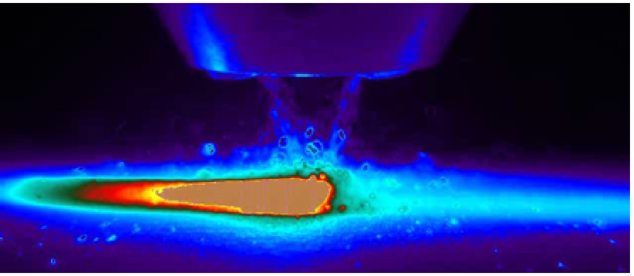
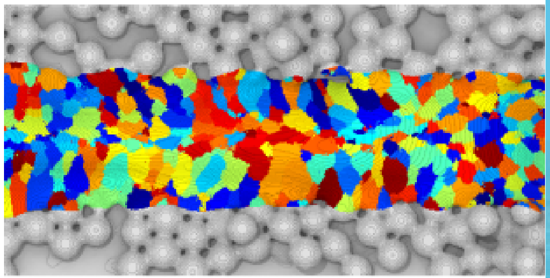
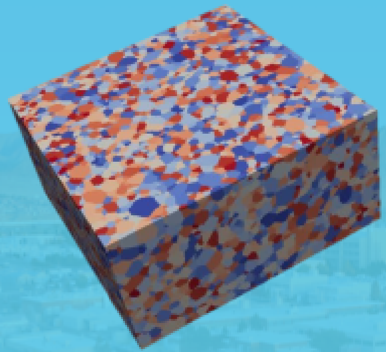
SAND2018-11694C

Sandia National Laboratories

Multiscale Modeling of Microstructure and Damage Evolution in the Performance of Additively Manufactured Parts







PRESENTED BY

*Kyle Johnson, **Jonathan D. Madison,** Theron Rodgers, Joseph Bishop, Bradley Jared, and John Emery*

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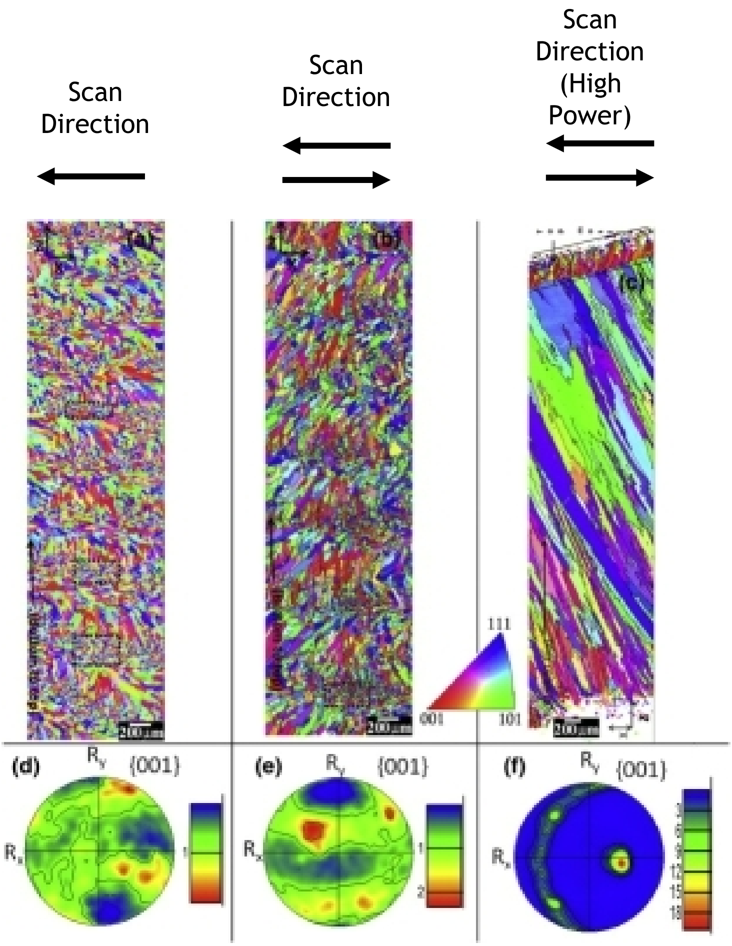
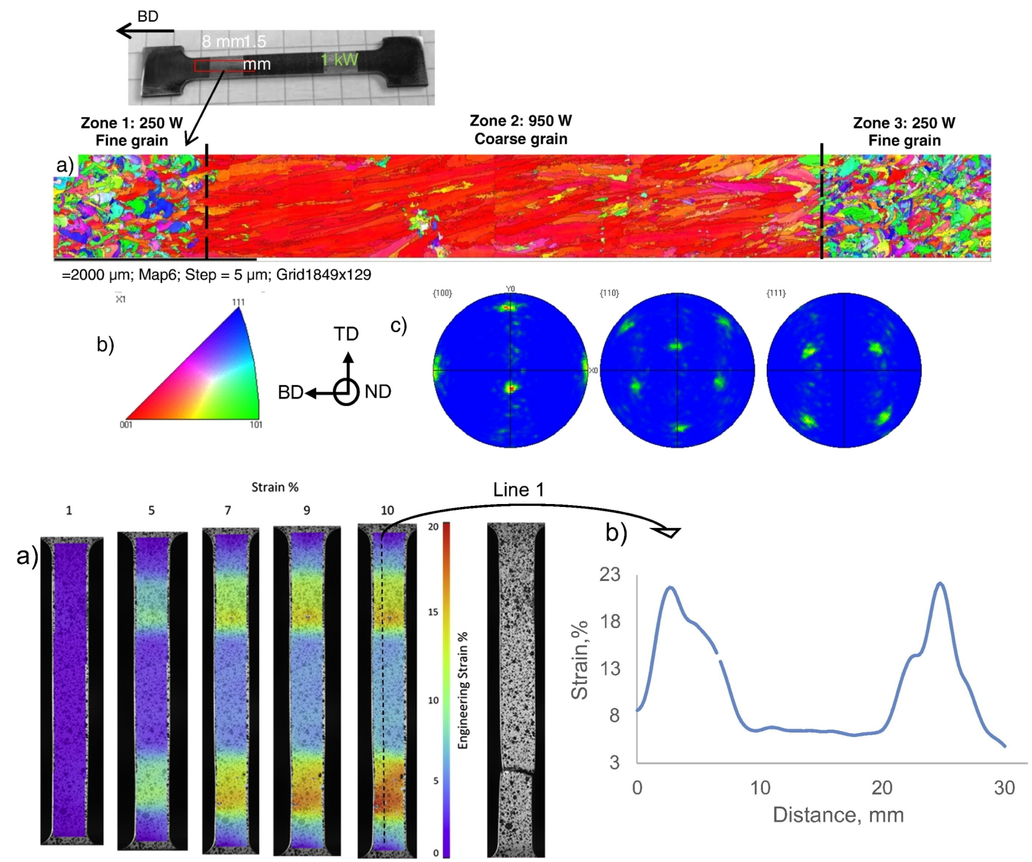
OUTLINE

- Background
- Microstructure Prediction
- Upscaling Microstructure Data
  - Direct Numerical Simulations
  - Error Estimation Techniques
- Implementing Voids and Damage
- Summary

Different Process Settings Cause Different Microstructures and Performance

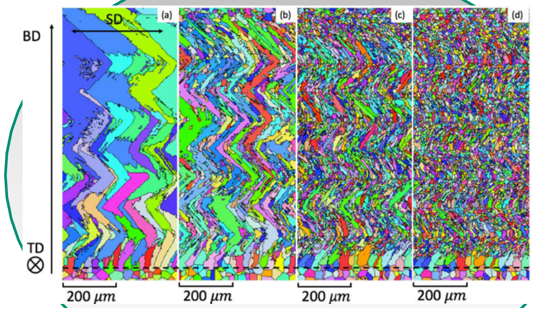




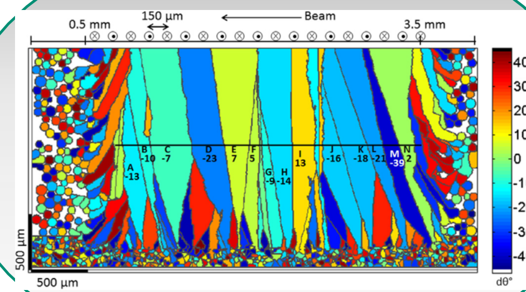
Parimi et al., Materials Characterization 2014

Popovich et al., Materials & Design 2017

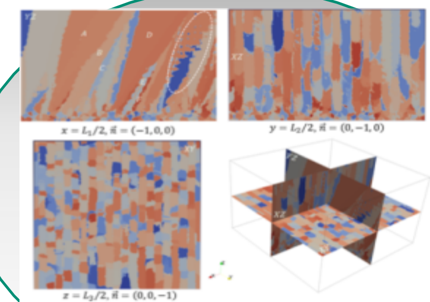
Microstructure Prediction – Cellular Automata Approaches



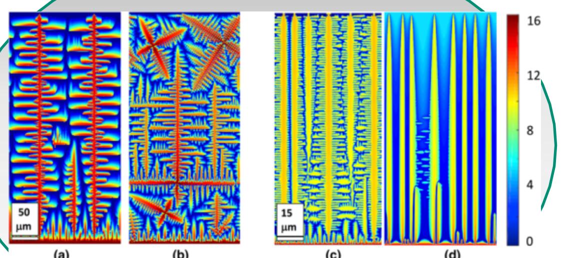
X. Li and W. Tan (U of Utah), SFFS 2017



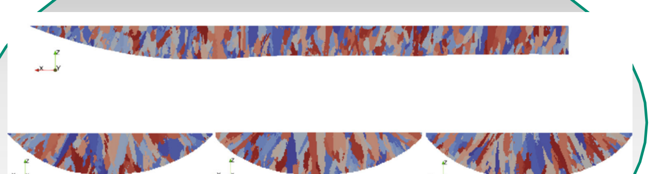
Rai and Körner (U. Erlangen), Add Manu 2017



Zinovieva et al (U. of Bremen), CMS 2017



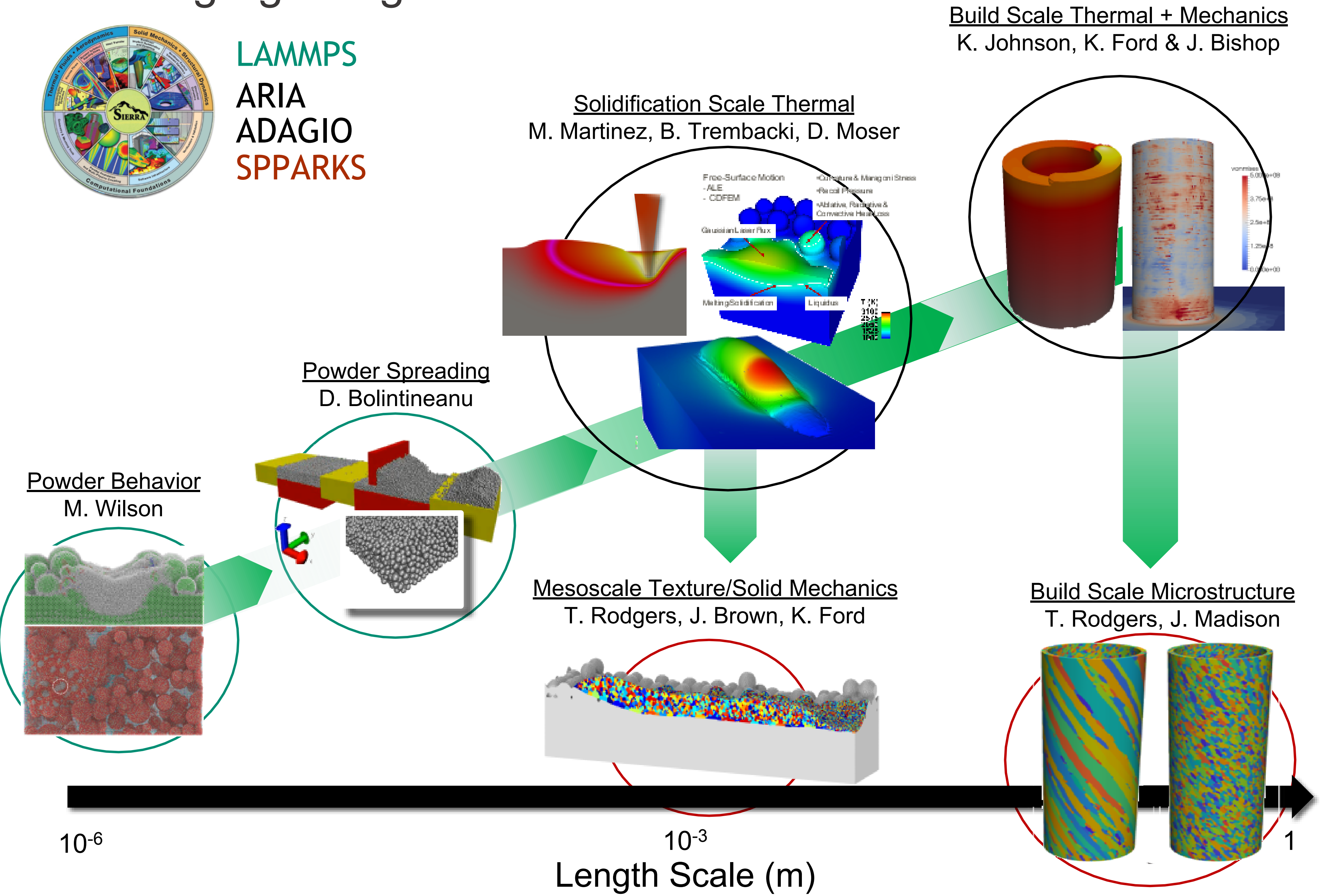
Rolchigo and LeSar (ISU), Met Trans A 2017



Lian and Wagner (Northwestern), Comp. Mech 2017

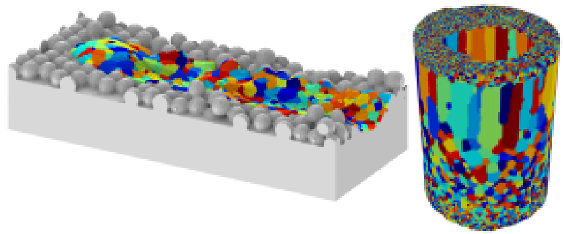
Publication	Pros/Included physics	Cons/Missing physics
Li & Tan	• Nucleation • 3D • Multi-pass/Layer • Coupled thermal solver	• No solid state evolution • Not parallelized (?) • Closed source • No fluid flow
Lian and Wagner	• Parallelized • Nucleation • 3D • Coupled thermofluid solver	• Single-pass/layer • No solid state evolution • Closed source
Zinovieva et al	• Texture • 3D • Multi-pass/Layer • Coupled thermal solver	• No solid state evolution • No nucleation • Closed source • No fluid flow
Rai and Körner	• Texture • Multi-pass/Layer • Coupled thermofluid solver (LBM)	• No solid state evolution • No nucleation • 2D • Closed source
Rolchigo and LeSar	• Microscale Dendrite model • Component segregation	• Single-pass/layer • No solid state evolution • 2D • Closed source

Bridging Length Scales – Informed Relevance

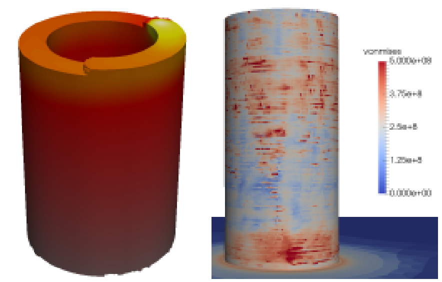


Process – Structure – Property – Performance Linkages via ***Microstructurally Aware Simulation***

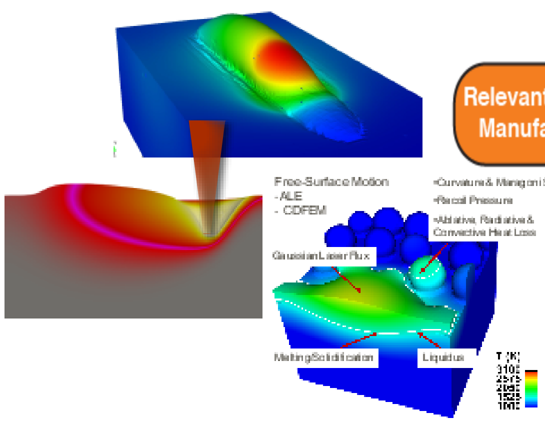
Mesoscale Texture/Solid Mechanics/CX
T. Rodgers, J. Brown, K. Ford

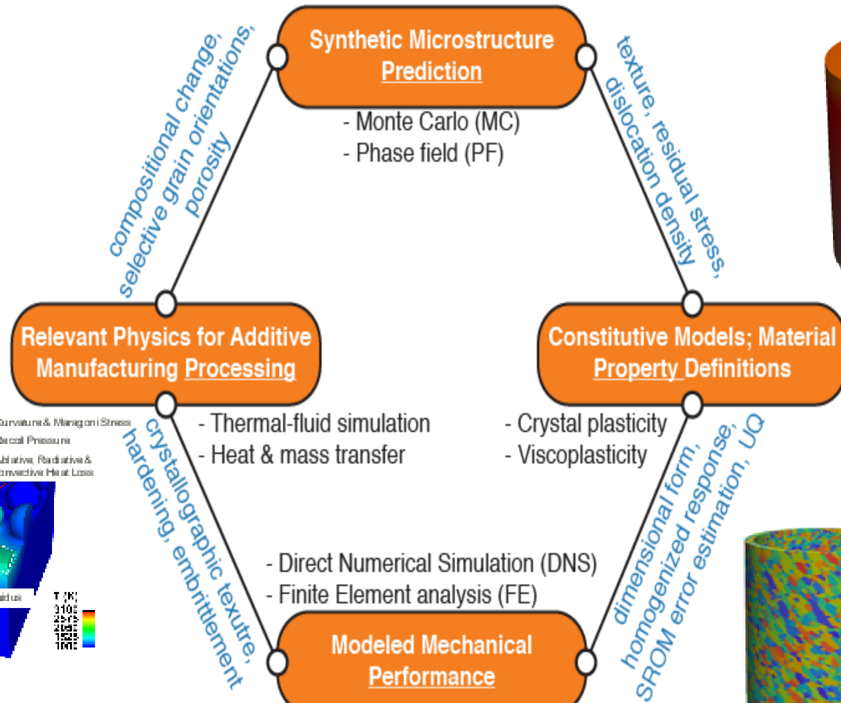


Build Scale Thermal + Mechanics
Kyle Johnson, Kurtis Ford & Joe Bishop

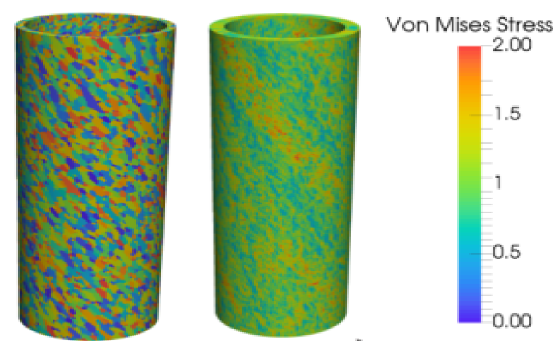


Solidification Scale Thermal
M. Martinez, B. Trembacki, D. Moser

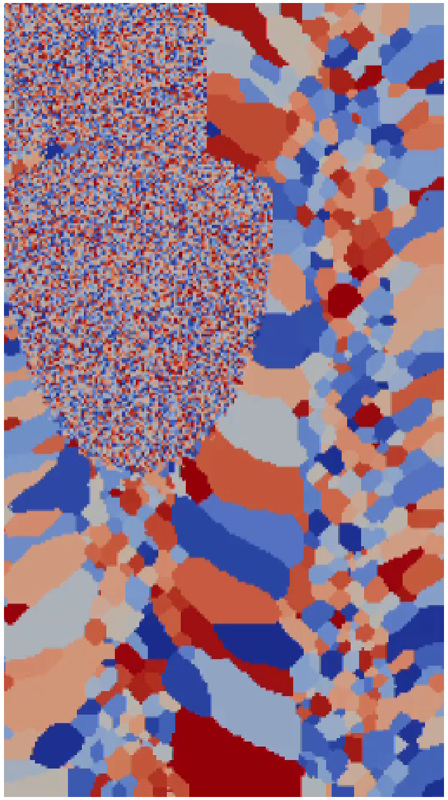




Direct Numerical Simulation
Theron Rodgers, Joe Bishop & Jon Madison

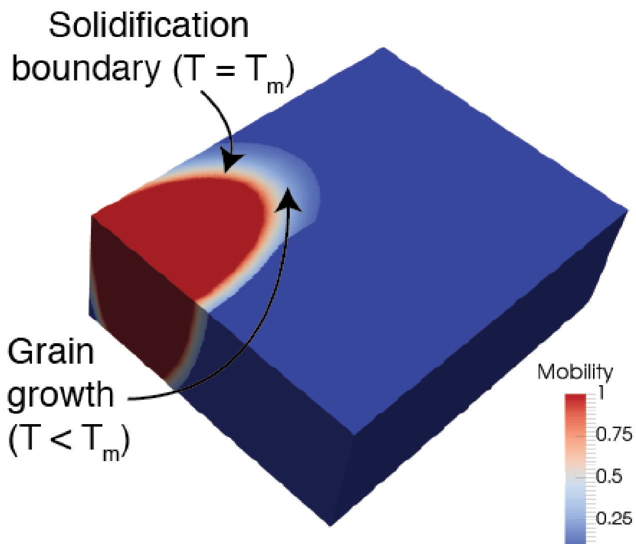


Microstructure Prediction in **S**tochastic **P**arallel **PAR**ticle **K**inetic **S**imulator (SPPARKS)



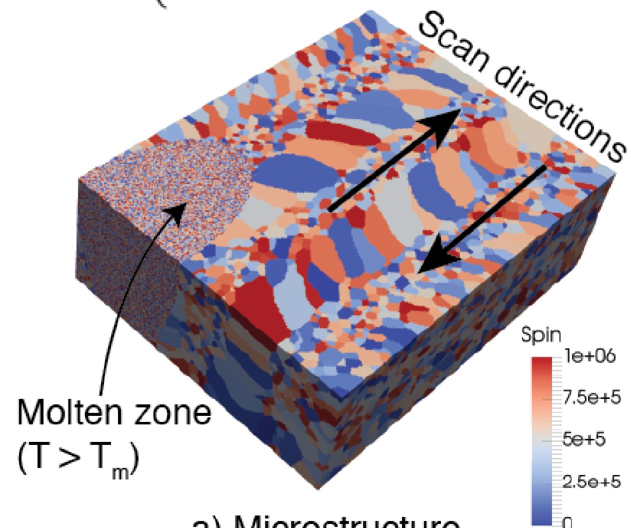
kMC & Solidification Structure

$$M(T) = M_o \exp\left(\frac{-Q}{RT}\right)$$



b) Mobility field

$$P = \begin{cases} M(T)\exp\left(\frac{-\Delta E}{k_B T_s}\right), & if\ \Delta E > 0 \\ M(T), & if\ \Delta E \le 0 \end{cases}$$

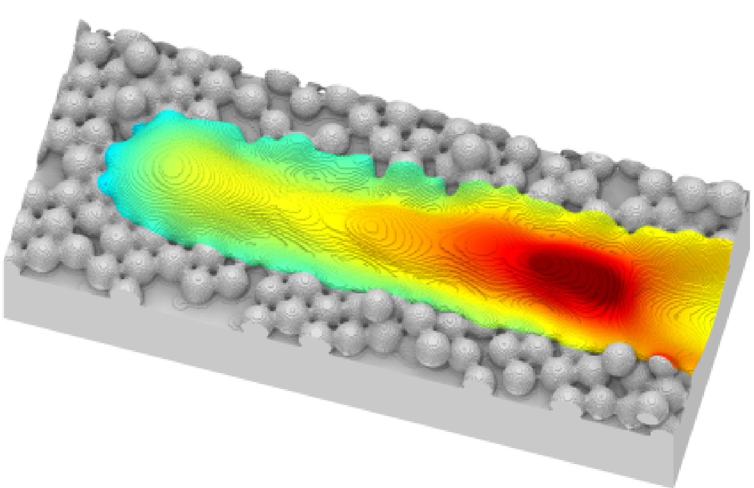


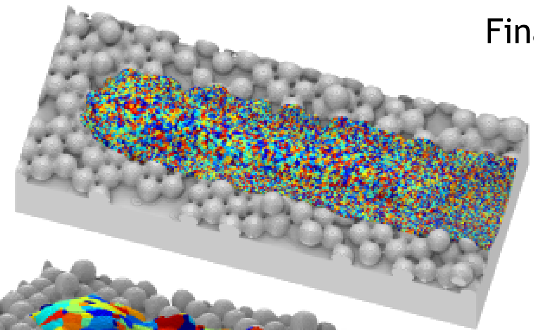
a) Microstructure

- The molten zone randomizes grain identities when it enters a region.
- Along the trailing surface, voxels either join existing columnar grains or form new grains.
- The temperature gradient creates a corresponding gradient of grain boundary mobilities via an Arrhenius relationship.

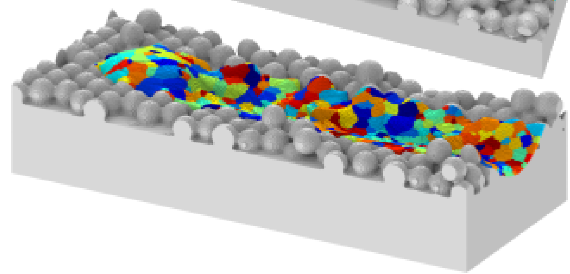
Sandia – Powder Bed Melt Model + Grain Prediction

Final temperature field of thermofluid simulation (M. Martinez)

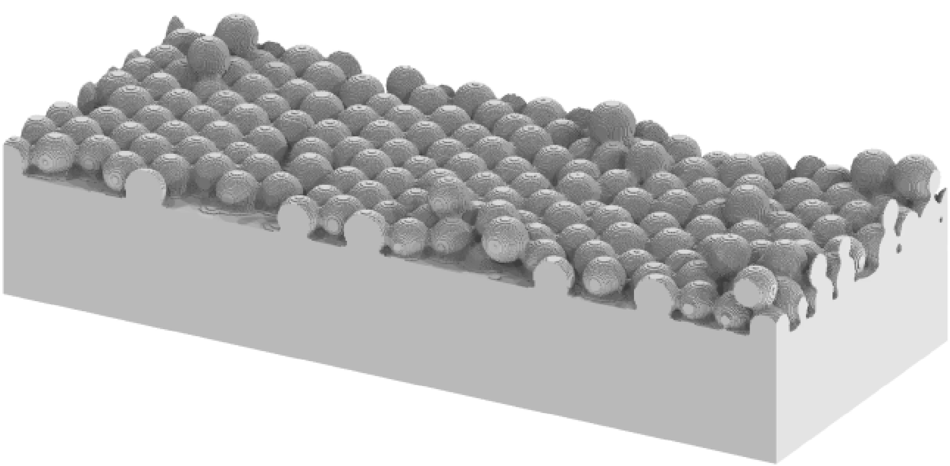




Final microstructure with old nucleation



Final microstructure with N_o = 10^{15}



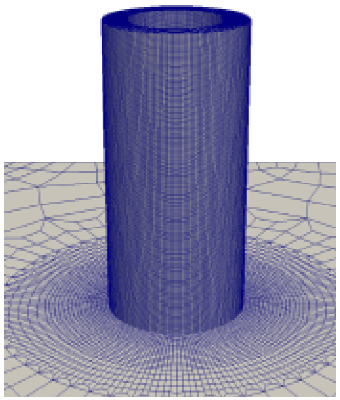
<u>Effect of nucleation site density:</u>

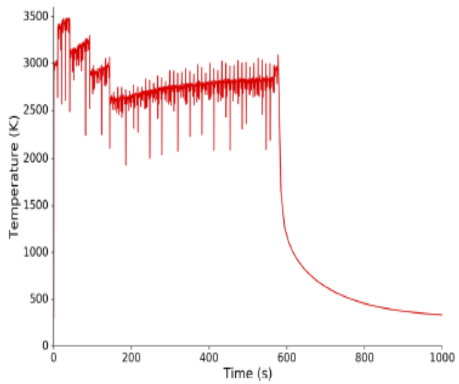
Particle-scale powder bed simulations used a much smaller lattice size than previous work (0.75 µm vs ~20 µm). With the old nucleation approach, these led to a large overprediction of nucleating grains, which resulted in a fine equiaxed structure (top).

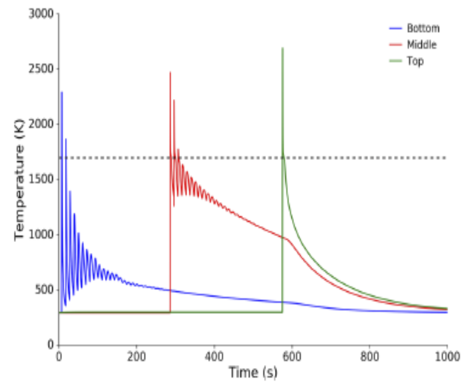
Introducing a N_o-dependent nucleation rule allowed only 1 nucleation site per 2,500 lattice sites and resulted in larger grains that grew from the substrate structure.

M. Martinez, T. Rodgers

Sandia – Conduction & Radiation Model

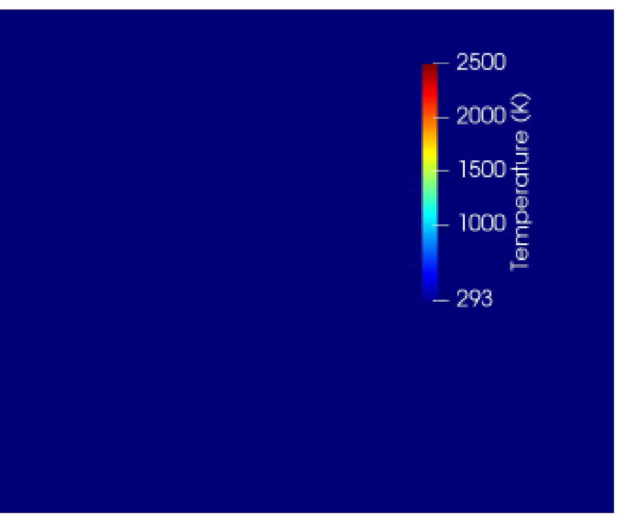




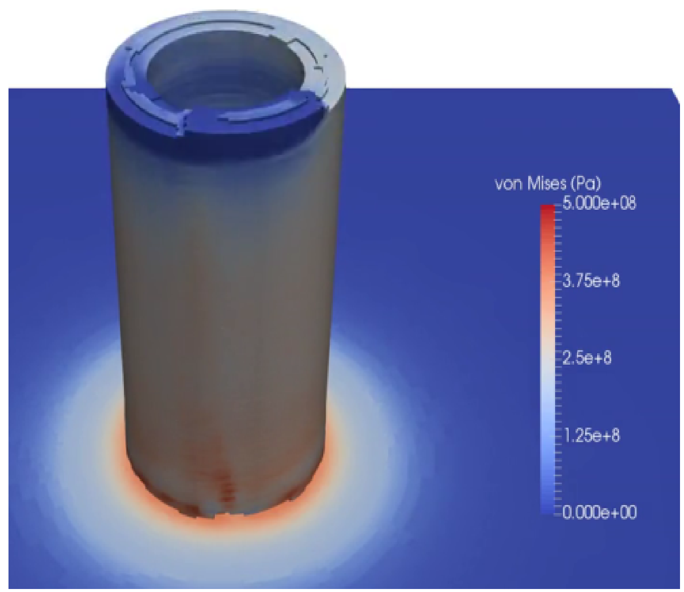


Using a radiative, conduction model we can estimate not only the build scale thermal field and history, but also the effective residual stresses within the build as a function of thermal history.

This goes beyond the local melt-scale solidification front phenomena to provide build scale understanding across appreciable intervals of time and physical space.



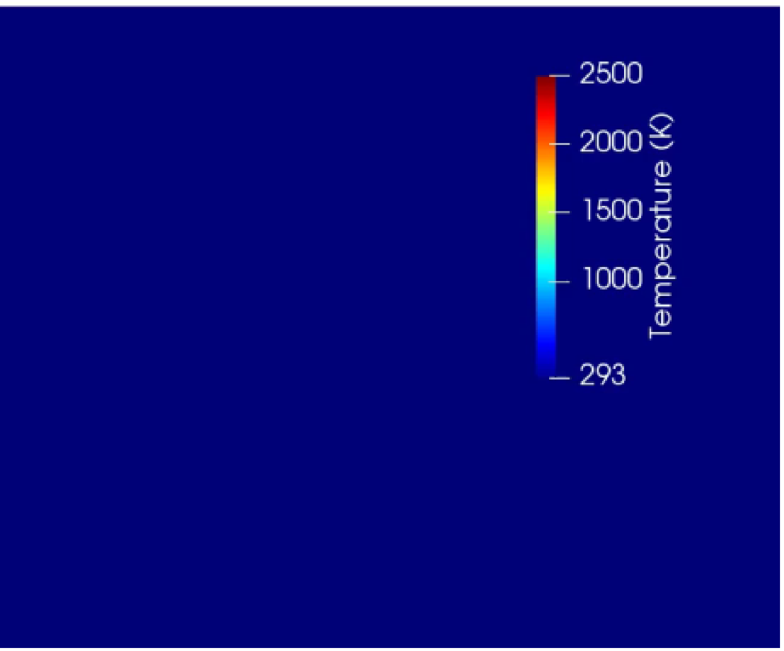
thermal

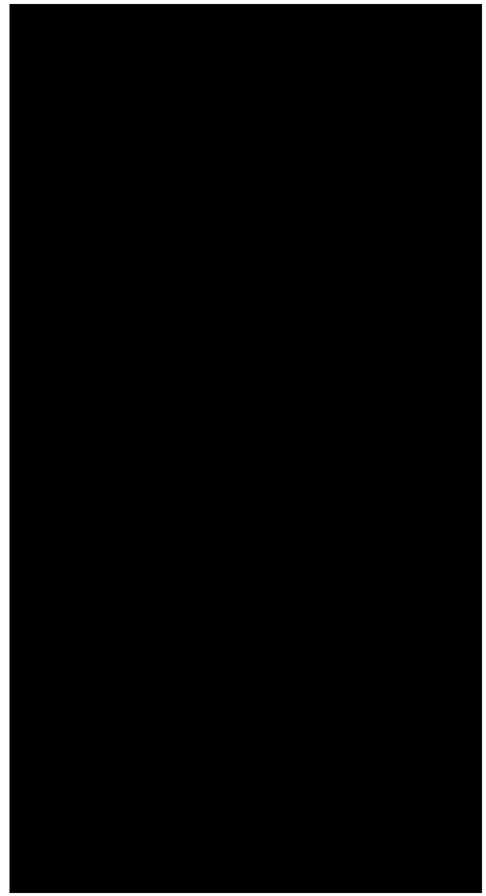


residual stress

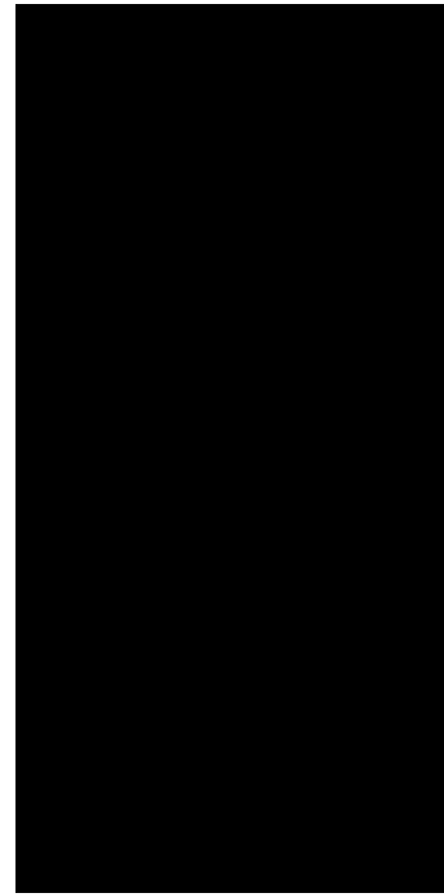
Johnson *et al.*, *Computational Mechanics 2018*

Sandia – Conduction & Radiation Model + Grain Prediction





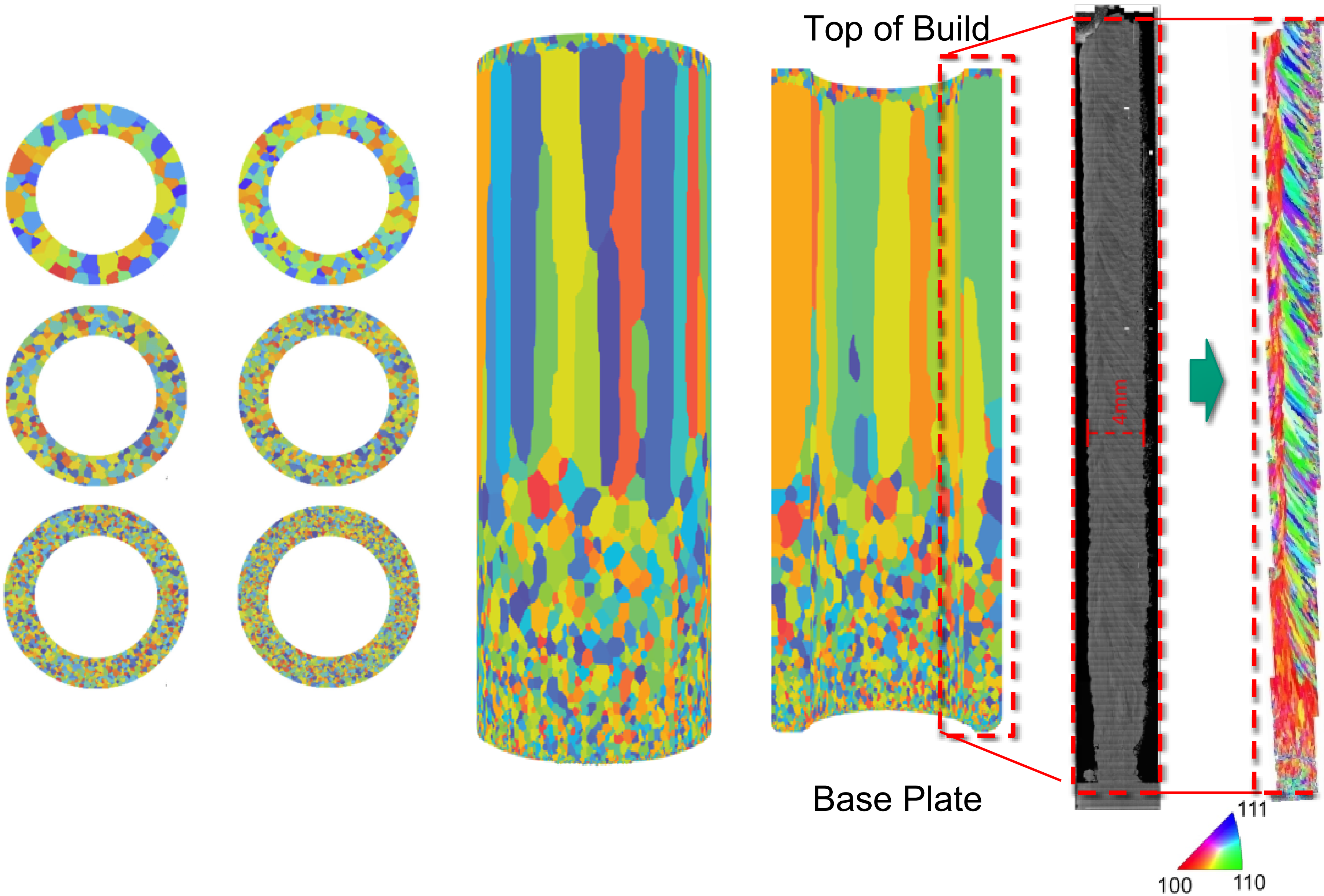
Single Continuous Build



Double Build (8 second delay in between layers)

Johnson *et al.*, *Computational Mechanics 2018*

Sandia – Comparison with Experiment



Johnson *et al.*, *Computational Mechanics 2018*

Direct Numerical Simulation on Additive Microstructures

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Direct numerical simulations in solid mechanics for understanding the macroscale effects of microscale material variability

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Received 13 October 2014; received in revised form 15 January 2015; accepted 27 January 2015
Available online 7 February 2015

JOM, Vol. 68, No. 5, 2016
DOI: 10.1007/s11837-016-1857-6

Direct Numerical Simulations in Solid Mechanics for Quantifying the Macroscale Effects of Microstructure and Material Model-Form Error

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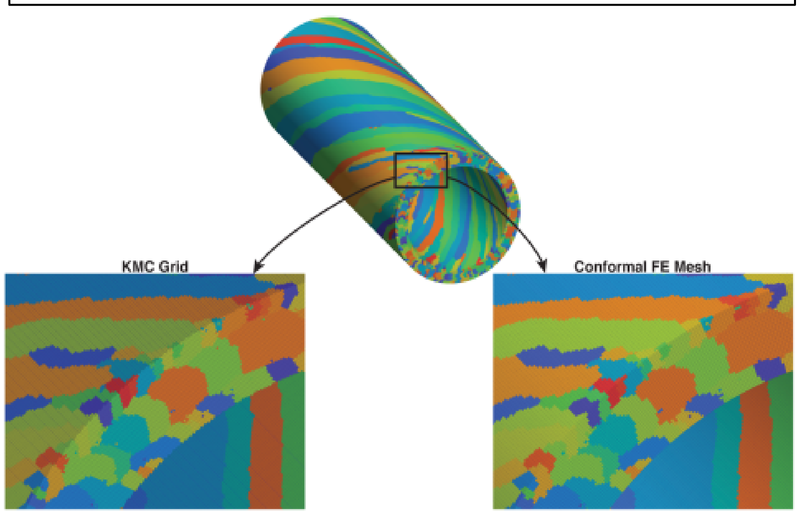
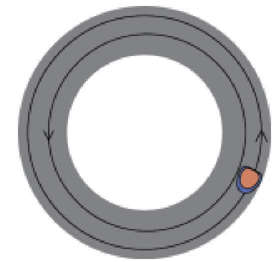
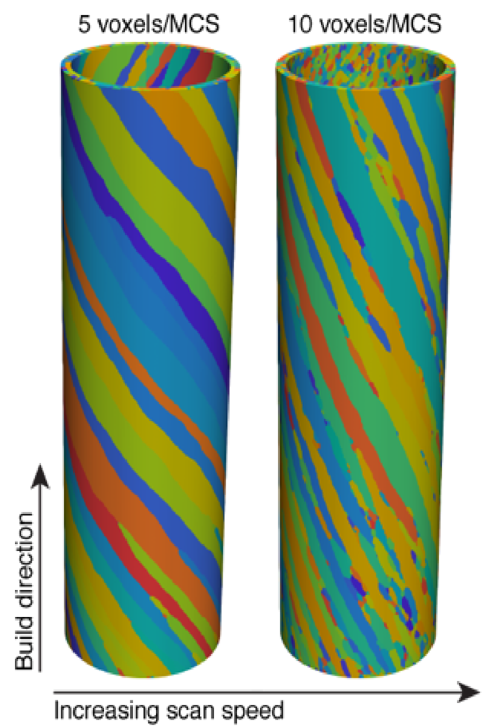


Synthetic AM builds



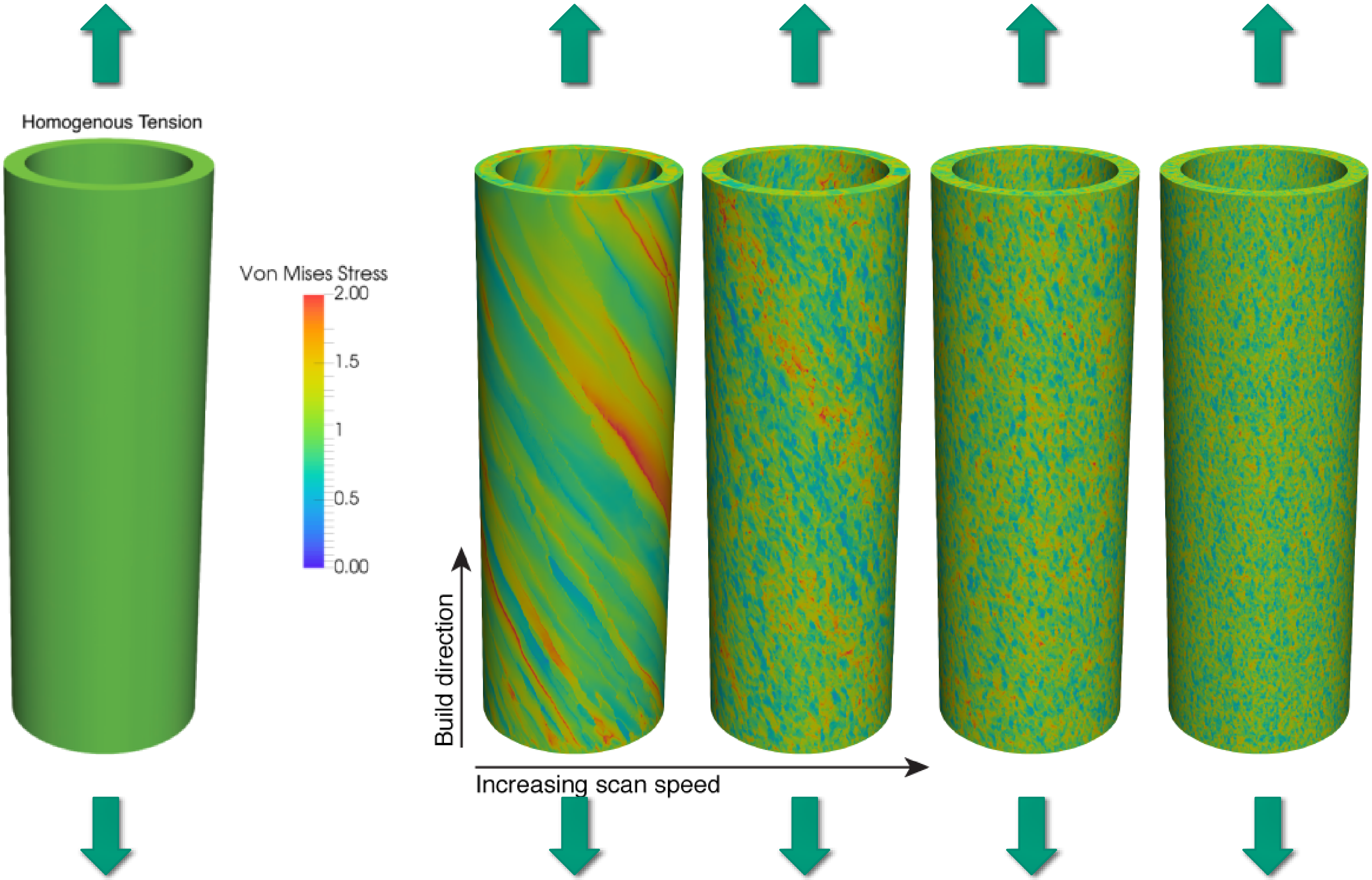
- 4 scan velocities.
- 2 concentric circular scan paths per layer.
- Idealized molten pool
- Significant microstructure variation w.r.t. scan velocities and w.r.t. wall thickness.



Wall Mid-plane

Rodgers, Bishop, and Madison, MSMSE 2018

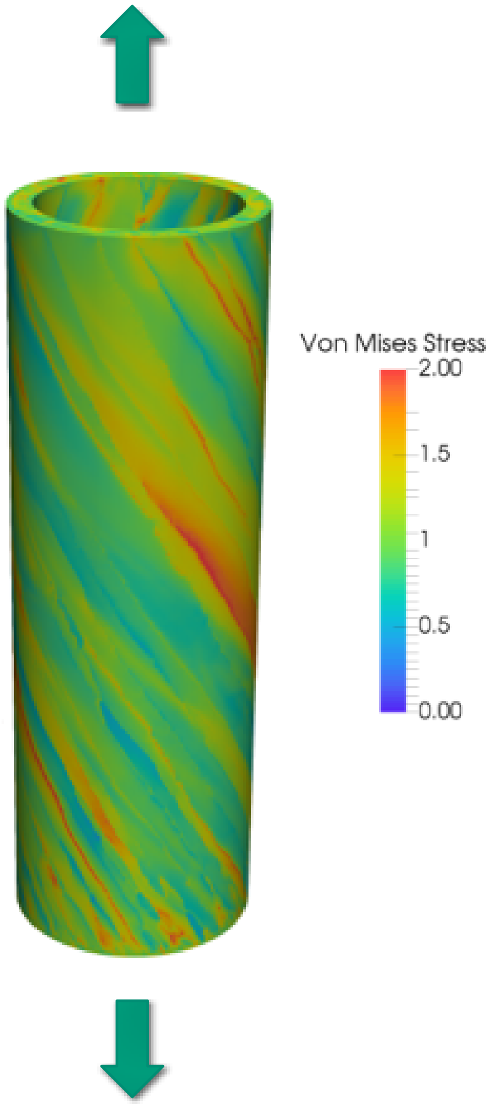
Direct Numerical Simulation on Additive Microstructures

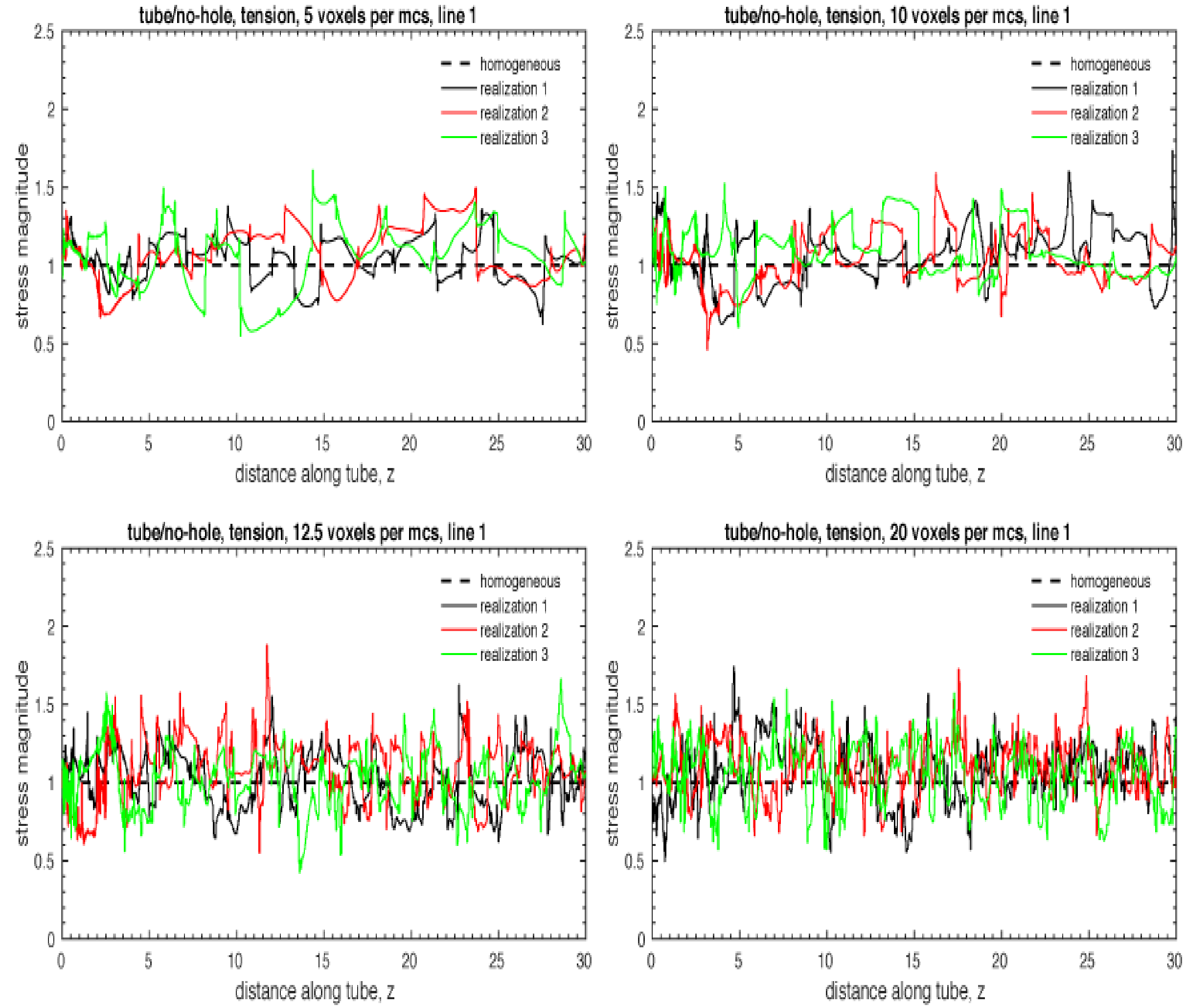


Stress response in tension

Rodgers, Bishop, and Madison, MSMSE 2018

Direct Numerical Simulation on Additive Microstructures

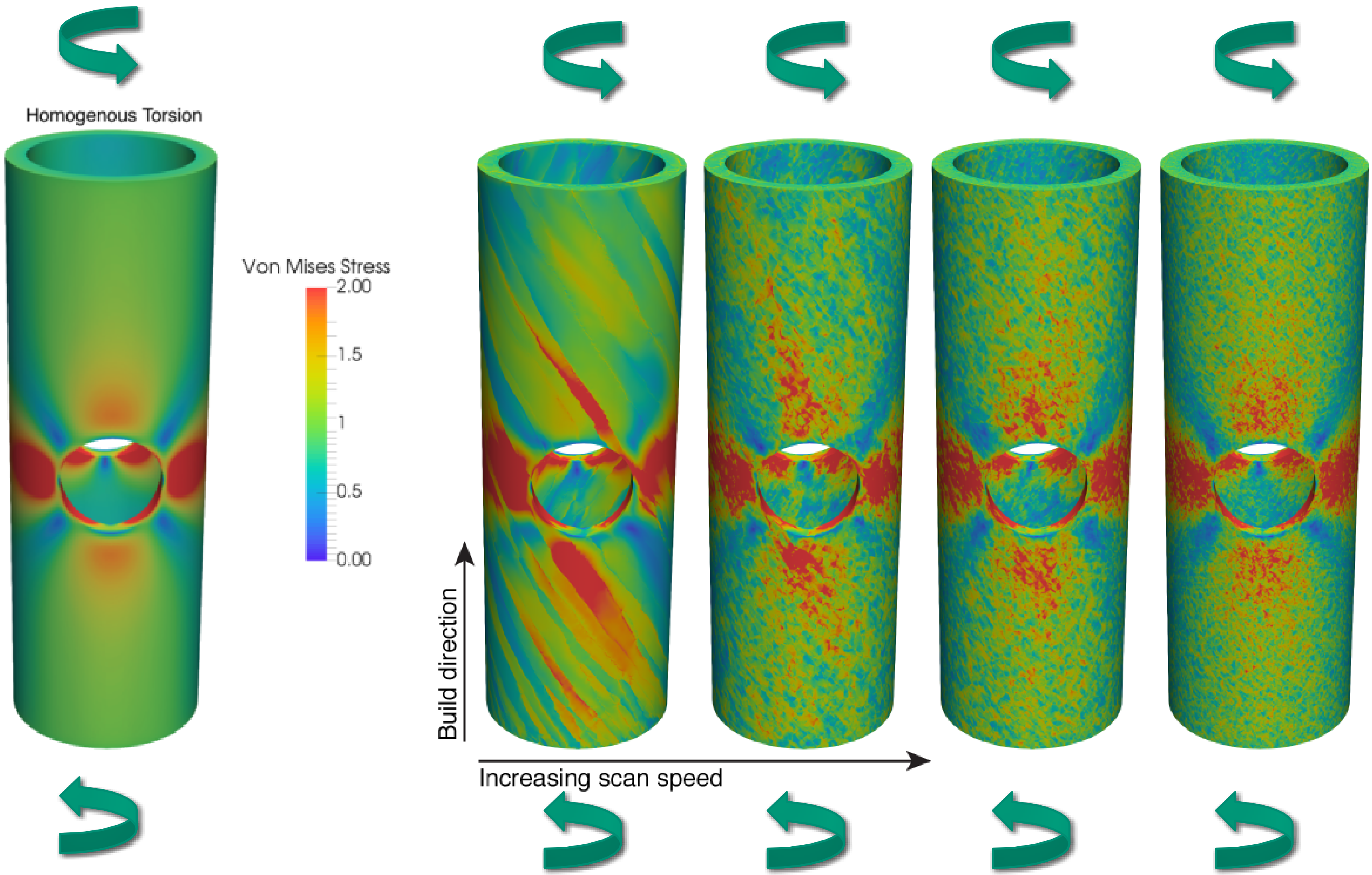




Stress response in tension

Rodgers, Bishop, and Madison, MSMSE 2018

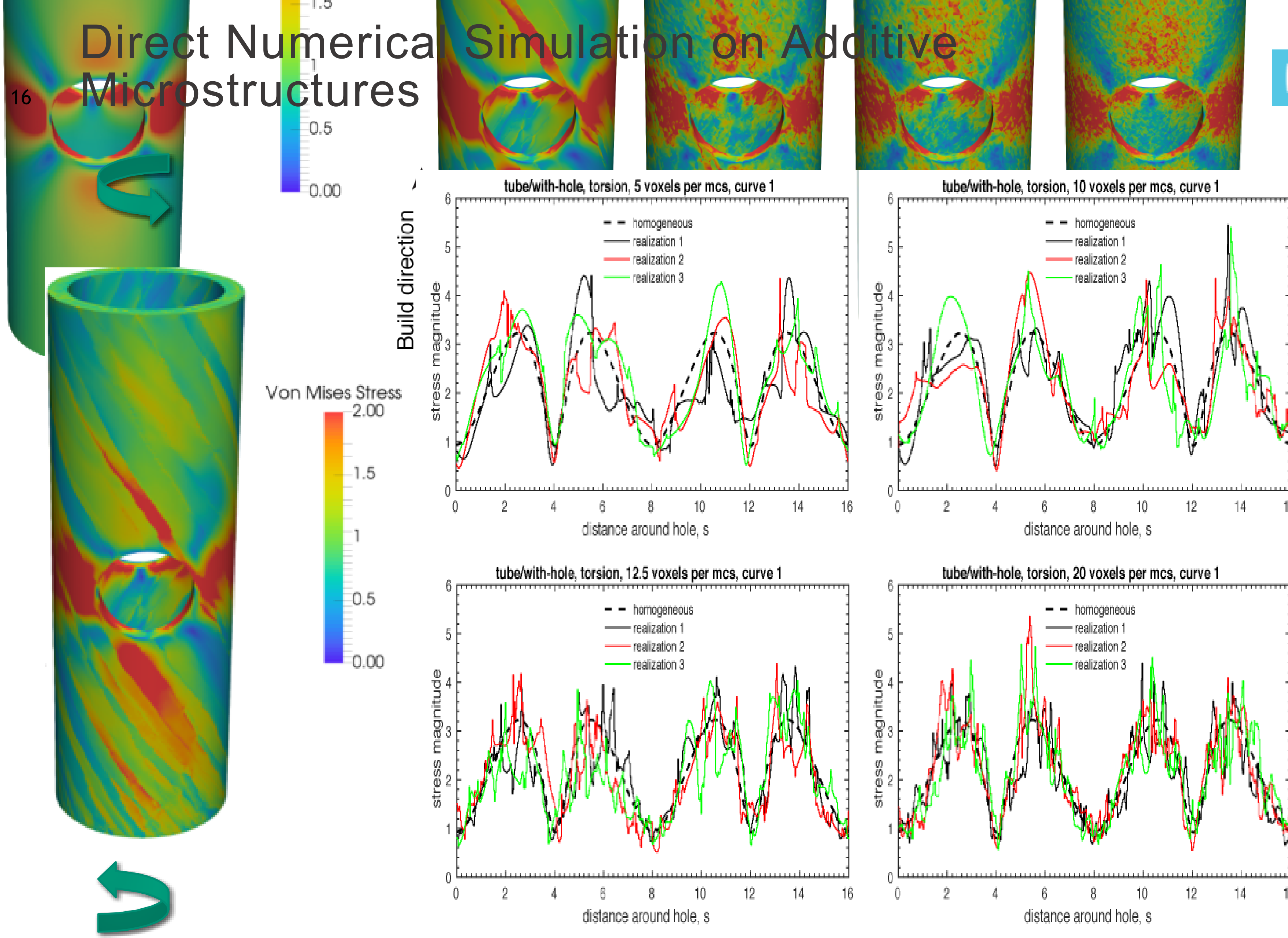
Direct Numerical Simulation on Additive Microstructures



Stress response in torsion

Rodgers, Bishop, and Madison, MSMSE 2018

Direct Numerical Simulation on Additive Microstructures



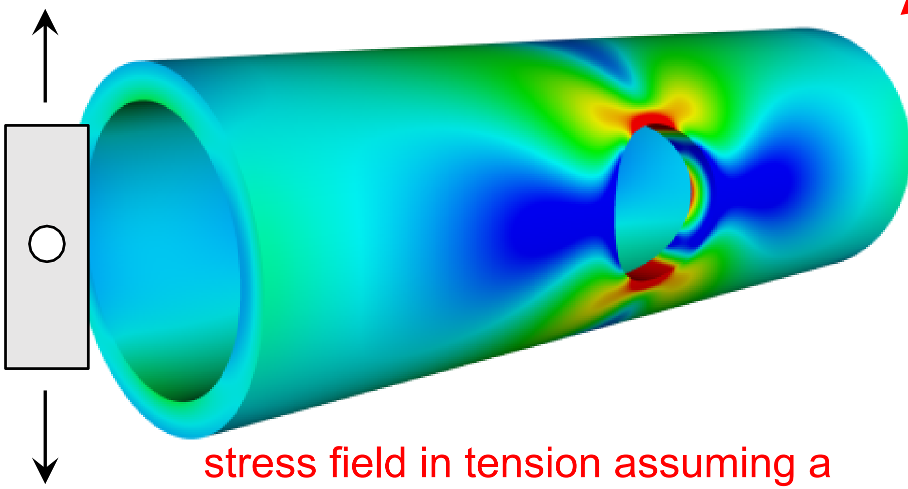
Stress response in torsion

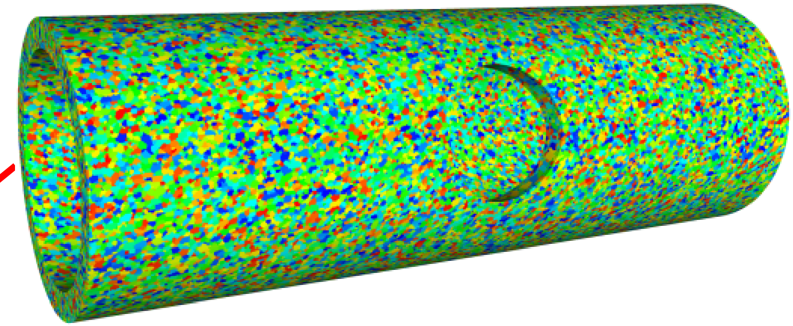
Rodgers, Bishop, and Madison, MSMSE 2018

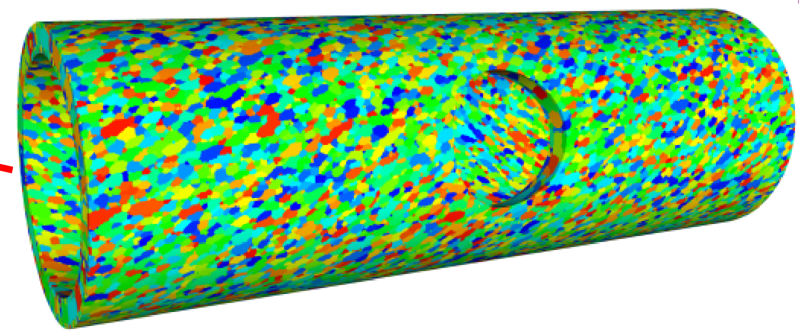
Error estimation as UQ

variable microstructure

- simple macroscale model
- deterministic (simulate once)
- assess error *a posteriori*





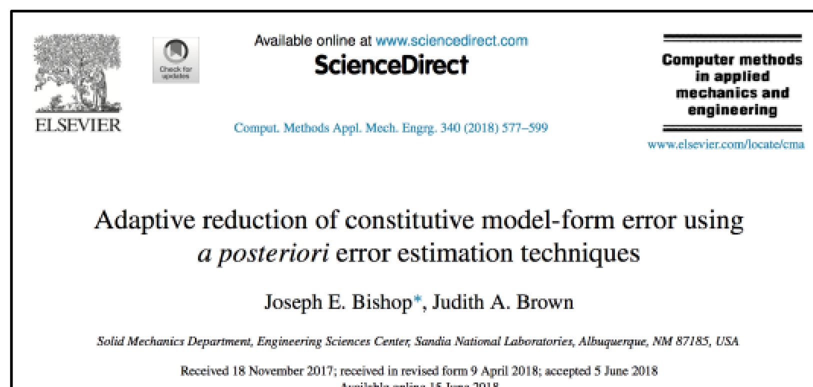


stress field in tension assuming a homogeneous isotropic material

time to failure

stochastic bound

$$t_{\mathrm{f}}(\omega) \longrightarrow t_f \leq \eta(\omega)$$



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Adaptive reduction of constitutive model-form error using *a posteriori* error estimation techniques

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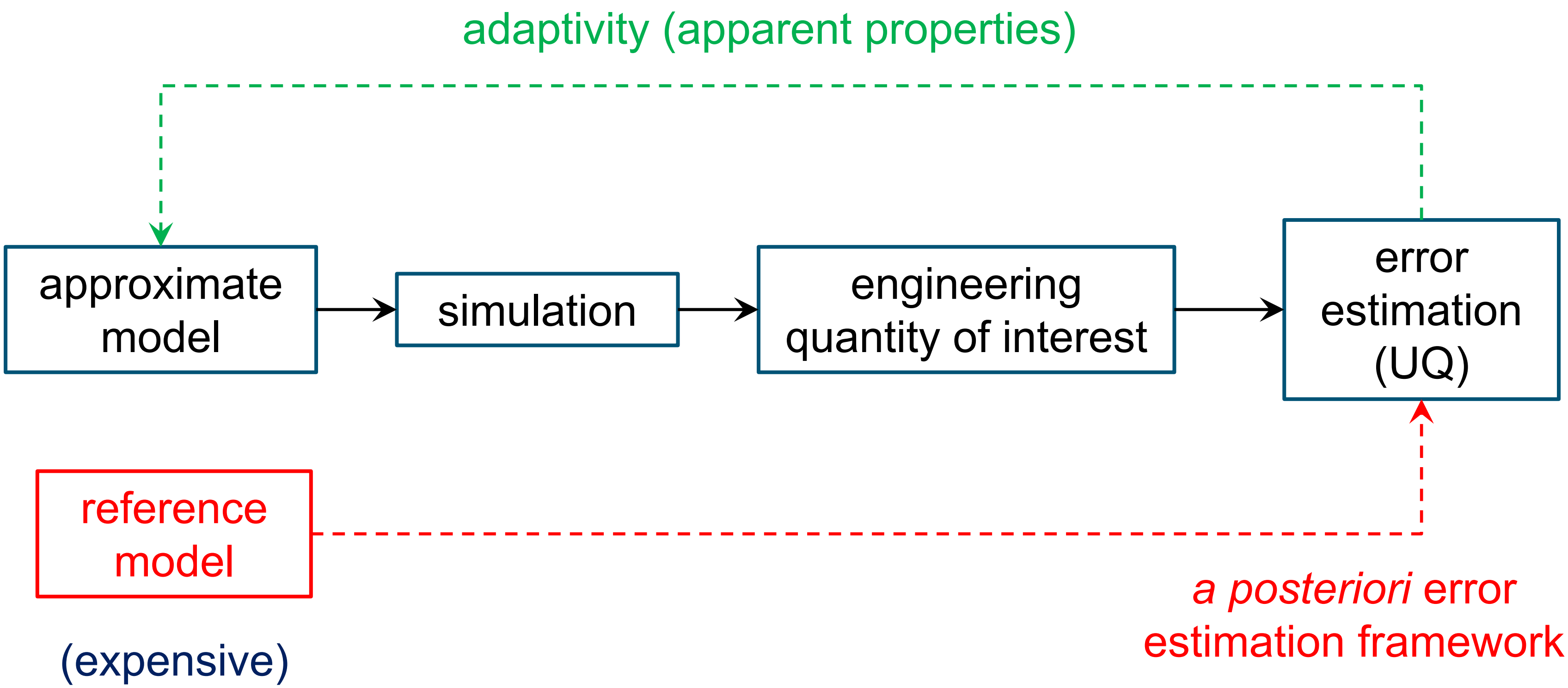
Received 18 November 2017; received in revised form 9 April 2018; accepted 5 June 2018
Available online 15 June 2018

Error estimation and adaptivity



time to failure

stochastic bound

$$t_{\mathrm{f}}(\omega) \longrightarrow t_f \leq \eta(\omega)$$

Error estimation: material-model error

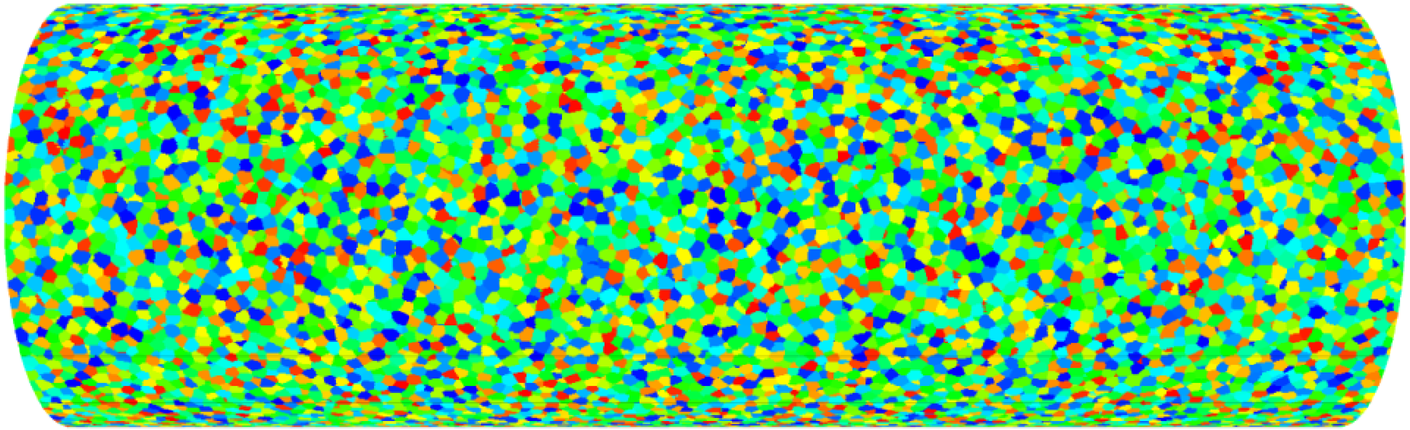
(Zohdi, Oden, Rodin, 1996, “Hierarchical modeling of heterogeneous bodies”, CMAME)

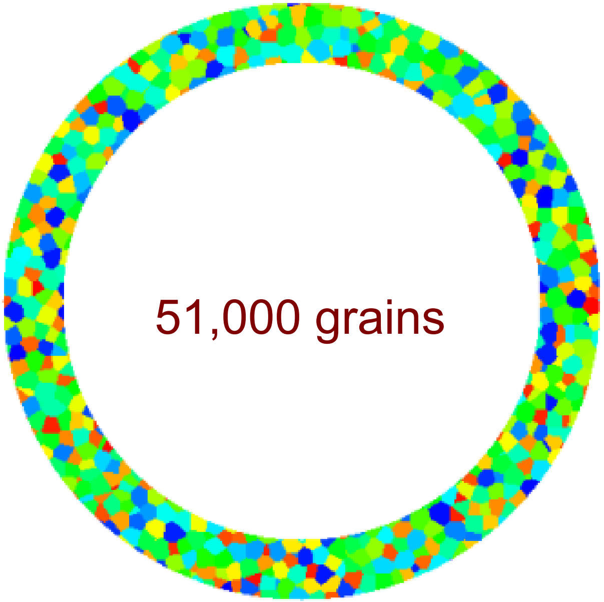
$$||\mathbf{u} - \mathbf{u}^0||_E^2 \leq \int_\Omega (\boldsymbol{\varepsilon}^0 - \bar{\boldsymbol{\varepsilon}}) : (\bar{\boldsymbol{\sigma}} - \boldsymbol{\sigma}^0)\, d\Omega$$

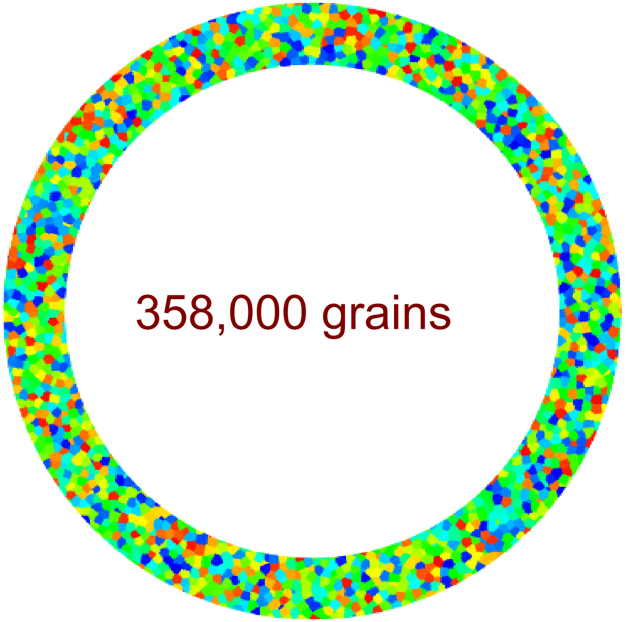
- displacement field using true material model ($\mathbf{u}$)
- approximate displacement field from simplified or approximate material model ($\mathbf{u}^0$)
- strain field resulting from approx. stress field but true material model ($\bar{\boldsymbol{\varepsilon}}$)
- stress field resulting from approx. strain field but true material model ($\bar{\boldsymbol{\sigma}}$)

<u>Key point</u>: Can bound error using only known quantities from the approximate simulation. Don’t need to run “true” model simulation.

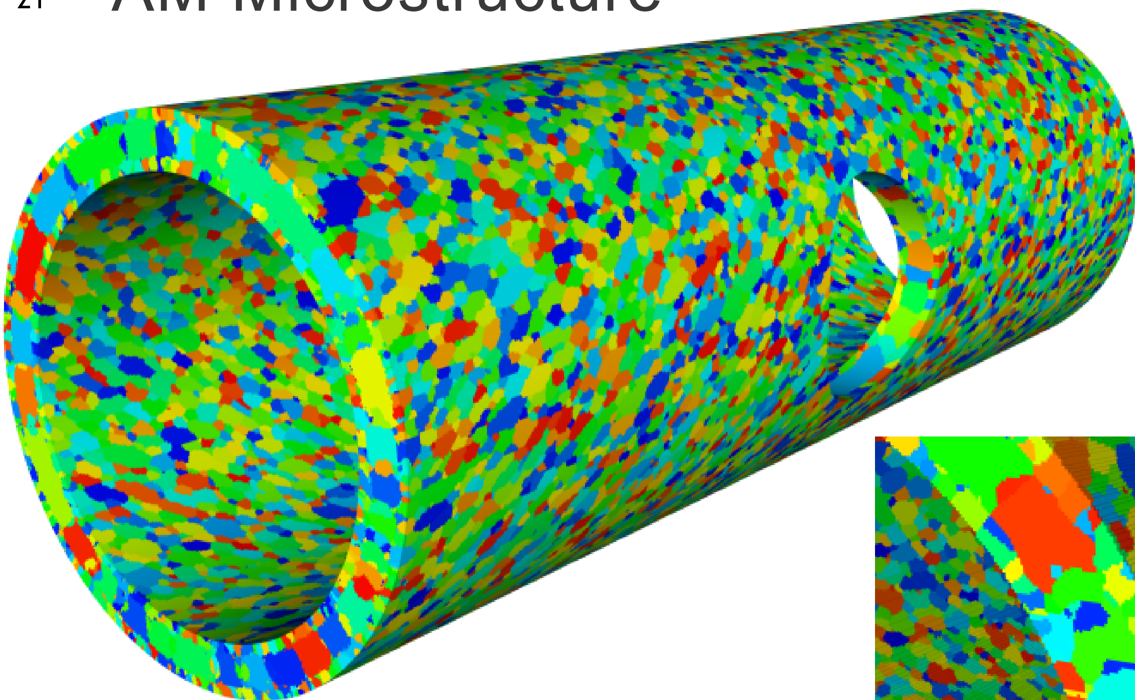
Equiaxed microstructure

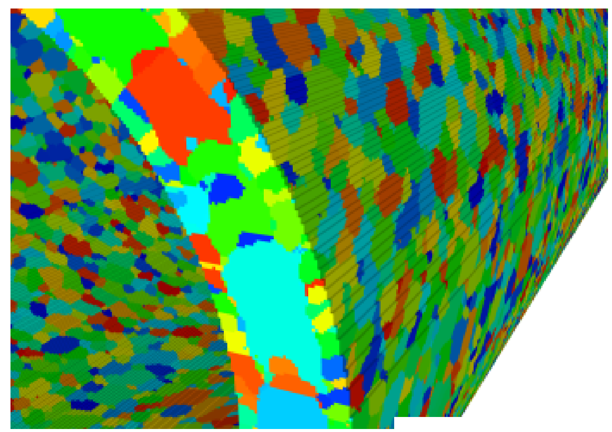




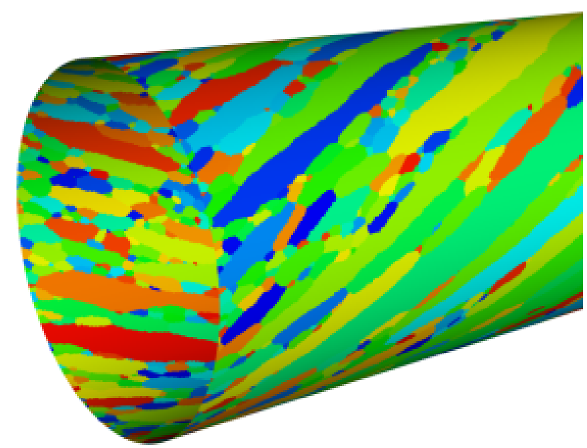


AM Microstructure



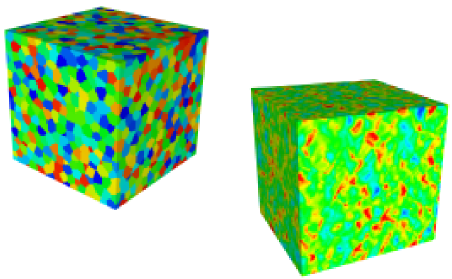


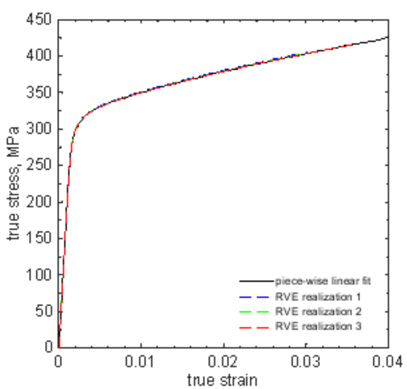
- KMC (SPPARKS) voxelated geometry
- 55M voxels
- two laser passes per layer (difference between surface and interior microstructure)
- map to conformal finite-element mesh
- 30M finite elements



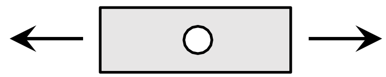
Homogenization-Localization Duality

Homogenize Using Crystal Plasticity (filter fine scale)

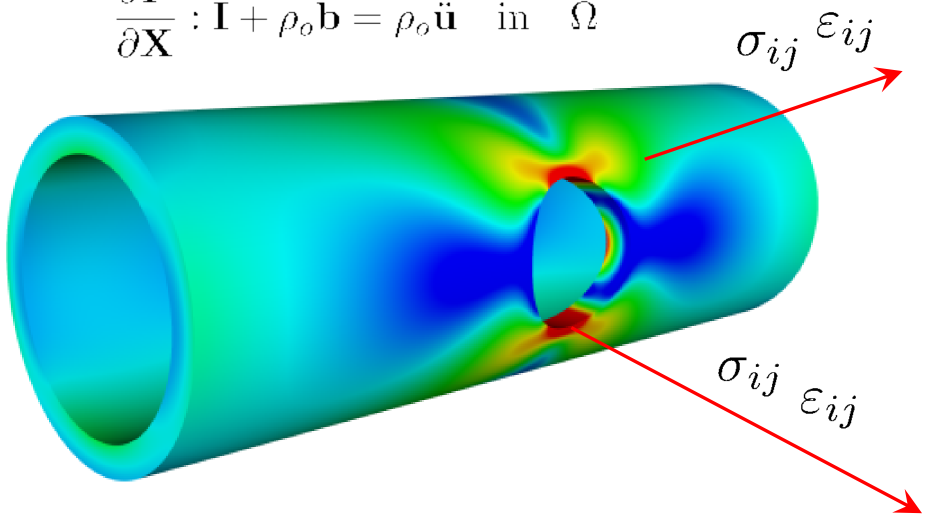




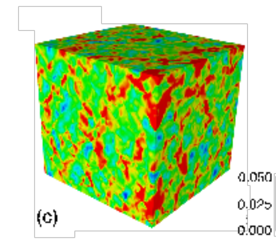
Macroscale simulation

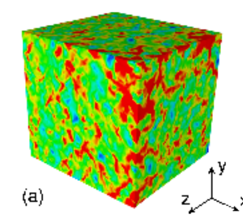


$$\frac{\partial \mathbf{P}}{\partial \mathbf{X}} : \mathbf{I} + \rho_o \mathbf{b} = \rho_o \ddot{\mathbf{u}} \quad \text{in} \quad \Omega$$



Localization (recover fine scale)

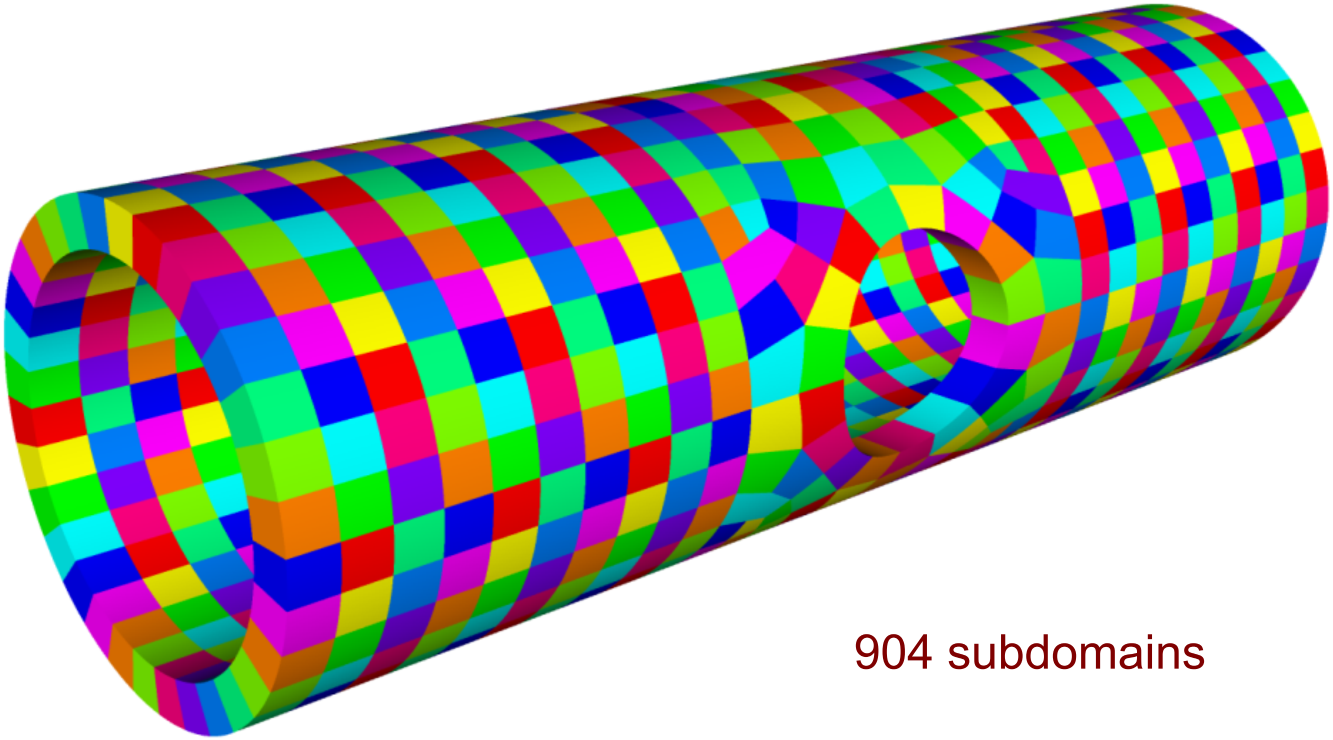




Assumptions:

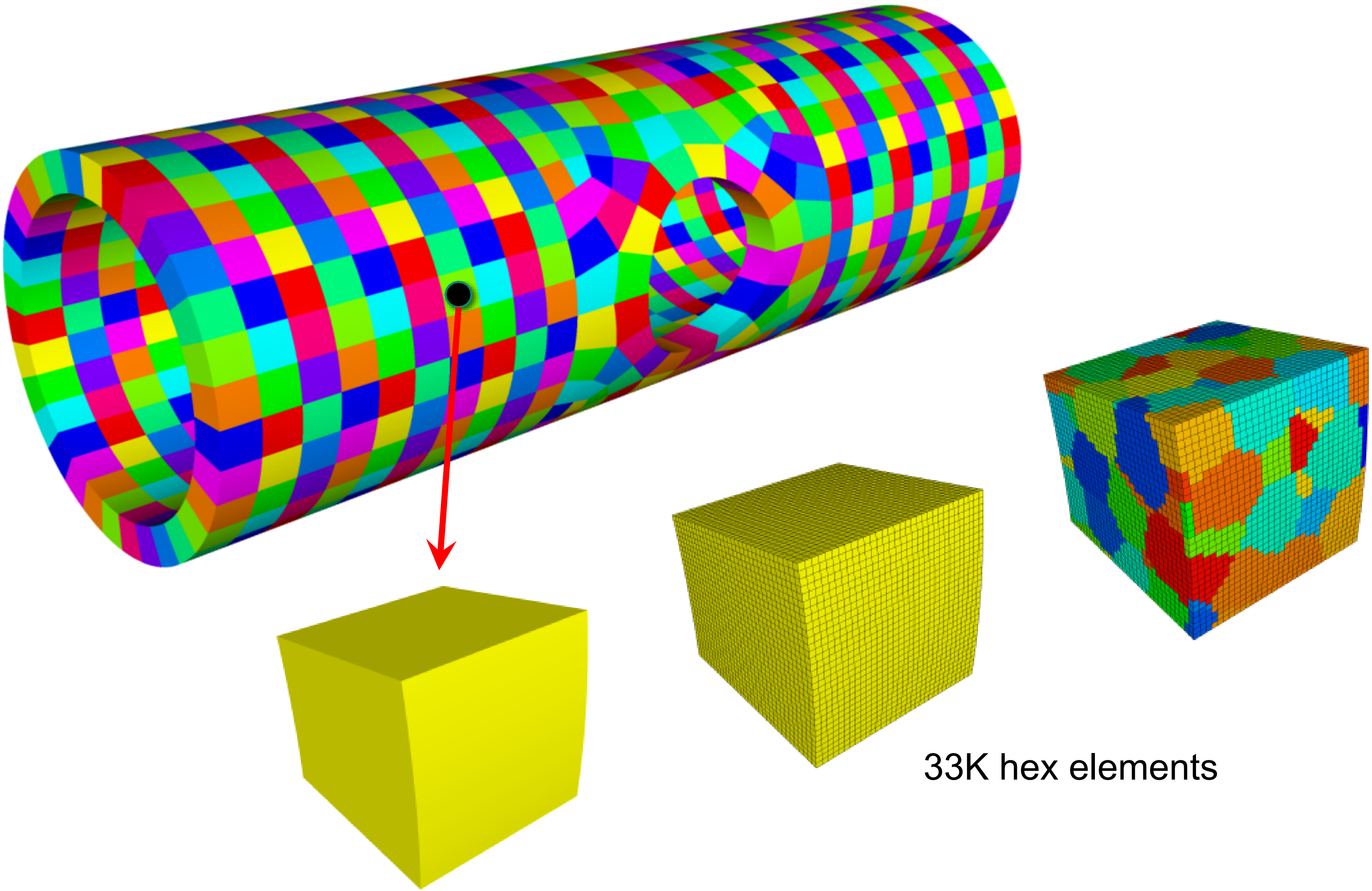
- scale separation
- RVE well defined
- no surface effects

First, partition structure into non-overlapping subdomains.



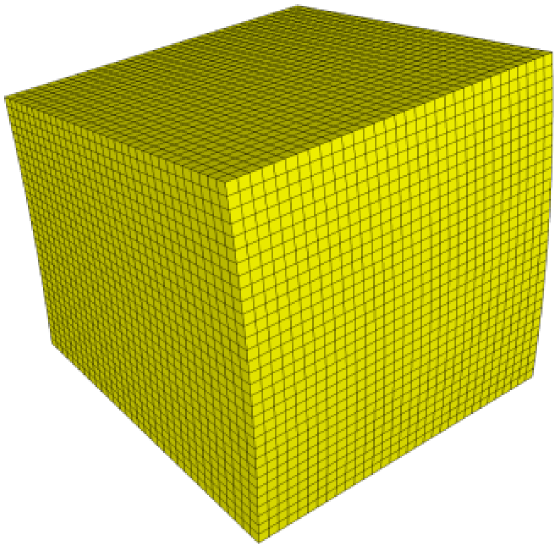
904 subdomains

Type 1 localization



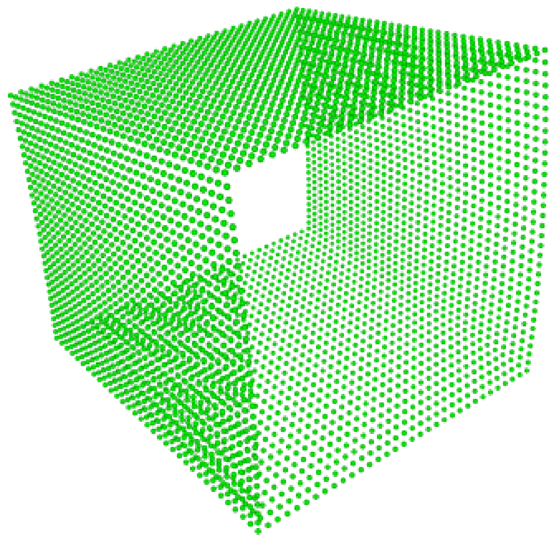
Type 1 localization

submodel

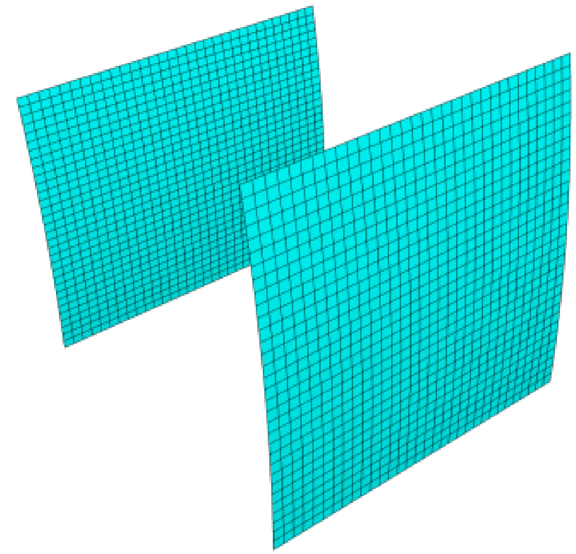


33K hex elements

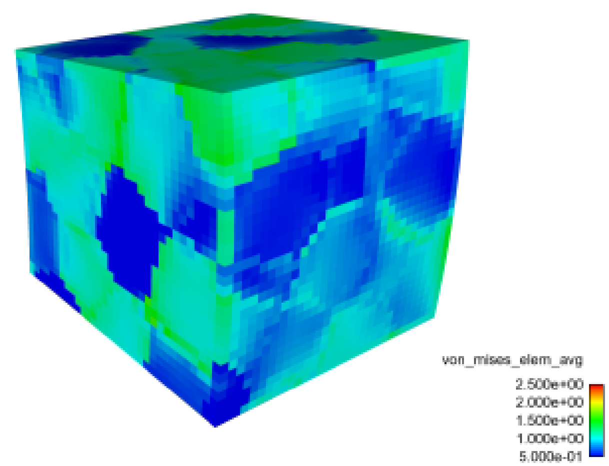
displacement b.c.s



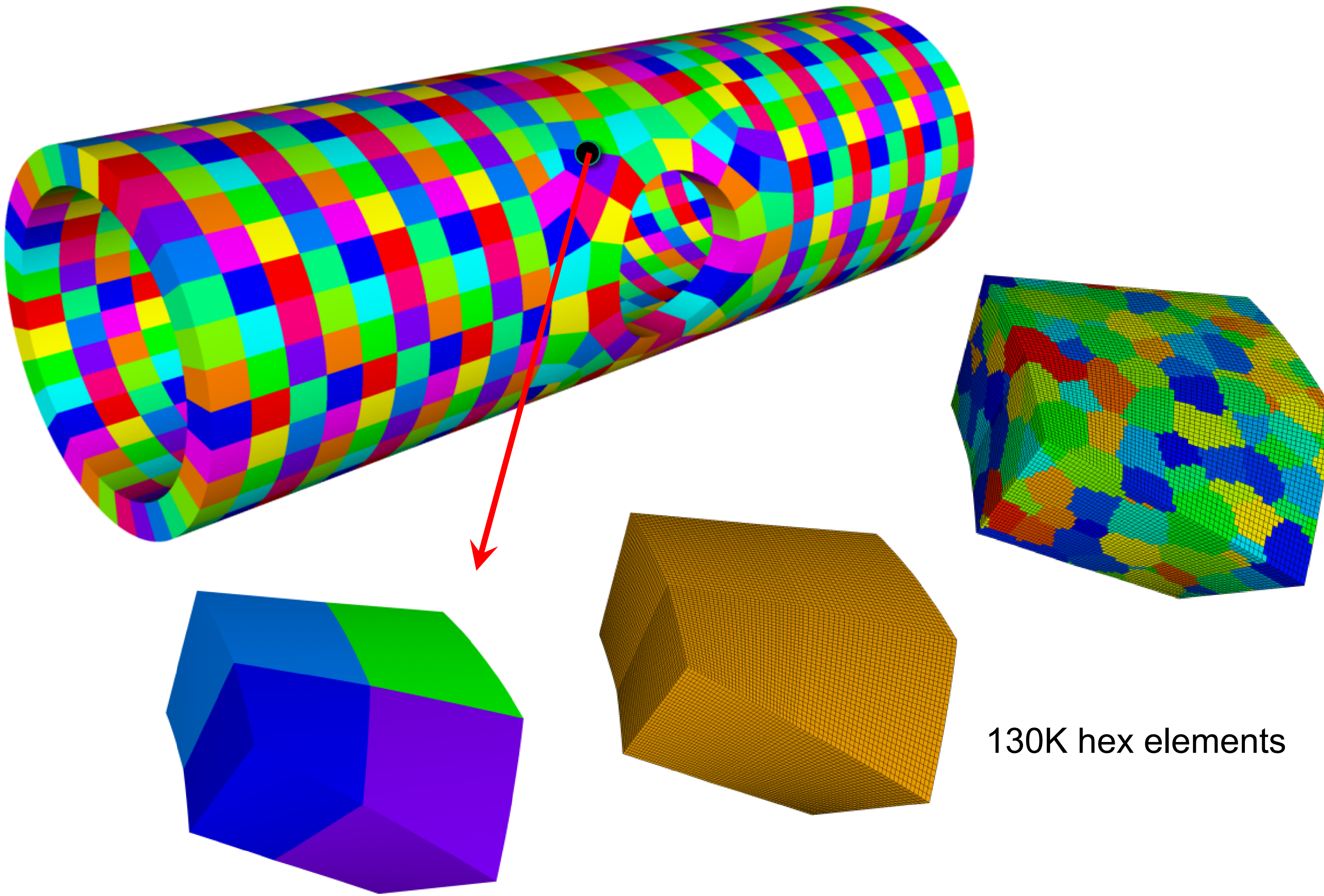
traction b.c.s



local stress field

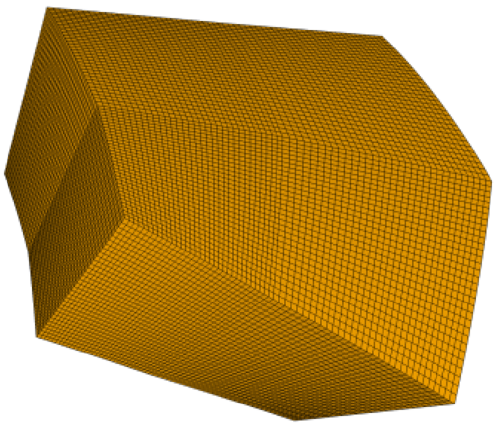


Type 2 localization (overlapping)

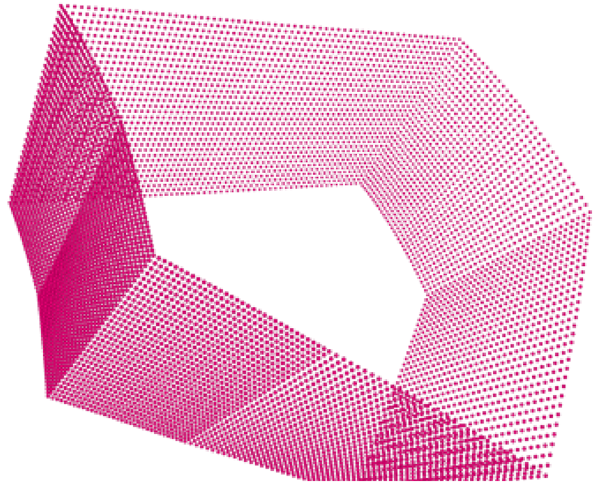


Type 2 localization

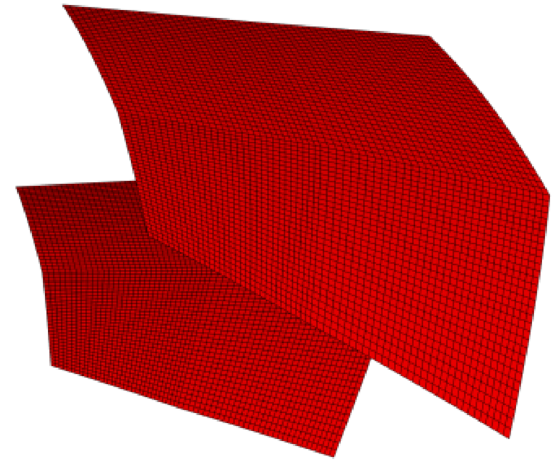
submodel



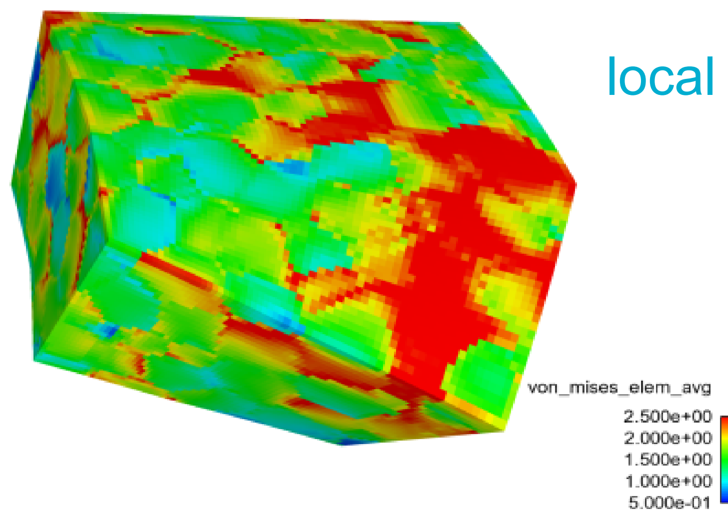
displacement b.c.s



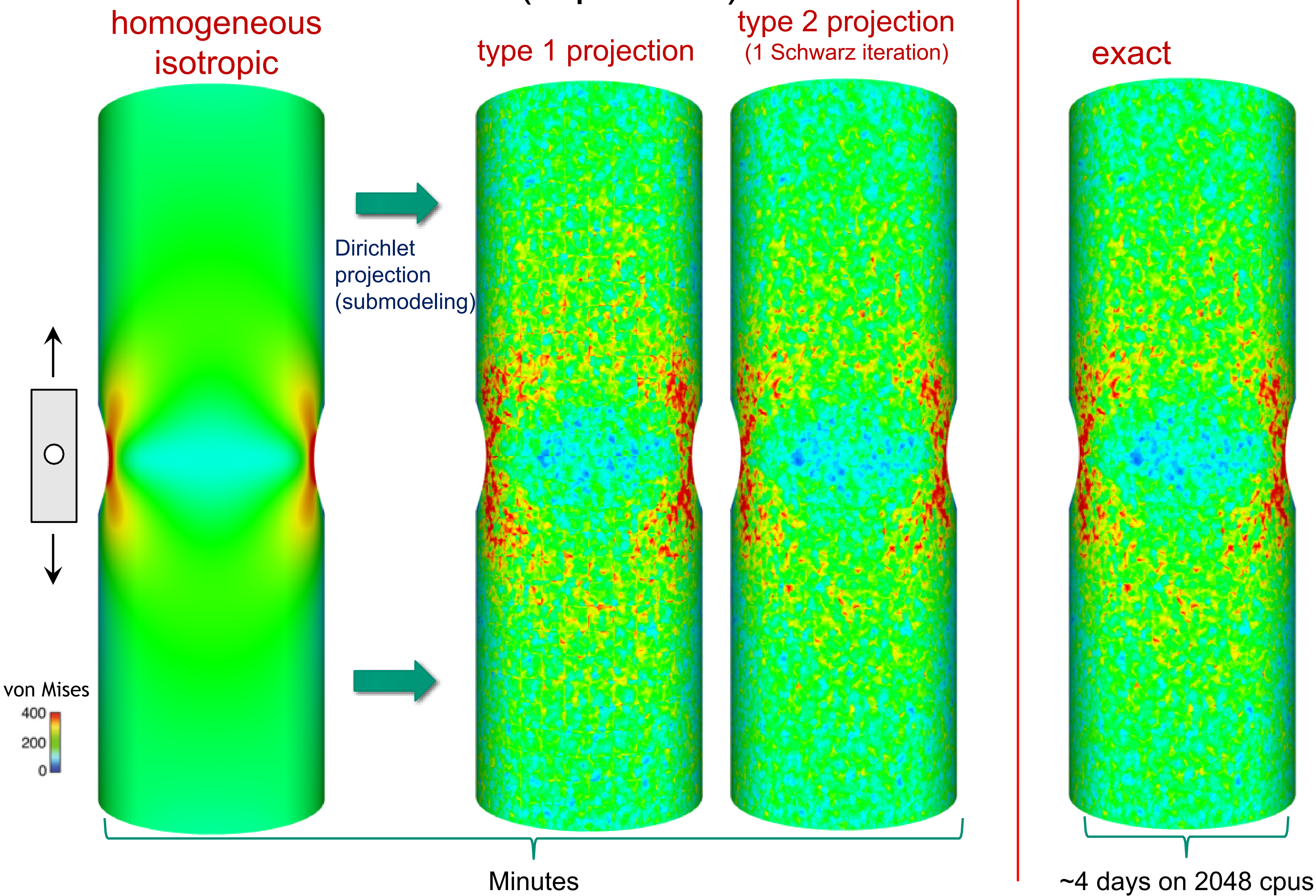
traction b.c.s



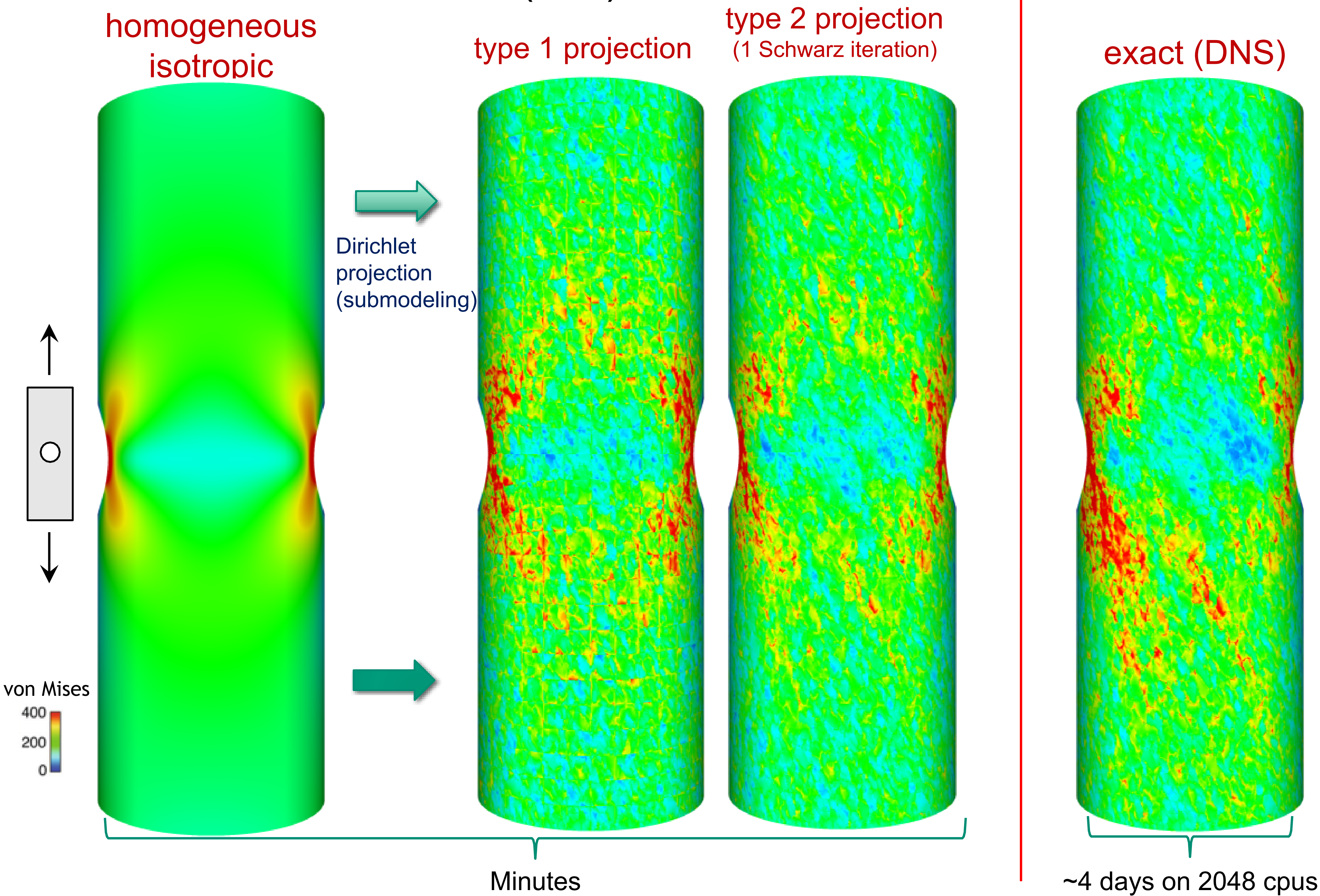
local stress field



Localization results (equiaxed)

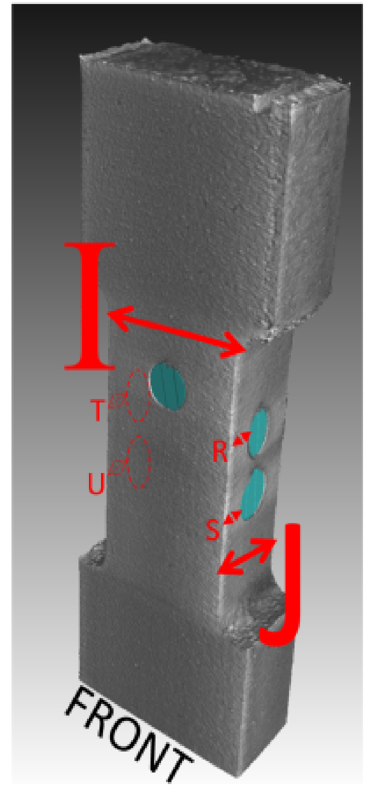


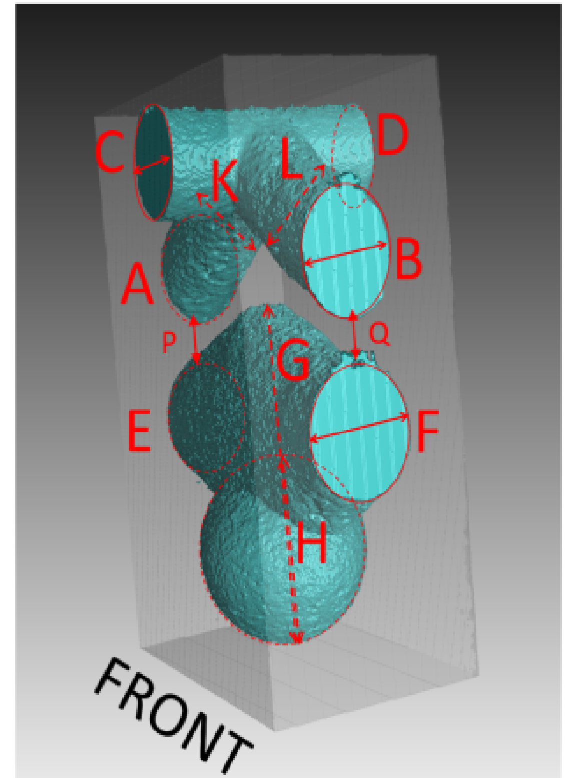
Localization results (AM)

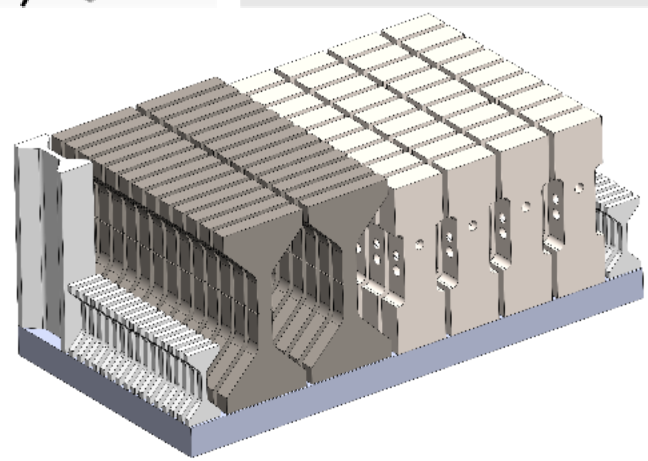


Sandia Fracture Challenge

- 316L Stainless Steel LPBF Part
- Complex geometry with internal channels and spherical cavity
- Loaded in tension
- Given CT data along with smooth tension and notched tension data
- Challenge Questions:
    - Force at four different displacements
    - Force and log strain at four points on front face
    - Total force-displacement curve
    - Force and log strain along four horizontal lines on front face
    - Images of front surface at crack initiation and complete failure
- 21 Participant Teams







Kramer, Boyce et al., *IJF (In preparation), Johnson* et al. *IJF (In preparation)*

Sandia/NM Predictive Approach

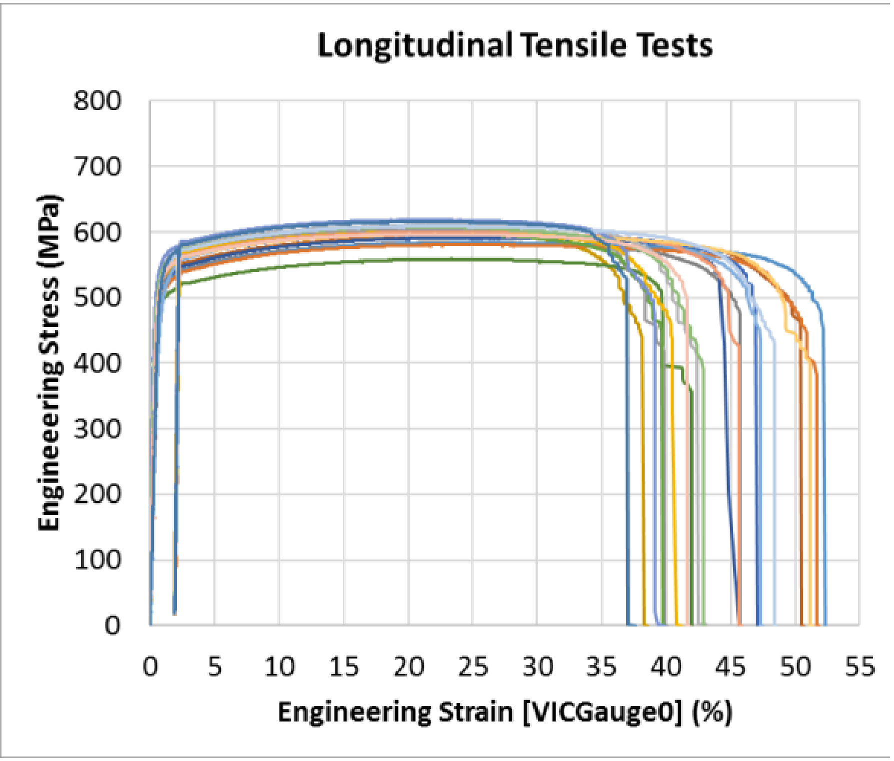
1. Fit robust plasticity model to calibration test data with porosity distributions as initial damage
2. Run many iterations of challenge geometry with many porosity distributions
3. Perform statistical analysis on results to enrich result distributions

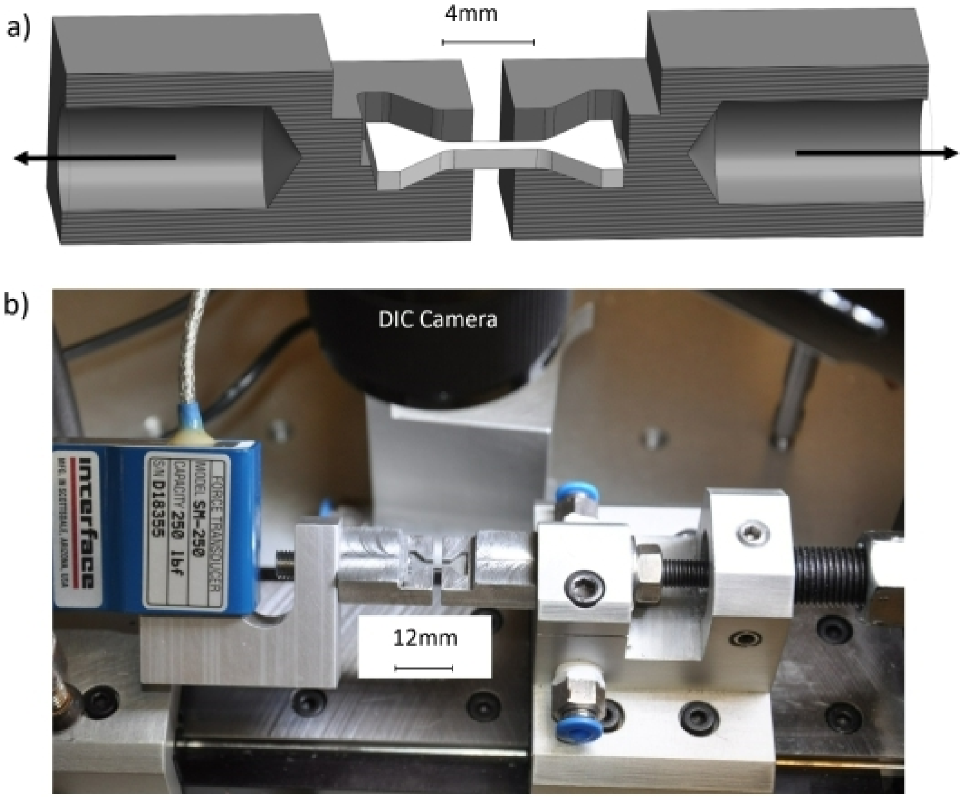
SNL/NM Team Members: Kyle Johnson, John Emery, Kurtis Ford, Joe Bishop, Judy Brown, Chris Hammetter, Spencer Grange

Additional help from Kyle Karlson (SNL/CA)

Kramer, Boyce et al., *IJF (In preparation), Johnson* et al. *IJF (In preparation)*

Tension Data Was Taken Using High Throughput Test Method





a) Model of Additive Manufactured Tensile Specimen in grips (cut-away). b) Mechanical Test Set-up. [Salzbrenner, *et.al,* JMPT 2017]

Kramer, Boyce et al., *IJF (In preparation), Johnson* et al. *IJF (In preparation)*

BCJ Material Model

- Temperature and history-dependent viscoplastic internal state variable model
- Stress is dependent on damage ϕ and evolves according to

$$\dot{\sigma} = \left(\frac{\dot{E}}{E} - \frac{\dot{\phi}}{1-\phi}\right)\sigma + E(1-\phi)(\dot{\epsilon} - \dot{\epsilon_p})$$

- Flow rule includes yield stress and internal state variables for hardening and damage

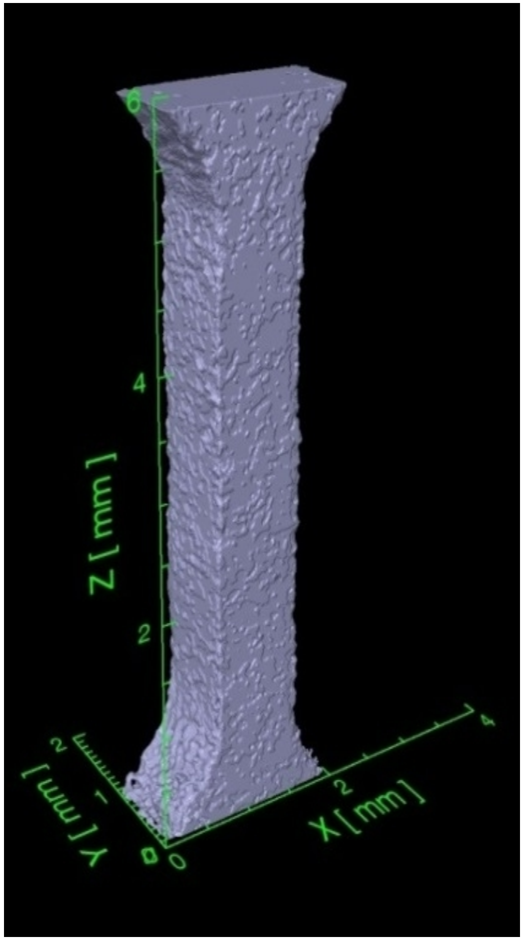
$$\dot{\epsilon}_p = f\,sinh^n\left(\frac{\frac{\sigma_e}{1-\phi} - \kappa}{Y} - 1\right)$$

- The isotropic hardening variable κ evolves in a hardening minus recovery form.

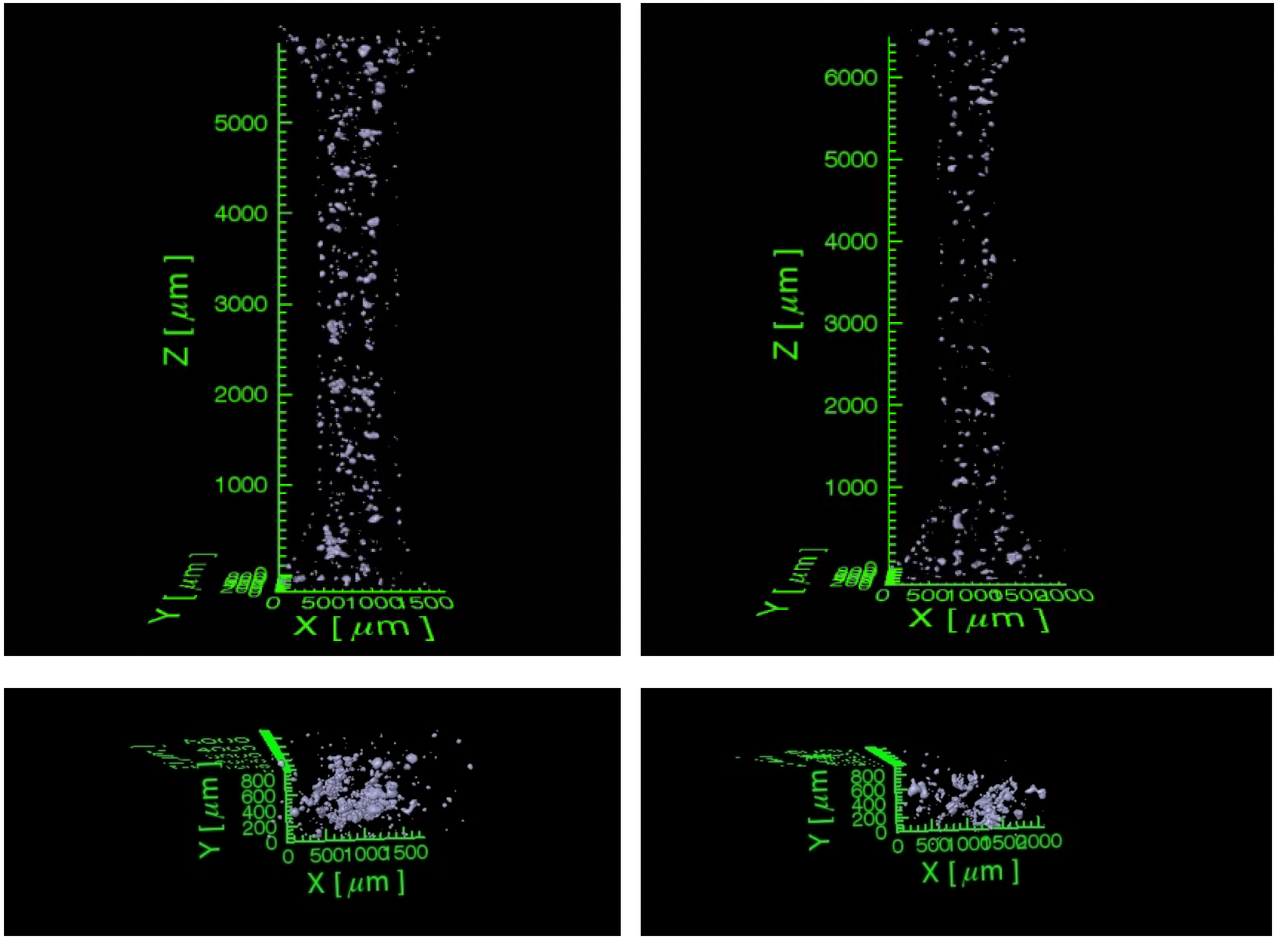
$$\dot{\kappa} = \kappa\frac{\dot{\mu}}{\mu} + (H(\theta) - R_d(\theta)\kappa)\dot{\epsilon}_p$$

Kramer, Boyce et al., *IJF (In preparation), Johnson* et al. *IJF (In preparation)*

3D Reconstruction & Characterization of Pore Defects



3D μCT surface render

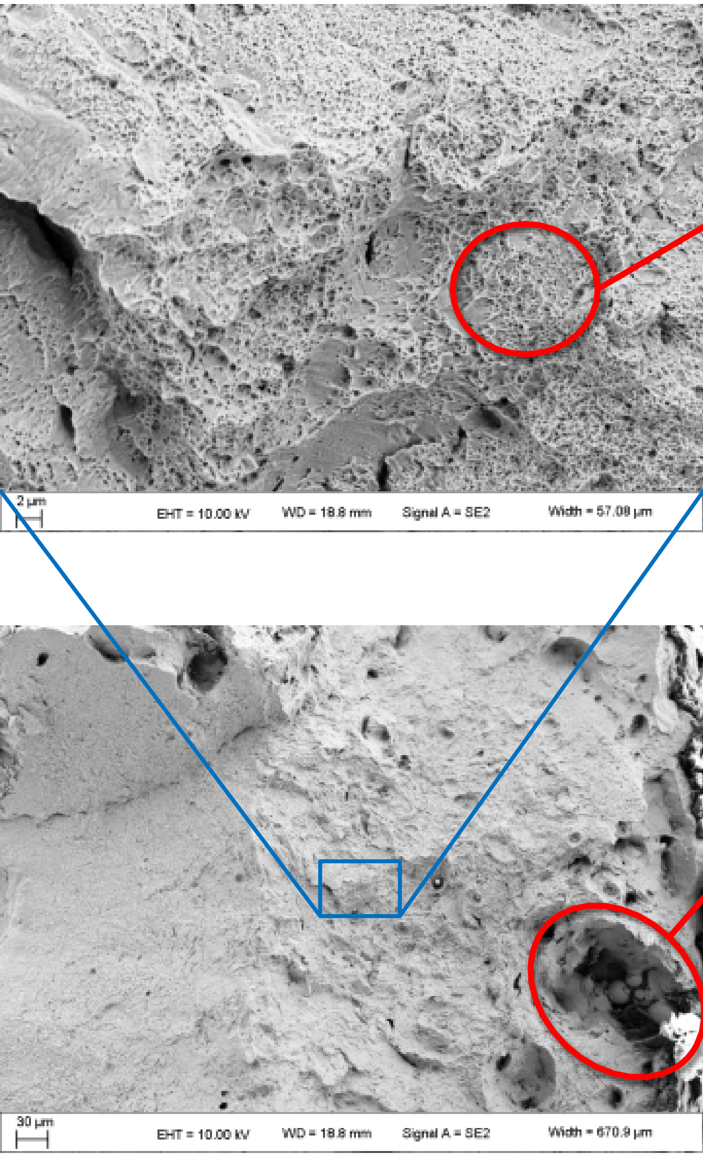


3D μCT internal porosity

Tremendous variation in pore content from sample to sample
Pore locations reminiscent of AM laser raster pattern

J. Madison, T. Ivanoff, O. Underwood

Incorporating porosity as initial damage



<u>Void Nucleation</u>

Fine scale voids (< 1μm) indicate nucleation

$$\dot{\eta} = \eta \dot{\epsilon}_p \left(N_1 \left[\frac{4}{27} - \frac{J_3^2}{J_2^3} \right] + N_2 \frac{J_3}{J_2^3} + N_3 \frac{\langle p \rangle}{\sigma_e} \right)$$

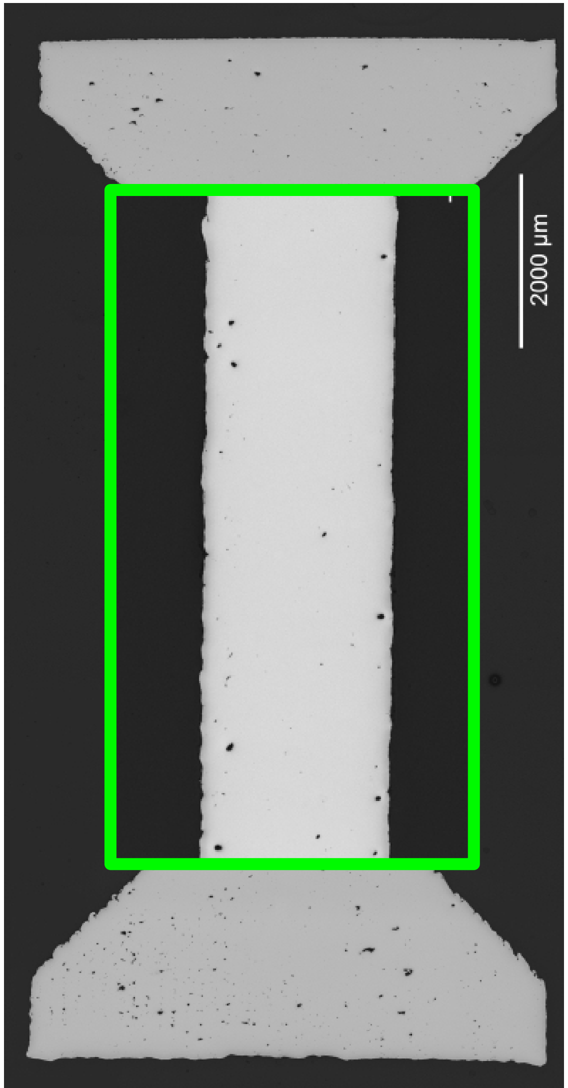
<u>Void Growth</u>

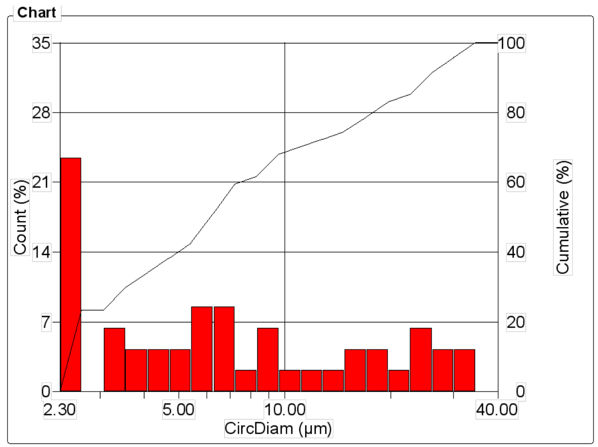
Pre-existing voids captured by void growth

$$\dot{\phi} = \sqrt{\frac{2}{3}} \dot{\epsilon}_p \frac{1 - (1 - \phi)^{m+1}}{(1 - \phi)^m} \sinh \left[\frac{2\,(2m - 1)}{2m + 1} \frac{\langle p \rangle}{\sigma_e} \right]$$

Kramer, Boyce et al., *IJF (In preparation), Johnson* et al. *IJF (In preparation)*

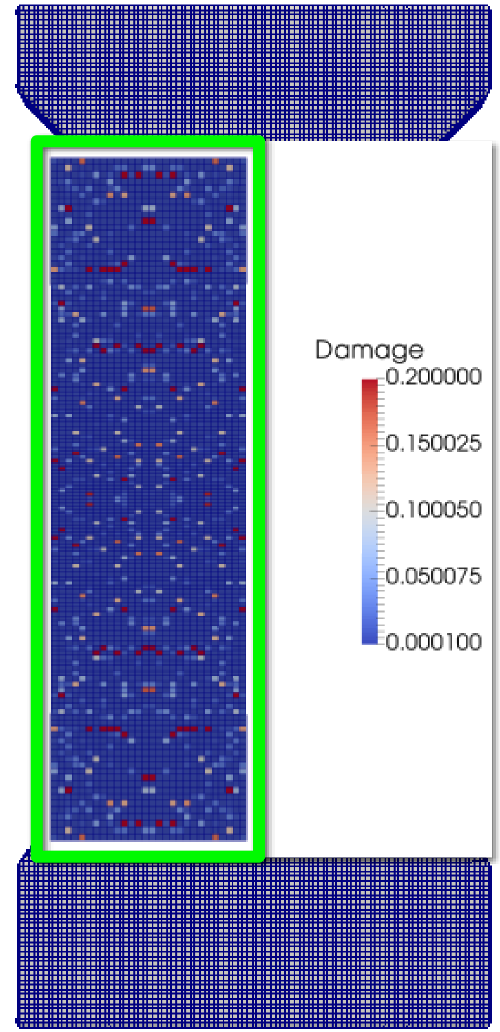
Porosity Distribution Directly Mapped to Mesh





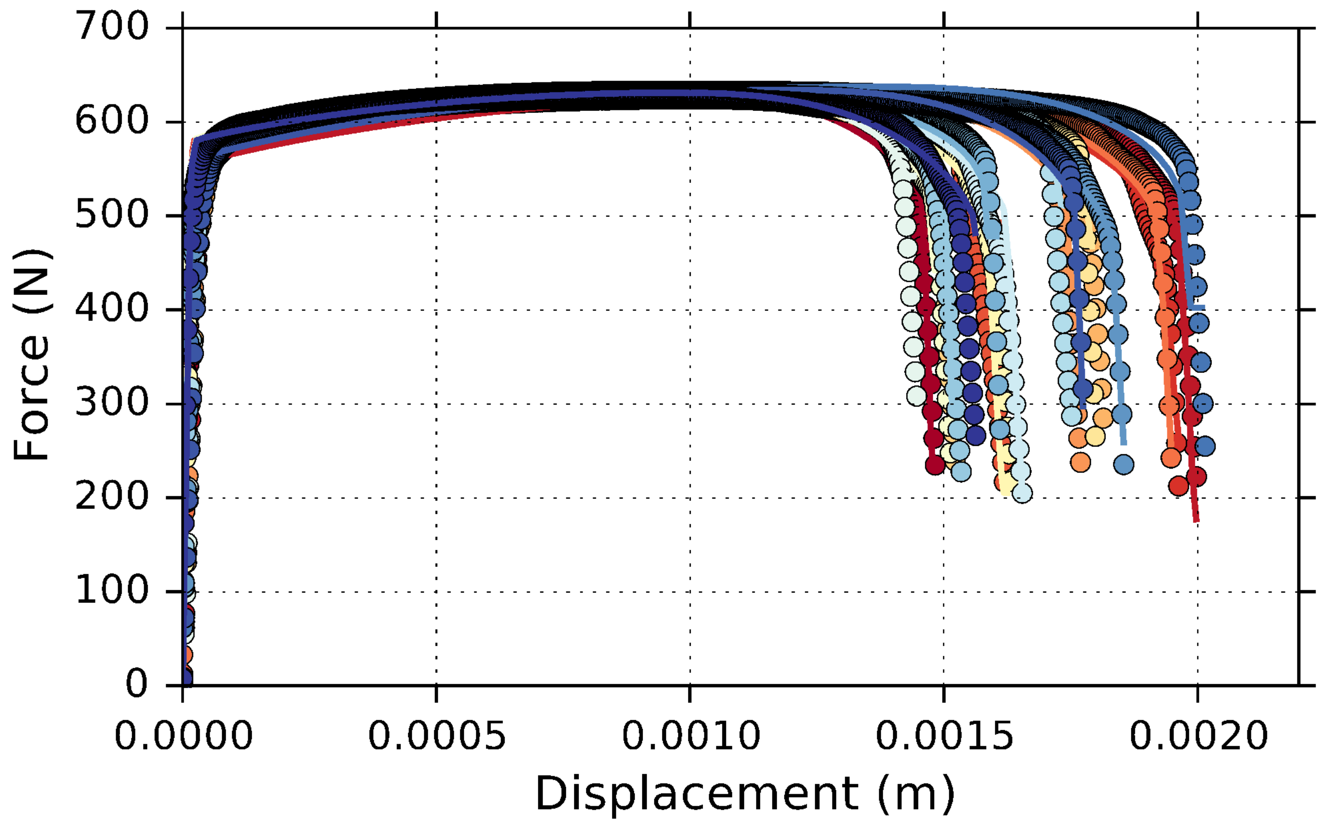
Porosity Mapping

x,y,z,r_{pore}



Kramer, Boyce et al., *IJF (In preparation), Johnson* et al. *IJF (In preparation)*

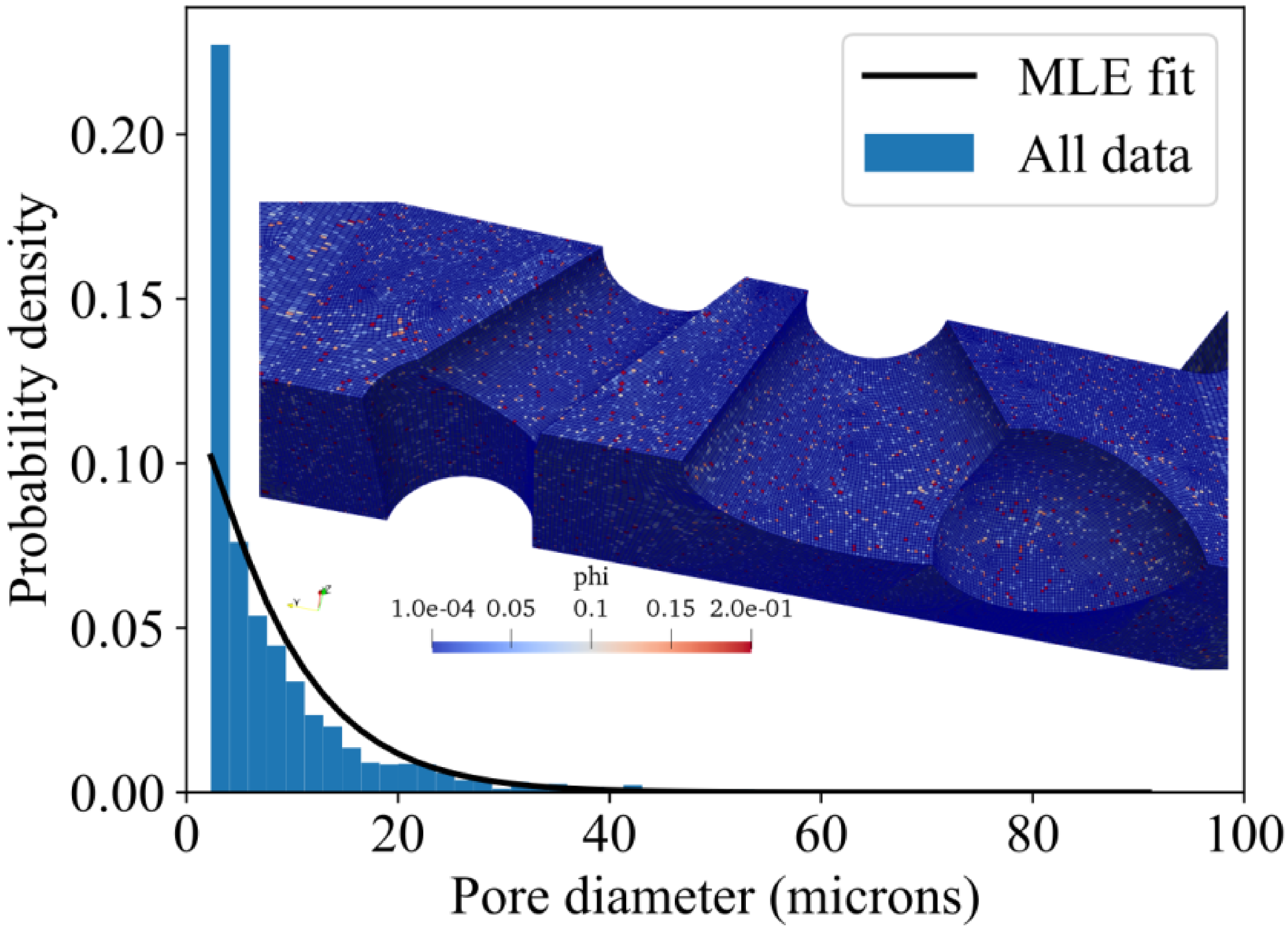
Calibration Results With Void Growth and Nucleation



- Each test has unique parameter set

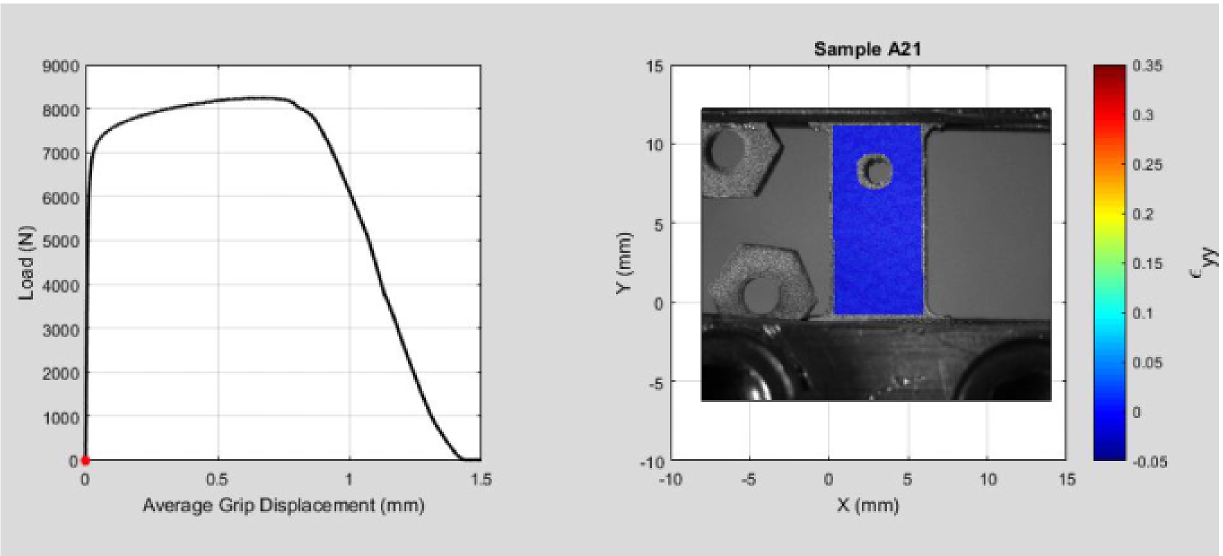
Kramer, *Boyce* et al., *IJF (In preparation)*, *Johnson* et al. *IJF (In preparation)*

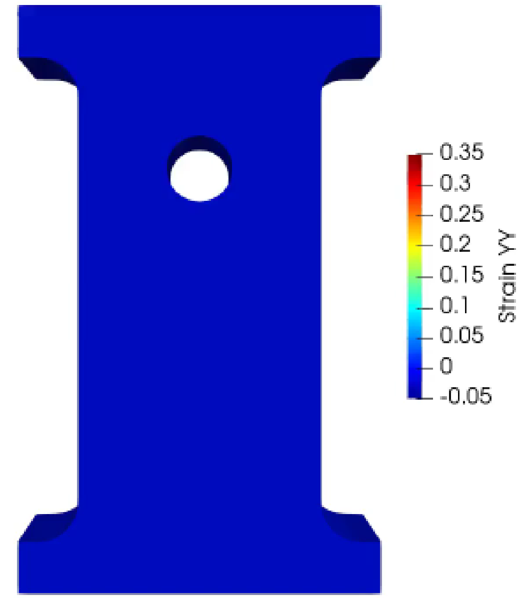
Porosity Distribution Directly Mapped to Challenge Geometry



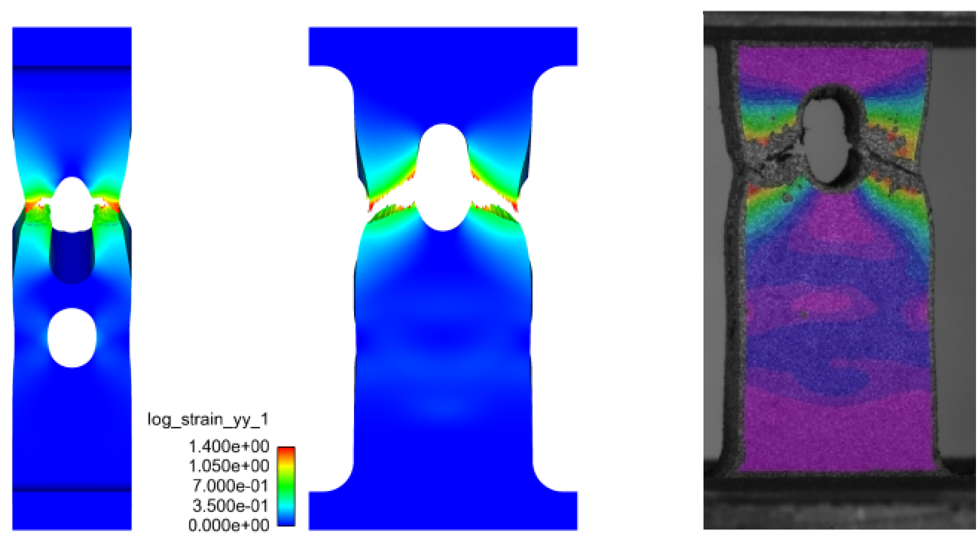
Kramer, Boyce et al., *IJF (In preparation), Johnson* et al. *IJF (In preparation)*

Performance Prediction and Experiments





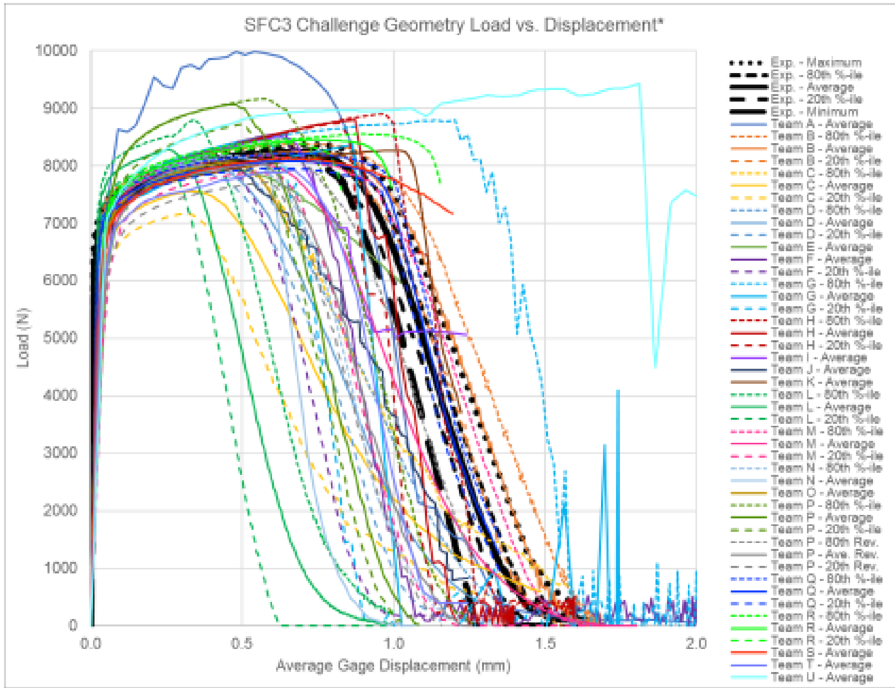
Crack initiation and propagation matches experiments well



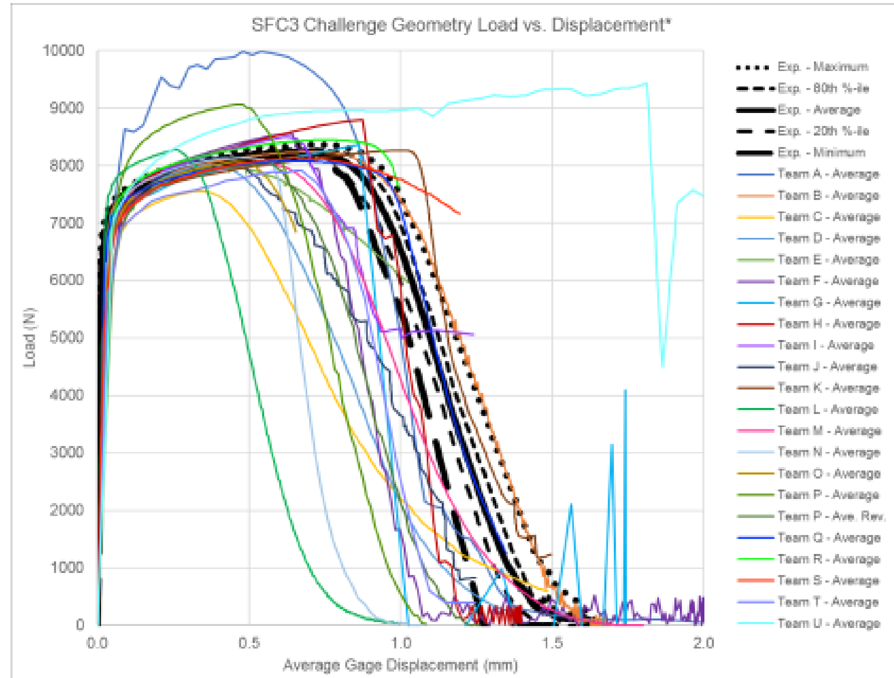
Kramer, Boyce et al., *IJF (In preparation), Johnson* et al. *IJF (In preparation)*

21 Participant Predictions Covered A Wide Range of Responses

21 Predictions and Bounds with Exp. Average and Bounds

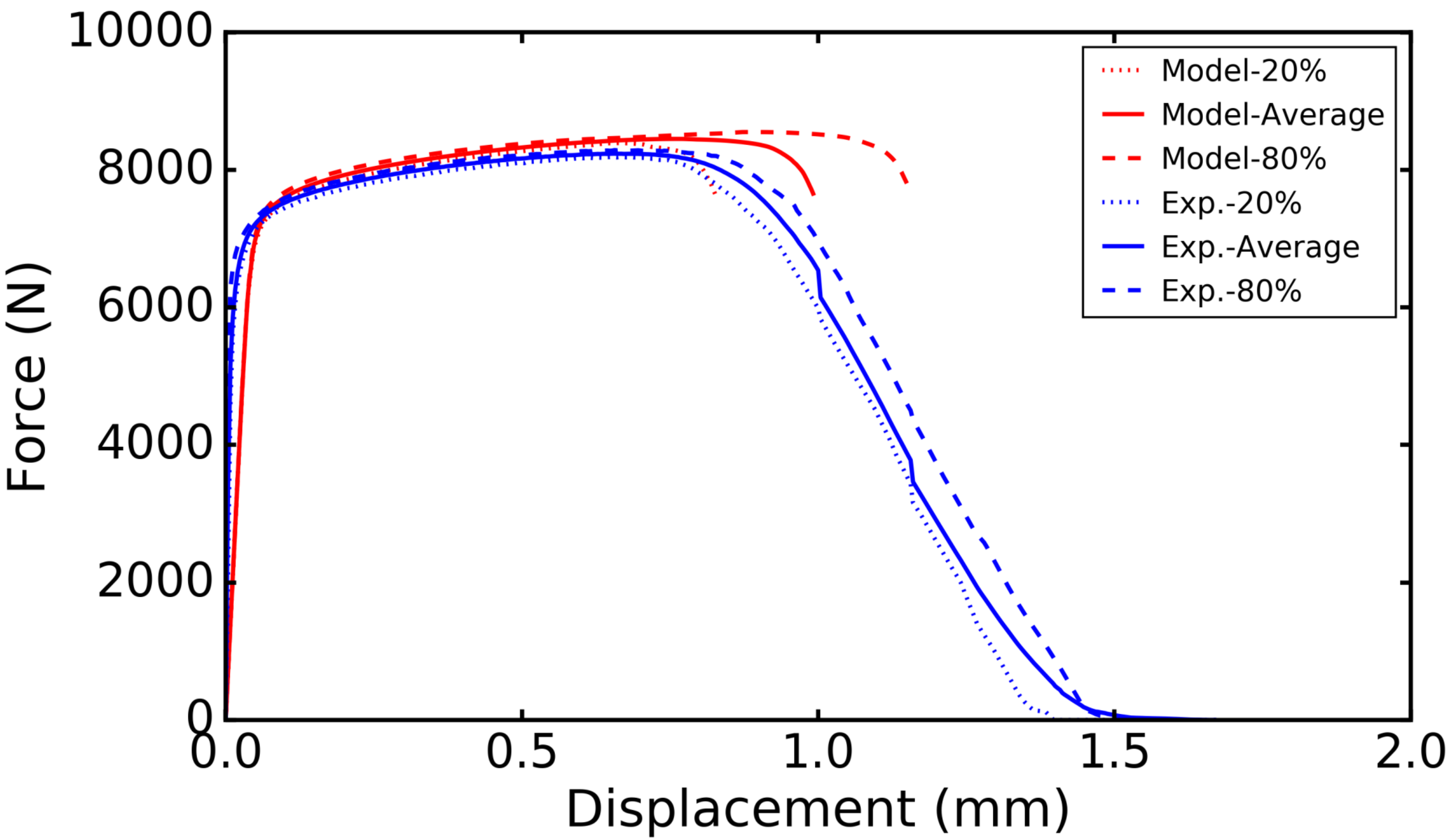


21 Nominal Predictions with Exp. Average and Bounds



Kramer, Boyce et al., *IJF (In preparation), Johnson* et al. *IJF (In preparation)*

Blind Predictions of Force-Displacement Curves Compare Reasonably Well With Experiments



Kramer, Boyce et al.*, IJF (In preparation), Johnson* et al. *IJF (In preparation)*

Summary

- Process models offer insight into phenomena such as melt pool dynamics, thermal histories, and residual stress
- Microstructure prediction using SPPARKS code has been performed at several different length scales and AM processes
- Texture prediction is being incorporated
- Initial approaches of coupling microstructure to continuum models show importance of microstructure consideration
- Investigating use of a posteriori error estimation techniques for quantifying homogenization errors and other model-form errors
- Continuum scale modeling of AM part performance compared well in blind predictions
- Porosity can be accounted for using a damage formulation