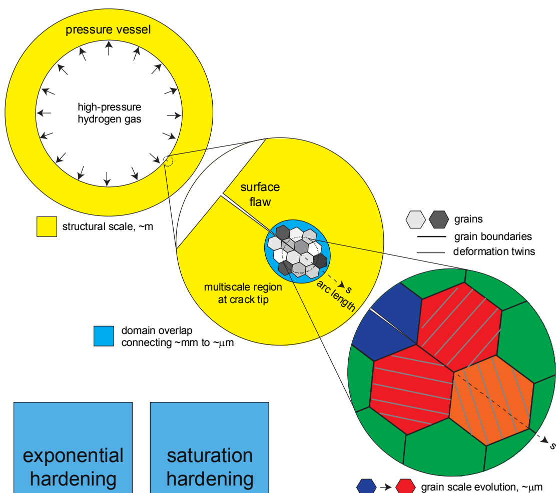
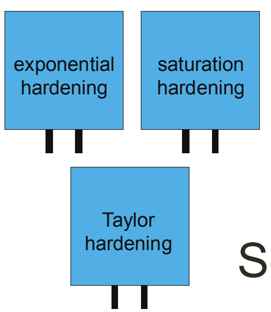
SAND2016-10116C

Concurrent multiscale modeling of microstructural effects on localization behavior in finite deformation solid mechanics





James Foulk
Coleman Alleman
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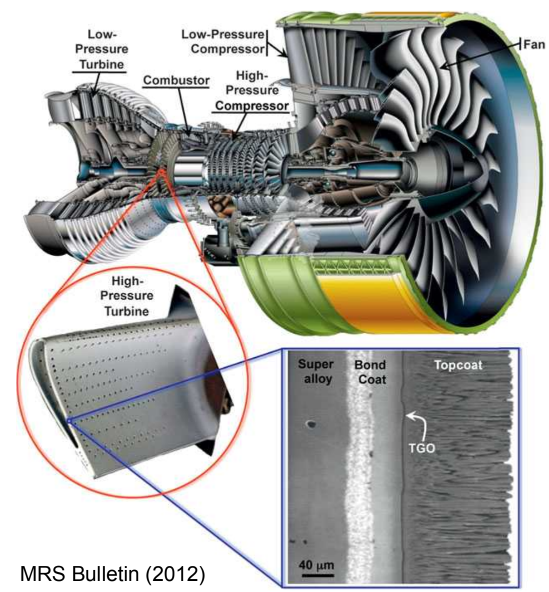

Collaborators: Irina Tezaur, Jake Ostien

MRS Bulletin (2012)

Society of Engineering Science 53rd Annual Technical Meeting

October 4, 2016

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT

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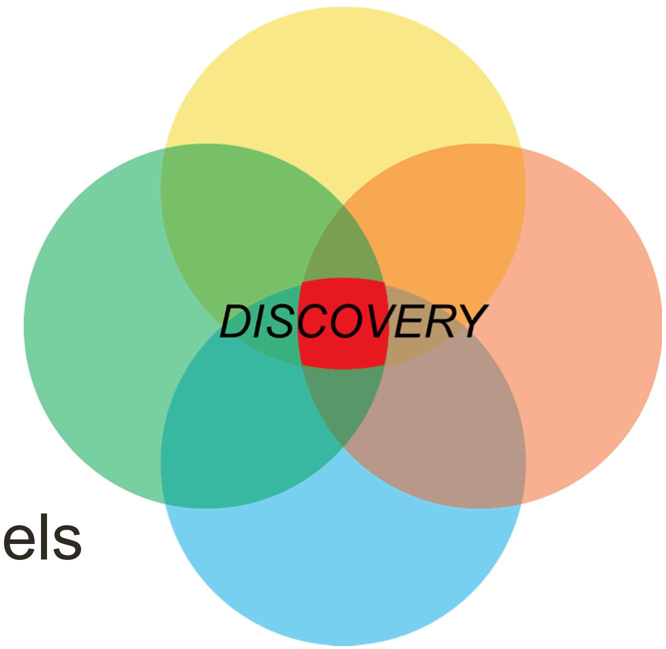
Sandia National Laboratories

Overview

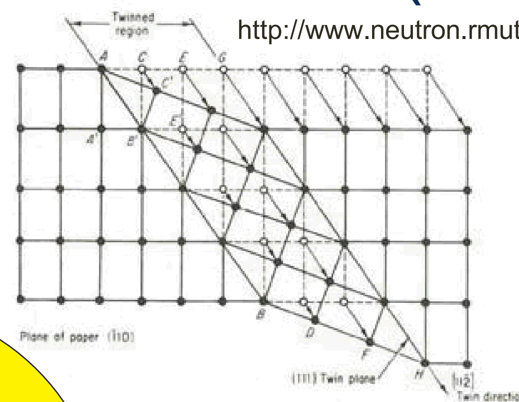
Developing strong, concurrent, multiphysics, multiscale coupling to understand the impact of microstructural mechanisms on the structural scale

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

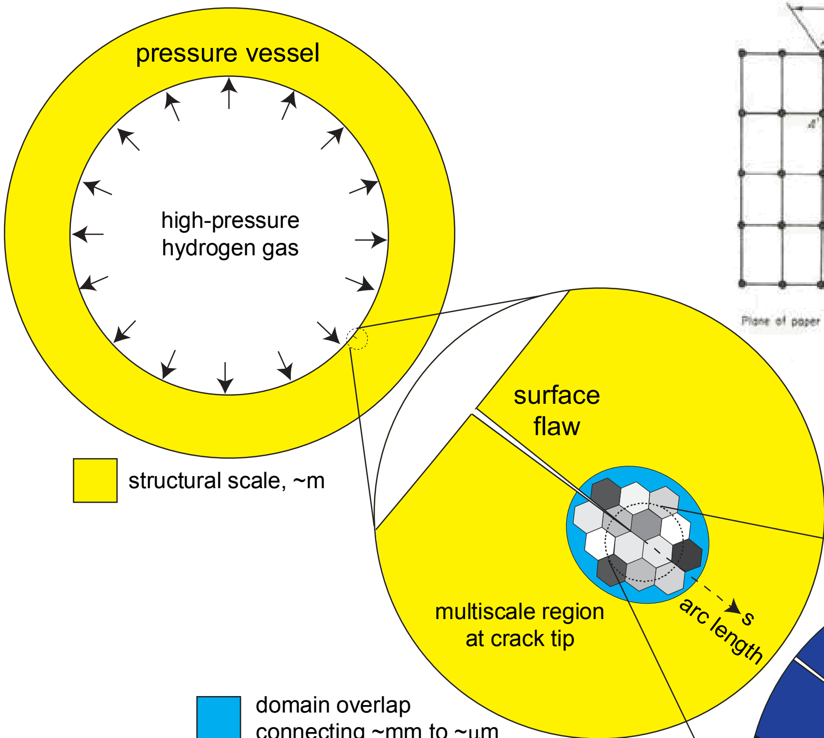


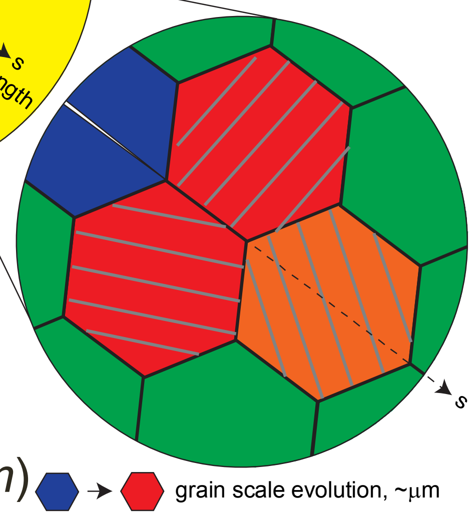
Goal: Predict void nucleation at the microscale

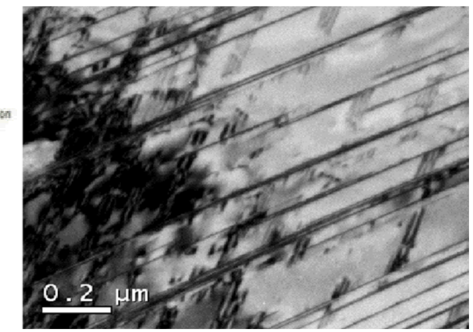
Hydrogen activates microstructure (stainless steel)



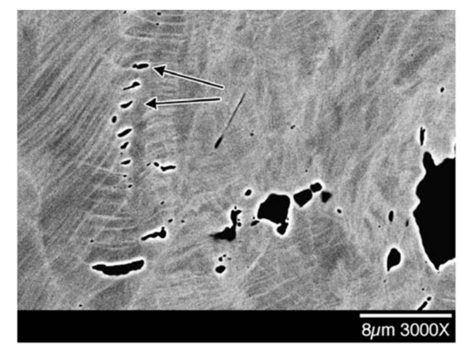
http://www.neutron.rmutphysics.com







extensive slip and deformation twinning



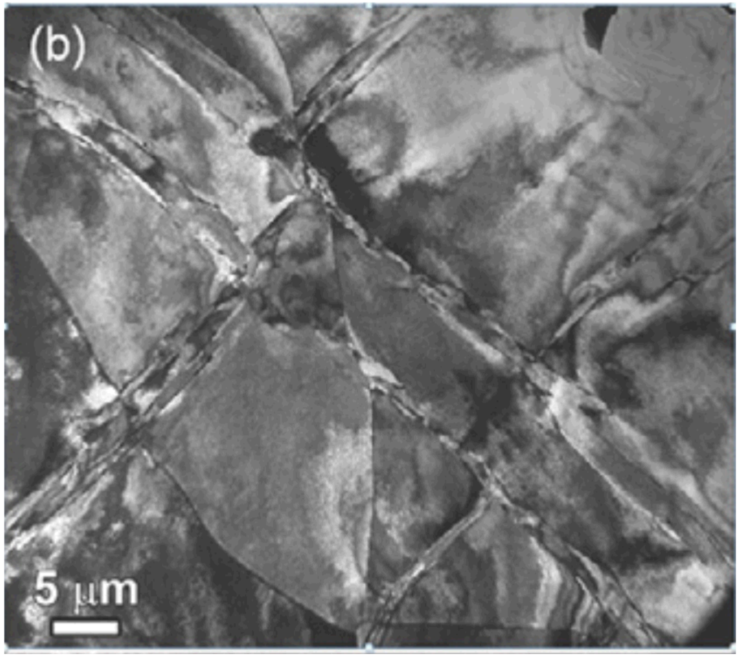
premature void nucleation*

Hydrogen *activates* microstructure

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

*Nibur, Somerday, Balch, San Marchi, The role of localized deformation in hydrogen-assisted crack propagation in 21Cr–6Ni–9Mn stainless steel, Acta Materialia, 2009.

Temperature/strain-rate activates microstructure (Ta)



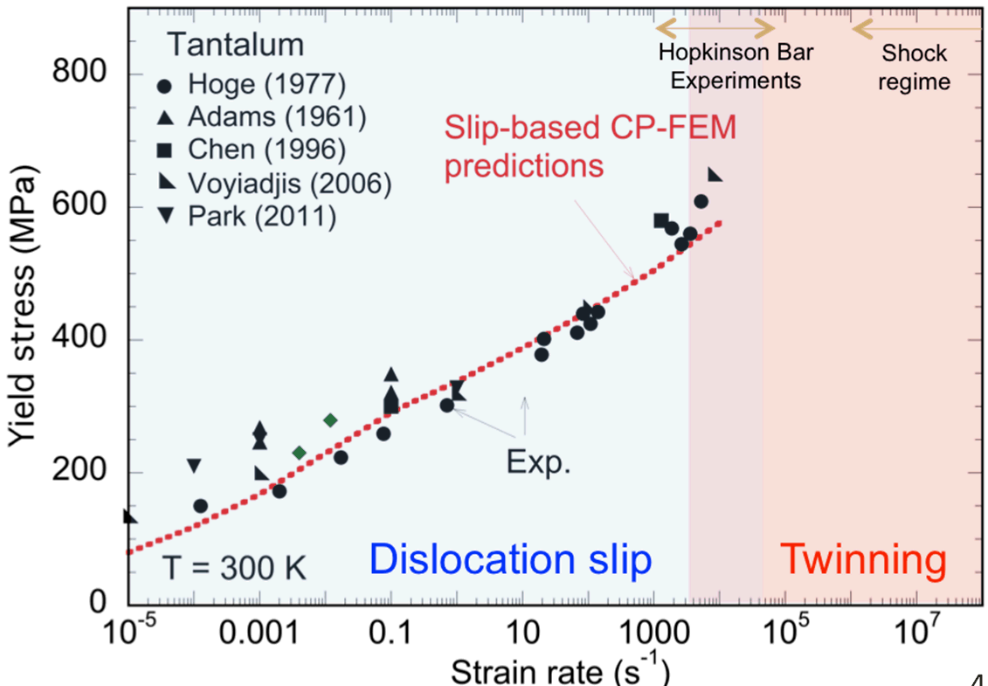
TEM micrograph of deformation twins in Ta[1] (T=77 K and $\dot{\varepsilon}$ =2.2x10^4 s^{-1}).

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*

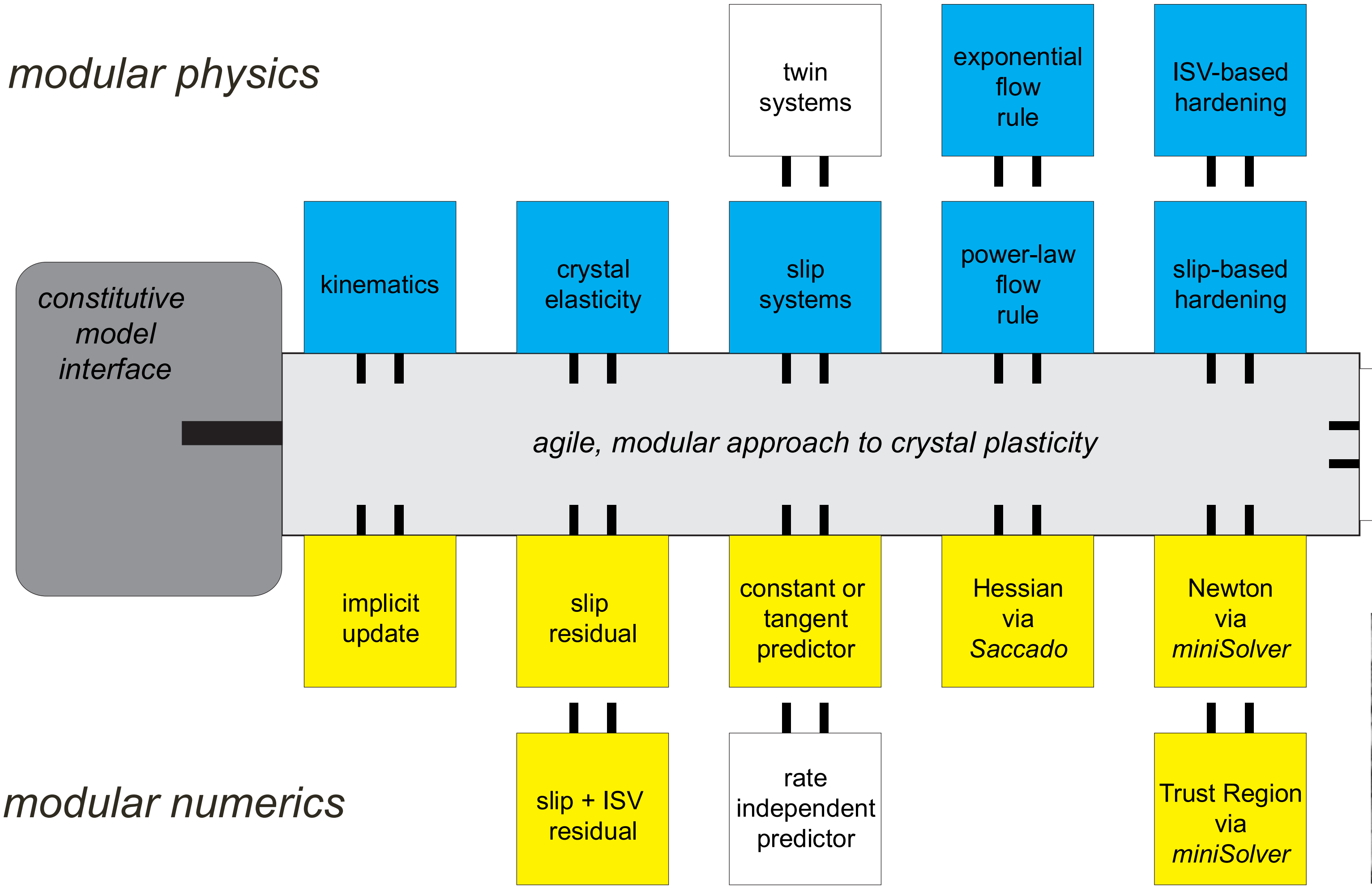
- Extensive slip within grains
- Twins evolve within steep gradients



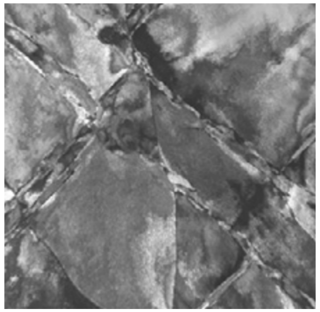
[1]Chen, C. Q., Hu, G., Florando, J. N., Kumar, M., Hemker, K. J., Ramesh, K. T., Interplay of dislocation slip and deformation twinning in tantalum at high strain rates, *Scripta Materialia* 69 (2013) 709 – 712.

Agile components of crystal plasticity

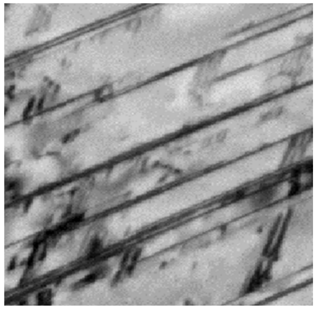
modular physics



modular numerics



localization in tantalum



localization in stainless steel

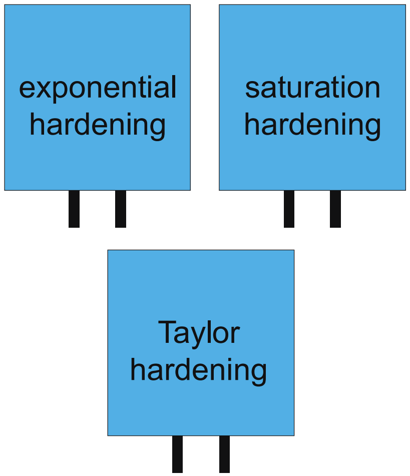
Multiple methods facilitate learning and lower the barrier for new advances.

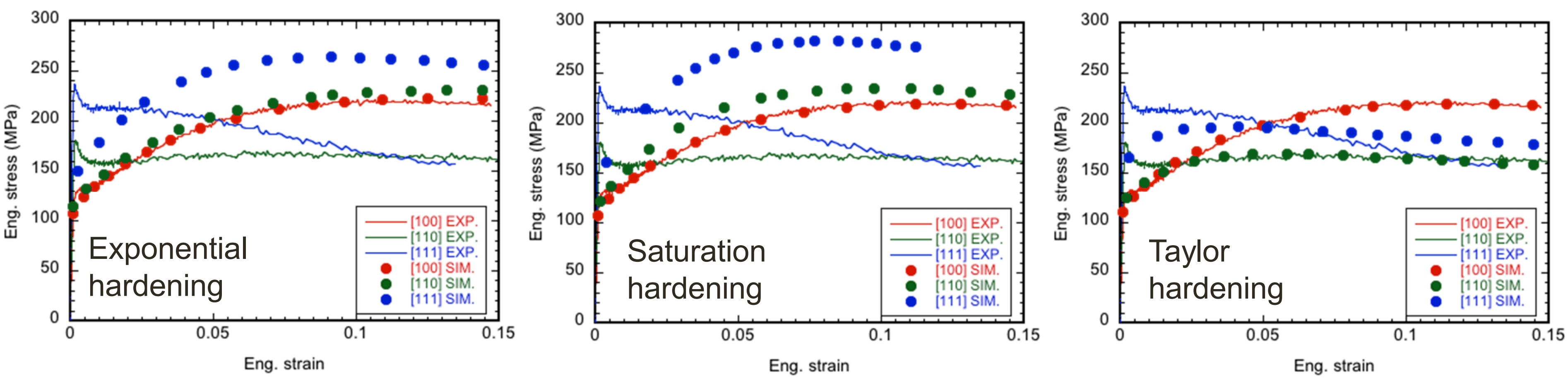
Predictions in single crystal Ta with physics++

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

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

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





- 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.

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

implicit update

Hessian via *Saccado*

minimal coding required!

FEM solver

Standard constitutive model evaluation

returns stress $\boldsymbol{P}$

Evaluate with automatic differentiation

returns derivative information $\dfrac{\partial \boldsymbol{P}}{\partial \boldsymbol{F}}$

Crystal plasticity model

Standard residual evaluation

returns residual $\boldsymbol{r}$

Evaluate with automatic differentiation

returns derivative information $\dfrac{\partial \boldsymbol{r}}{\partial \gamma}$

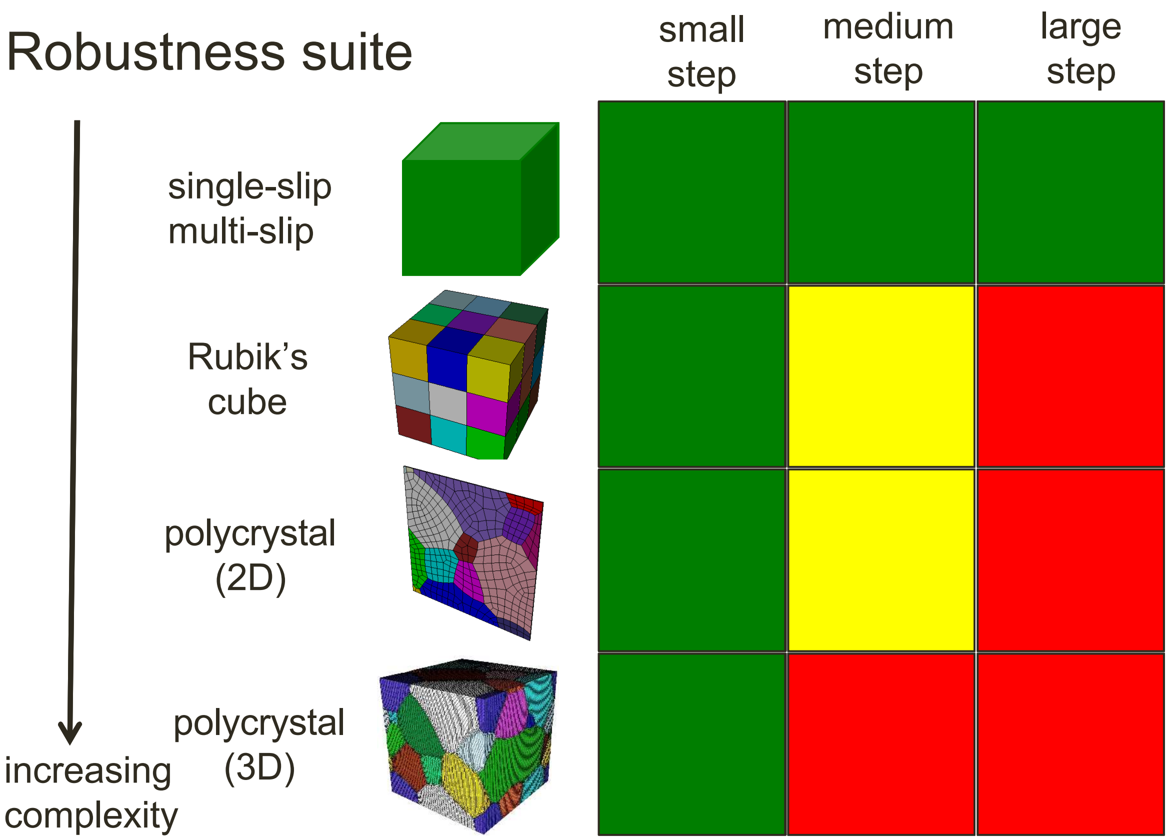
Residual Equation

Evaluates correctness of plastic slip values

Lessons learned: Powerful but requires idealized BVPs (single slip) to permit verification.

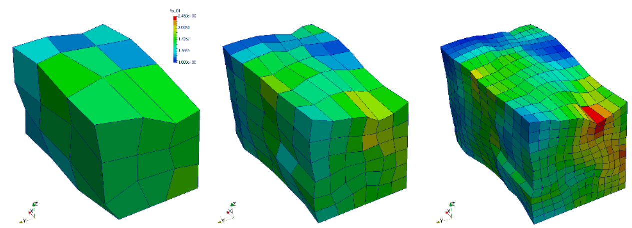
Measuring robustness through application

Robustness suite



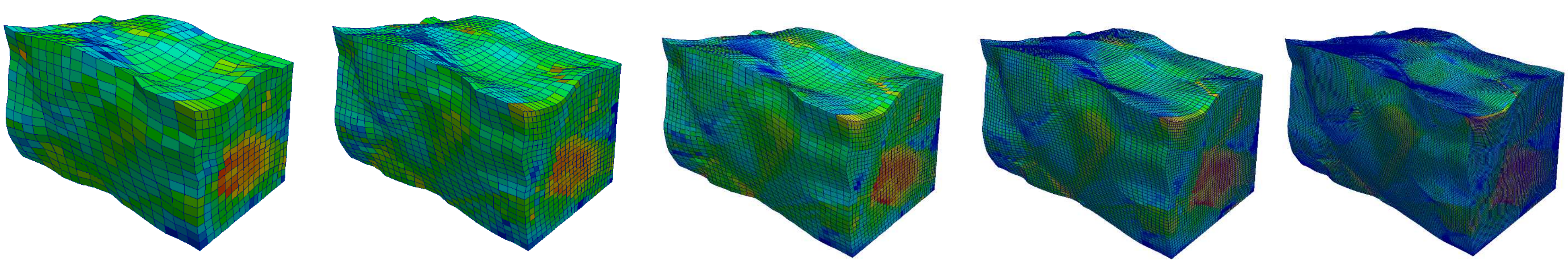
Rubik's cube case

- Random texture
- 100% engr. strain
- Vary elements/grain
- Vary step size
- Vary solution methods



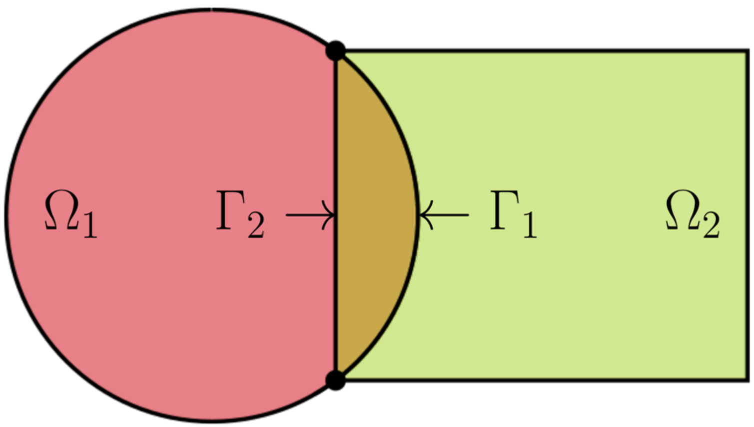
Sample microstructures with

- Voxelated grain boundaries
- Conformal grain boundaries



871 steps | 929 steps | 1062 steps | 1170 steps | 1545 steps

Update on the Schwarz alternating method



Hermann Schwarz (1870)

Initial conditions for Partial Differential Equation (PDE)

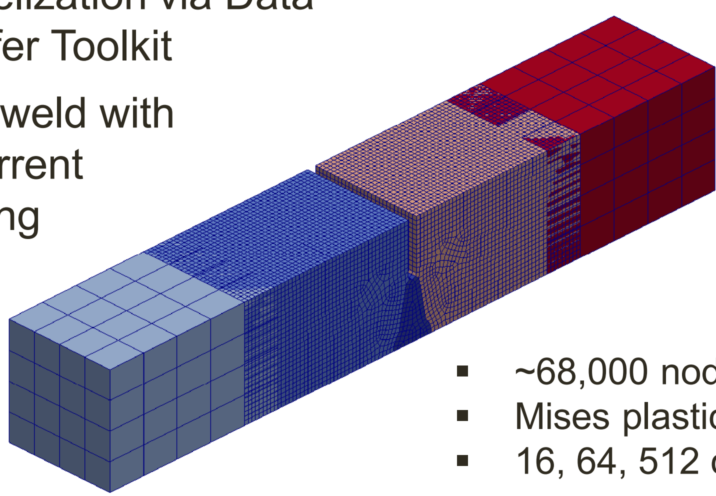
- Solve PDE by any method on Ω_1 using an initial guess for Dirichlet BCs on Γ_1.

Iterate

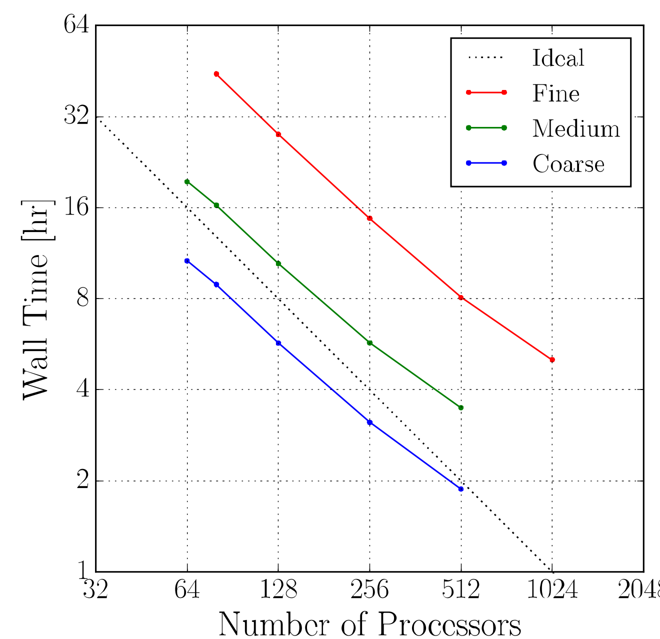
- Solve PDE by any method on Ω_2 using Dirichlet BCs on Γ_2 that are the values just obtained for Ω_1.
- Solve PDE by any method on Ω_1 using Dirichlet BCs on Γ_1 that are the values just obtained for Ω_2.0

Parallelization via Data Transfer Toolkit

Laser weld with concurrent coupling



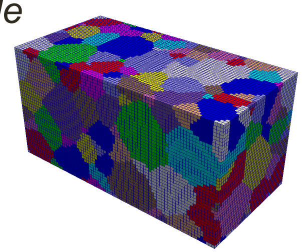
- ~68,000 nodes
- Mises plasticity
- 16, 64, 512 cores



Ingredients of a Schwartz analysis

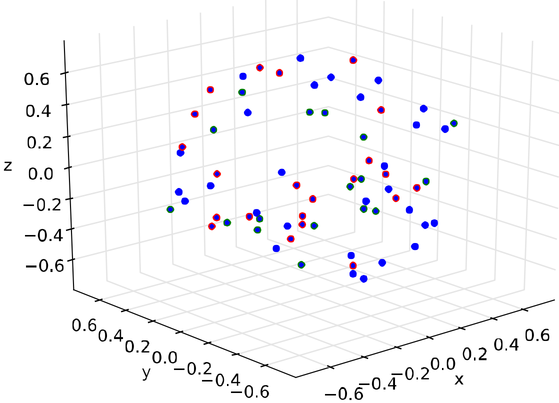
1 part mesoscale

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



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

s

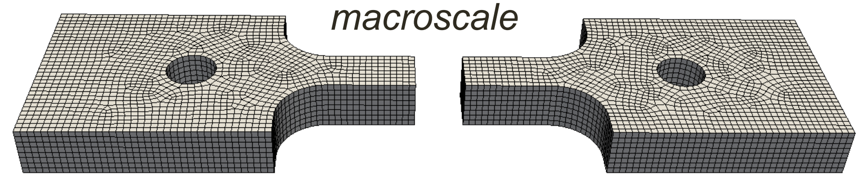


151 axial vectors from 3 of the 10 ensembles of random rotations (blue, green, red)

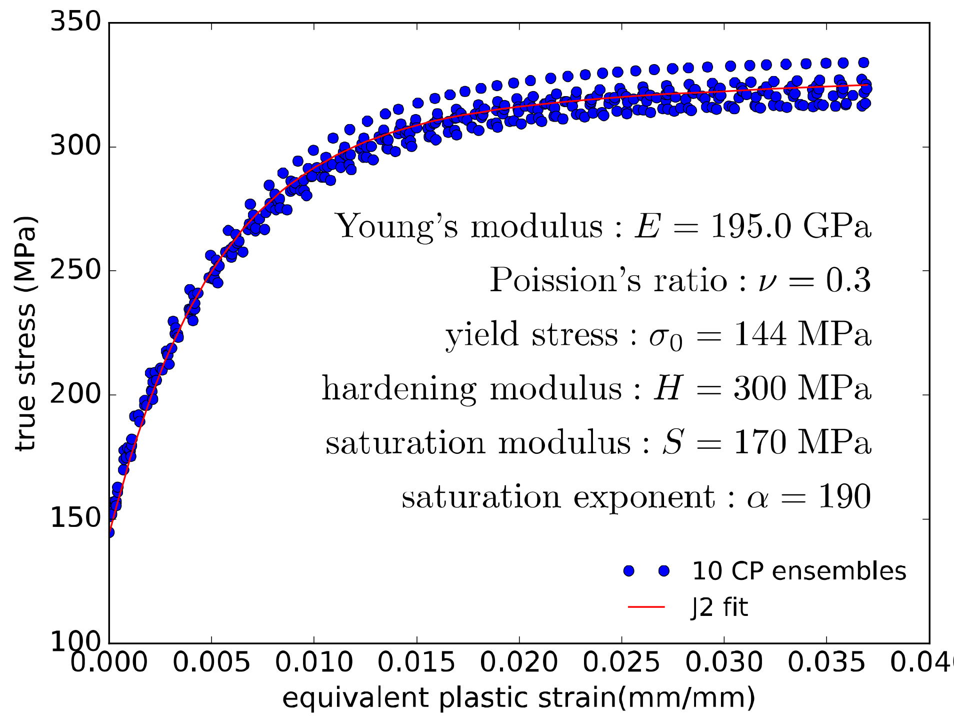
Point of collaboration with Multiscale Reliability LDRD

+

2 parts macroscale

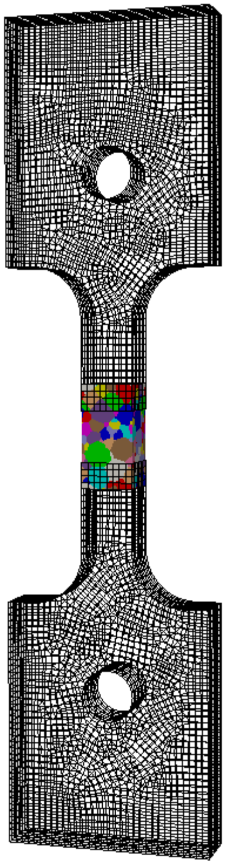


- Load microstructural ensembles in uniaxial stress
- Convert load/displacements to flow curves
- Fit flow curves with a macroscale J_2 plasticity model

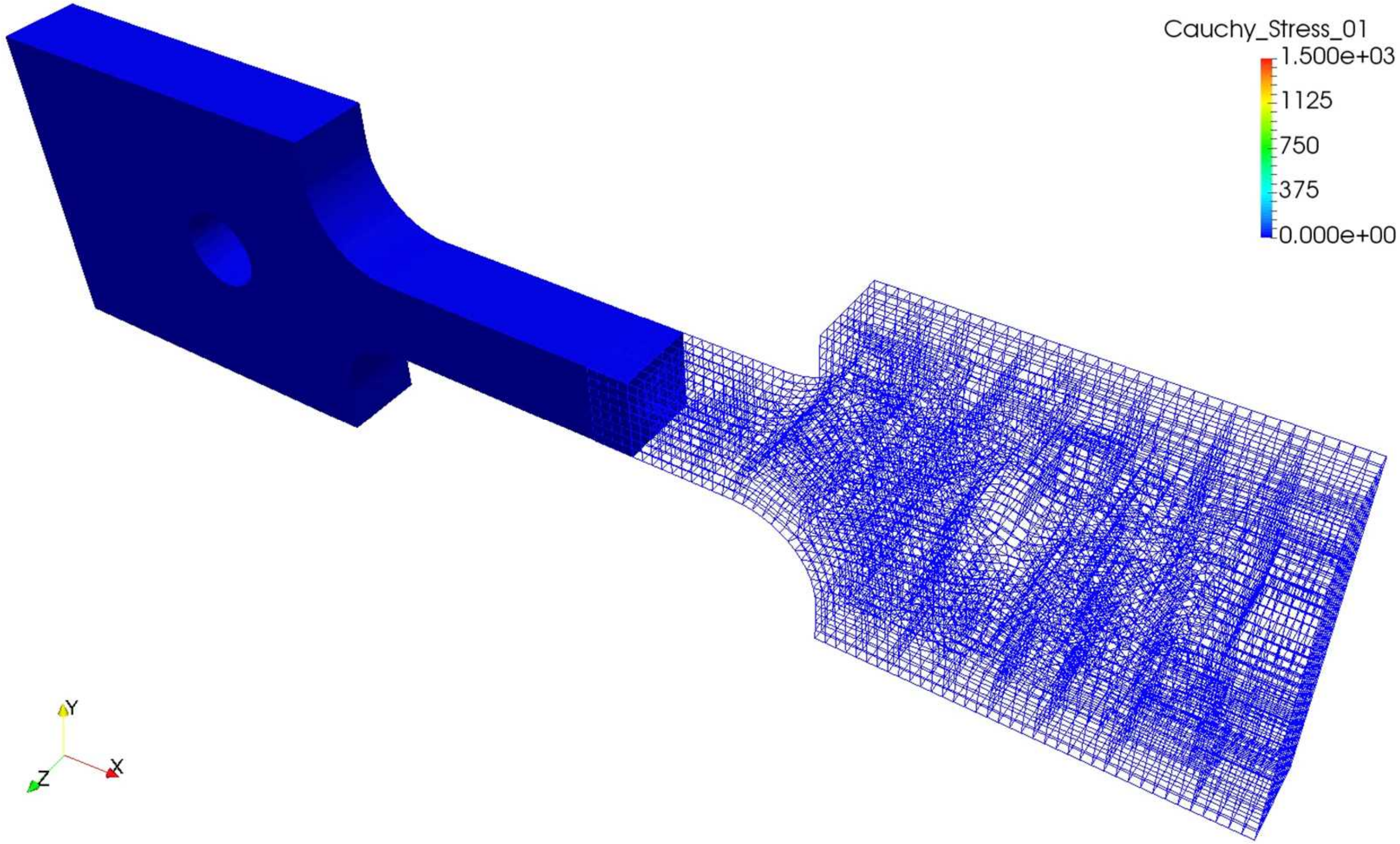


$$\sigma_y = \sigma_0 + H\epsilon_p + S(1 - e^{-\alpha\epsilon_p})$$

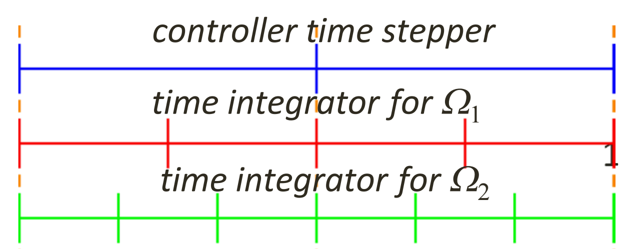
Coupling components to microstructure



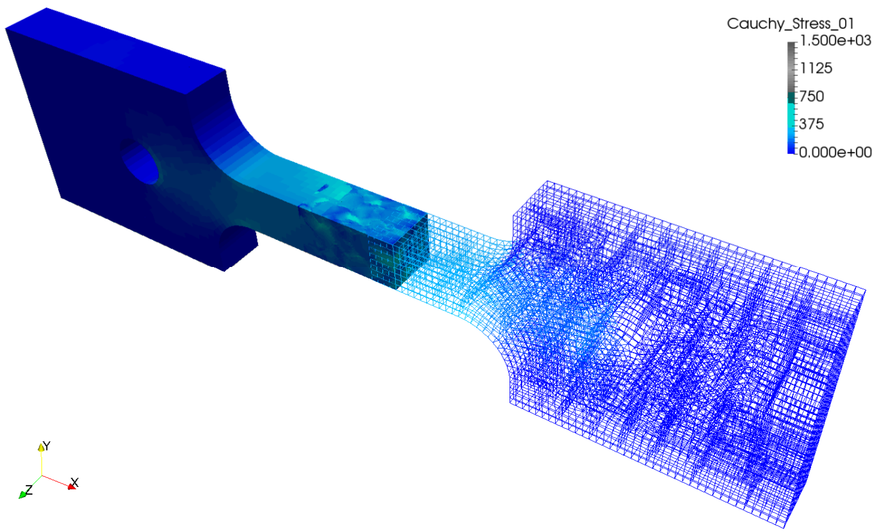
Embed microstructure in ASTM tensile geometry

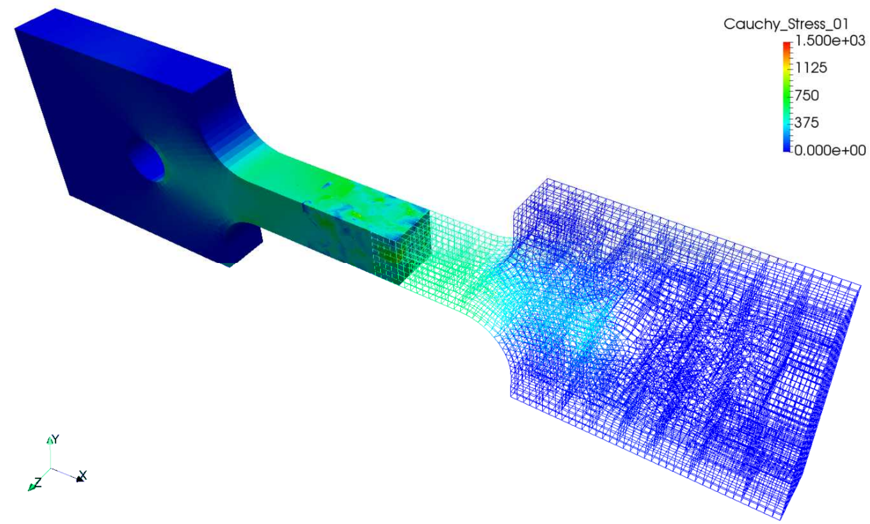


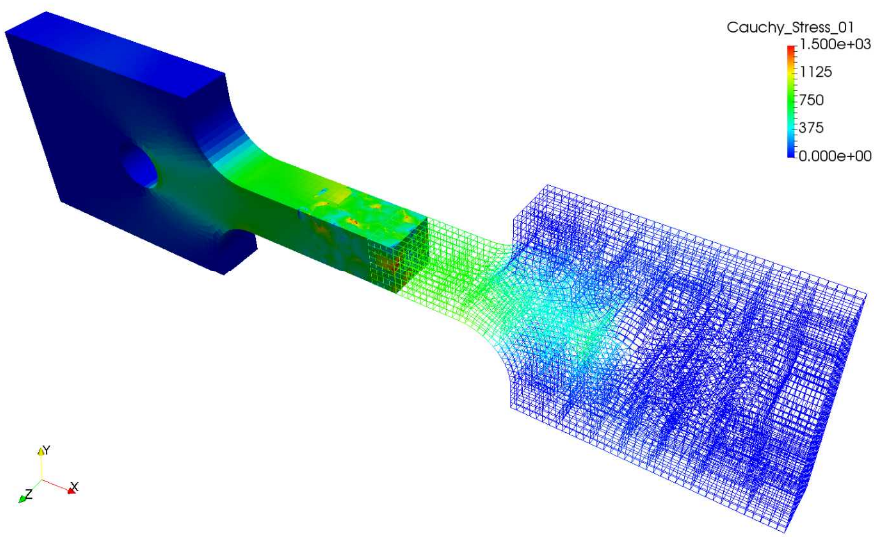
- Currently extending Schwarz coupling to dynamics
- Extending approach to multiphysics

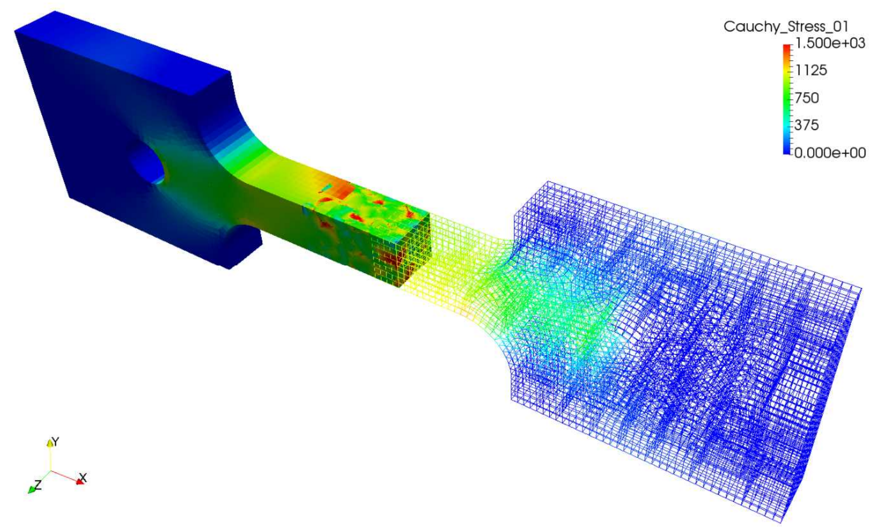


Coupling components to microstructure









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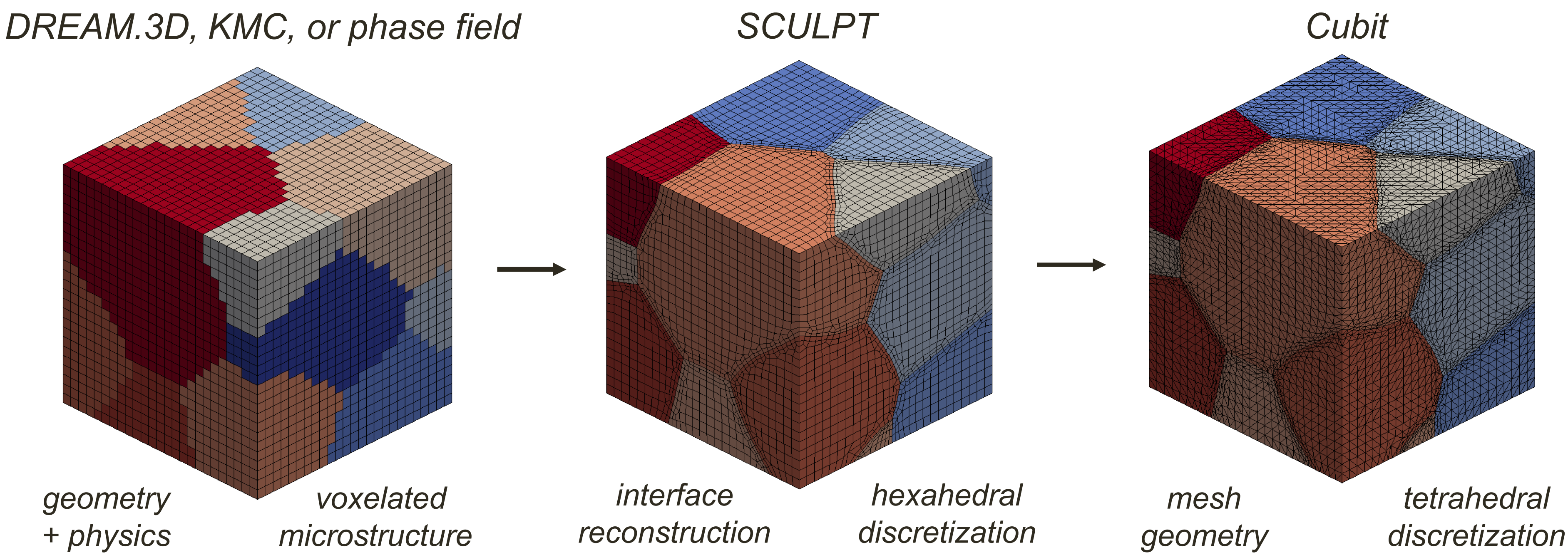
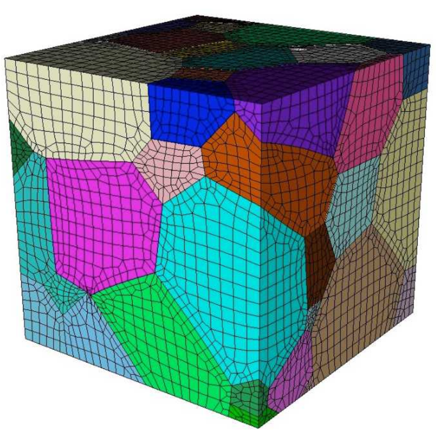
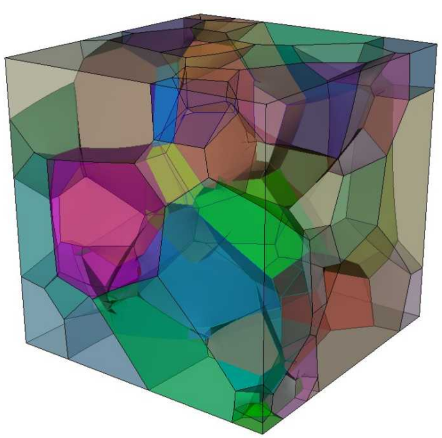
SCULPT, conformal boundaries, tet meshing

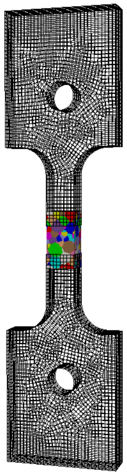


- SCULPT powerful tool for microstructure
- Performs interface reconstruction & meshing
- All-hex meshes can be problematic
- Mesh refinement requisite for solution
- Move from reconstruction to geometry
- Export STL or // tet mesh in SCULPT
- Leverage new surface & volume tet meshers

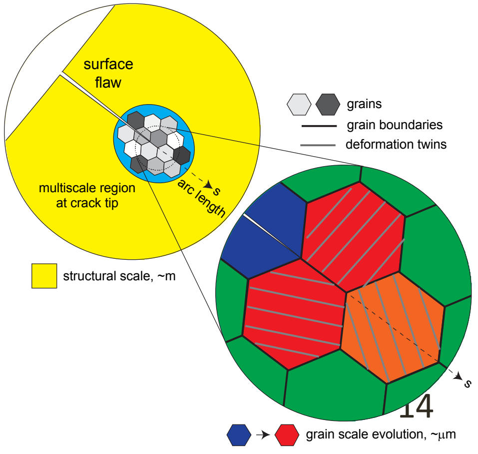

hexes problematic


geometry for tets

Filling gaps and overcoming barriers



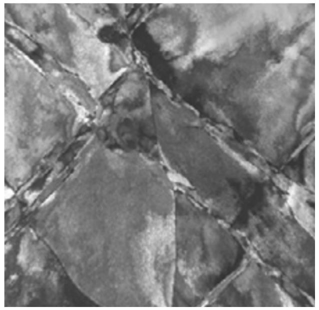
- Develop a more fundamental understanding of localization in
  - Austenitic stainless steel structures exposed to hydrogen gas
  - Tantalum structures subjected to high rates of loading
- Discovery enabled through
  - Intimate connection between structure and microstructure (Schwarz)
  - Strong multiphysics 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.

Additional slides

Intersection of materials science, engineering science, and computer science

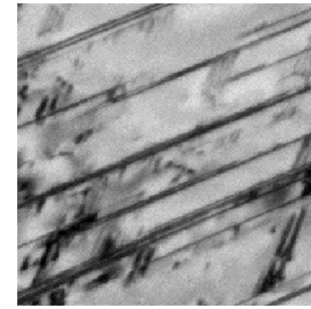


localization in tantalum

Trilinos

Phalanx for multiphysics

Albany

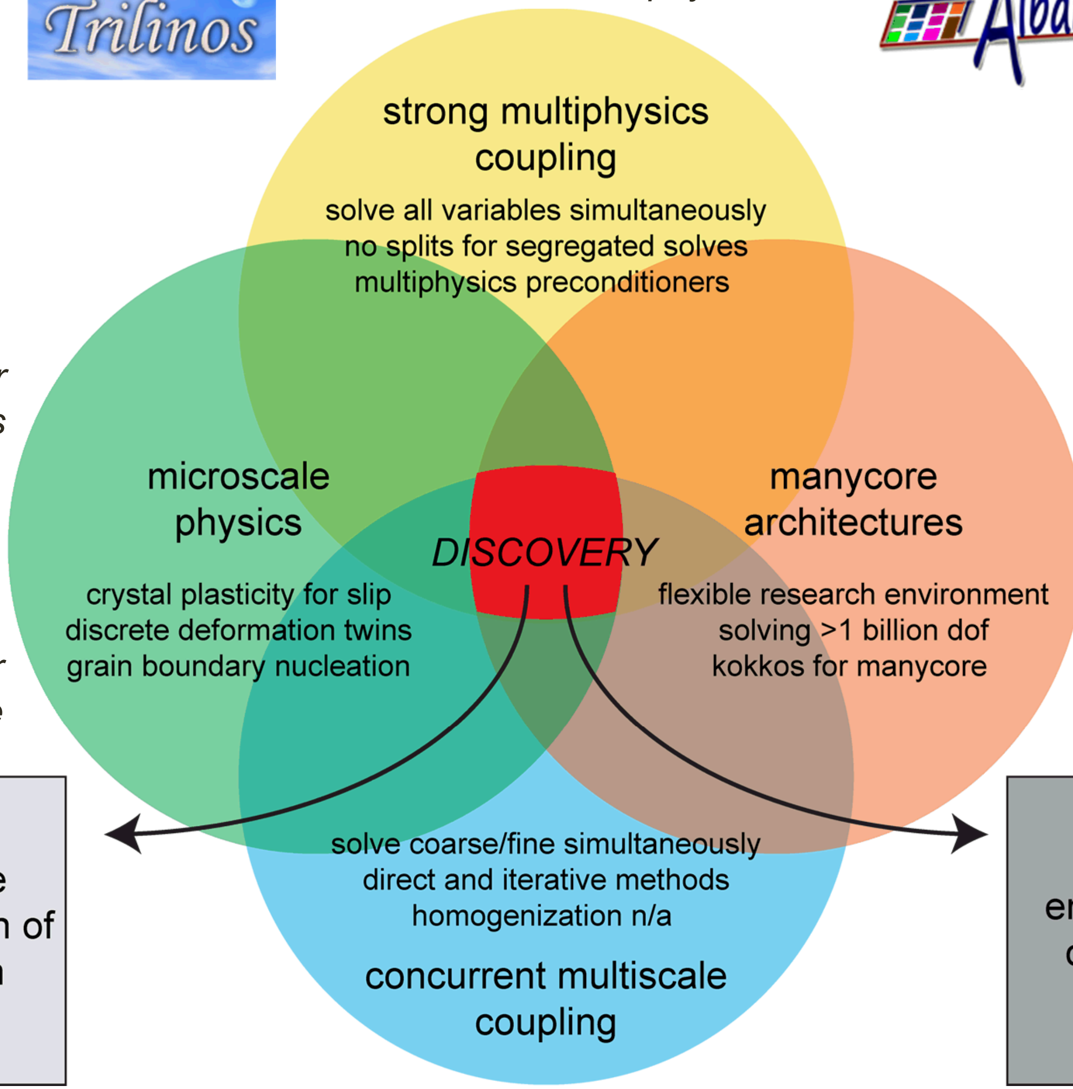


localization in stainless steel

miniTensor for mechanics

Sacado for the Hessian

miniSolver for constitutive update



Intrepid for element library

Massively parallel solvers

Kokkos for next generation platforms

high-rate deformation of tantalum

hydrogen embrittlement of stainless steels

Teko & Data Transfer Toolkit for spatial multiscale

Finite deformation, strong, multiphysics coupling

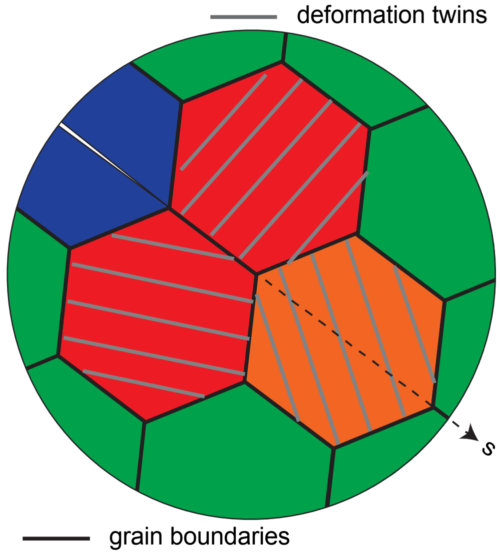
Fox and Simo (1990), Callari, Armero, Abati (2010)

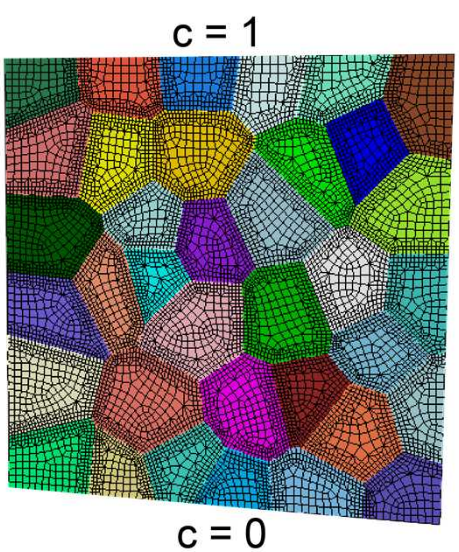
redefine space $$\boldsymbol{X} = \boldsymbol{\Phi}(\xi^1, \xi^2, \xi^3) = \bar{\boldsymbol{\Phi}}(\xi^1, \xi^2) + \boldsymbol{N}(\xi^1, \xi^2)\xi^3$$

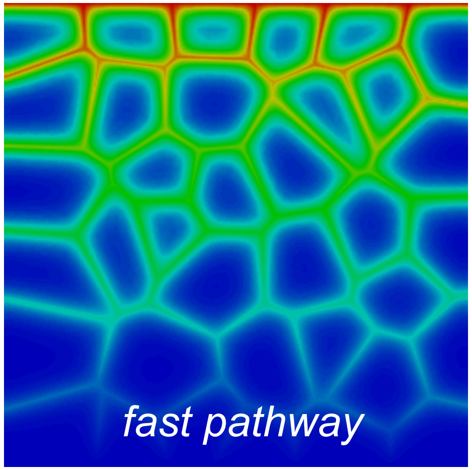
include jump in concentration $$C(\boldsymbol{X}) = \bar{C}(\phi[\xi^1, \xi^2]) + \frac{[\![C]\!](\phi[\xi^1, \xi^2])}{h}\xi^3$$

$$\boldsymbol{G}_i = \boldsymbol{\Phi}_{,i} = \frac{\partial \boldsymbol{X}}{\partial \xi^i} \qquad \nabla_{\boldsymbol{X}} C = (\nabla \boldsymbol{\Phi})^{-T} \frac{\partial C}{\partial \xi^i}$$

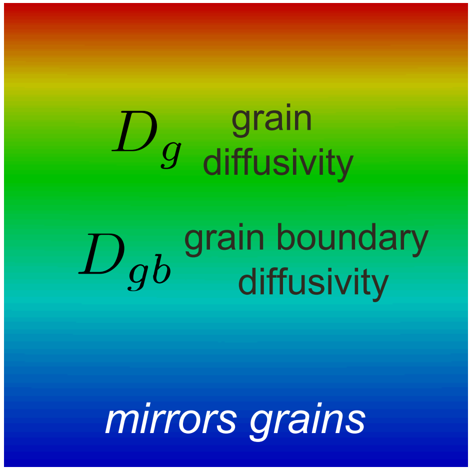
finite element implementation is straightforward



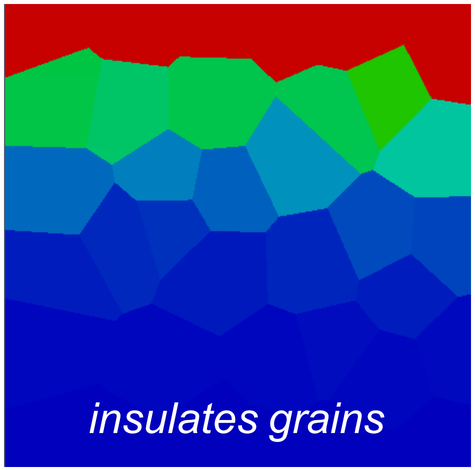




$D_{gb} = 1 \times 10^5 D_g$



$D_{gb} = D_g$



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

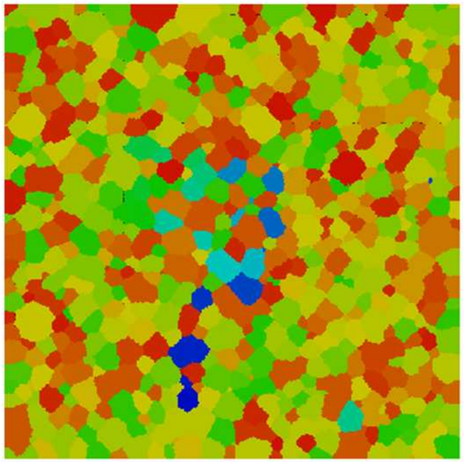
Lessons learned: Block solves require robust methods for scaling. Work in progress.

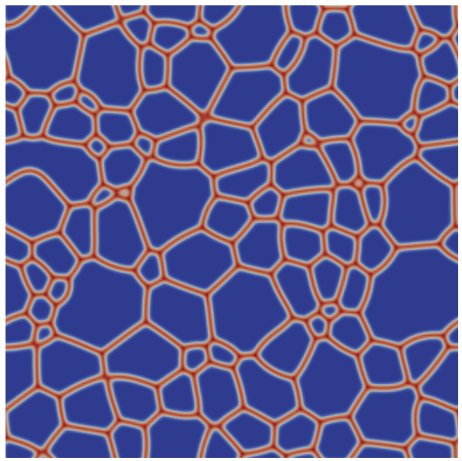
Collaboration through Georgia Tech

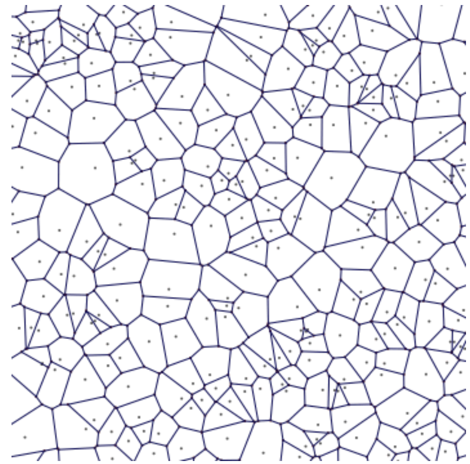
Exploring microstructure-mechanical property relationship using statistical data analysis

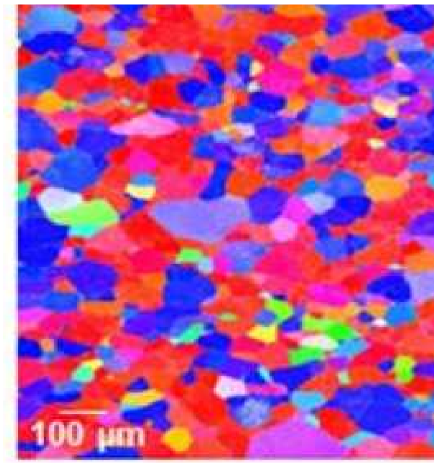
Multiscale/multiphysics LDRD. SNL PI: Hojun Lim. GT PI: Professor Surya Kalidindi

Rigorous statistical quantification of polycrystalline microstructures

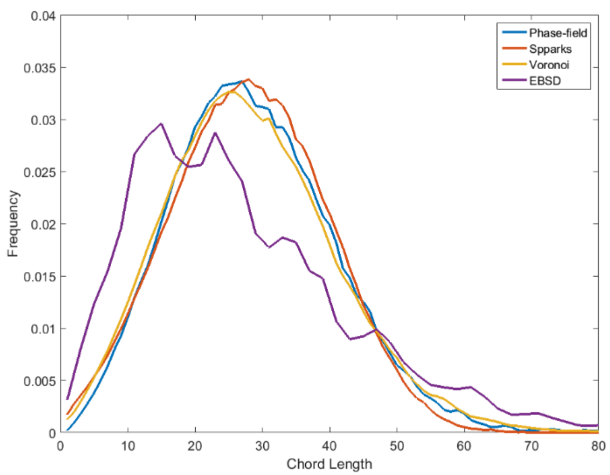

KMC grain growth


Phase field grain growth


Voronoi tessellation



EBSD



grain boundary chord lengths

Future work w/ focus on *Data Science* (~100K)

- Method for creating statistically equivalent microstructures from 2-D EBSD data (03/17)
- Conduct CP-FEM simulations of Ta and stainless steel using statistically generated 3-D polycrystalline microstructures (09/17)
- At least two papers will be submitted to archival journals and a final report with the same information will be submitted (09/17)

Professor: S. Kalindini, Postdoc: E. Popova, PhD student: D. Patel