Exceptional service in the national interest

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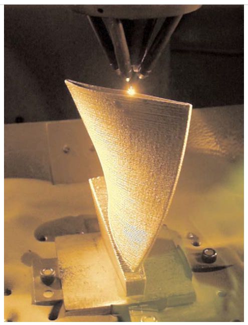
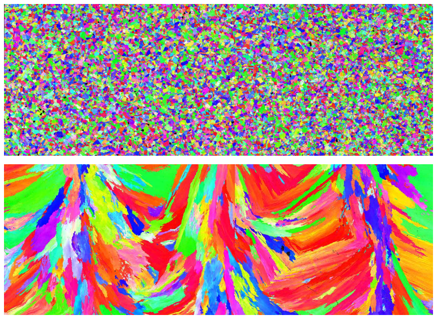
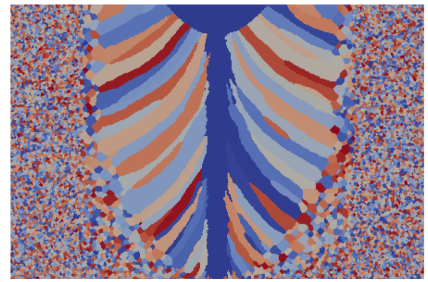
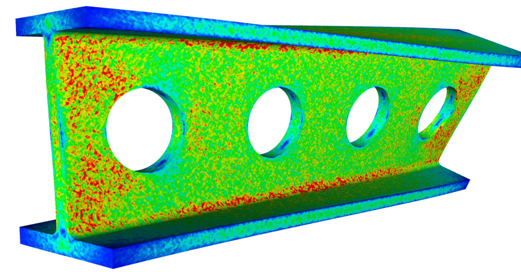

Additive Manufacturing Challenges for Computational Solid Mechanics

Joe Bishop

Sandia National Laboratories

A Workshop on Predictive Theoretical and Computational Approaches for Additive Manufacturing
National Academy of Sciences
Washington, DC
October 7-9, 2015

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Mechanical Response of Additively Manufactured (AM) Stainless Steel 304L across a Wide Range of Strain Rates

David P. Adams (SNL)
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Acknowledgements:

Predictive Performance Margins Project

Goal: Provide a science-based foundation for design and analysis capabilities that links nanoscale mechanisms and microscopic variability to stochastic performance.

Collaborators:

John Emery
John Madison
David Littlewood
Rich Field
Corbett Battaile
Brad Boyce
Jay Foulk

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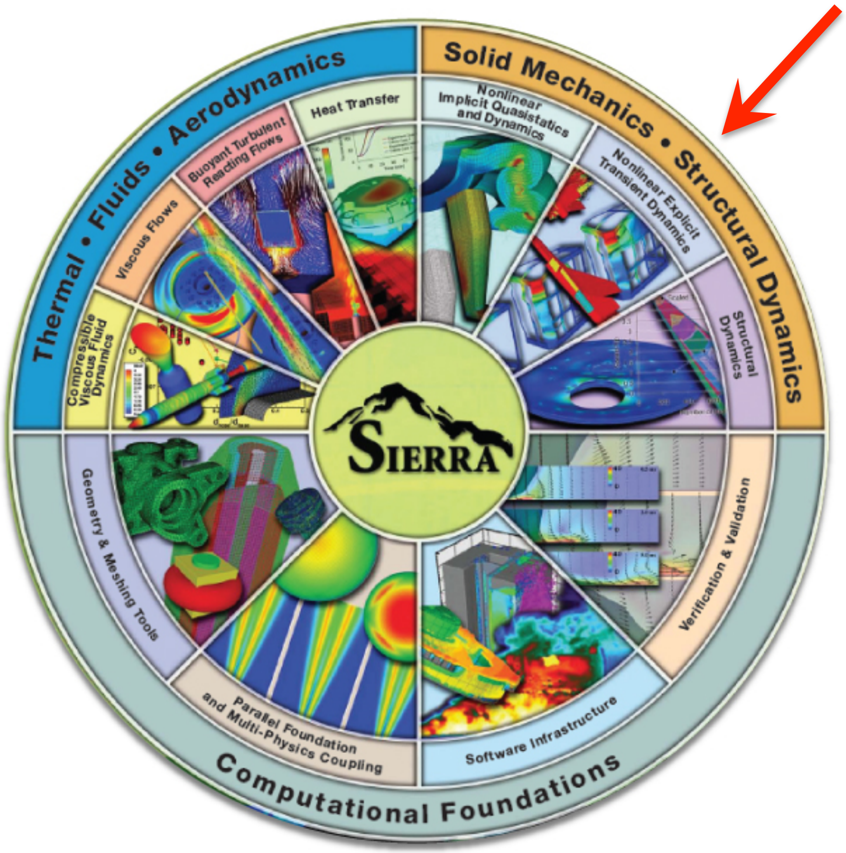
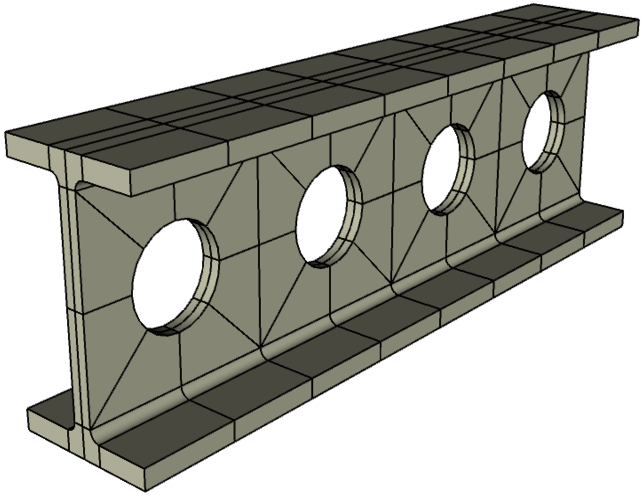
Using the solid-mechanics FEA module within DOE ASC code Sierra/SM.

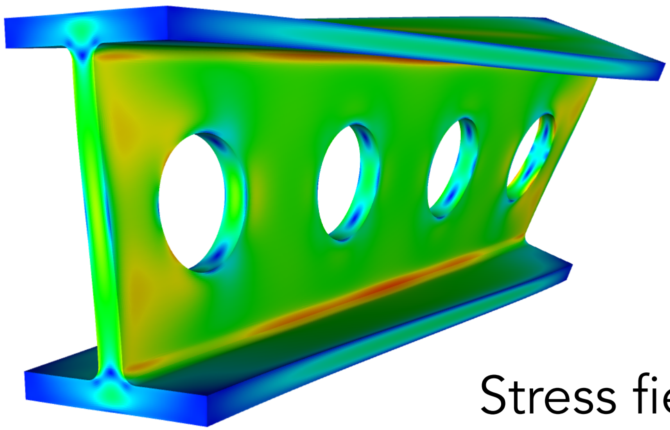


Questions to be answered:

1. -
2. How to leverage HPC spanning scientific discovery to ensembles of engineering solutions?
3. -
4. -
5. What analytical, experimental, and software tools are needed?
6. -
7. What opportunities exist for HPC, in order to provide fundamental scientific discovery of the process-properties-performance relationship relevant to AM?
8. What are those drivers and fundamental advancements are needed for computational methods and optimization techniques?

Macroscopic vision
(process-property-performance)





Stress field

1. Temperature history at each material point.
2. As-manufactured state using an advanced viscoplastic material model with internal state variables capable of representing processing history (e.g. recrystallization)
   - Residual-stress field
   - Initial yield-stress (field), hardening parameters, failure parameters, etc.
3. Predict part performance with error estimation and UQ in quantities of interest

A. Brown, D. Baumann, 2012, ``Validation of a model for static and dynamic recrystallization in metals,"
Int. J. of plasticity, 32-33, pp. 17-35.

AM challenges and opportunities for computational solid mechanics

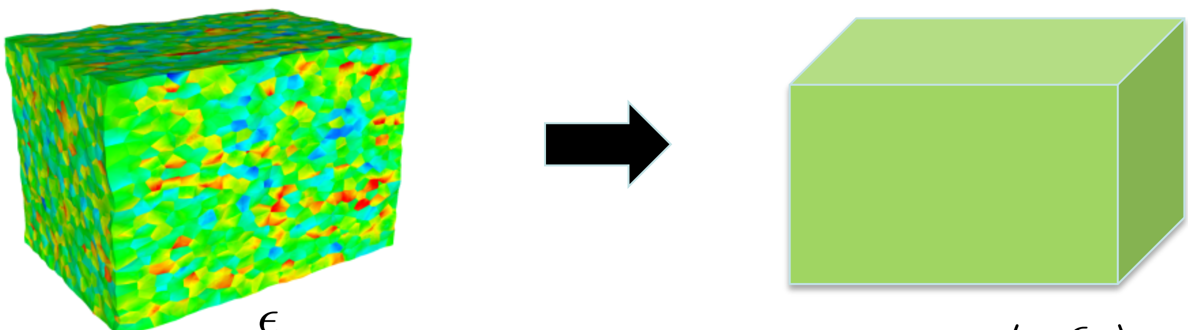
1. Is the concept of a ``material property'' appropriate for AM parts?
2. The residual-stress field must be quantified with its uncertainty.
3. Data science as an enabler for predictive modeling.
4. Fast simulations for industrial use.

Is the concept of a ``material property'' appropriate for AM parts?

Is the concept of a ``material property'' an accurate approximation for AM materials?

- Material property and macrostructure are no longer separable.
- Process/material/part must be qualified concurrently.
- What is the accuracy of homogenization theory for AM materials?
  - scale separation
  - texture/anisotropy
  - surface effects
- Need to apply concepts from *a posteriori* error-estimation to quantify errors inherent in homogenization and material-model form error.

Homogenization

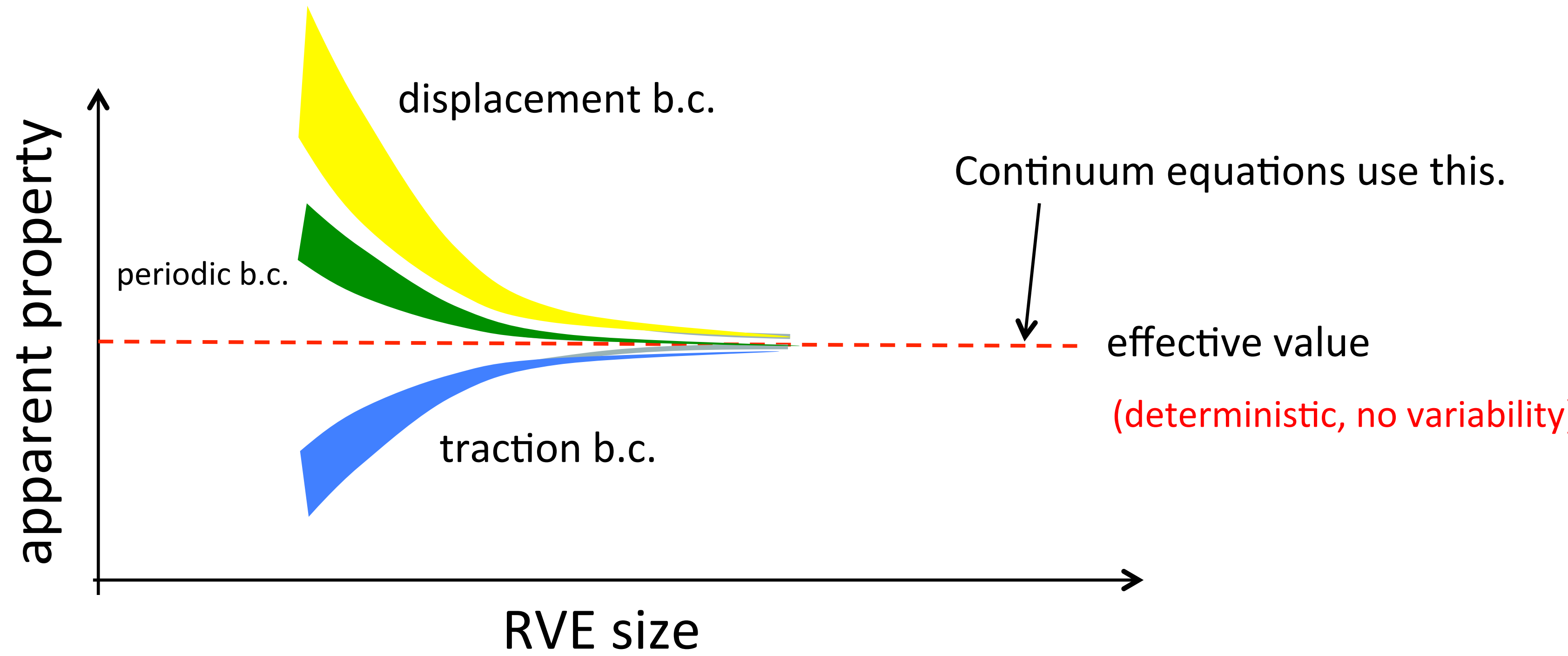


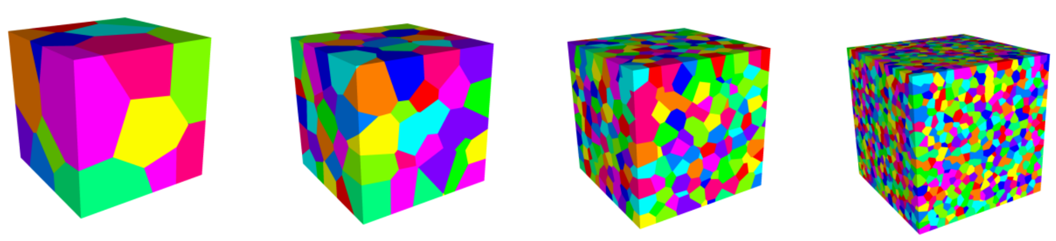
σ_{ij}^{ϵ} $\qquad$ $\sigma_{ij} = \langle \sigma_{ij}^{\epsilon} \rangle$

fine-scale fluctuations $\qquad$ replaced with mean behavior

Apparent vs. effective material properties

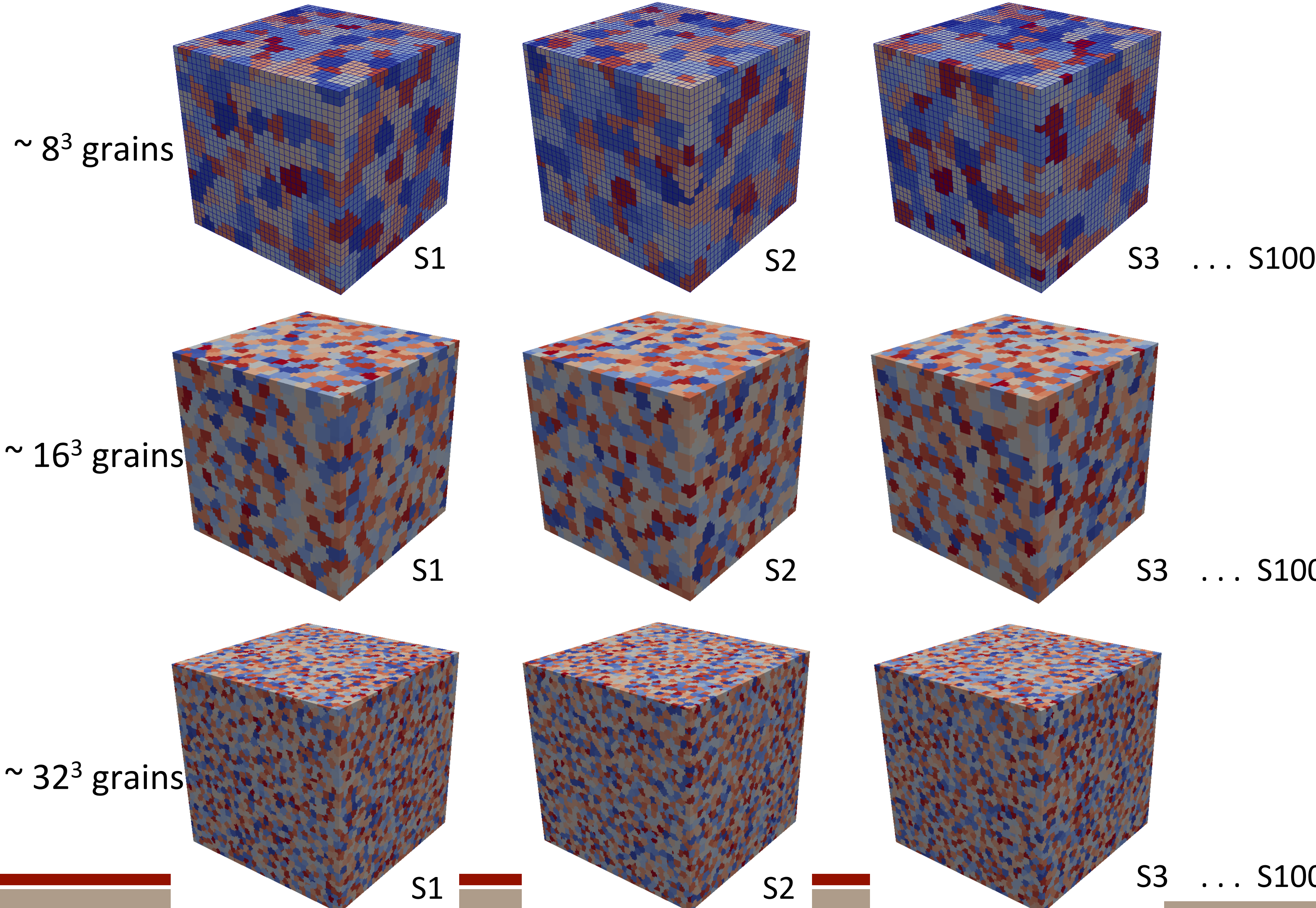
Huet, C. (1990). "Application of variational concepts to size effects in elastic heterogeneous bodies." *Journal of the Mechanics and Physics of Solids,* 38(6): 813-841.



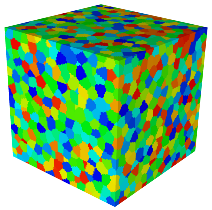
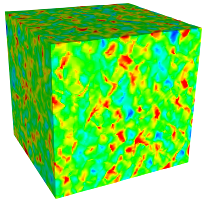


$\varepsilon = 0.32$ $\varepsilon = 0.16$ $\varepsilon = 0.08$ $\varepsilon = 0.04$

From SVEs to RVEs



Convergence to effective isotropic elastic properties

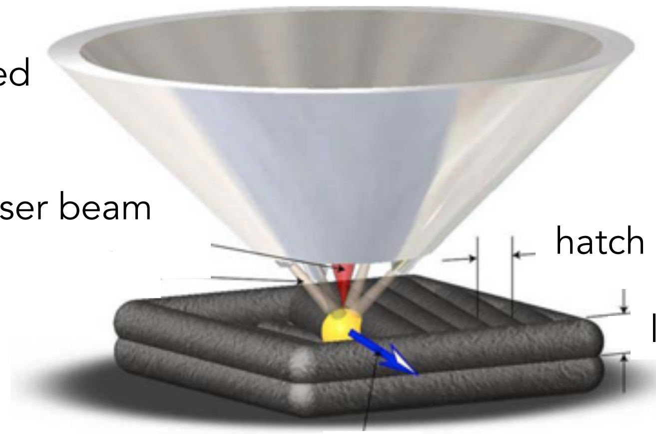



- mean of 100 simulations at each "grain level"
- rational function extrapolation to ∞

number of grains	apparent Young's Modulus (GPa)	apparent Poisson's ratio
~4^3 grains	185.2	0.307
~8^3 grains	190.5	0.301
~16^3 grains	193.9	0.298
~32^3 grains	195.7	0.296
∞	197.6	0.294

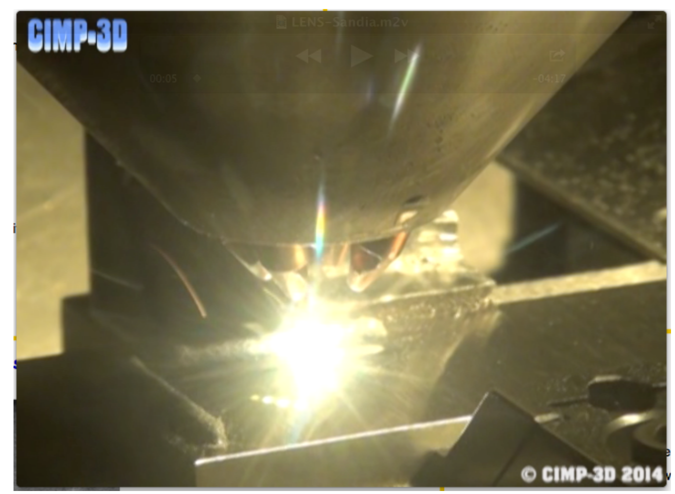
These values will be used as the homogenized, isotropic, elastic properties.

LENS®, Laser Engineered Net Shaping



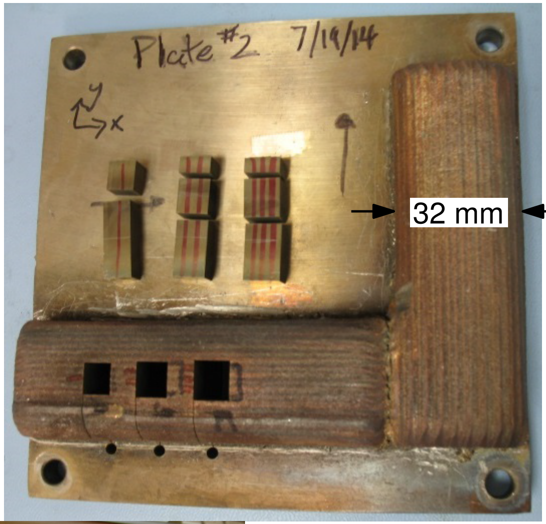
LENS® deposition

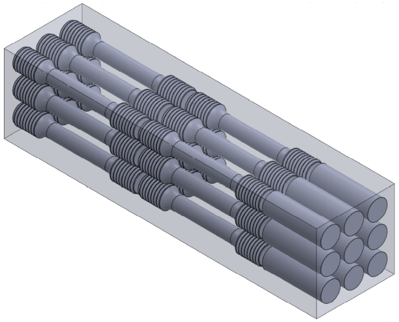
(T. Palmer, PSU)



Wrought stainless steel 304L bar

LENS build, 304L 3.8kW





Large area views of microstructure of AM SS-304L (2.0 kW)

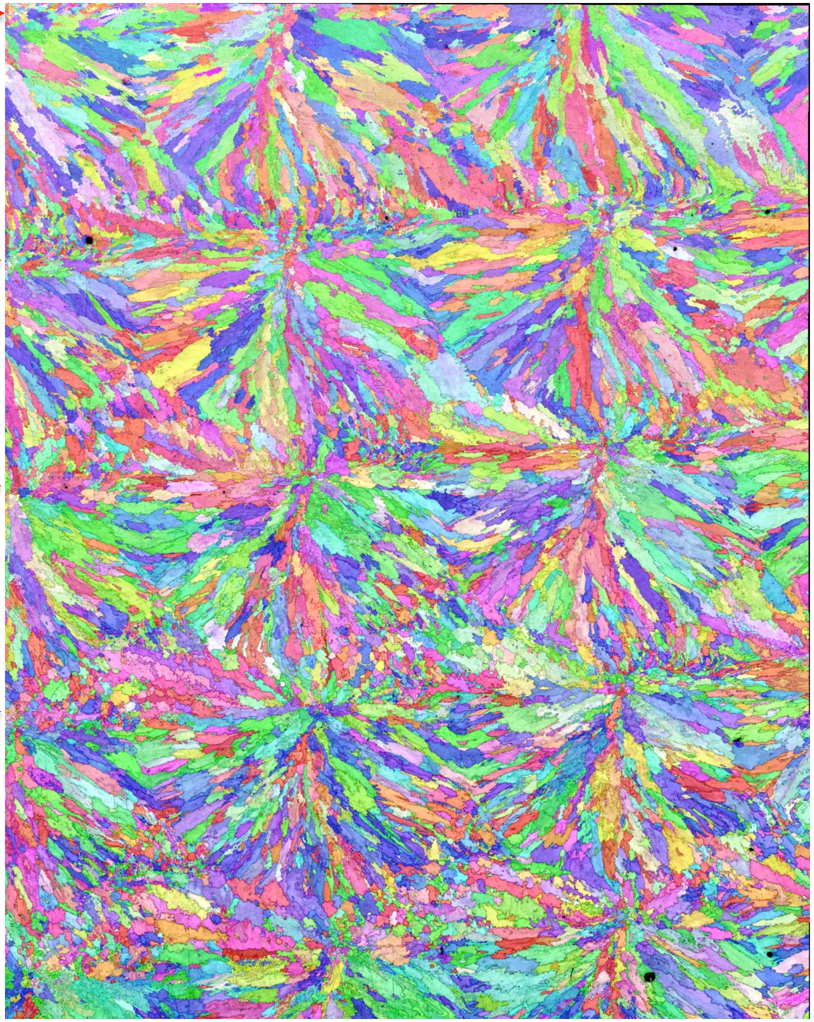
(D. Adams, SNL)

- Electron backscatter diffraction (EBSD) maps of electropolished surface.
- Built using a cross-hatch pattern.
- Density has been confirmed at 99.8 (Archimedes method).

How to homogenize to get a ``material properties"?

- Assume periodicity?
- Assume statistically homogeneous?
- anisotropic

6 mm X 10 mm

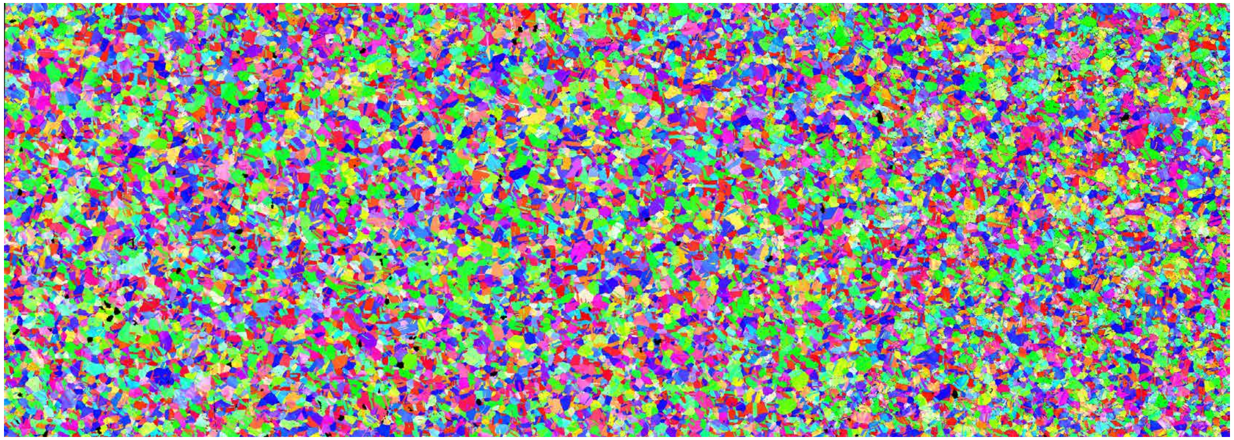


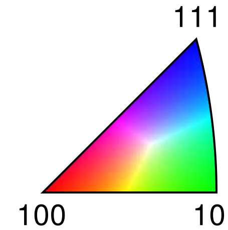
Laser direction

(J. Michael, SNL)

Microstructure comparison

Wrought

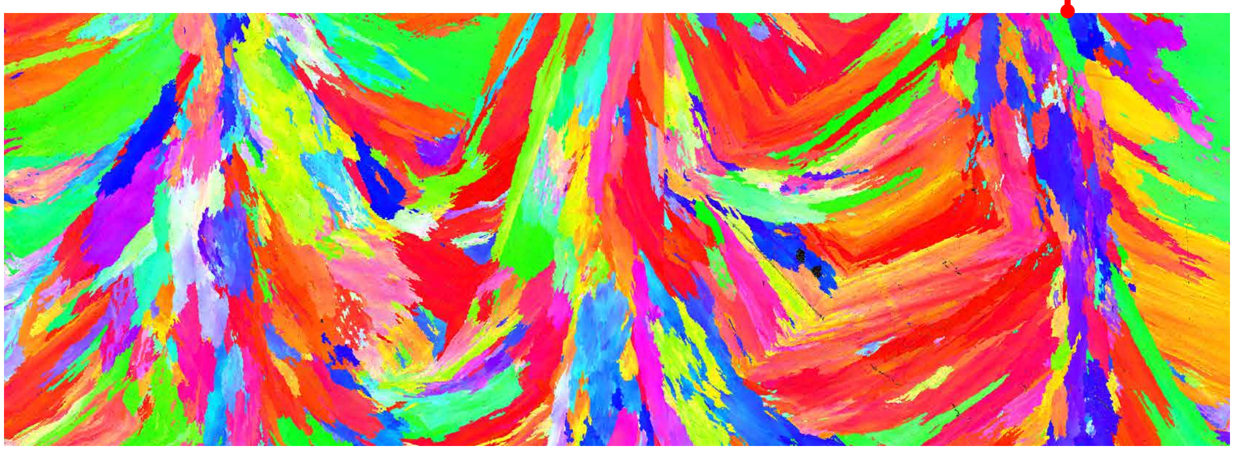


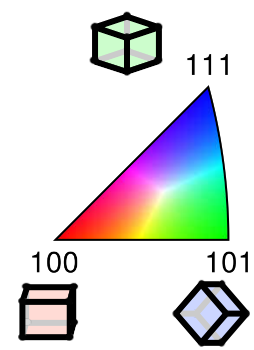


1.0 mm

Laser Beam

3.8 kW LENS

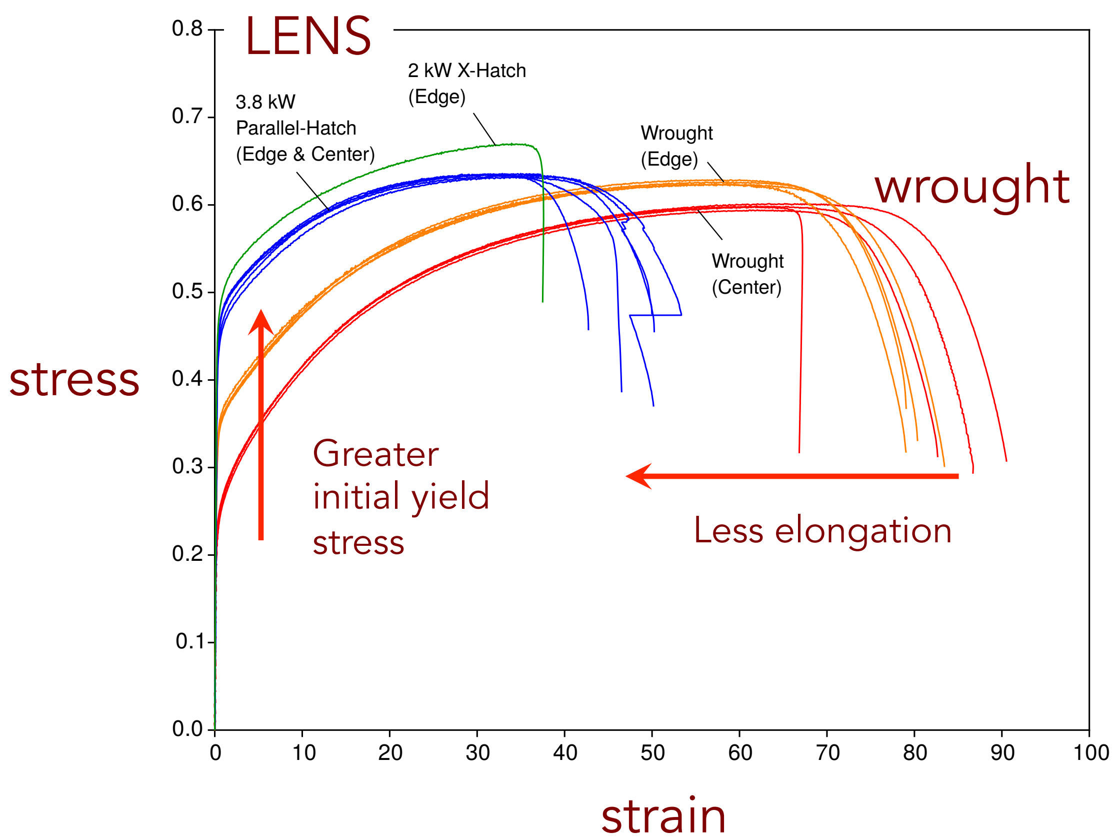




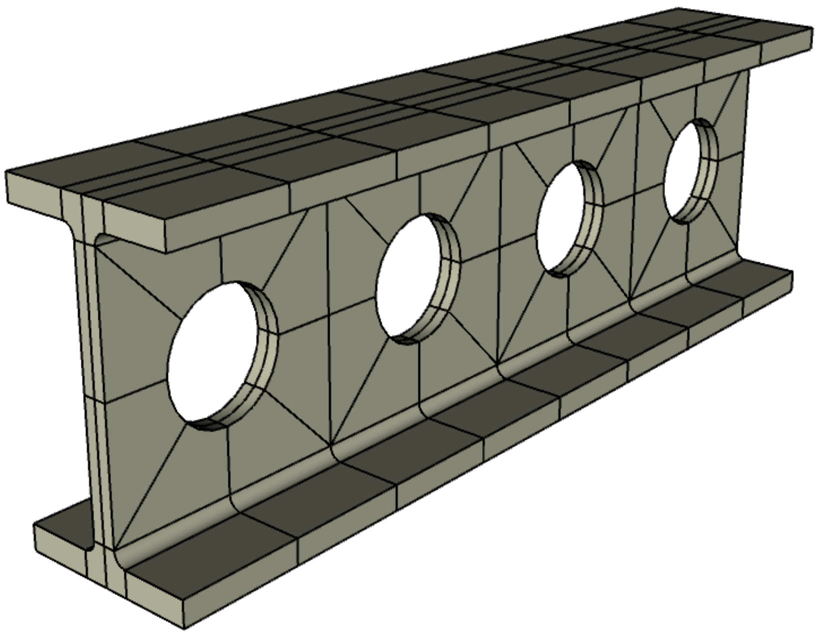
1.0 mm

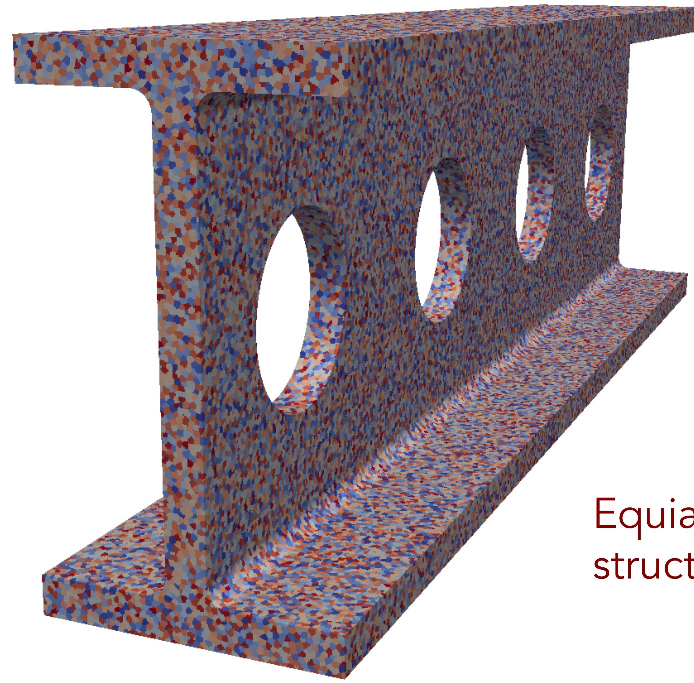
Stress-strain response

(J. Carroll, SNL)



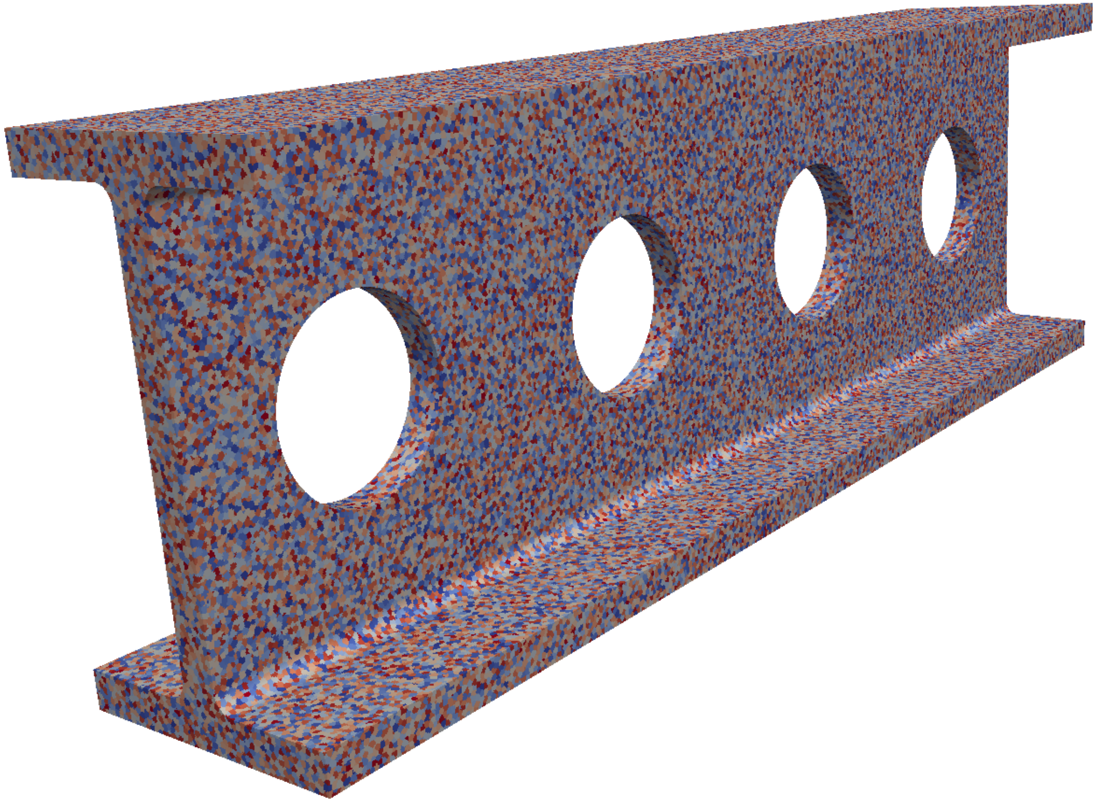
Do we resort to Direct Numerical Simulation (multiscale modeling)?

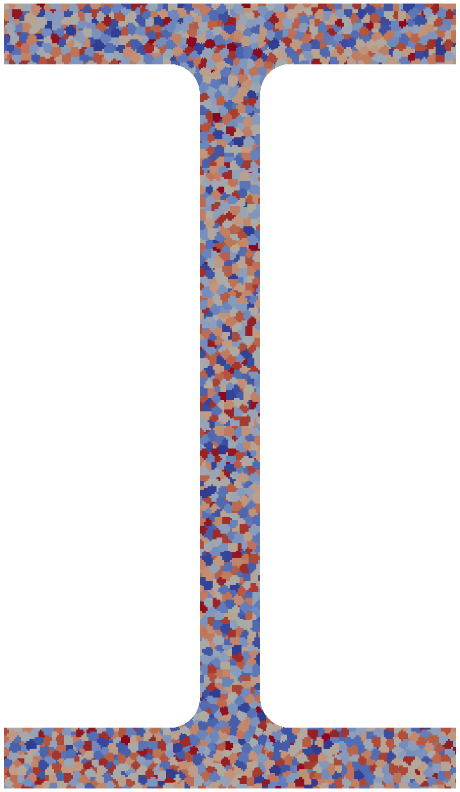




- Model the grain structure directly within the engineering-scale FEA model.
- Uses crystal-plasticity material models for each grain.
- Can incorporate as-manufactured state (e.g. texture, residual stress)
- Requires massively parallel FEA framework.
- Useful for understanding errors in homogenization and "data-science" studies.

Example: I-beam in torsion





- ~420,000 grains
- Web thickness to grain ratio = 8
- uniformly random crystal orientations (no texture)
- 35M finite elements

FCC crystal plasticity model

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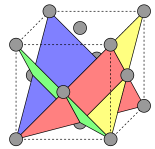
(K. Matous, A. Maniatty, 2004, *IJNME*)

plastic velocity gradient: $$L^p = \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha P^\alpha$$



Schmid tensor: $$P^\alpha = m^\alpha \otimes n^\alpha$$

slip system slip rates: $$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left(\frac{\tau^\alpha}{g}\right)^{1/m} \cdot \mathrm{sign}(\tau^\alpha)$$

slip system hardening: $$g = g_o + (g_{so} - g_o)\left[1 - \exp\left(-\frac{G_o}{g_{so} - g_o}\gamma\right)\right]$$

$$\gamma = \sum_{s=1}^{N} |\gamma^s|$$ (sum over slip systems)

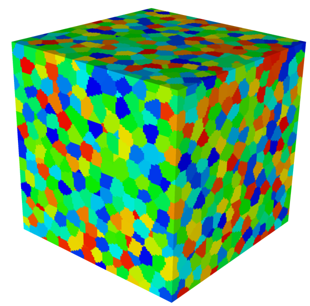
Single crystal elastic constants (austenite)

$$C_{11} = 204.6 \ \ \mathrm{GPa}$$
$$C_{12} = 137.7 \ \ \mathrm{GPa}$$
$$C_{44} = 126.2 \ \ \mathrm{GPa}$$

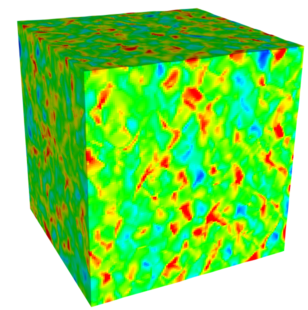
Not considering:

- grain boundary effects (Hall-Petch effect)
- twinning
- dislocation substructures
- latent hardening

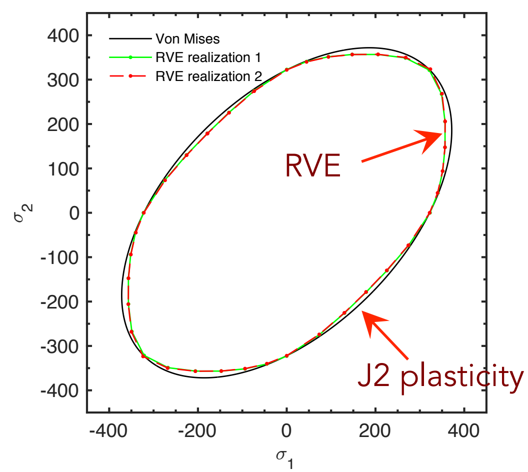
Representative Volume Element (RVE) response



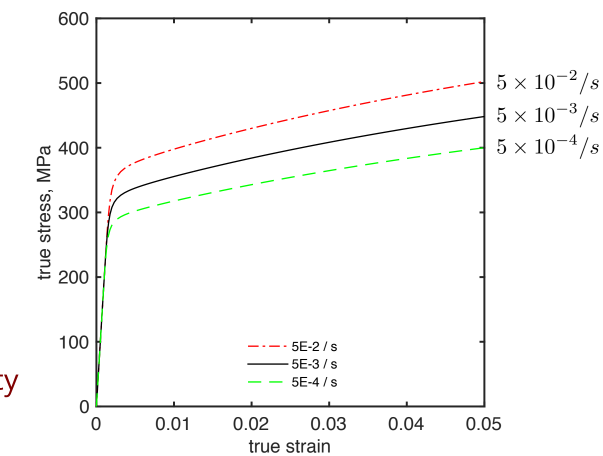
plastic response



yield surface

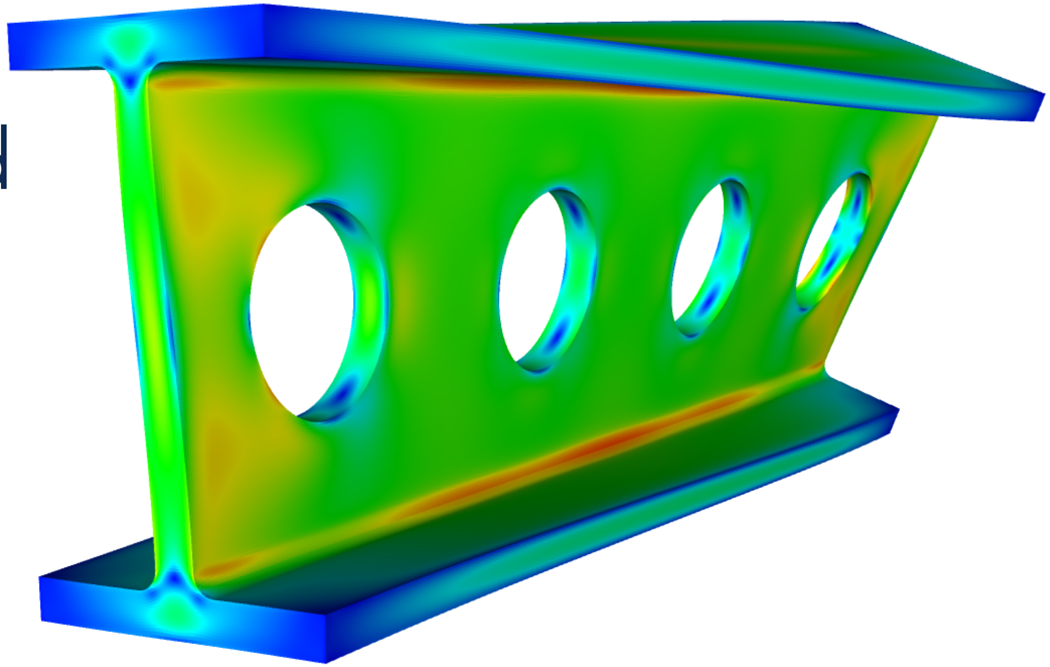


strain-rate dependence

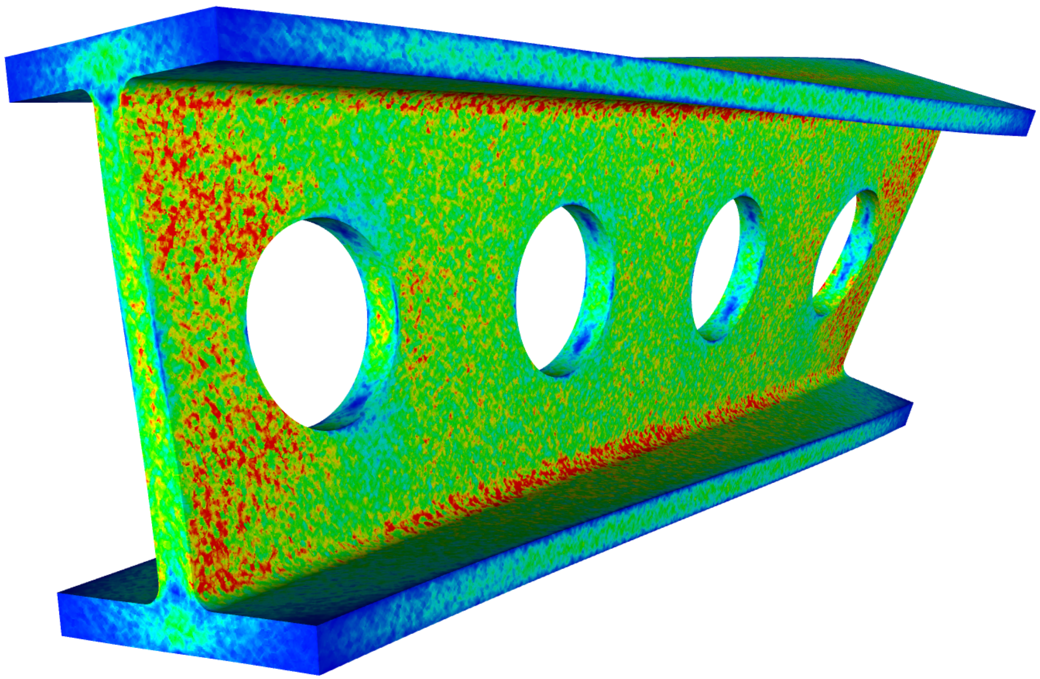


VonMises stress field

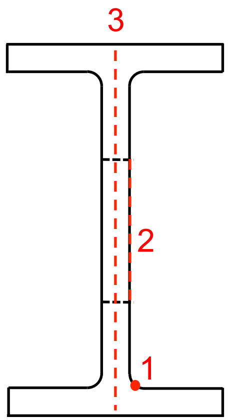
Homogenization solution

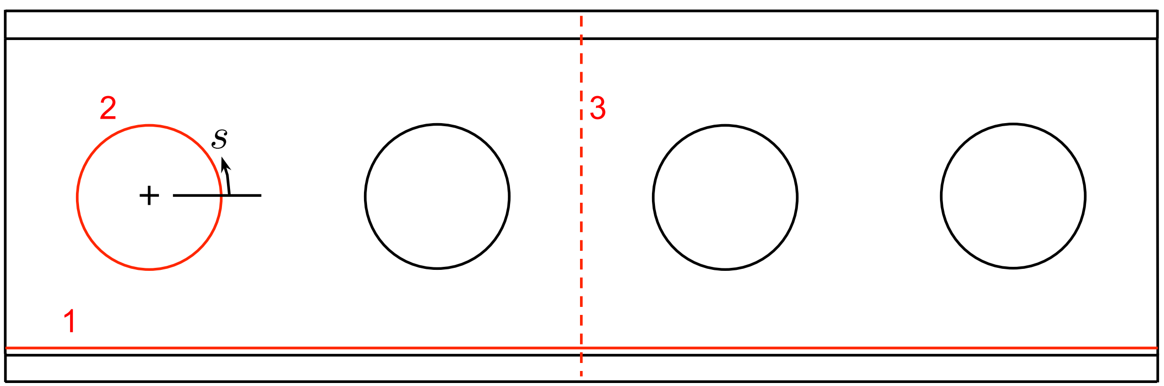


Multi-scale modeling
(direct numerical simulation, DNS)



Stress extraction lines/curves

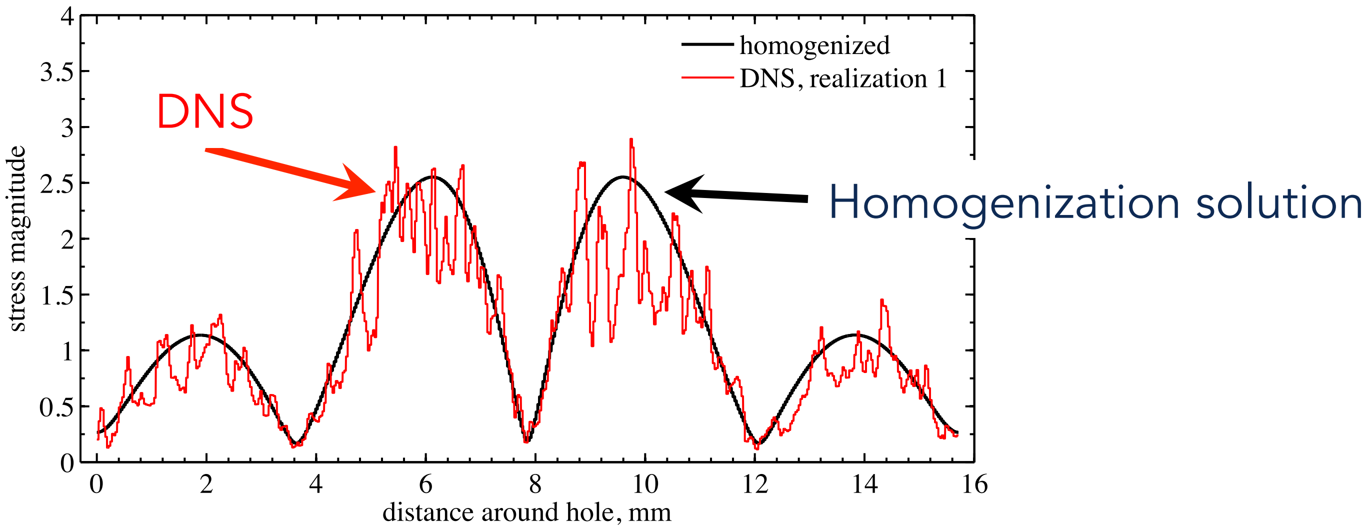




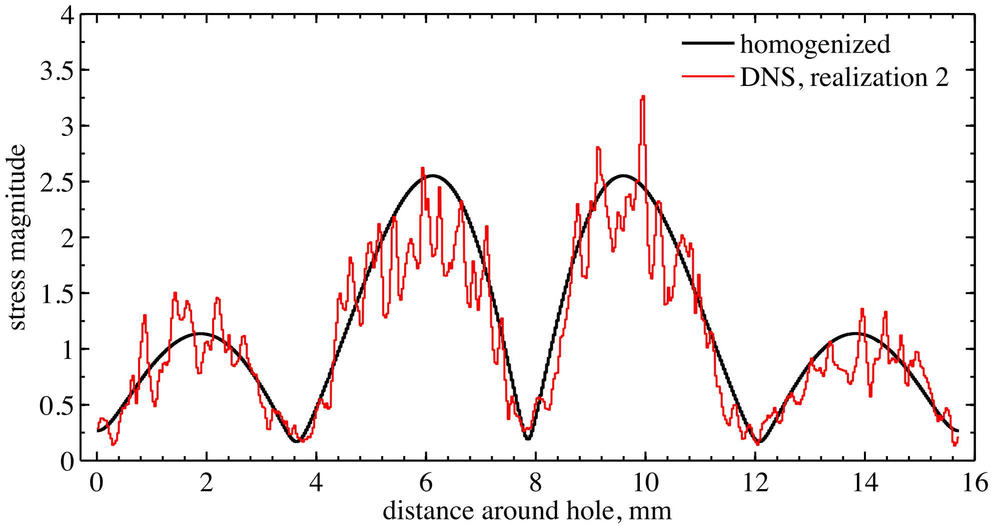
Homogenization solution vs. DNS

Stress magnitude around hole

realization 1



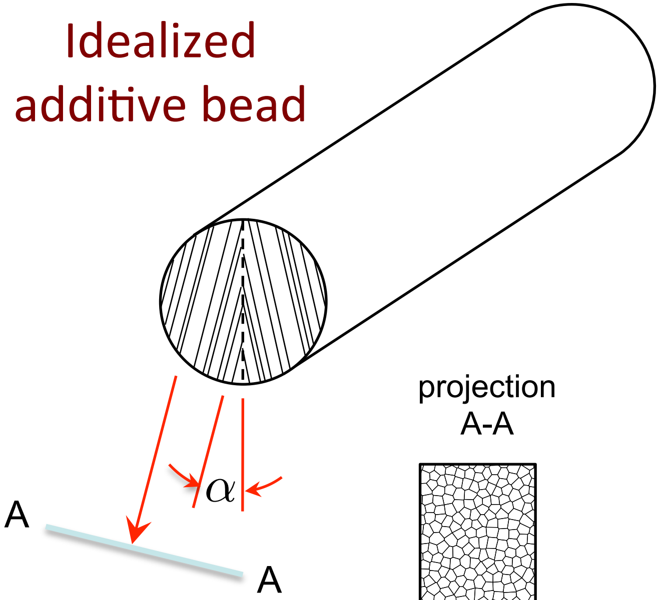
realization 2



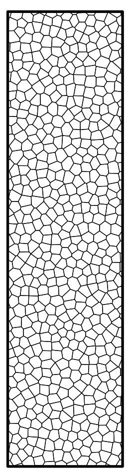
What about modeling the LENS microstructure?

Idealized LENS microstructures

Idealized additive bead

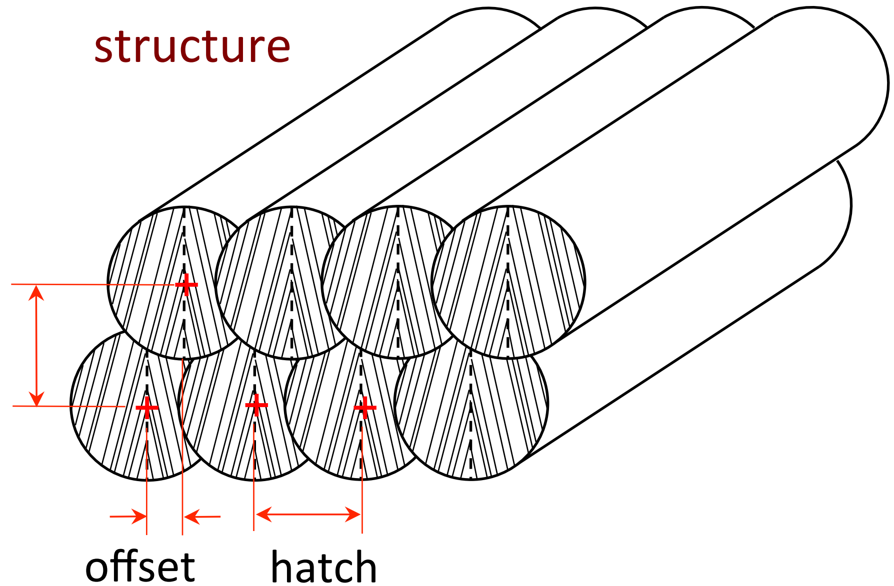


projection A-A



random Voronoi through MPS sampling

Idealized LENS structure



texture?

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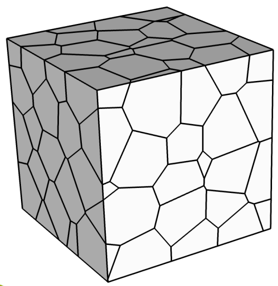
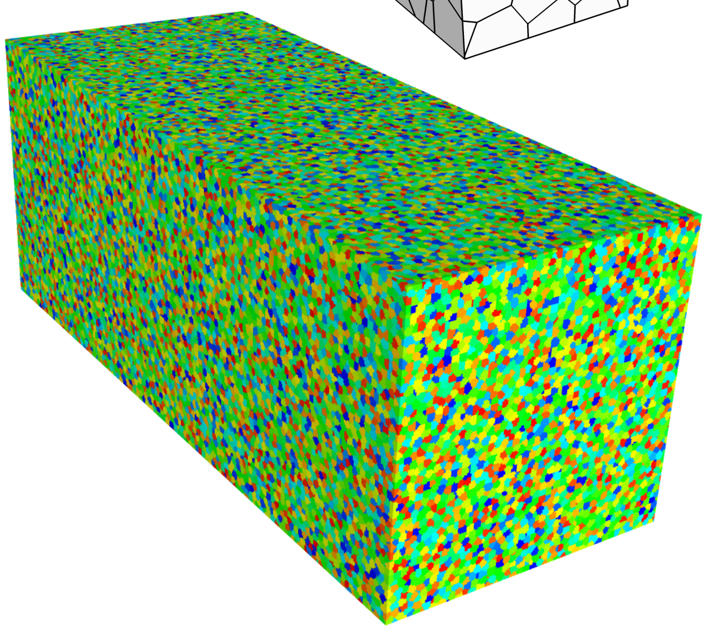
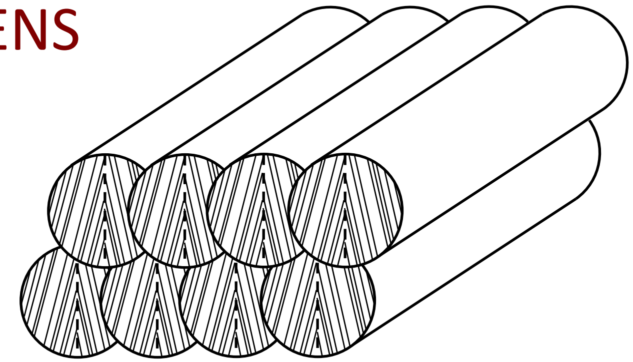
equiaxed



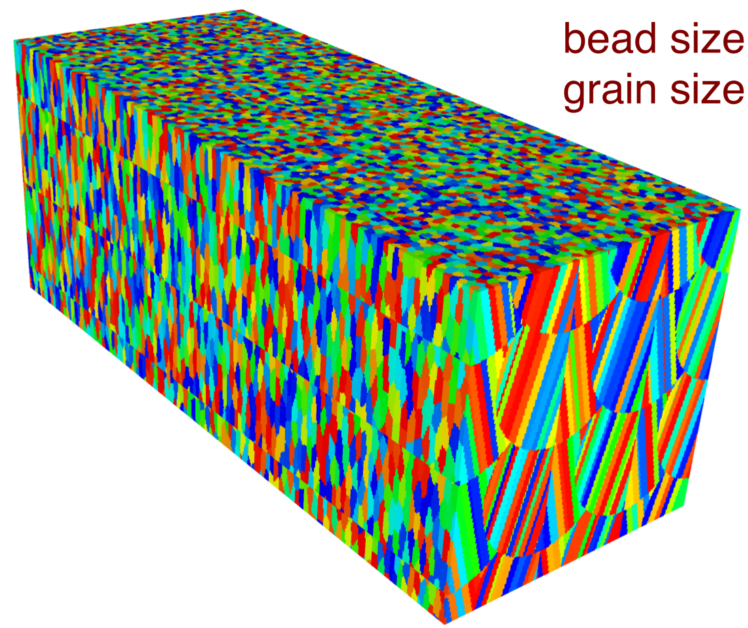


grain size = 40 microns

additive, LENS

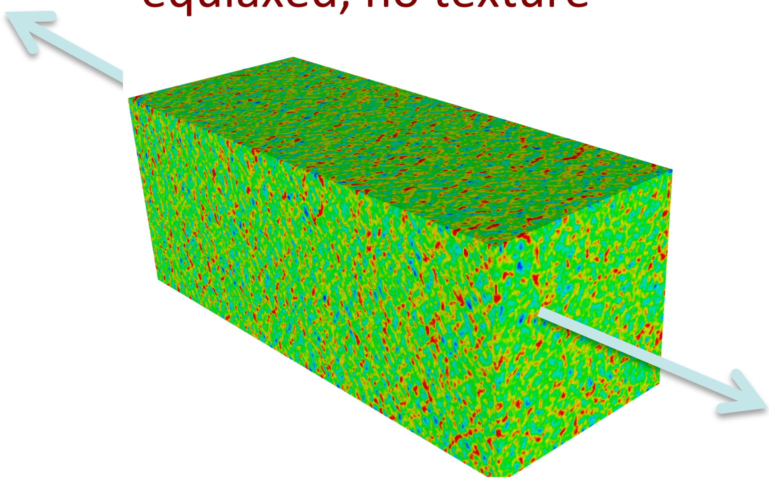


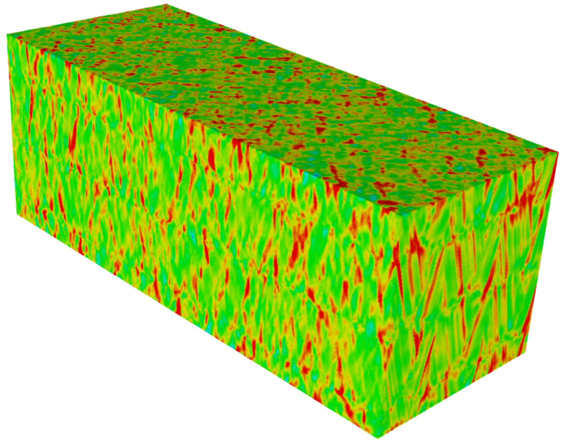
bead size = 1 mm
grain size = 40 microns



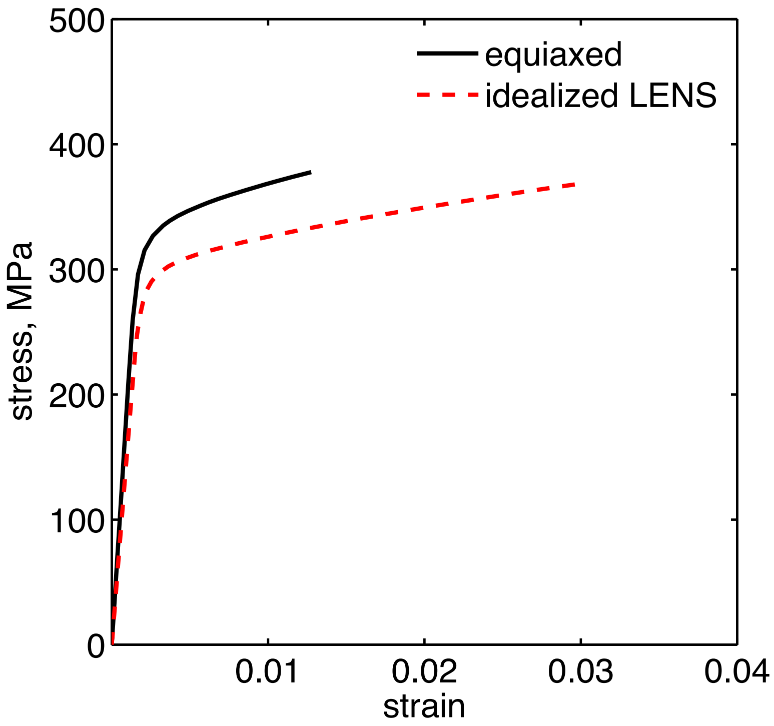
Stress-strain response

equiaxed, no texture



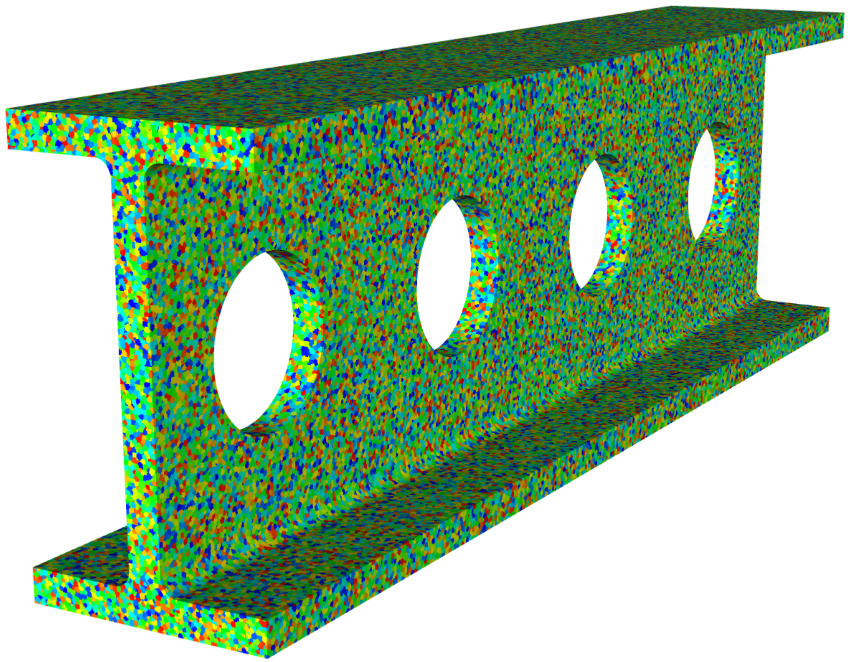


additive, LENS

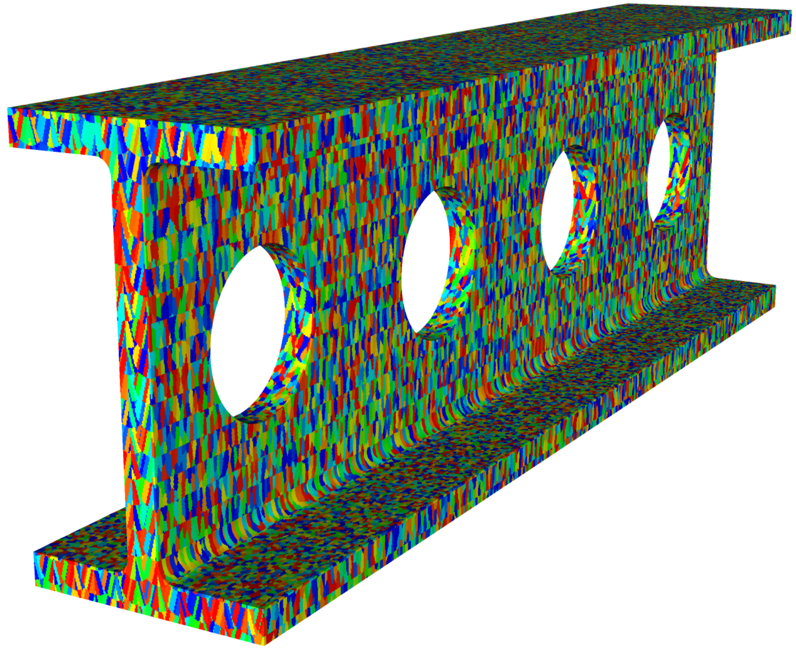


Idealized microstructures

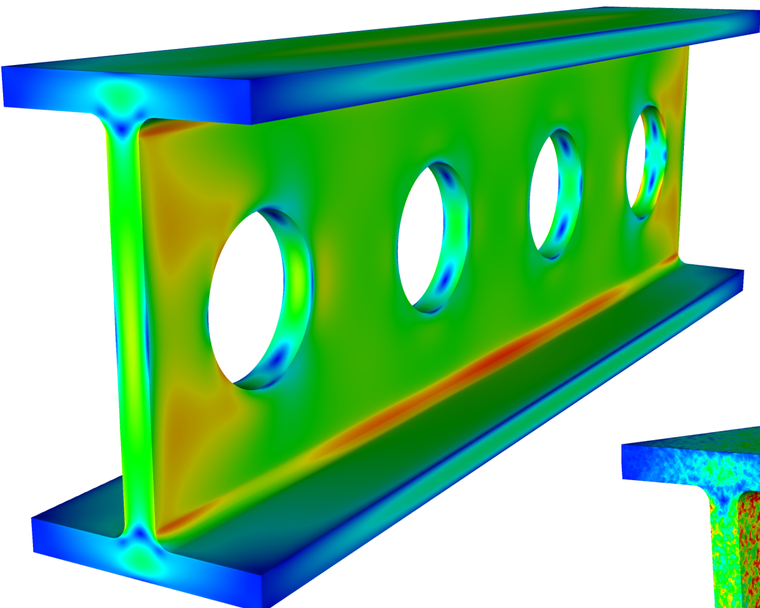
equiaxed



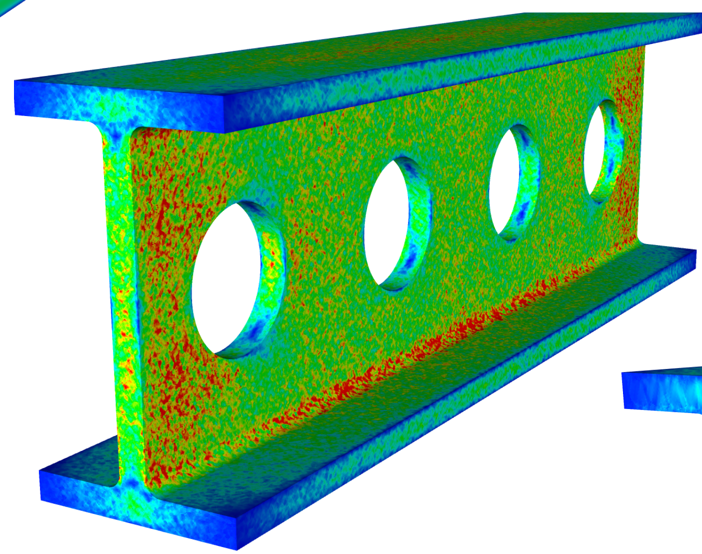
LENS



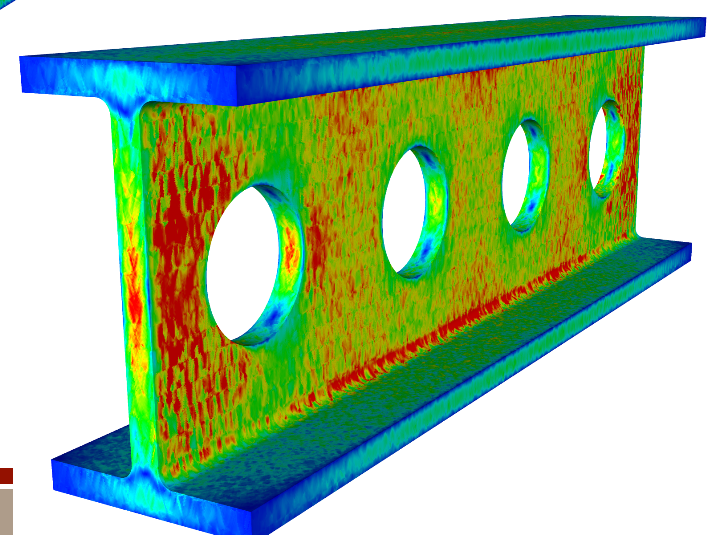
Macroscopic stress field



homogeneous, isotropic



equiaxed, no texture, isotropic

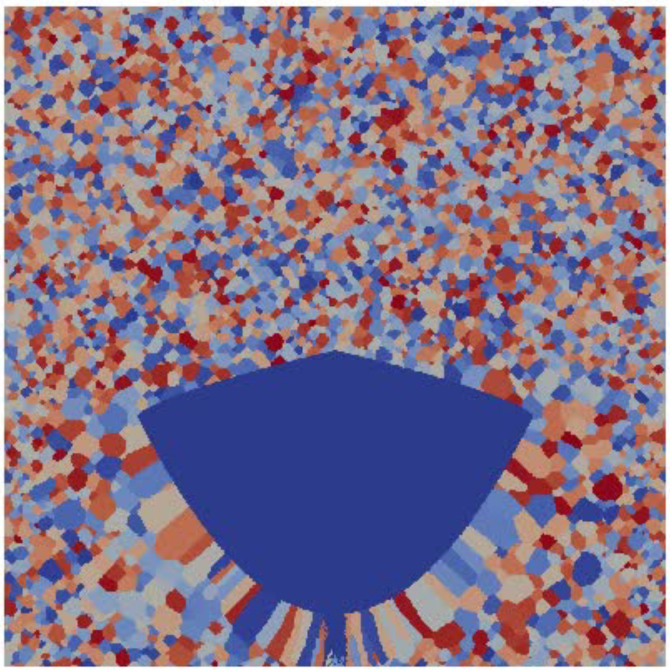


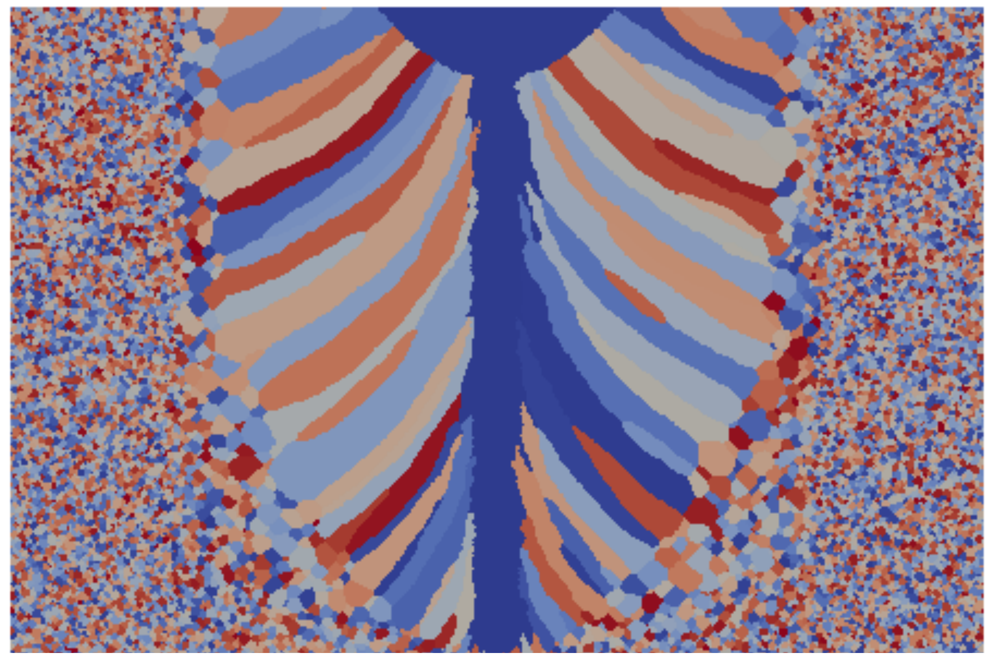
idealized LENS

What about AM microstructures?

(V. Tikare, J. Madison, SNL) (http://spparks.sandia.gov)

- Kinetic Monte Carlo (KMC)
- Laser-welding simulation





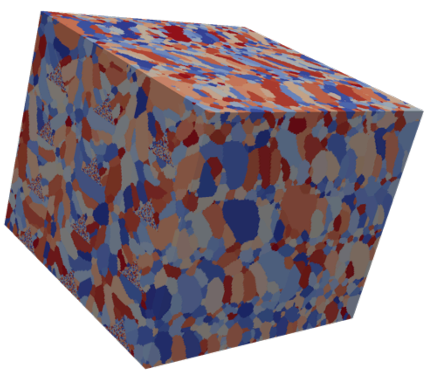
Microstructure generation

(T. Rodgers, J. Madison, V. Tikare, SNL) (http://spparks.sandia.gov)

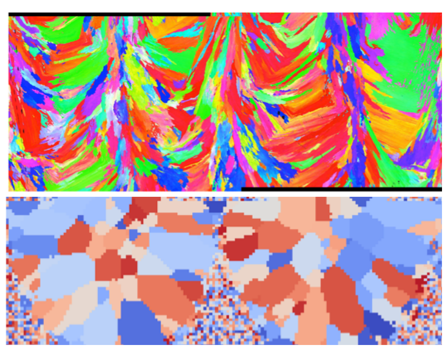
For additive manufacturing applications, two of the most important properties for KMC:

1. melt pool velocity
2. shape of the hot-zone trailing the melt pool's path

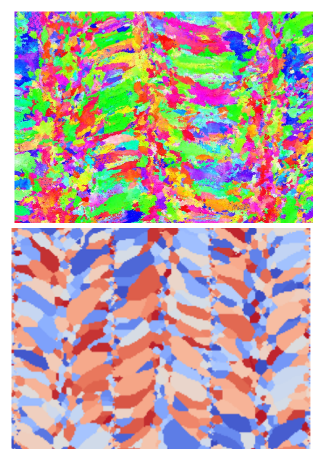
Comparison with LENS 3.8 kW EBSD results



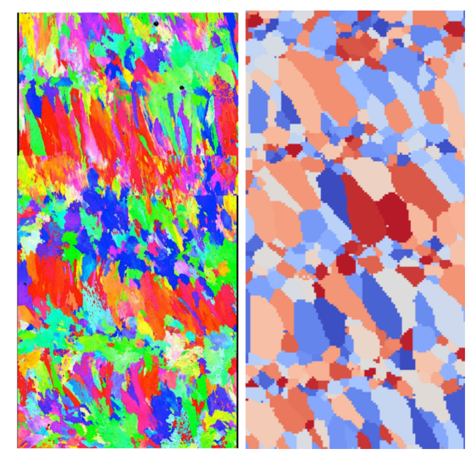
YZ plane



XY plane



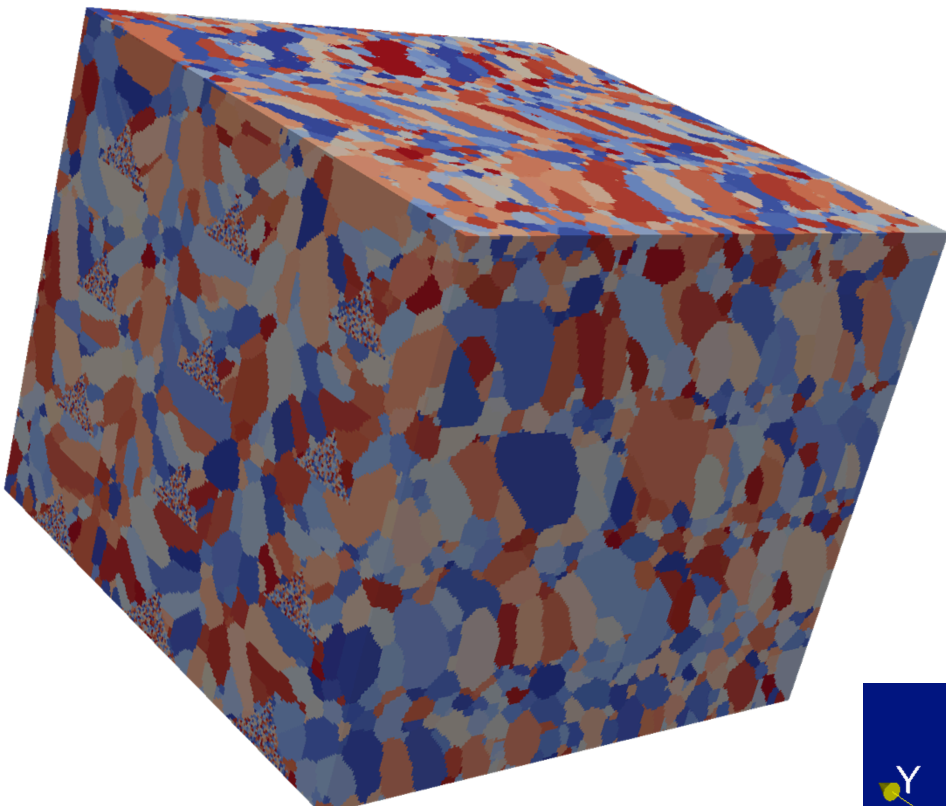
XZ plane



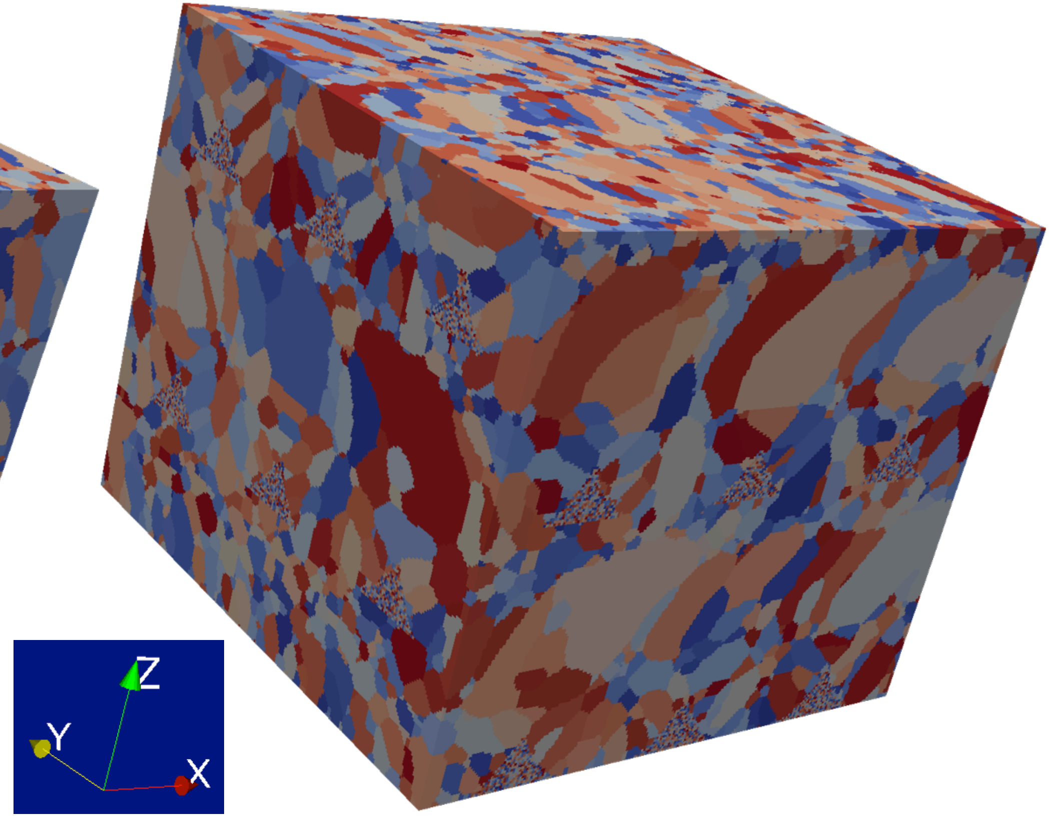
Comparison of AM scan patterns

(T. Rodgers, J. Madison, V. Tikare, SNL)

X only



X and Y, alternating layers



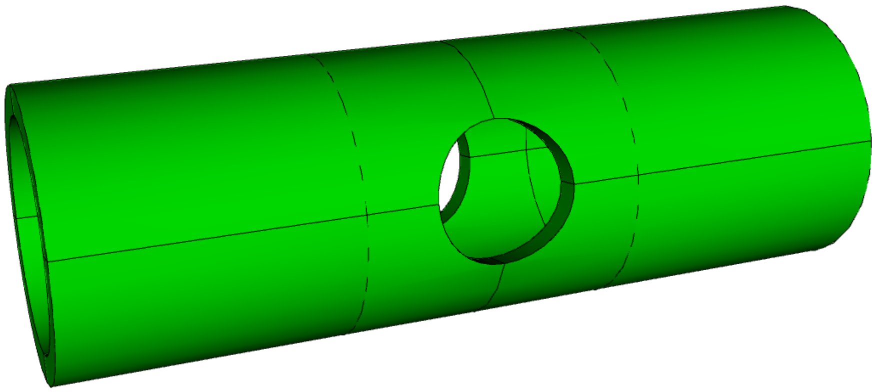
Data science as an enabler for predictive modeling

Data science as an enabler for predictive modeling

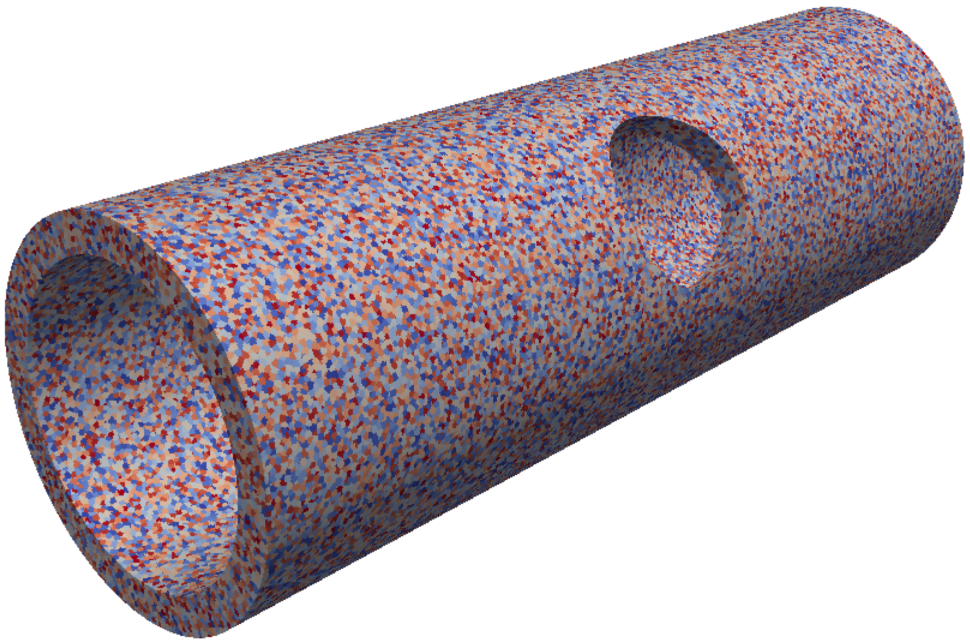
- High through-put material testing
  - UQ, statistical learning
  - pattern recognition for material-failure precursors
- 3D digital volume correlation (DVC) using micro-CT
  - Internal speckle pattern?
- Statistical learning, pattern recognition, emergent behavior

Stainless-steel tube under axial loading

Geometry



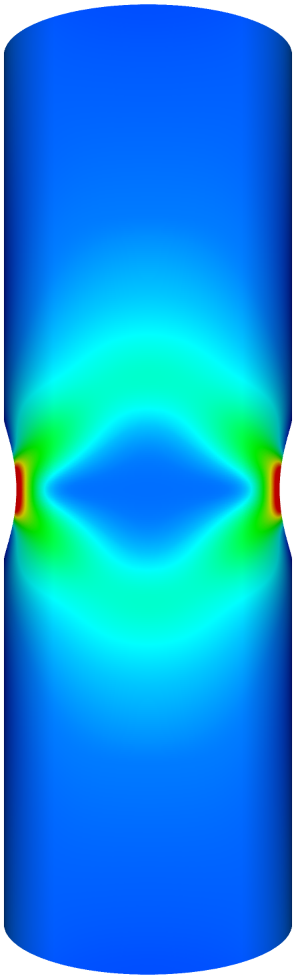
Part with embedded microstructure



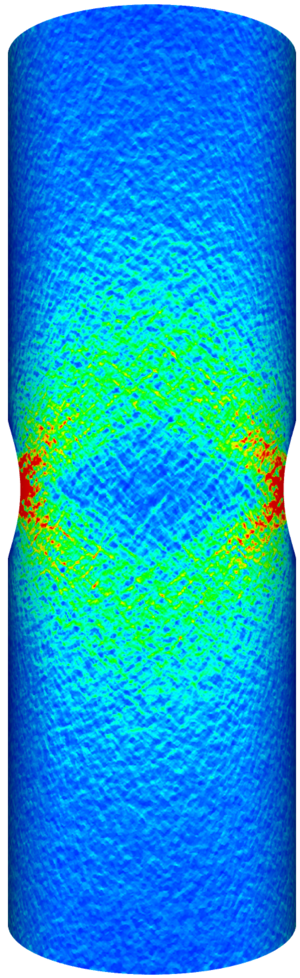
- thickness/grain ratio = 8
- 352,000 equi-axed grains
- uniformly random crystal orientations (no texture)

Pattern recognition?

Axial load, plastic regime, 2% strain

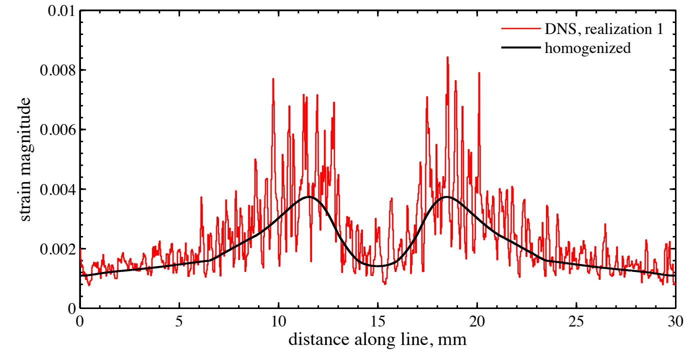


Homogenization

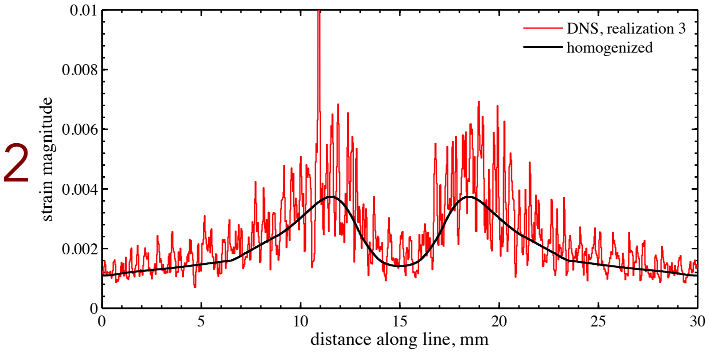


Multiscale

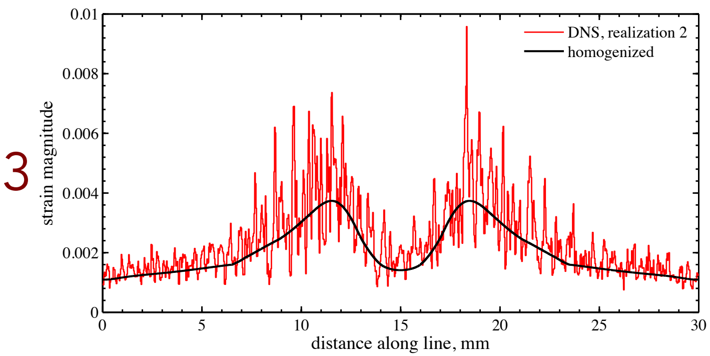
realization 1



realization 2

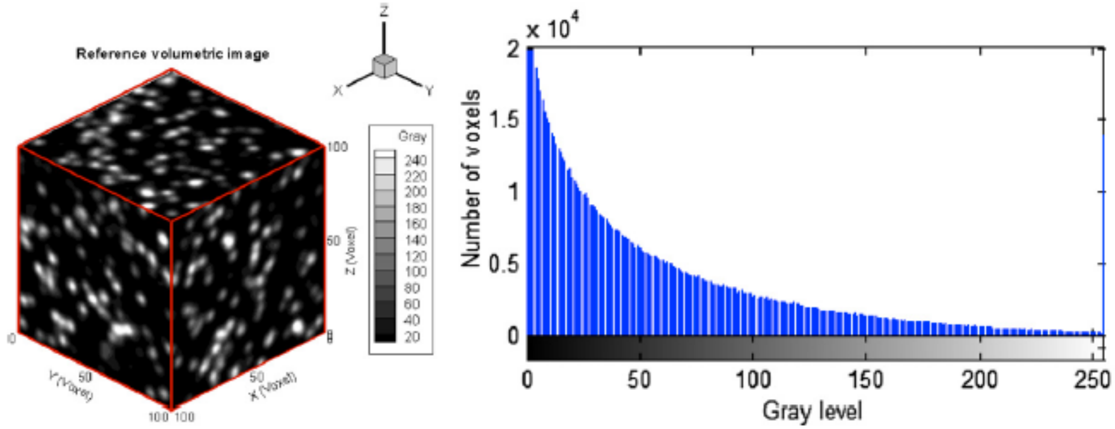


realization 3



3D, Digital Volume Correlation (DVC)

Synthetic data



Pan, etal, Meas. Sci. Technol. 23 (2012) 045002

- Internal speckle pattern for metal AM?
- Invoke statistical learning, pattern recognition for discovery in material failure modeling.

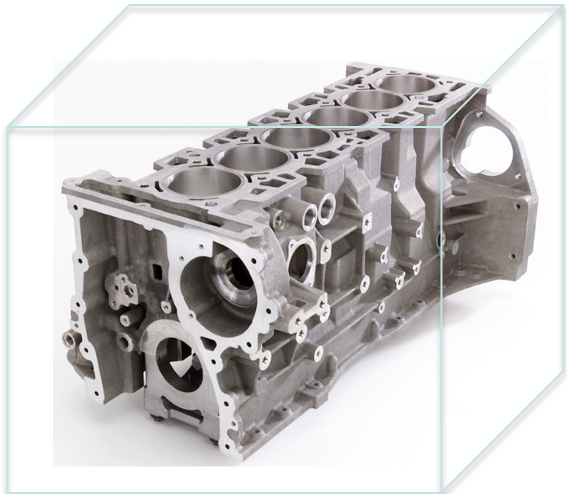
Fast simulations for industrial use.

Fast simulations for industrial use.

- Need to develop specialized computational tools that are extremely efficient, instead of relying on general purpose computational tools.
- Opportunity to break out of current CAD-analysis paradigm.
- Focus on implicit representations of geometry.
- Focus on implicit representations of approximation spaces so that meshing process is eliminated.
  - Fictitious-domain methods, finite-cell methods, FFT methods
  - Mesh-free methods
- *A posteriori* error estimation in engineering quantities-of-interest
  - Heuristics in FEA are still state-of-the-art.

Instead of meshing the complex geometry explicitly, use an "embedded domain" paradigm

Sandia National Laboratories

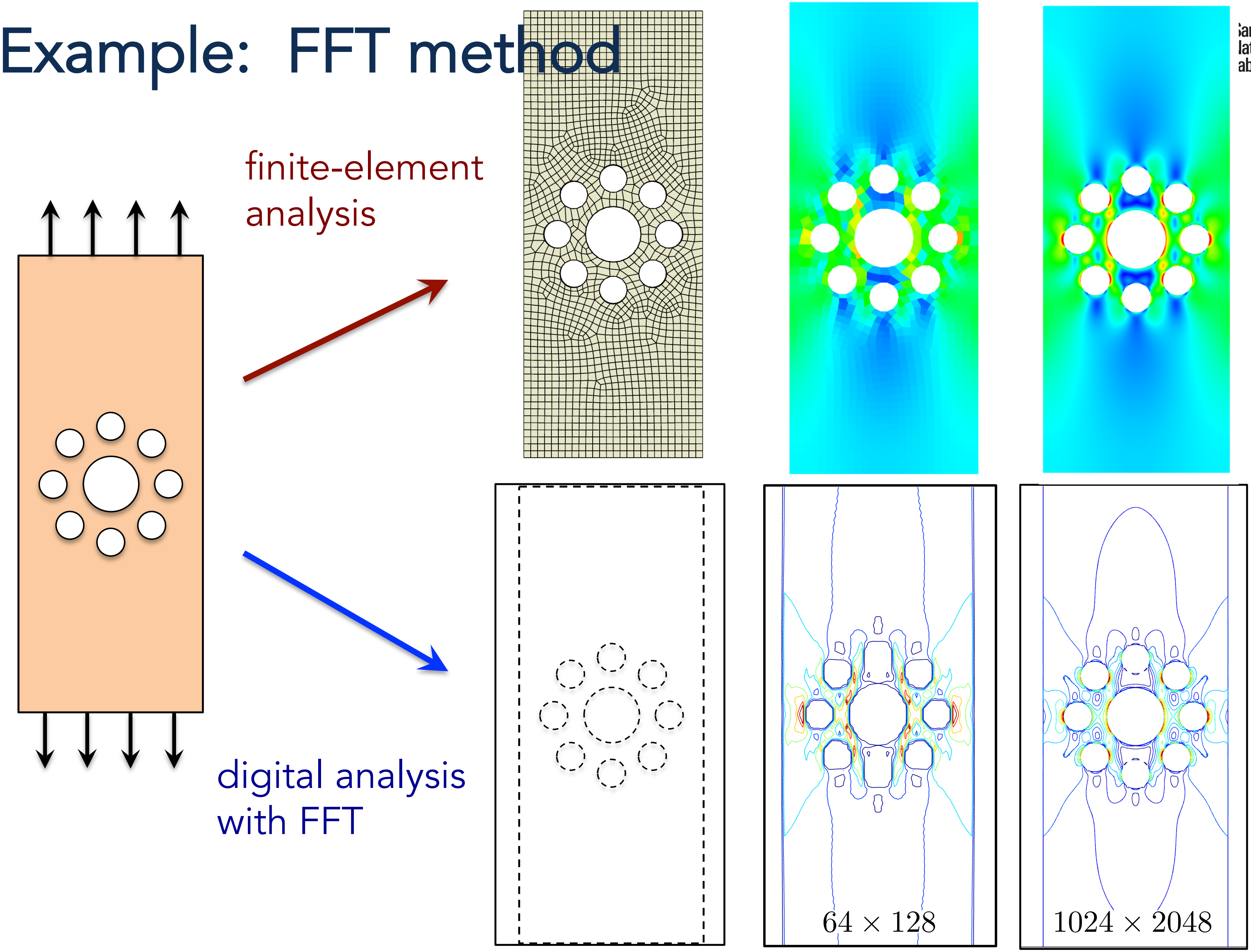


Bishop, 2004, ``Rapid stress analysis of geometrically complex domains using implicit meshing", Computational Mechanics, 30, 46-478.

FFT method

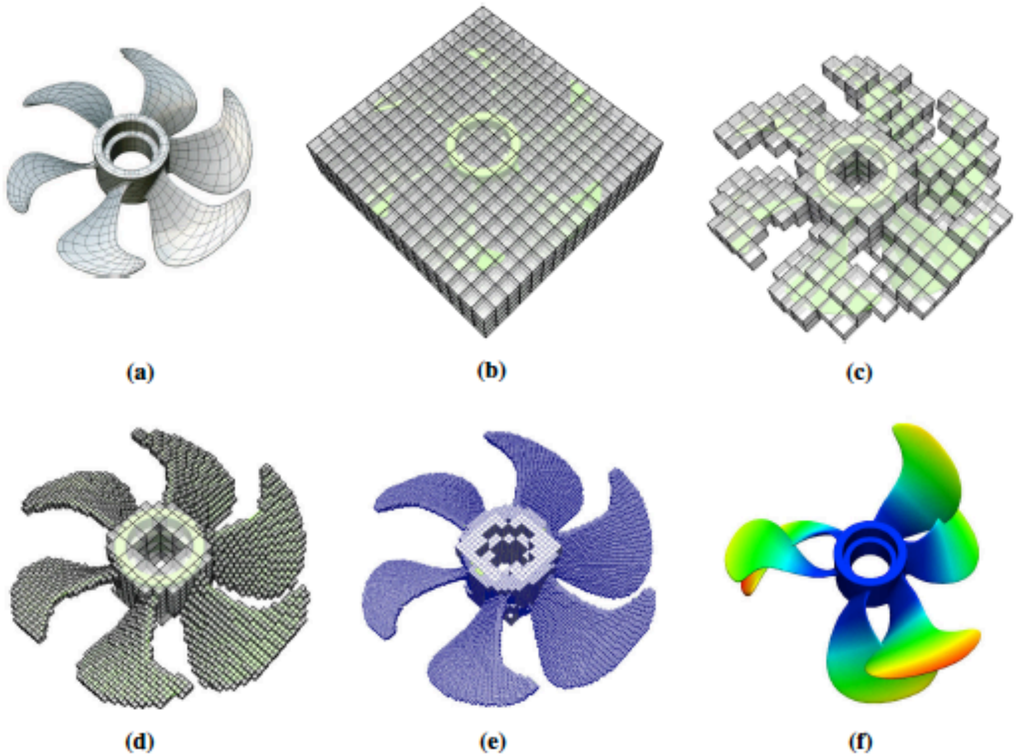
1. Embed complex structure in a box that is simple to mesh.
2. Discretize displacement field using a Fourier basis (voxelation of domain).
3. Use fixed-point iteration to solve governing PDEs using 3D FFT.

Example: FFT method



The Finite Cell Method: A Review in the Context of Higher-Order Structural Analysis of CAD and Image-Based Geometric Models

D. Schillinger & M. Ruess, Archive of Computational Methods in Engineering, 2014,



- Consistent with implicit representation of part geometry
- Fast analysis (no explicit meshing)

Goals to advance predictive methods in AM

Short term

- Continue development of advanced viscoplastic macroscopic material models with internal-state variables capable of representing changes to microstructure due to complex processing history.
- Process modeling (T, stress) for full-field residual-stress state determination
- Measurement and inversion techniques for full-field residual-stress state determination

Goals to advance predictive methods in AM

Long term

- Error estimation in engineering quantities of interest for quantifying material model form error, discretization error, and homogenization error.
- Process models for microstructure predictions, e.g. KMC, phase field.
- Multiscale material models that represent microstructure explicitly, e.g. through concurrent homogenization with crystal-plasticity models.
- Development of crystal-plasticity models; advanced calibration methods.
- Data science enabled by high-throughput testing and digital-volume correlation.
- Development of implicit geometry representations and computational techniques.
- Fast simulations tools for industrial use.