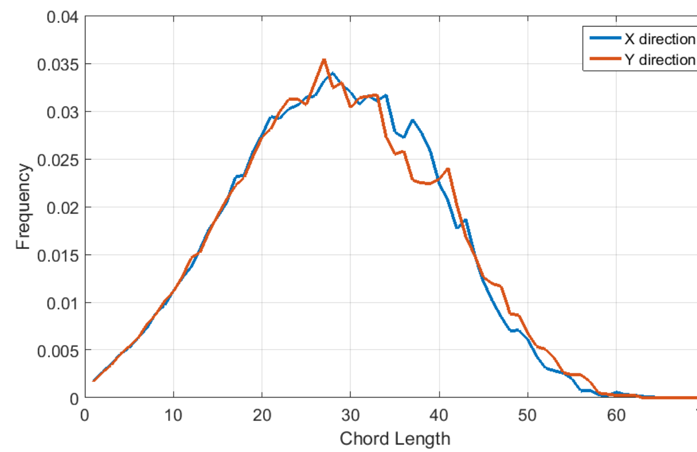
Phase Field Grain Growth model



Electron back scattered diffraction

Rigorous statistical quantification of polycrystalline microstructures

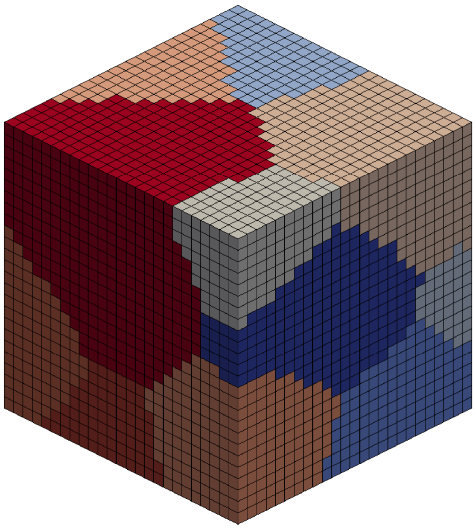
Distribution of grain boundary chord lengths in a candidate microstructure

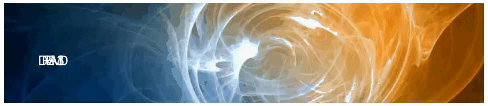


Exploring microstructure-mechanical property relationship using statistical data analysis

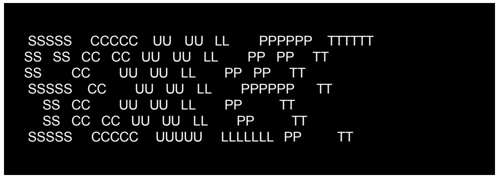
Multiscale/multiphysics LDRD. SNL PI: Hojun Lim. GT PI: Professor Surya Kalidindi

Finite Element Meshing Workflow

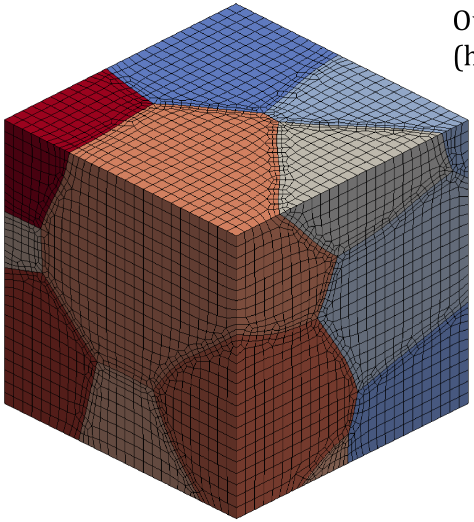


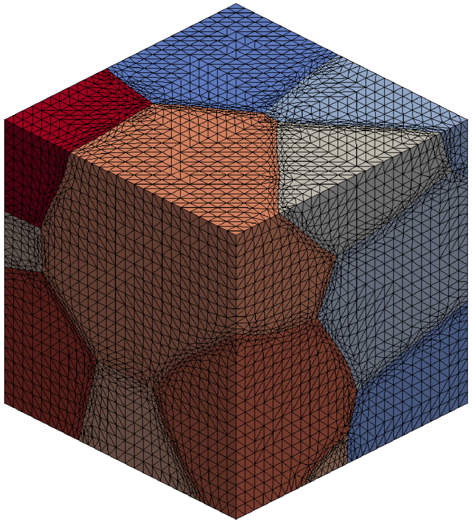


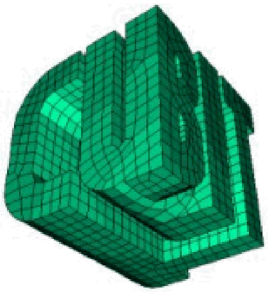
DREAM.3D
Input: microstructure statistics
Output: voxelized microstructure



SCULPT
Input: voxelized microstructure
Output: finite element mesh (hexahedral)

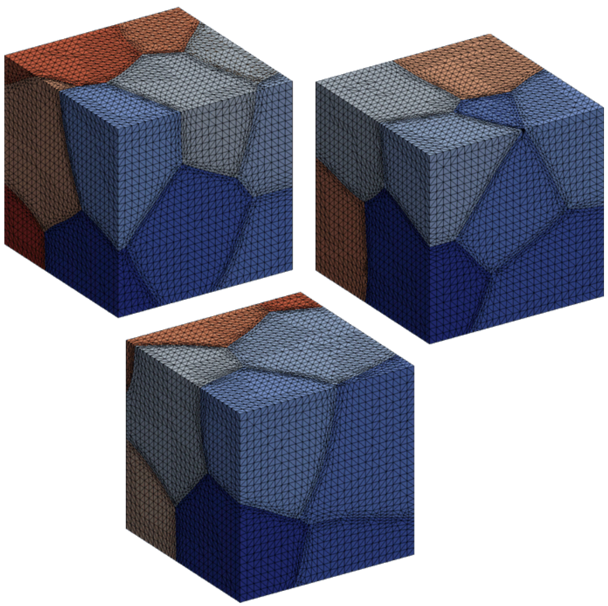




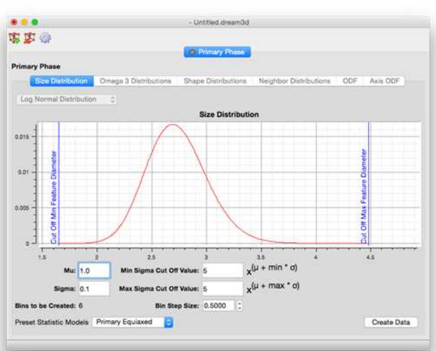


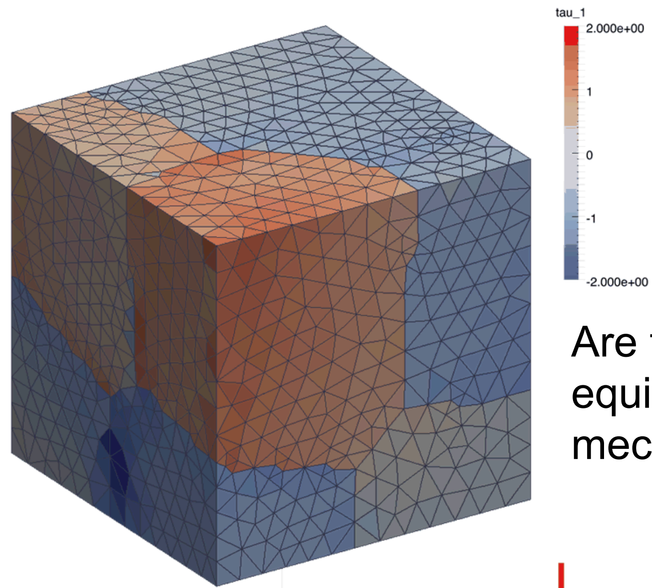
CUBIT
Input: finite element mesh (hexahedral)
Output: finite element mesh (e.g., tetrahedral)

Microstructural Parametrization

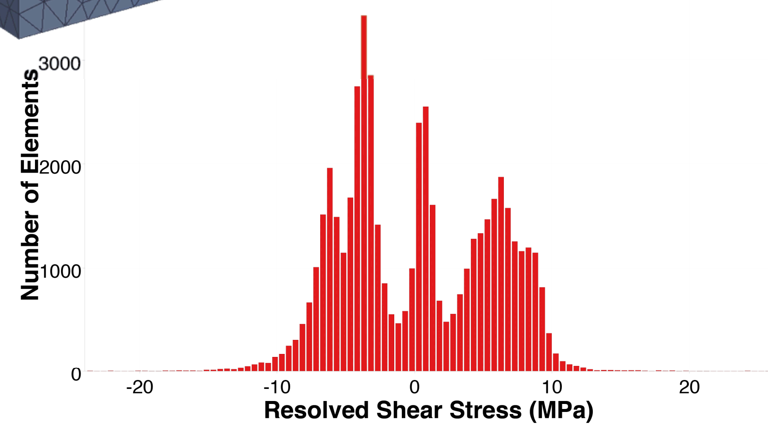


Microstructural realizations from a single set of underlying morphological statistics



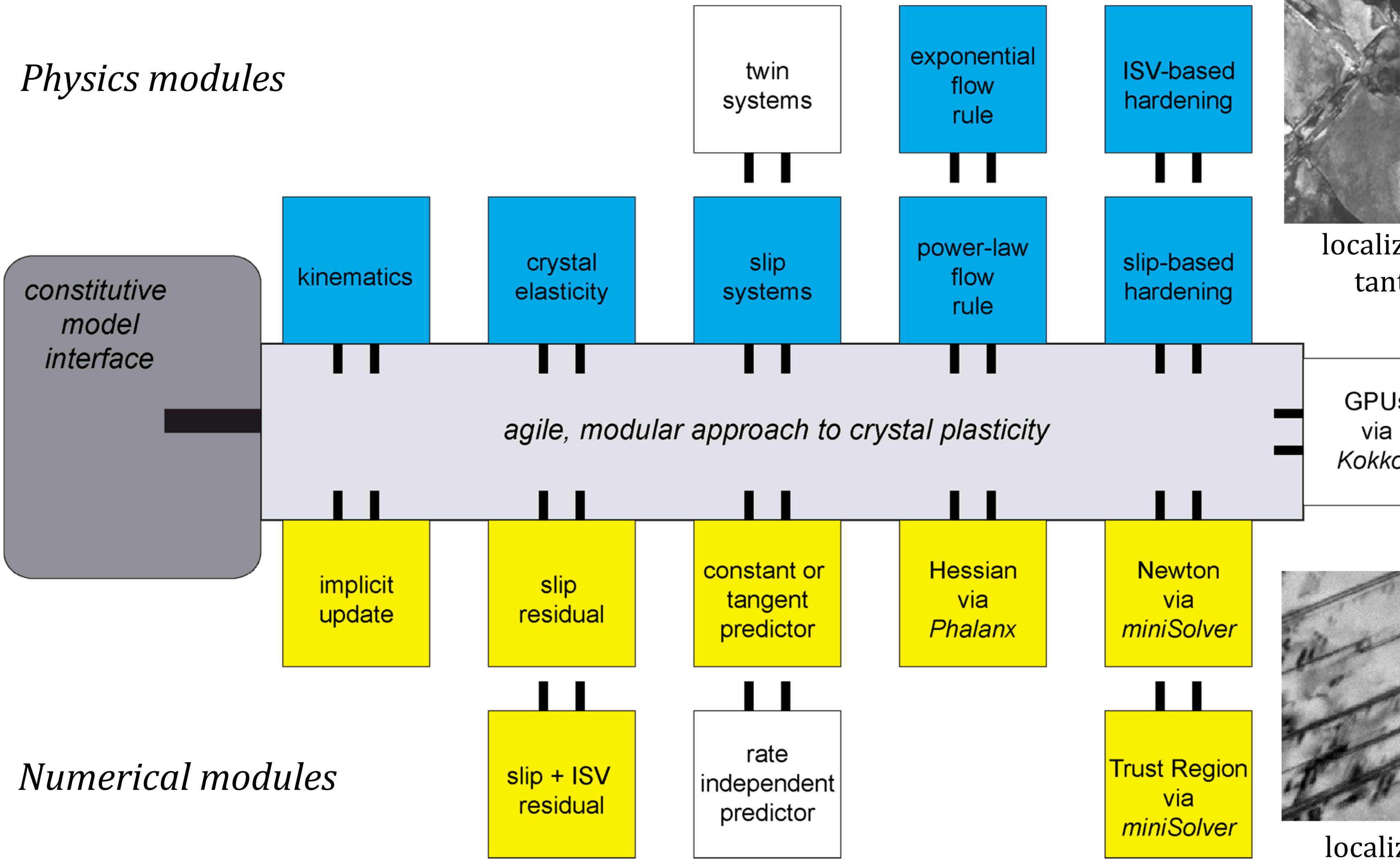


Are the realizations equivalent in terms of mechanical response?

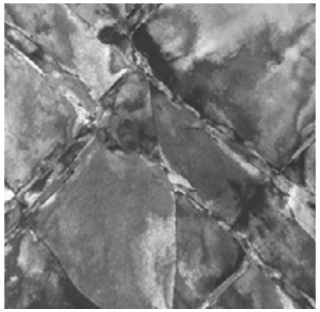


Agile components of crystal plasticity

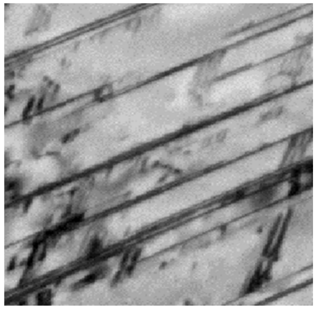
Physics modules



Numerical modules



localization in tantalum

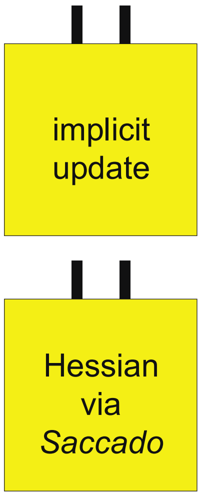


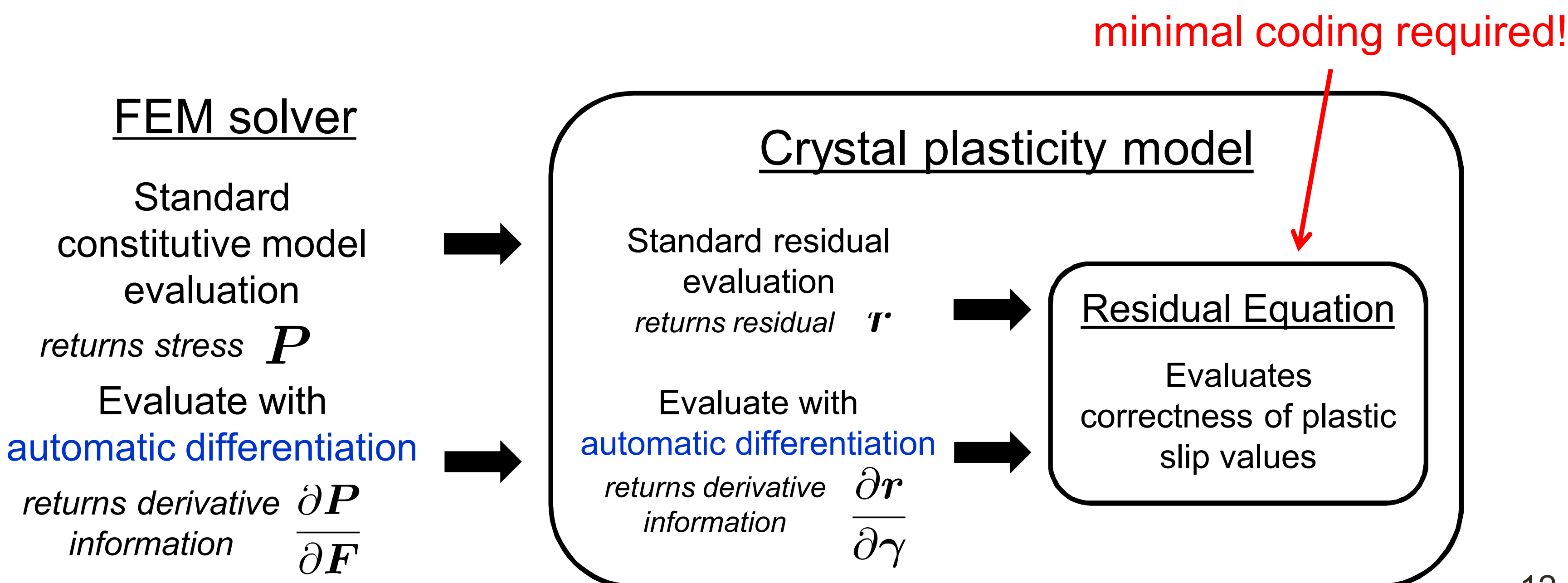
localization in stainless steel

Multiple methods facilitate learning and lower the barrier for new advances.

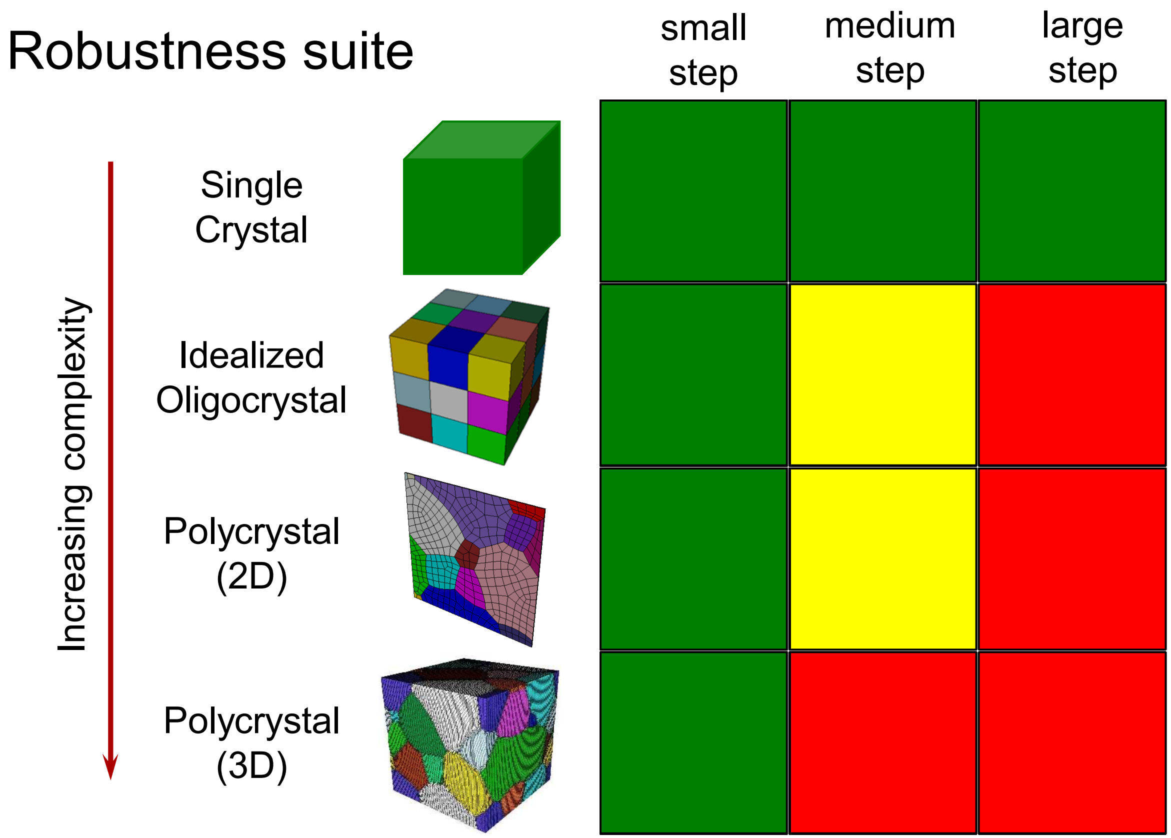
Automatic differentiation enables modularity

- *Goal*: Allow users to mix and match crystal plasticity features
  - Crystal structure, flow rule, hardening law, etc.
- *Challenge*: Altering the crystal plasticity equations requires difficult changes to the model's state update routine (implicit update)
- *Strategy*: Automatic differentiation using the *Sacado* package dramatically reduces the required changes to material model





Measuring Robustness Through Application



Automated evaluation of model performance for various problems of interest

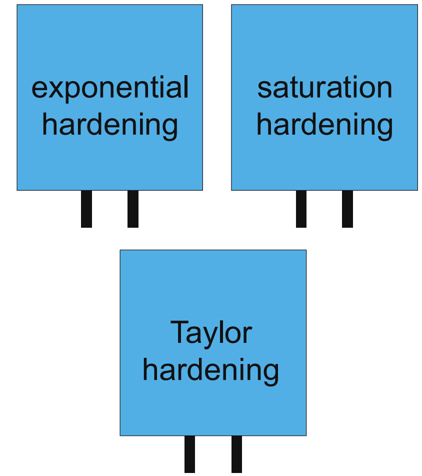
- Usability – Code users less burdened with implementation details
- Confidence – Verified solutions within realistic problem space

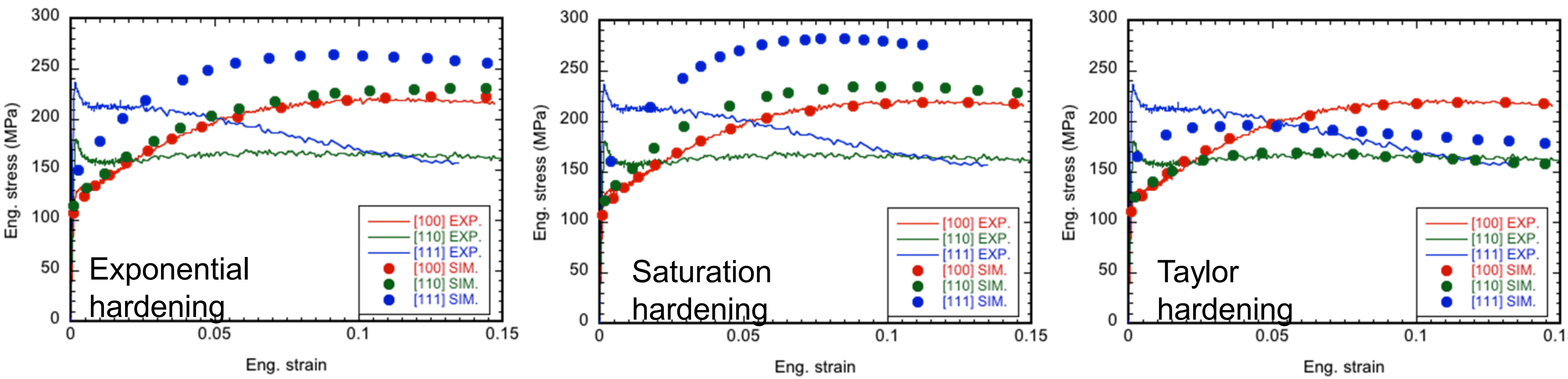
Predictions in single crystal Ta

Exponential hardening $g^\alpha = H_0 + \frac{H_1}{H_2}\left(1 - \exp(-H_2 \varepsilon^\alpha)\right)$

Saturation hardening $\dot{g}^\alpha = \dot{g}_0 \left(\frac{g_s - g^\alpha}{g_s - g_0}\right) \sum_\beta 2 \left|\mathrm{S}^\alpha_{ij}\mathrm{S}^\beta_{ij}\right| \left|\dot{\gamma}^\beta\right| \qquad g_s = g_{s_0} \left|\frac{\dot{\gamma}}{\dot{\gamma}_0}\right|^\omega$

Taylor hardening
(dislocation density) $g^\alpha = A\mu b \sqrt{\sum_{\beta=1}^{24} \mathbf{H}^{\alpha\beta}\rho^\beta} \qquad \dot{\rho}^\alpha = \left(\kappa_1 \sqrt{\sum_{\beta=1}^{\mathrm{NS}} \rho^\beta} - \kappa_2 \rho^\alpha\right) \cdot \left|\dot{\gamma}^\alpha\right|$





- Increment physics through an array of hardening models in crystal plasticity framework
  - Parameterize through BCC Ta single crystal experiments in [100] orientation
  - Predict response in [110] and [111] orientations.
- *Dislocation density based Taylor hardening model* most accurately reflects anisotropy.

Role of Boundary Representation

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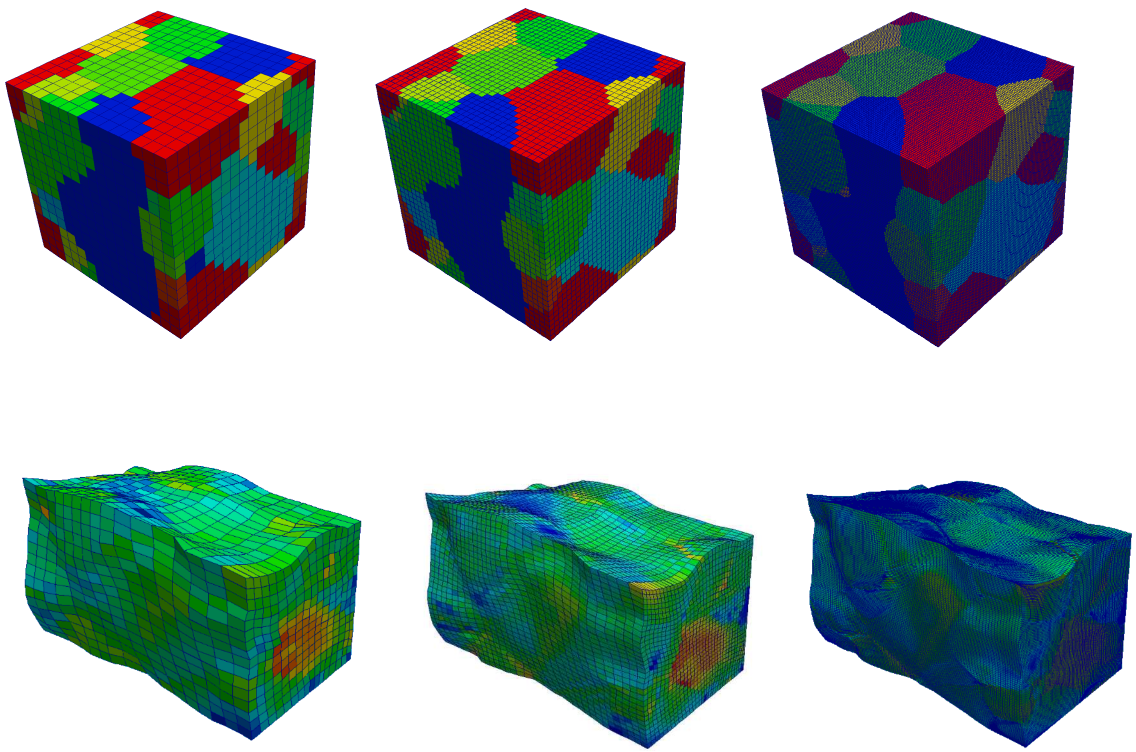
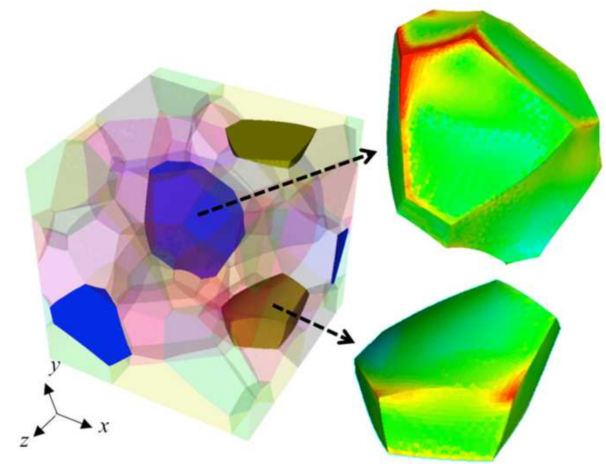
3D polycrystal with 30 grains generate through phase-field modeling. Voxelated grain boundaries.

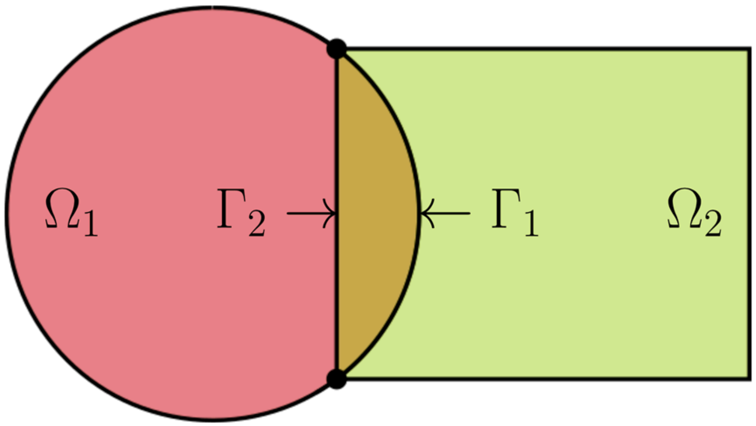


Phase-field microstructures



Conformal boundaries w/ focus on higher-order tets

Schwarz Alternating Method for Multiscale Coupling in Quasistatics



Concept of solution scheme

- Solve PDE by any method on Ω_1 using an initial guess for Dirichlet BCs on Γ_1.
- Solve PDE by any method (can be different than for Ω_1) on Ω_2 using Dirichlet BCs on Γ_2 that are the values just obtained for Ω_1.
- Solve PDE using Dirichlet BCs on G_1 that are the values just obtained for Ω_2.

- Mathematical proof of convergence for solid mechanics problem
- Allows coupling of nonconforming domains with different element types and levels of refinement
- Information is exchanged concurrently among two or more subdomains
- Different solvers can be used for each subdomain
- Different material models can be coupled provided that they are compatible

Convergence: Overlap and Refinement

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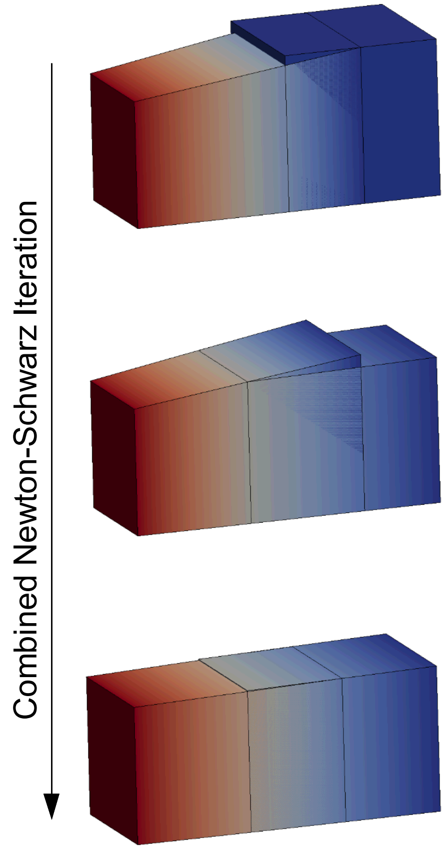
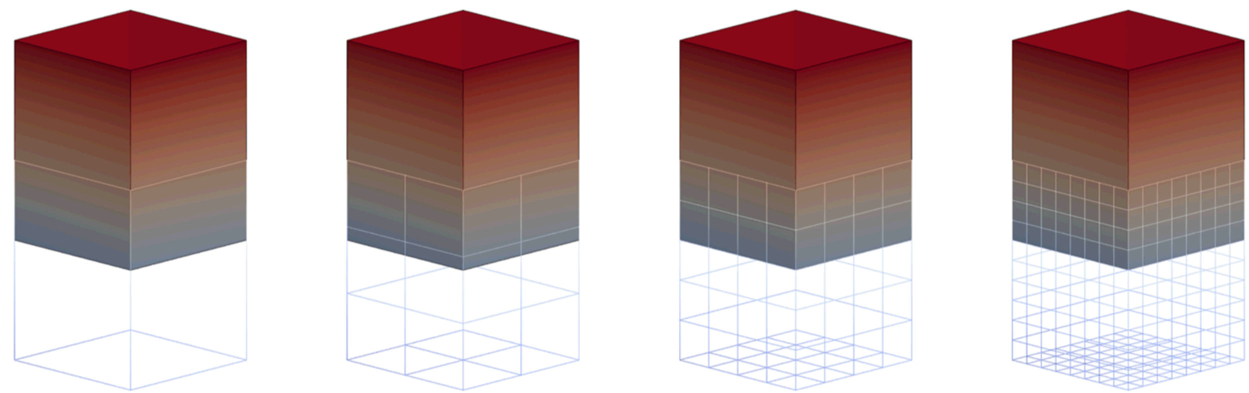
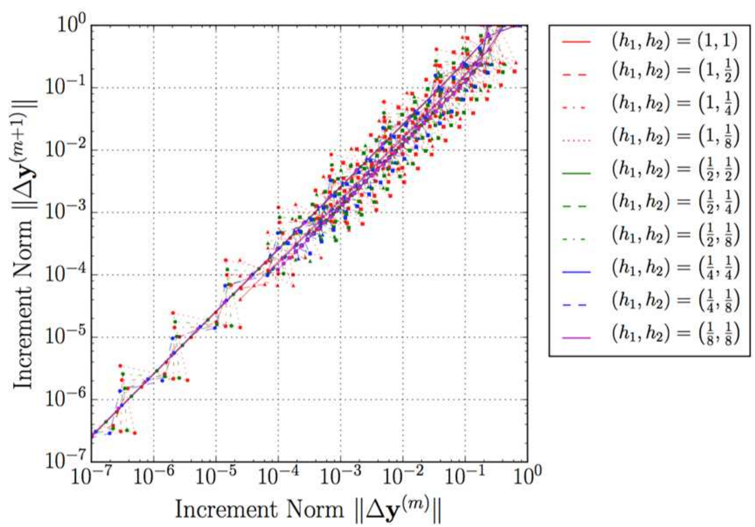
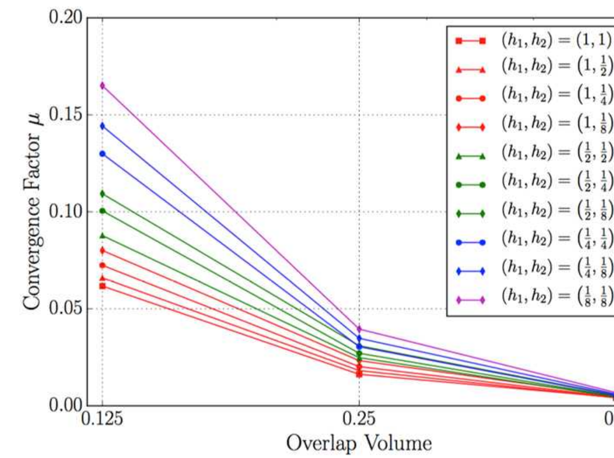






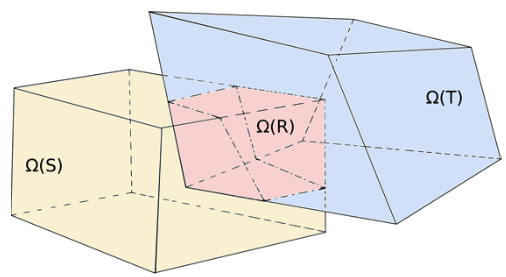


Schwarz Alternating Method in Albany

- Schwarz method implemented in Sandia's open-source Albany code within the LCM project.
- Use of components in code design for rapid development of capabilities.
- Extensive use of libraries from the open-source TRILINOS project.
  - PHALANX package to decompose complex problem into simpler problems with managed dependencies.
  - SACADO package for automatic differentiation. The stiffness is neither derived nor implemented explicitly.
  - TEKO package for block preconditioning.
- Parallel implementation uses the Data Transfer Kit (DTK).
- All software available on GitHub.

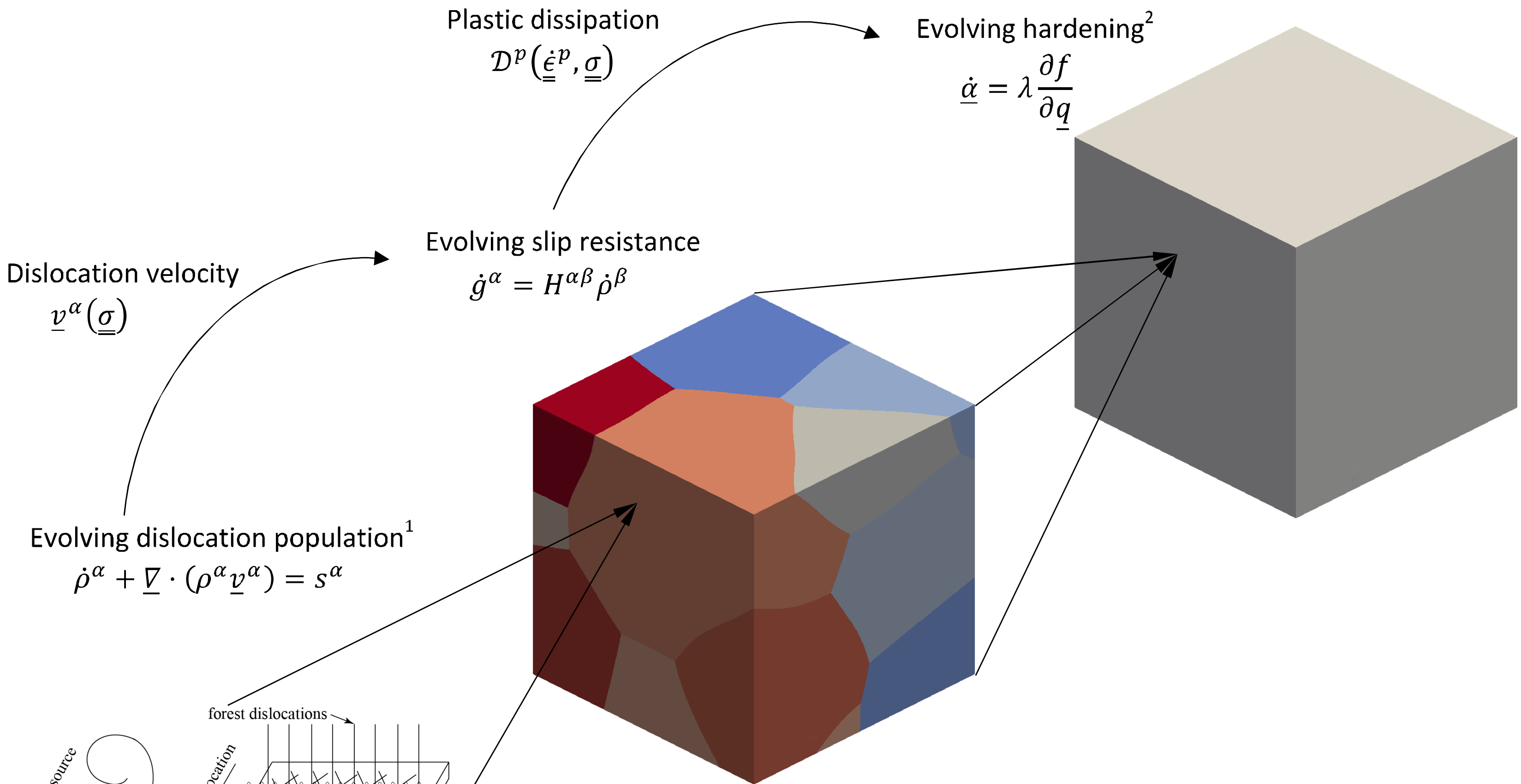
https://github.com/trilinos/trilinos

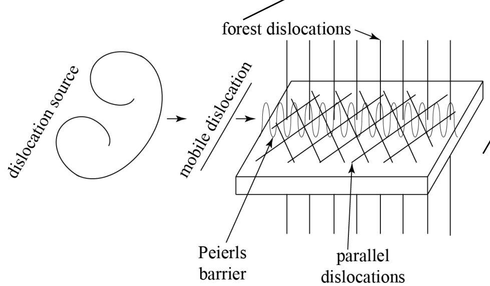
https://github.com/gahansen/Albany



https://github.com/ORNL-CEES/DataTransferKit

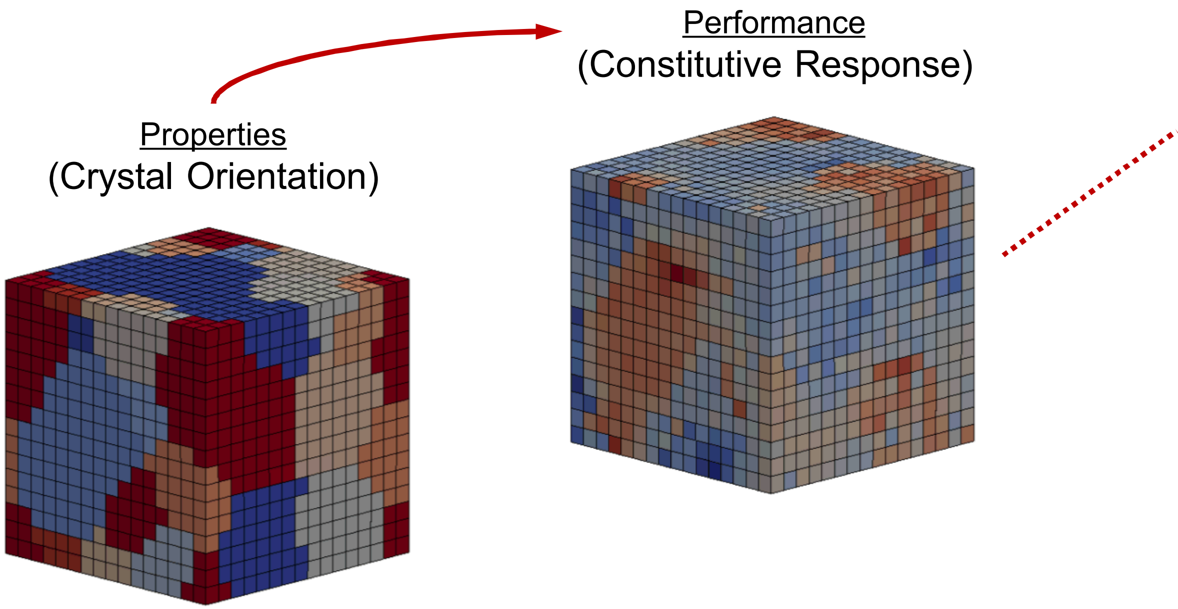
Meso-Continuum Scale Hierarchy

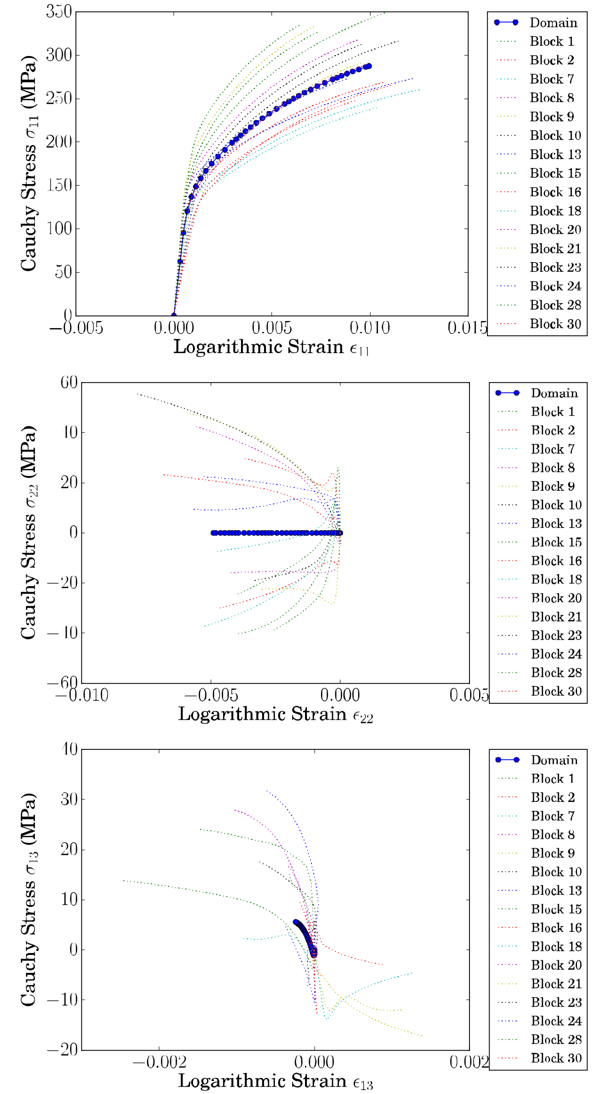




[1]D.J. Luscher, et. al., Int. J. Plasticity, 76, 2016, 111-129.
[2]J.C. Simo and T.J.R. Hughes, Computational Inelasticity, 1998.

Microstructurally-Derived Constitutive Response





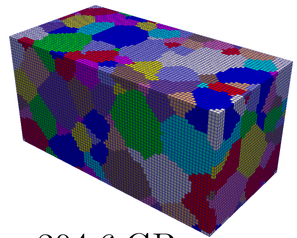
Predicting performance from measured properties requires:

- Characterization of properties
  - Develop microstructure metrics beyond average grain size
- Characterization of response
  - Develop metrics for heterogeneity
    - No grain experiences uniaxial stress state, but domain-averaged response is nearly uniaxial
- Mapping from property metrics to response metrics
  - Develop framework to upscale microscale response

Ingredients of a Schwartz analysis

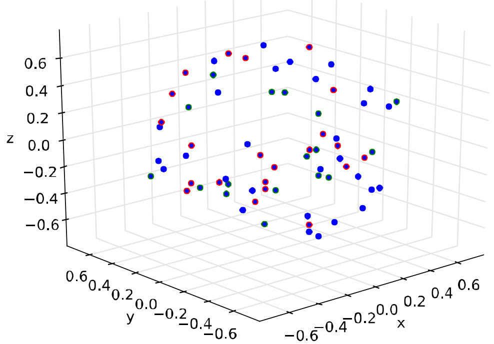
Mesoscale

voxelated microstructure derived from phase-field evolution (F. Abdeljawad)



$$\text{cubic elastic constant}: C_{11} = 204.6 \text{ GPa}$$
$$\text{cubic elastic constant}: C_{12} = 137.7 \text{ GPa}$$
$$\text{cubic elastic constant}: C_{44} = 126.2 \text{ GPa}$$
$$\text{reference shear rate}: \dot{\gamma}_0 = 1.0 \text{ 1/s}$$
$$\text{rate sensitivity factor}: m = 20$$
$$\text{hardening rate parameter}: \dot{g}_0 = 2.0 \times 10^4 \text{ 1/s}$$
$$\text{initial hardness}: g_0 = 90 \text{ MPa}$$
$$\text{saturation hardness}: g_s = 202 \text{ MPa}$$
$$\text{saturation exponent}: \omega = 0.01$$

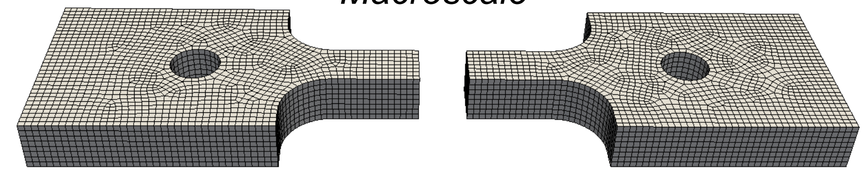
les



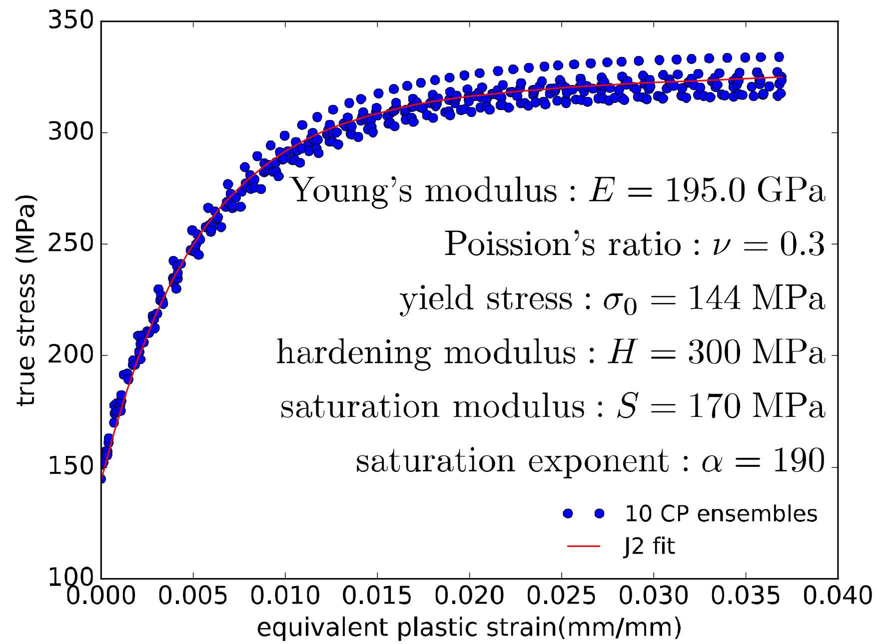
151 axial vectors from 3 of the 10 ensembles of random rotations (blue, green, red)

+

Macroscale

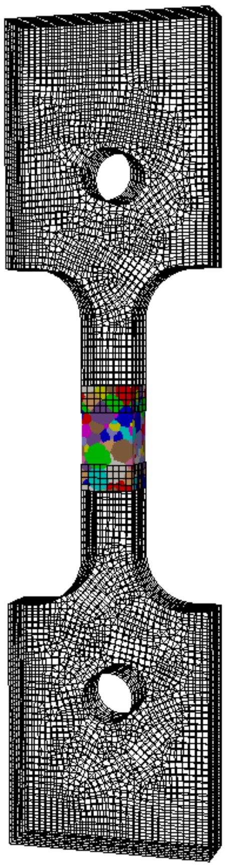


- Load microstructural ensembles in uniaxial stress
- Convert load/displacements to flow curves
- Fit flow curves with a macroscale J_2 plasticity model

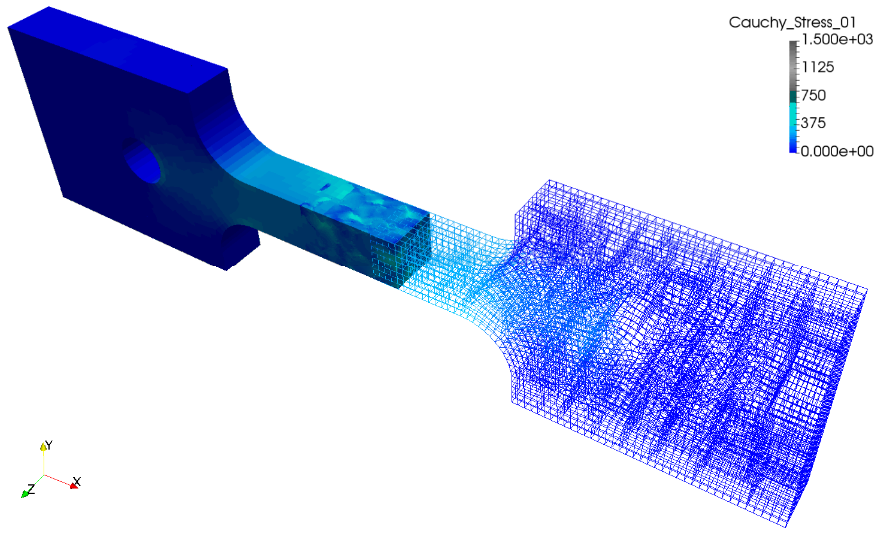


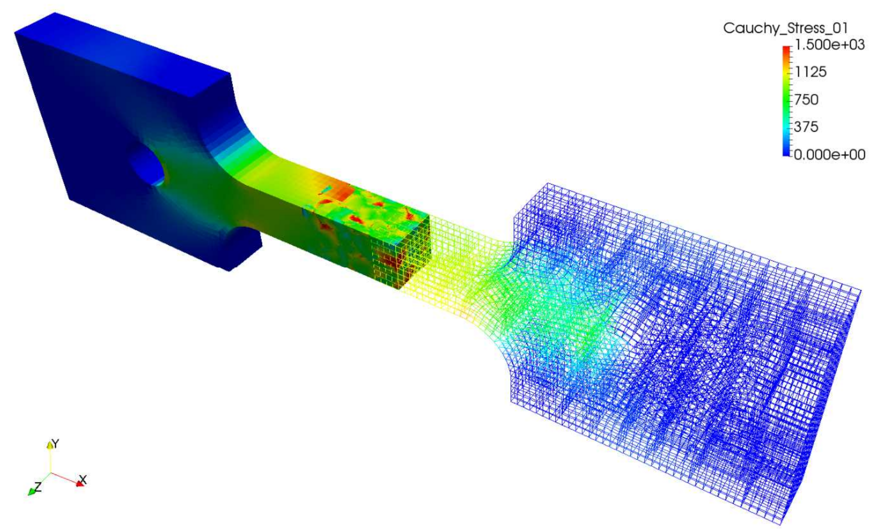
$$\sigma_y = \sigma_0 + H\epsilon_p + S(1 - e^{-\alpha \epsilon_p})$$

Coupling components to microstructure



Embed microstructure in ASTM tensile geometry



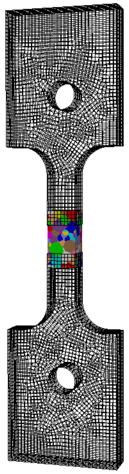


Key R&D Milestones for FY17

- *Strong multiphysics and concurrent multiscale*
  - Novel methods for multiphysics & multiscale coupling
  - Extend multiscale to dynamics
- *Microscale physics*
  - Develop/implement models for twinning
  - Develop/implement thermal/transport models for boundaries/twins
  - Publish developments in both physics and robustness
  - Develop/implement models that capture effects of hydrogen/temperature
- *New architectures*
  - Investigate/improve scalability of Kokkos in LCM
- *Applications*
  - Model discrete twins in stainless steel
  - Simulate the high-rate loading of tantalum
  - Couple microstructural scale to structural scale
  - Through ensembles of microstructures, investigate void nucleation

Progress and future work

- Develop a more fundamental understanding of localization in
  - Austenitic stainless steel structures exposed to hydrogen gas
  - Tantalum structures subjected to high rates of loading
- Discovery enabled through
  - Intimate connection between structure and microstructure (Schwarz)
  - Strong multiphysics capable of capturing autocatalytic processes
  - Systematically increasing microstructural physics
  - Robust solution methods for increasing complexity
  - Extension to next generation platforms



Part of a top down strategy (macro to micro) to provide context, identify disconnects, and provide drivers.