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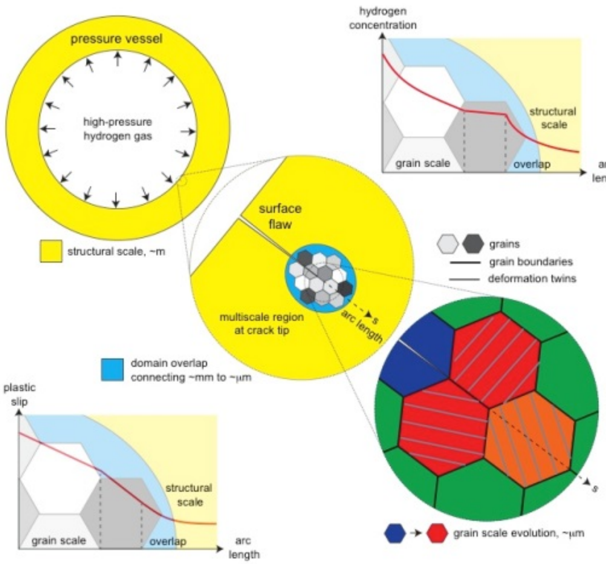

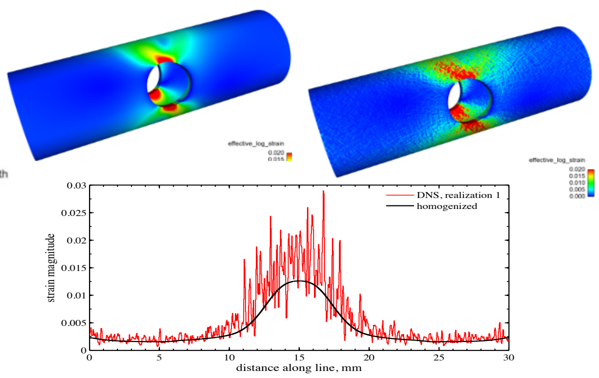

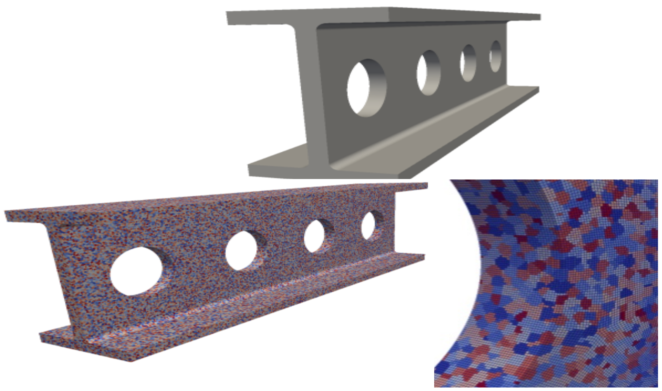

Top Down Multiscale Strategies for Solid Mechanics Applications

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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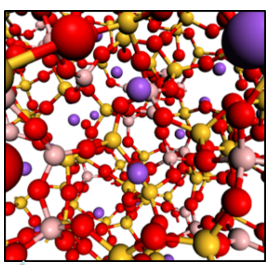
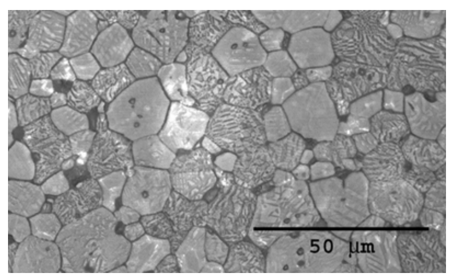
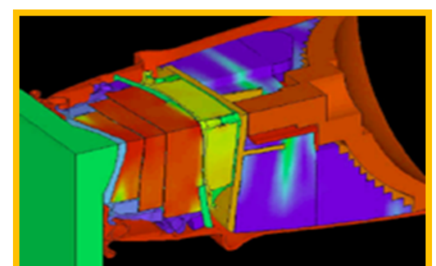
What Do We Mean by Multiscale for Solid Mechanics?

- In the computational sciences multiscale has many meanings
- Our definition
  - Applications of mathematical models, numerical methods, tools, and expertise explicitly connecting length scales to enrich engineering scale models with substructural response
  - Geometric, materials, and multiphysics aspects
- Enabling progress in multiscale structural requires advances in both **Methods** and **Physics**



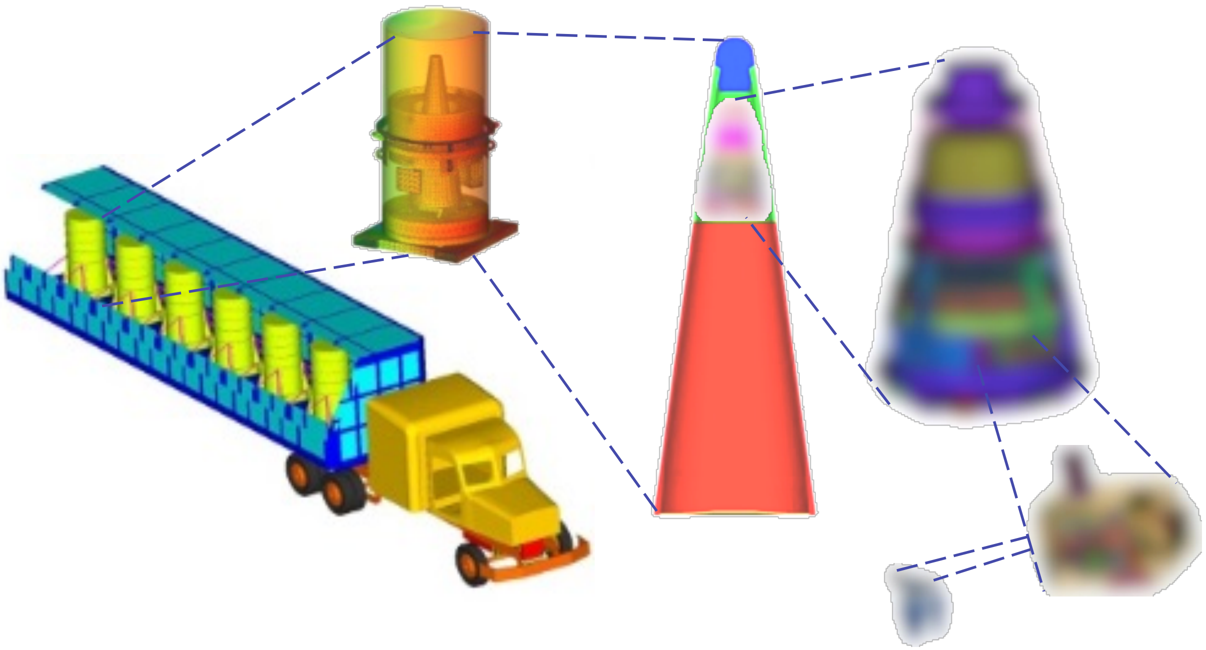




Methods and Physics Across and Linking Length Scales

Drivers and Needs

- Sandia fields system with a tremendous span of geometrical scales
- In order to asses these systems we need efficient methods and algorithms for:
  - Coupling across length scales
  - Asses the impact of lower length scale physics
  - Incorporating and propagating lower length scale uncertainties and variabilities



Multiscale Strategy: R&D Thrusts

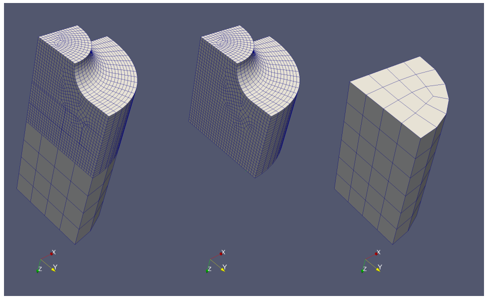
1. Computational **Methods**
   - Scale Coupling – Methods to pass information between geometric scales
   - Physics Coupling – Methods to coupling physical laws
   - Variability/Uncertainty Propagation – Methods to pass statistical information across scales
   - Experimental Diagnostics – Methods for discovery
2. Scale Dependent **Physical Models**
   - Balance Laws – Lower length scales involve richer physics
   - Local Physical Mechanisms – Determining dominant physical mechanisms requires experimental discovery
   - Micro/Sub-structural heterogeneity – Complexity of engineering materials requires representation of local spatial variability
   - Aging – Demonstrated fundamental understanding of physical behavior over long time scales

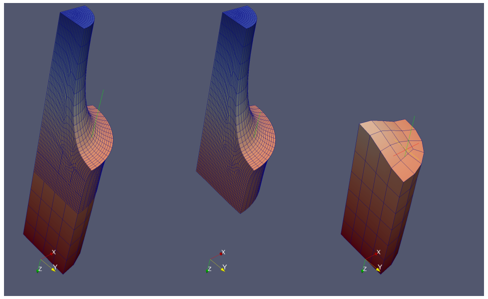
Multiscale Strategy: Objectives

1. Develop scale bridging technologies
   - Attack the use cases where we simply need more geometric resolution (not necessarily more physics), i.e. bolted joint in a structure.
   - Focus on theoretical foundation, robustness, efficiency
   - Investigate Homogenization and Concurrent methods for appropriate spaces
2. Leverage ongoing investments in lower length scale physics
   - Construct models using scale bridging technologies for specific drivers
   - Discover and verify the assertion that lower length scale physics has significant impact on the engineering scale.
3. Incorporate statistical information pertaining to material variability and uncertainty
   - Propagate material response between meso and continuum scale

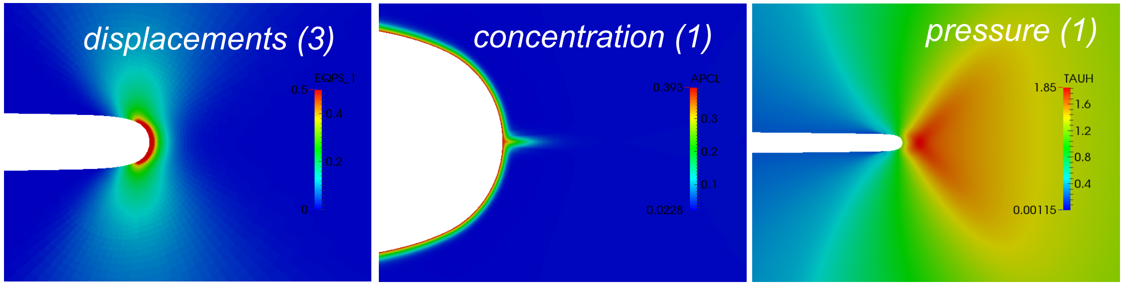
Implementation: Select Projects

- Multiscale methods for failure
  - Concurrent Coupling
  - Alternating Schwarz





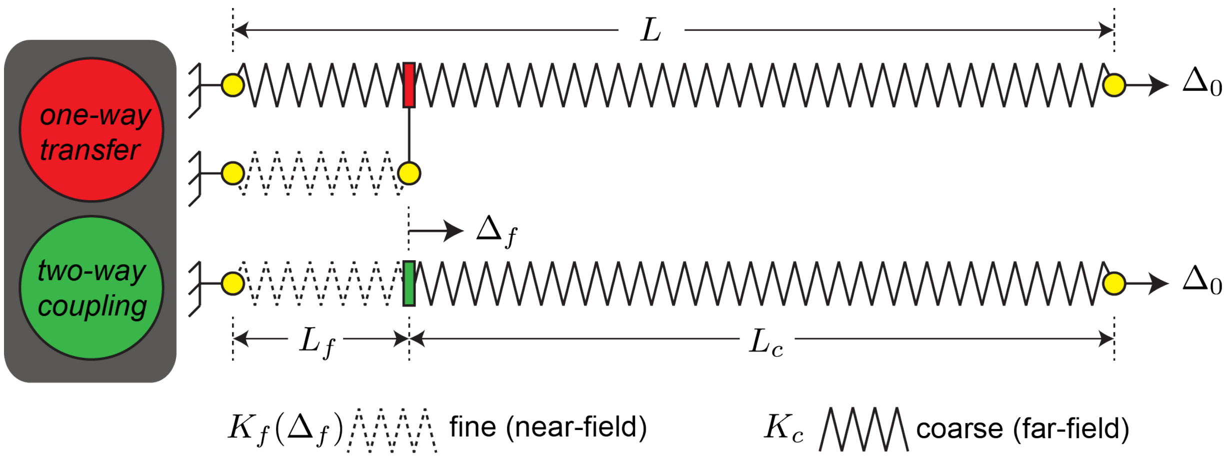
- Strong, concurrent, multiphysics and multiscale coupling
  - Failure mechanisms of hydrogen embrittlement in stainless steel
  - High rate deformation and twinning of tantalum

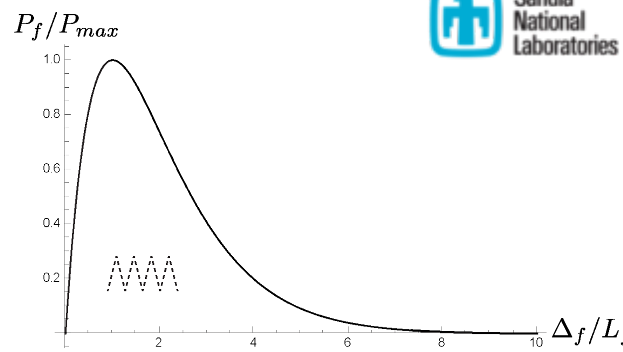


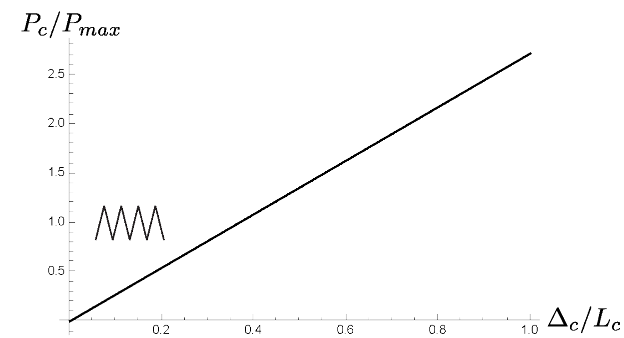
- Meso/Continuum Coupling
  - Investigating microstructural effects on bulk inelastic properties

A case for concurrent coupling

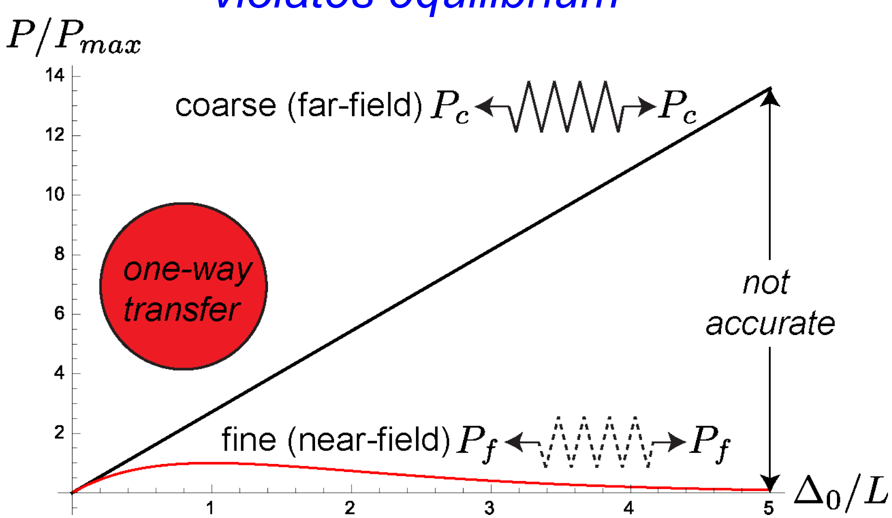
Q: Is a one-way transfer accurate? Conservative?
A: For failure processes involving localization, no.



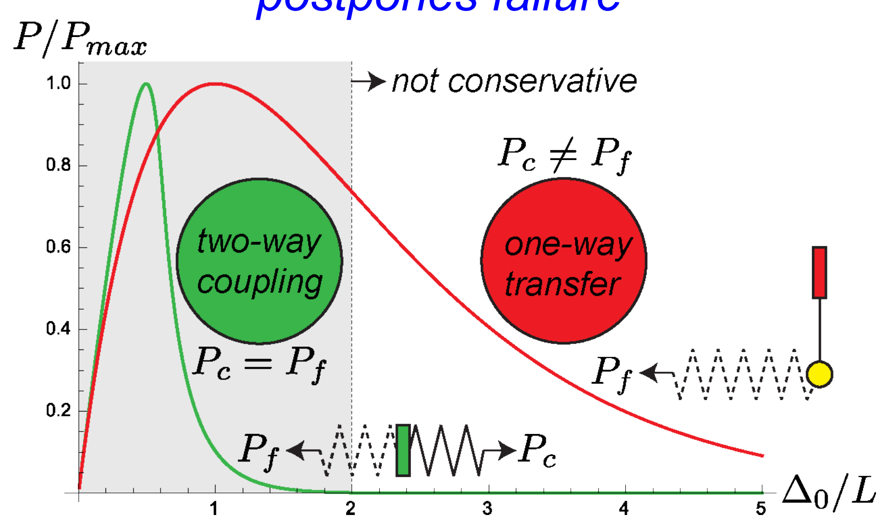




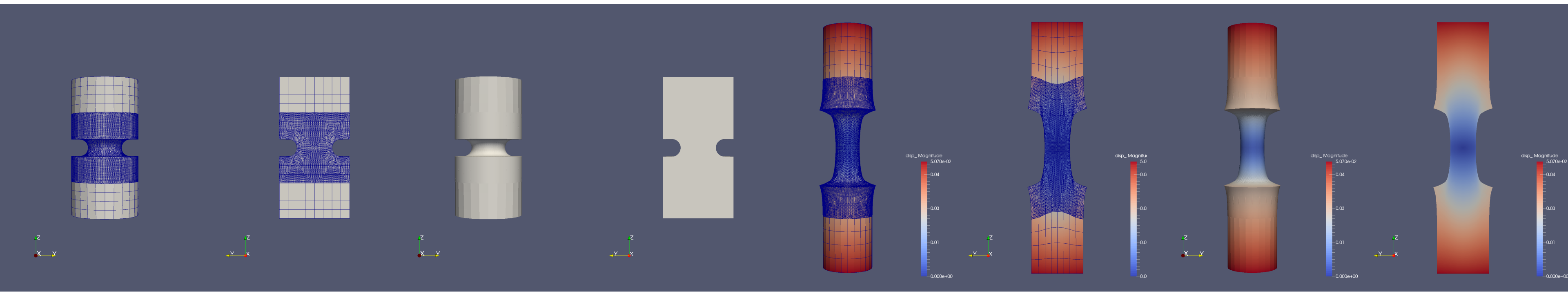
violates equilibrium



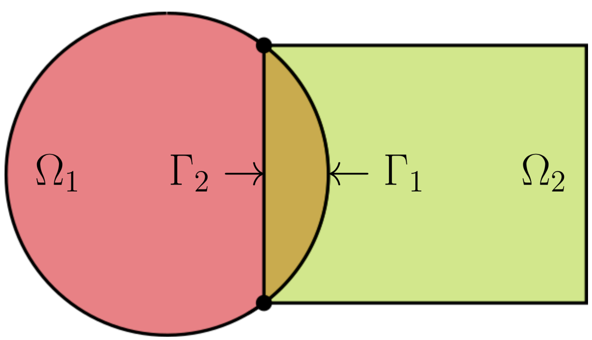
postpones failure



Coupling finite element meshes

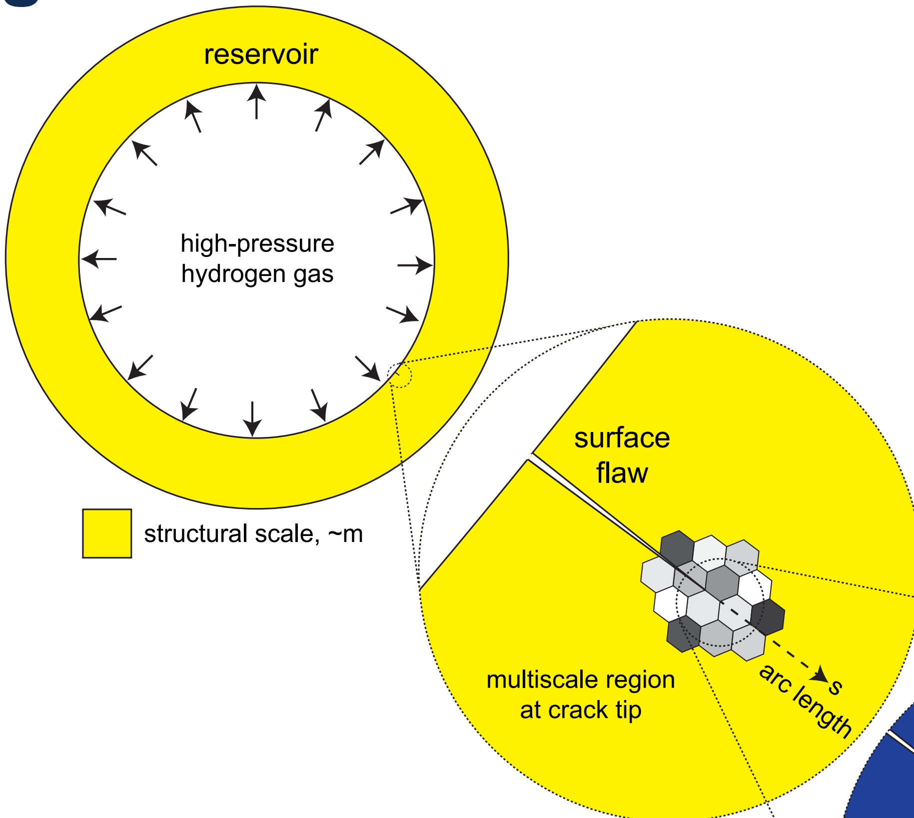


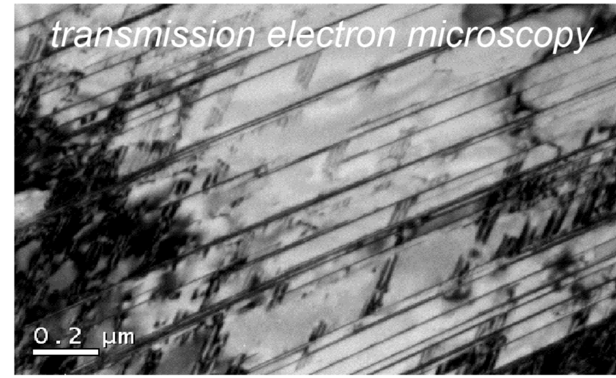
$$\begin{pmatrix} \boldsymbol{K}^1_{AB} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{K}^2_{AB} \end{pmatrix} \begin{Bmatrix} \triangle \boldsymbol{x}^1_B \\ \triangle \boldsymbol{x}^2_B \end{Bmatrix} = \begin{Bmatrix} -\boldsymbol{R}^1_A - \boldsymbol{K}^1_{Ab} \left(\boldsymbol{\chi}^1_b - \boldsymbol{x}^1_b \right) - \boldsymbol{K}^1_{A\beta} \left(P_{\Omega_2 \to \Gamma_1} [\boldsymbol{x}^2] - \boldsymbol{x}^1_\beta \right) \\ -\boldsymbol{R}^2_A - \boldsymbol{K}^2_{Ab} \left(\boldsymbol{\chi}^2_b - \boldsymbol{x}^2_b \right) - \boldsymbol{K}^2_{A\beta} \left(P_{\Omega_1 \to \Gamma_2} [\boldsymbol{x}^1] - \boldsymbol{x}^2_\beta \right) \end{Bmatrix}$$



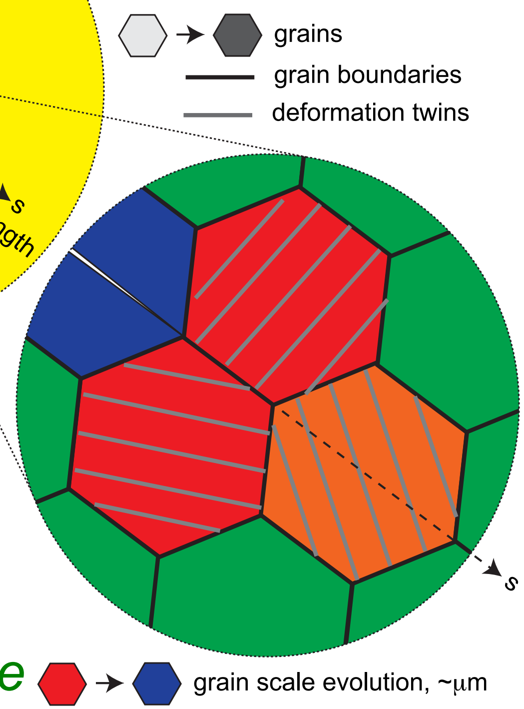
$$\begin{pmatrix} \boldsymbol{K}^1_{AB} & \boldsymbol{K}^1_{Ab} & \boldsymbol{K}^1_{A\beta} & & & \\ & \boldsymbol{I} & & & \boldsymbol{0} & \\ & & \boldsymbol{I} & & & \\ & & & \boldsymbol{K}^2_{AB} & \boldsymbol{K}^2_{Ab} & \boldsymbol{K}^2_{A\beta} \\ & \boldsymbol{0} & & & \boldsymbol{I} & \\ & & & & & \boldsymbol{I} \end{pmatrix} \begin{Bmatrix} \triangle \boldsymbol{x}^1_B \\ \triangle \boldsymbol{x}^1_b \\ \triangle \boldsymbol{x}^1_\beta \\ \triangle \boldsymbol{x}^2_B \\ \triangle \boldsymbol{x}^2_b \\ \triangle \boldsymbol{x}^2_\beta \end{Bmatrix} = \begin{Bmatrix} -\boldsymbol{R}^1_A \\ \boldsymbol{\chi}^1_b - \boldsymbol{x}^1_b \\ P_{\Omega_2 \to \Gamma_1} [\boldsymbol{x}^2] - \boldsymbol{x}^1_\beta \\ -\boldsymbol{R}^2_A \\ \boldsymbol{\chi}^2_b - \boldsymbol{x}^2_b \\ P_{\Omega_1 \to \Gamma_2} [\boldsymbol{x}^1] - \boldsymbol{x}^2_\beta \end{Bmatrix}$$

Hydrogen activates microstructure





deformation twins



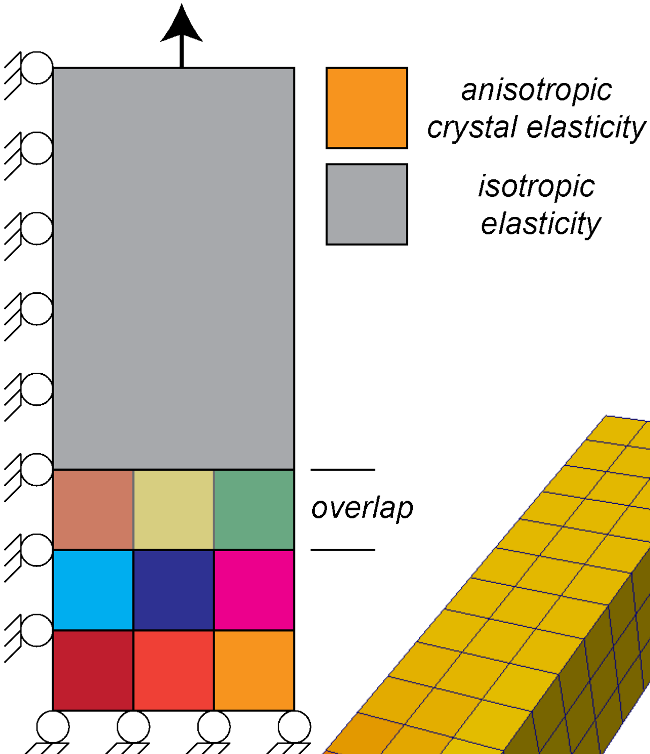
Hydrogen *activates* microstructure

- Aids deformation bands/twinning (*nm*)
- Activates phase transformations (*nm* – *μm*)
- Accentuates grain boundary interactions (*nm*)

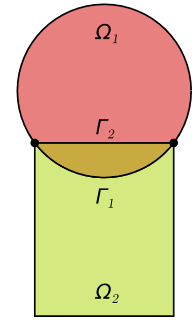
Material specifications focus on microstructure

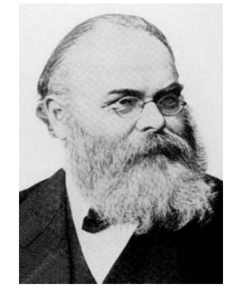
Strong coupling…

Demonstrate Concurrent Multiscale Coupling



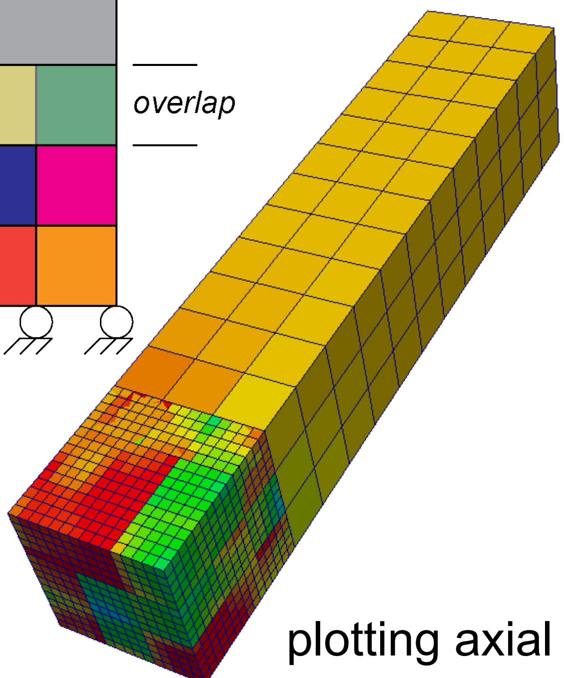
Two distinct bodies, the component scale and the microstructural scale, are coupled iteratively with alternating Schwarz





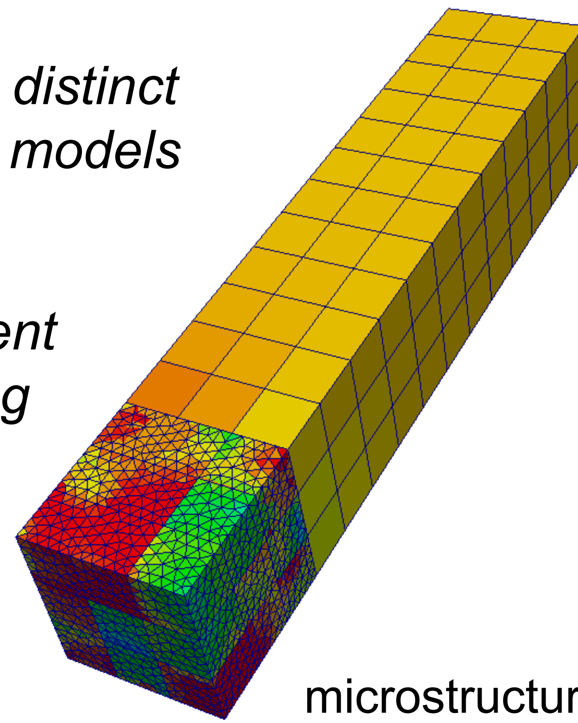
Schwarz

distinct models



concurrent coupling

plotting axial stress



component scale

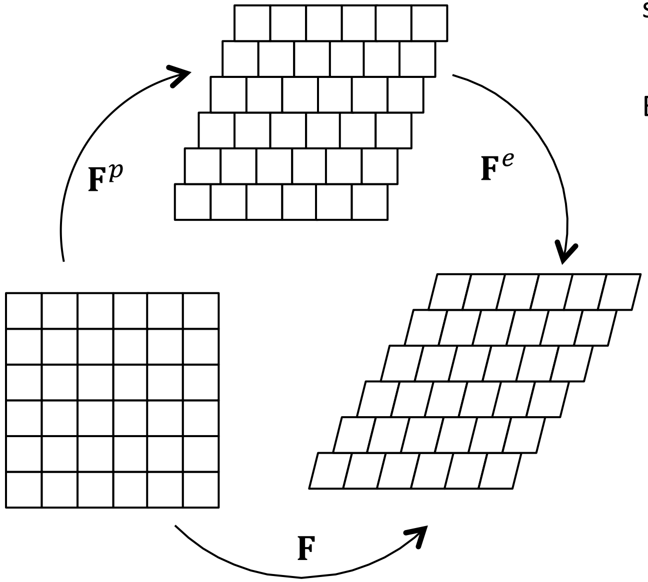
microstructural scale

Single crystal constitutive equations

Kinematics

Multiplicative decomposition of the deformation gradient

$$\mathbf{F}^e = \mathbf{F} \cdot (\mathbf{F}^p)^{-1}$$



Crystal elasticity

Second Piola-Kirchhoff stress in the intermediate configuration

$$\mathbf{T}^* = \mathbb{L}^c : \mathbf{E}^e$$

Elasticity tensor in the global coordinate system

$$\mathbb{L}^c = \mathbf{R}^T \cdot \mathbf{R}^T \cdot \mathbb{L} \cdot \mathbf{R} \cdot \mathbf{R}$$

Elastic Lagrangian strain

$$\mathbf{E}^e = \frac{1}{2}[(\mathbf{F}^e)^{\mathrm{T}}\mathbf{F}^e - \mathbf{I}]$$

Crystal Plasticity

Evolution of plastic part of deformation gradient

$$\dot{\mathbf{F}}^p = \mathbf{L}^{p*} \cdot \mathbf{F}^p$$

Plastic part of velocity gradient in the intermediate configuration

$$\mathbf{L}^{p*} = \sum_{\alpha} \dot{\gamma}^{\alpha} \mathbf{m}_0^{\alpha} \otimes \mathbf{n}_0^{\alpha}$$

Power-law flow rule for FCC materials

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left| \frac{\tau^{\alpha}}{\tau_0 + g^{\alpha}} \right|^k \mathrm{sign}(\tau^{\alpha})$$

Resolved shear stress

$$\tau^{\alpha} = [(\mathbf{F}^e)^{\mathrm{T}} \cdot \mathbf{F}^e \cdot \mathbf{T}^*] : \mathbf{m}_0^{\alpha} \otimes \mathbf{n}_0^{\alpha}$$

Evolving slip resistance

$$g^{\alpha} = \frac{H}{R_d}[1 - \exp(-R_d|\gamma^{\alpha}|)]$$

Microstructural equivalency

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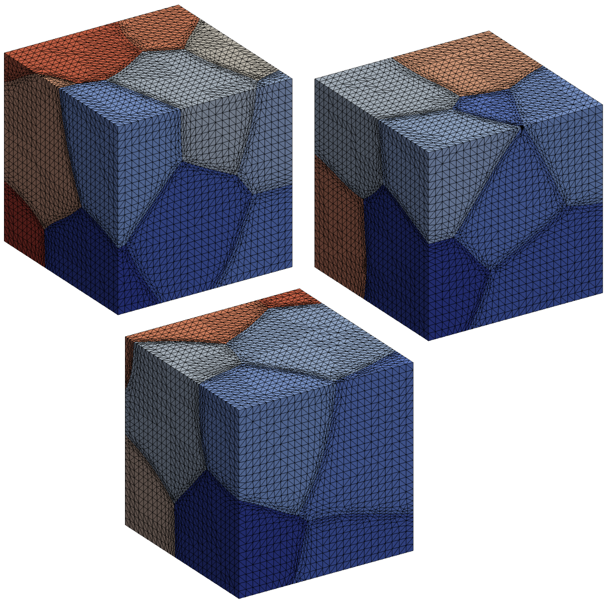
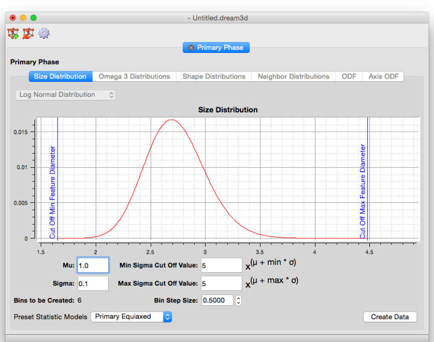
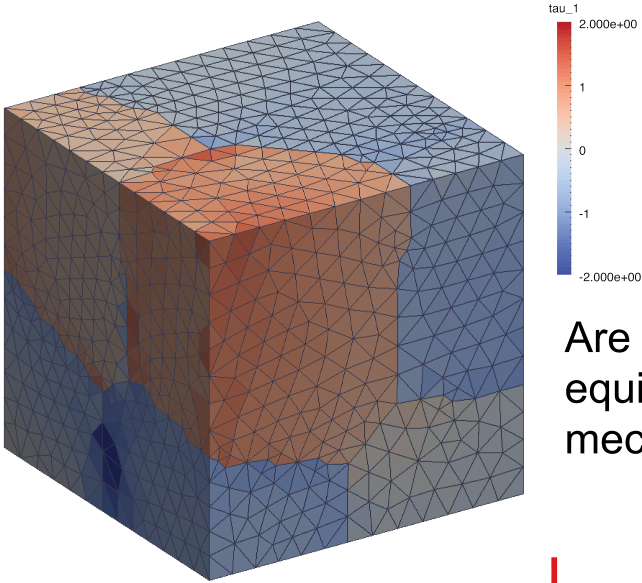
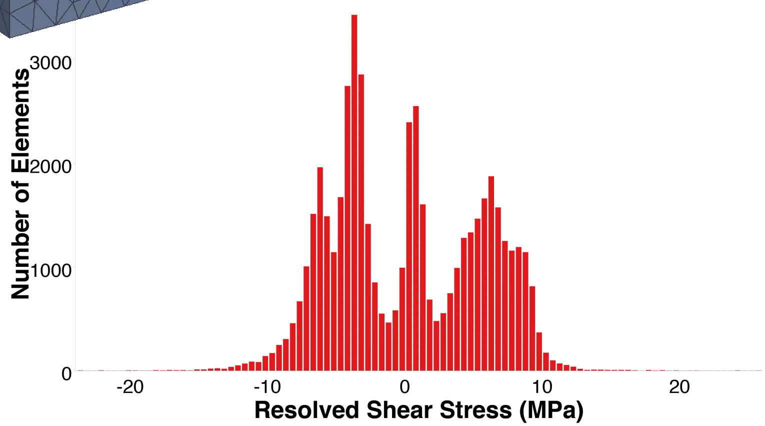


Microstructural realizations from a single set of underlying morphological statistics





Are the realizations equivalent in terms of mechanical response?



Summary

- Sandia modeling needs drive development of technologies for:
  - Scale bridging
  - Incorporating lower length scale response
  - Evaluating the effects of microstructure
- Current efforts include development in the areas of:
  - Concurrent coupling strategies
  - Microstructural tools, crystal plasticity models
  - Strong multiphysics coupling