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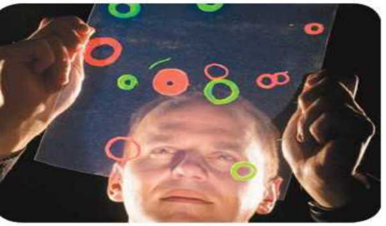

Optimization Under Uncertainty for Predicting Properties and Performance

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Uncertainty Quantification in Computational Solid and Structural Materials Modeling

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Baltimore, MD

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Context: Topology Optimization

Design Tools to Leverage Additive Manufacturing

Objective: Provide a *design environment* that can leverage existing simulation tools and emerging HPC architectures.

Forward Problem:

Design + Materials → Response

Inverse Problem:

Design + Materials ← Response

Approach: Use *topology optimization* to let performance objectives dictate the design

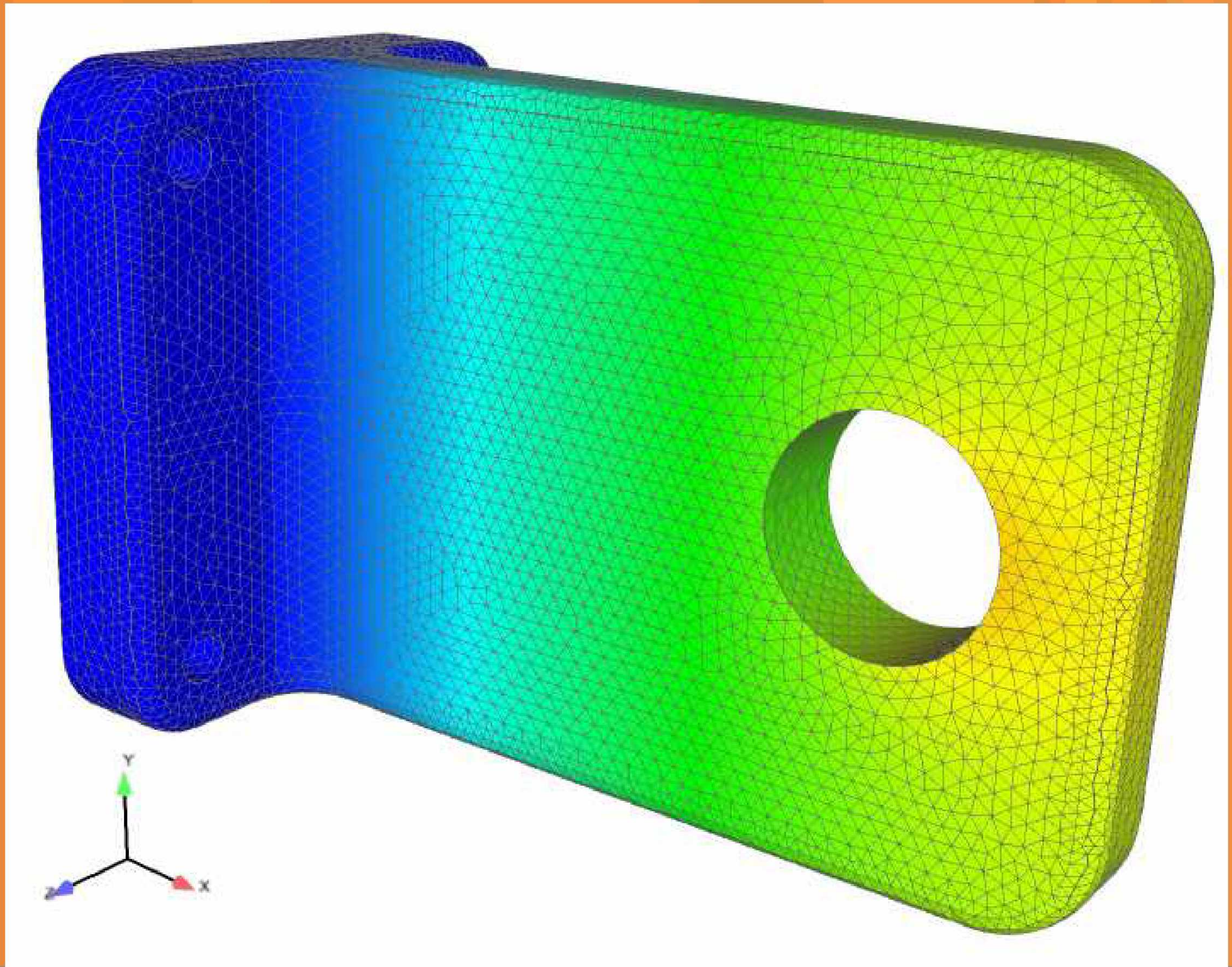
Objective: $\min_{\boldsymbol{z},\boldsymbol{x}} \sum_{\boldsymbol{i}} \alpha_i f_i(\boldsymbol{u}_i, \boldsymbol{z}, \boldsymbol{x})$

PDE Constraint: $\boldsymbol{g}_i(\boldsymbol{u}_i, \boldsymbol{z}, \boldsymbol{x}) = \boldsymbol{0}$

Inequality Constraint: $h(\boldsymbol{u}, \boldsymbol{z}, \boldsymbol{x}) \leq 0$

WATCHING DESIGNS EVOLVE THROUGH SIMULATION

Real time multi-physics design

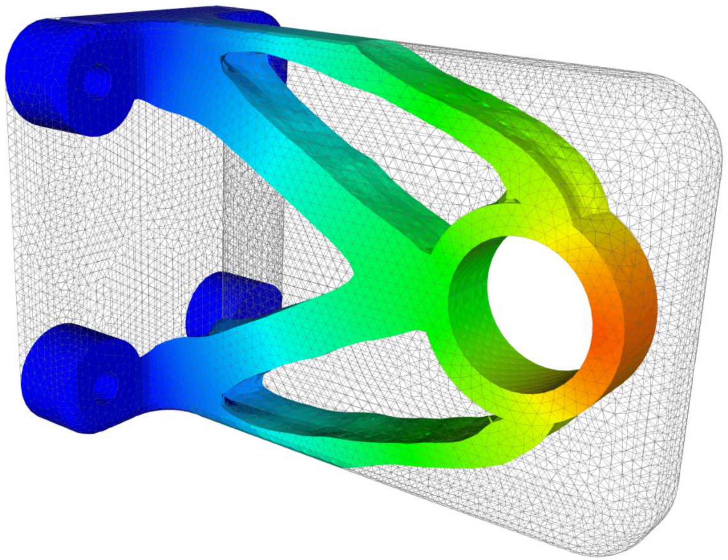


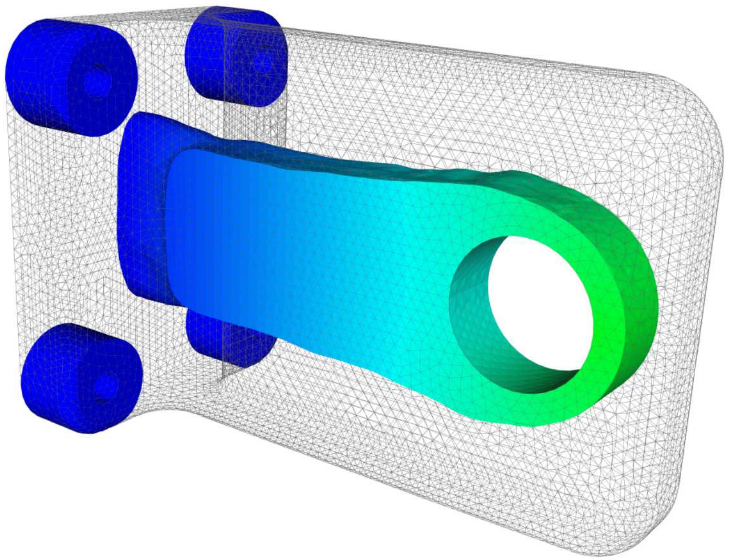
- GPU enabled solver package
- Optimized for stiffness and thermal conductivity
- Video is time is the real time to optimize the design

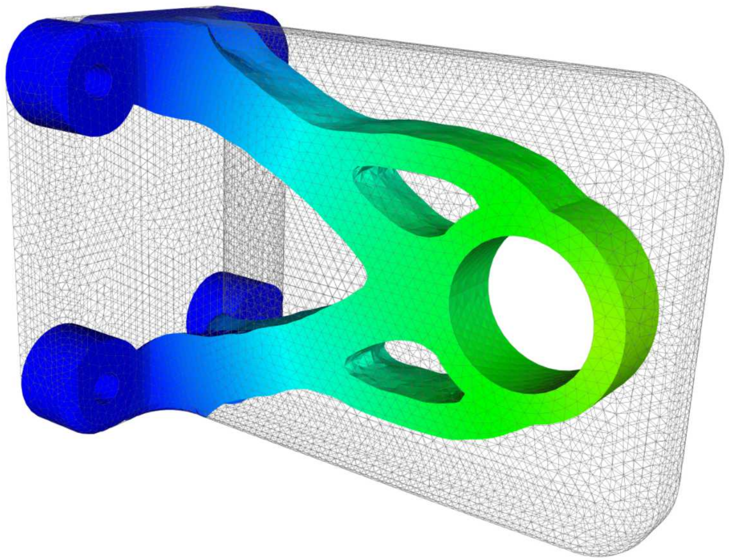
DIFFERENT PERFORMANCE OBJECTIVES LEADS TO DIFFERENT DESIGNS

Important to incorporate as much of the relevant physics as possible

Mechanical compliance minimization	Thermal compliance minimization	Mechanical and thermal compliance minimization







Constraint: *Equal mass in each design*

Note: Structure is disconnected from the mounts – no consideration was given to mechanical stiffness!

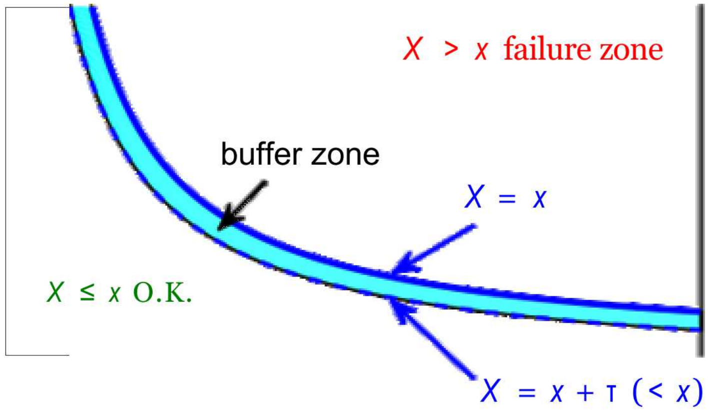
Incorporating Uncertainty

- **Probabilistic optimization**
  - Risk measures
  - Buffered probabilities
- **Material-aware optimization**
  - Continuum material anisotropy
  - Microstructure anisotropy due to additive manufacturing

Buffered Probabilities

Sandia National Laboratories

Incorporates conservatism due to large tail values

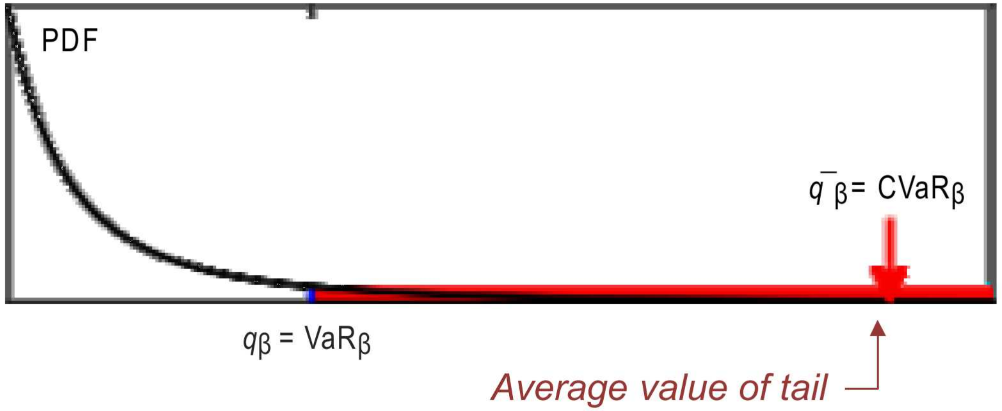


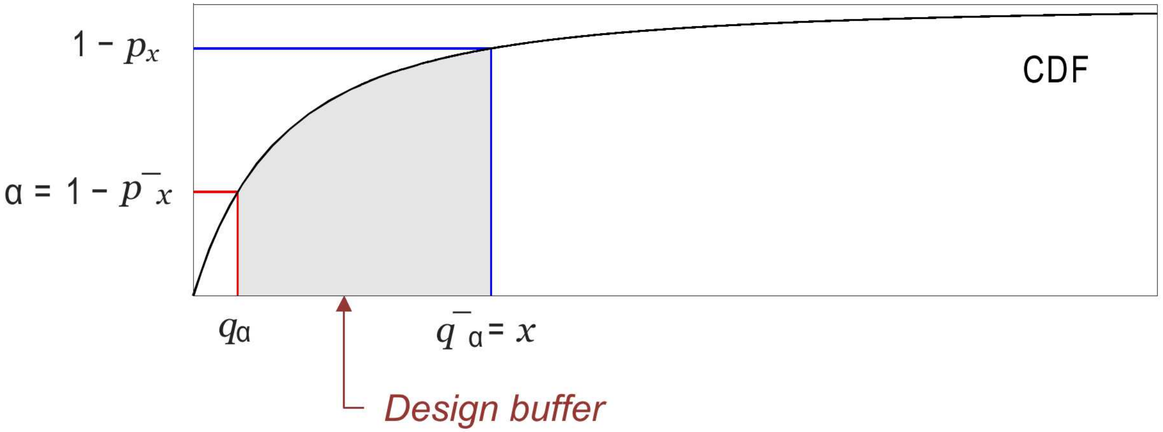
Buffered probability of exceedance: $R(X) = \bar{p}_x(X) = \mathrm{P}(X > \tau(x))$

where $\tau(x)$ is determined by $\mathrm{CVaR}_{(1-\bar{p}_x(X))}(X) = \mathrm{E}[\,X \mid X > \tau(x)\,] = x$

$$\boxed{\mathrm{bPOE}_x[X] = 1 - \alpha \quad \text{where } \alpha \text{ solves } \mathrm{CVaR}_\alpha[X] = x}$$

Conditional Value-at-Risk





Example: 3D Topology Optimization with Buffered Probability

Given compliance tolerance c_0, probability $p_0 \in (0, 1)$, order $q \geq 1$,

$$\min_{0 \leq z \leq 1} \int_D z \,\mathrm{d}x =: \mathrm{vol}(z) \quad \text{subject to} \quad \mathrm{bPOE}_{q,c_0}\left(\int_D F \cdot S(z)\mathrm{d}x \right) \leq 1 - p_o$$

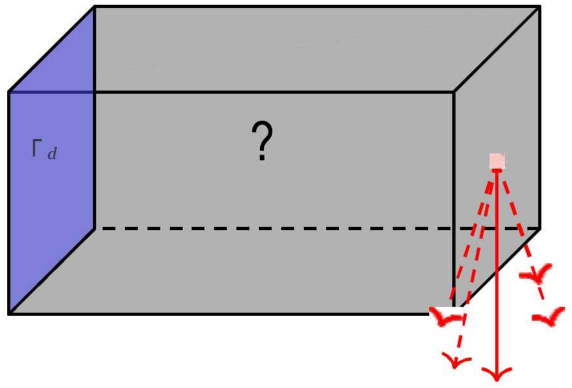
where $S(z) = u$ solves the **linear elasticity equations**

$$-\nabla \cdot (\mathbf{E}(z) : \varepsilon u) = F, \qquad \text{in } D$$

$$\varepsilon u = \tfrac{1}{2}\left(\nabla u + \nabla u^{\top}\right), \qquad \text{in } D$$

$$u = 0, \qquad \text{on } \Gamma_D$$

$$\varepsilon u : n = 0, \qquad \text{on } \partial D \setminus \Gamma_D$$



F: Three uncertain parameters

- Magnitude
- Polar and azimuthal angles

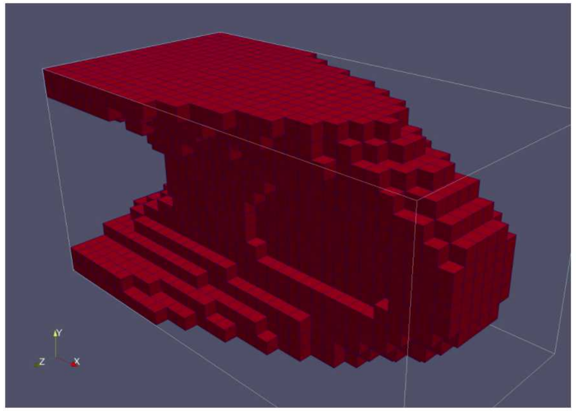
Numerical Results

Spatial Discretization: Q1 FEM on a uniform $32 \times 16 \times 16$ mesh

Stochastic Discretization: $Q = 120$ Monte Carlo samples

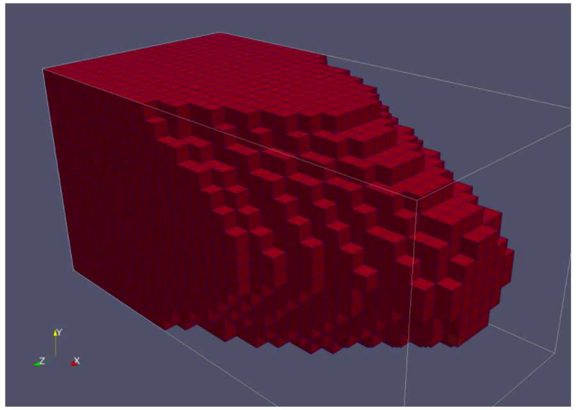
Problem Data: $p_0 = 0.75$ and $c_0 = 2\mathrm{E}\left[\int_D F \cdot S(\mathbf{1})\mathrm{d}x\right]$

Mean Value



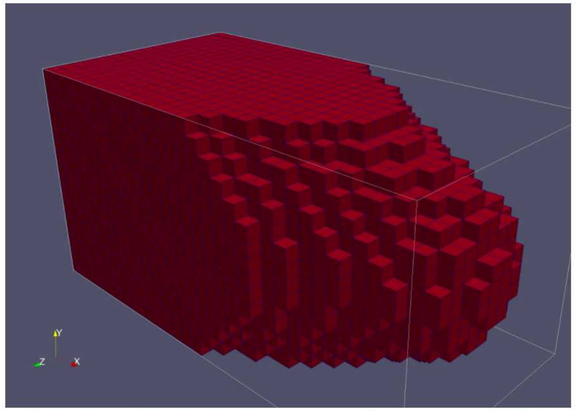
Deterministic

Risk Neutral



Constraint on average compliance

bPOE



Constraint on average of largest 25%

	Mean Value	Risk Neutral	bPOE
Volume Fraction	49.1%	47.6%	67.2%

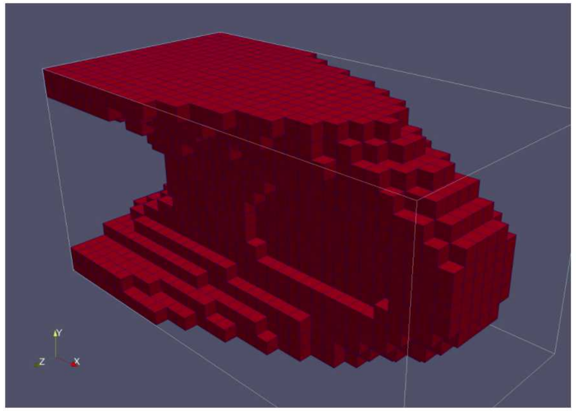
Numerical Results

Spatial Discretization: Q1 FEM on a uniform $32 \times 16 \times 16$ mesh

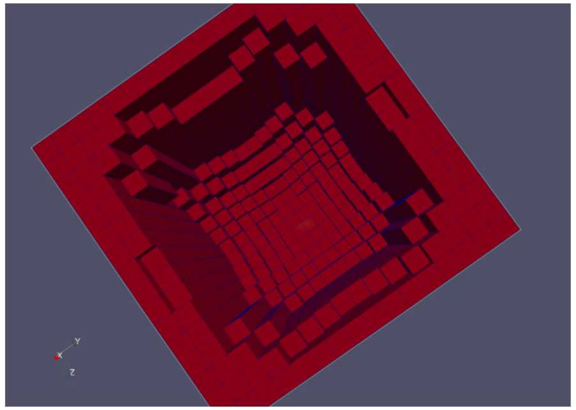
Stochastic Discretization: $Q = 120$ Monte Carlo samples

Problem Data: $p_0 = 0.75$ and $c_0 = 2\mathrm{E}\left[\int_D F \cdot S(\mathbf{1})\mathrm{d}x\right]$

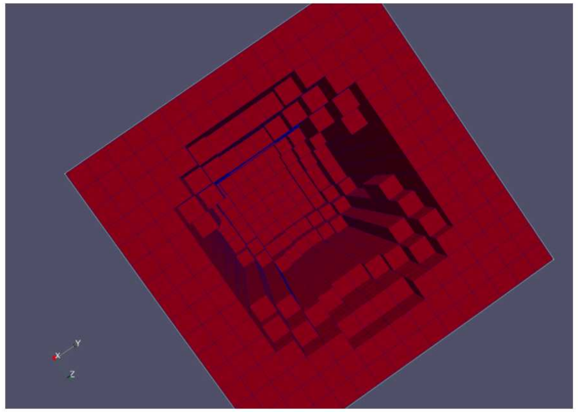
Mean Value



Risk Neutral



bPOE



Note: Topology changes from beam to shell!

	Mean Value	Risk Neutral	bPOE
Volume Fraction	49.1%	47.6%	67.2%

Incorporating Uncertainty

- **Probabilistic optimization**
  - Risk measures
  - Buffered probabilities
- **Material-aware optimization**
  - Continuum material anisotropy
  - Microstructure anisotropy due to additive manufacturing

Material-aware stress minimization

Example: Barlat model w/ anisotropic yield surface

Objective: $\min_{\boldsymbol{z},\boldsymbol{x}} f(\boldsymbol{u},\boldsymbol{z},\boldsymbol{x})$

PDE Constraint: $\boldsymbol{g}(\boldsymbol{u},\boldsymbol{z},\boldsymbol{x}) = \boldsymbol{0}$

Inequality Constraint: $h(\boldsymbol{u},\boldsymbol{z},\boldsymbol{x}) \leq 0$

$$f = \left[\frac{1}{V}\int_{\Omega}\left(\frac{\bar{\sigma}}{\sigma_y}\right)^p dV\right]^{1/p}$$

Yield function

$$\bar{\sigma} = \left(\frac{\phi(\mathbf{S}',\mathbf{S}'')}{4}\right)^{1/a}$$

$$\mathbf{s}' = \mathbf{C}'\mathbf{s}$$

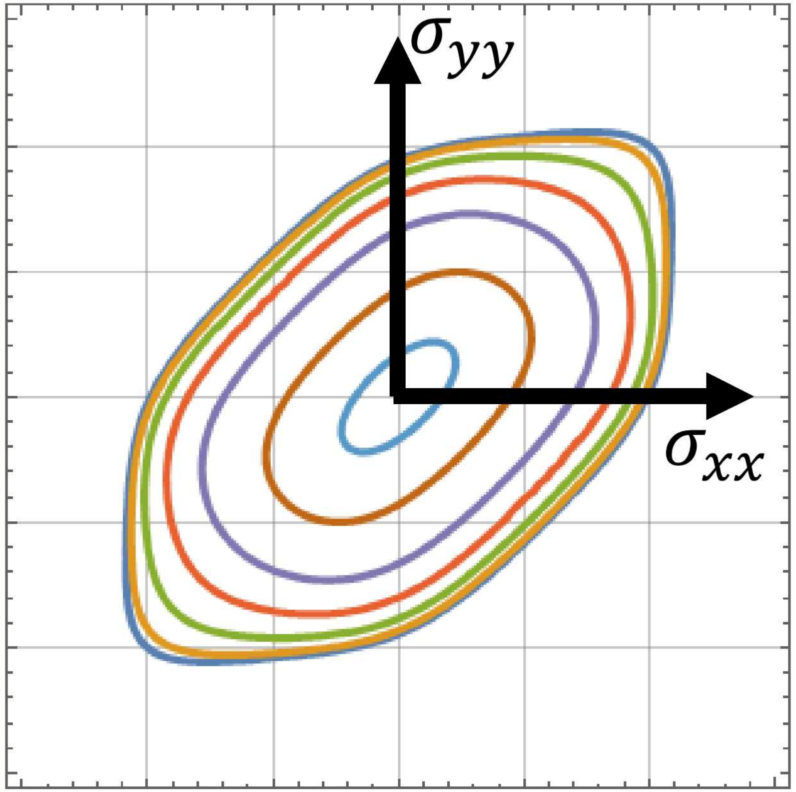
$$\mathbf{s}'' = \mathbf{C}''\mathbf{s}$$

$$\phi = \sum_{i=1}^{3}\sum_{j=1}^{3}\left|S_i' - S_j''\right|^a$$

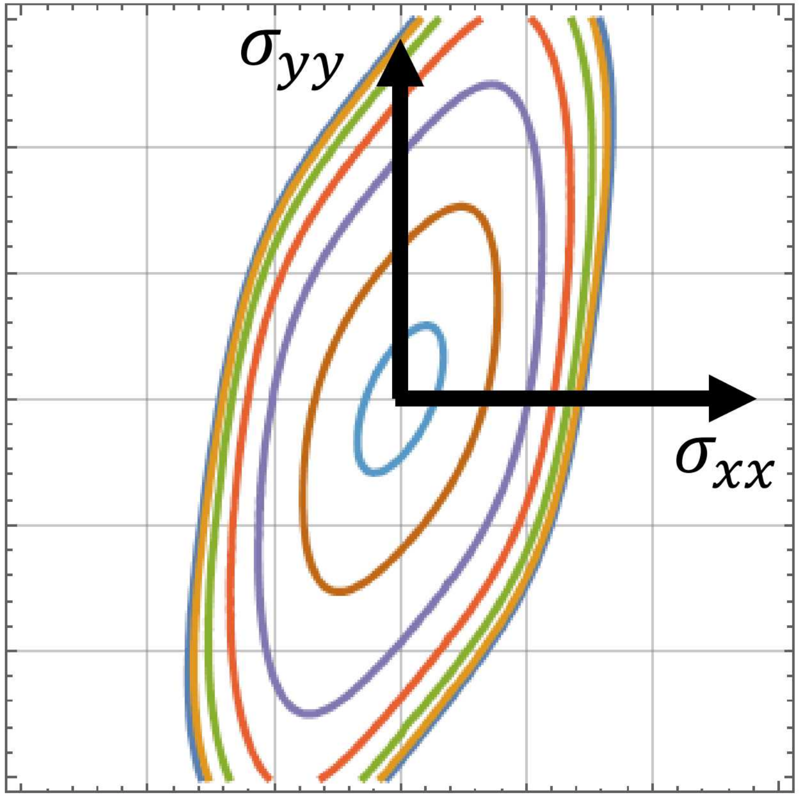
Material constants: $\mathbf{C}'$ $\mathbf{C}''$ a σ_y

Barlat et al. (2005), Int. J. Plasticity

Yield Surfaces



6111-T4 (Barlat, IJP, 2005)



Hypothetical material

Superposed Shear

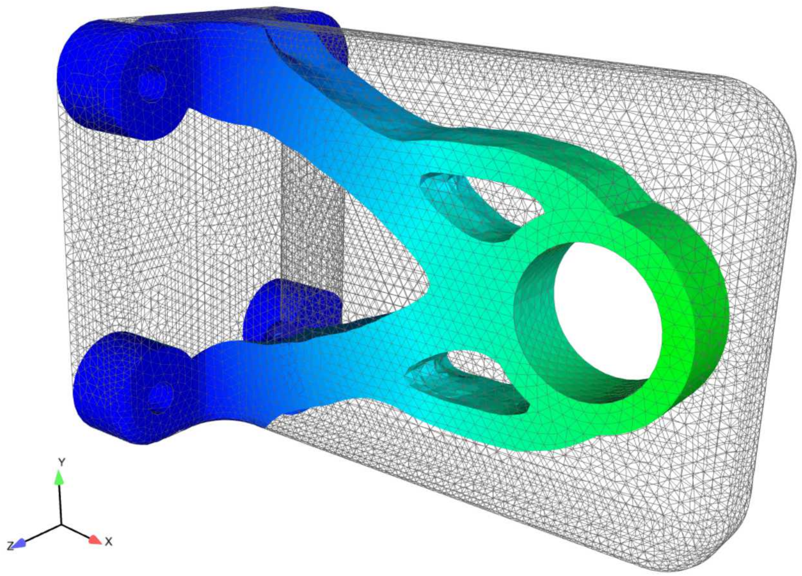
$\sigma_{xy} = 0.0$
$\sigma_{xy} = 0.1$
$\sigma_{xy} = 0.2$
$\sigma_{xy} = 0.3$
$\sigma_{xy} = 0.4$
$\sigma_{xy} = 0.5$
$\sigma_{xy} = 0.55$

Example: Material-aware compliance minimization

Thermal and mechanical compliance minimization

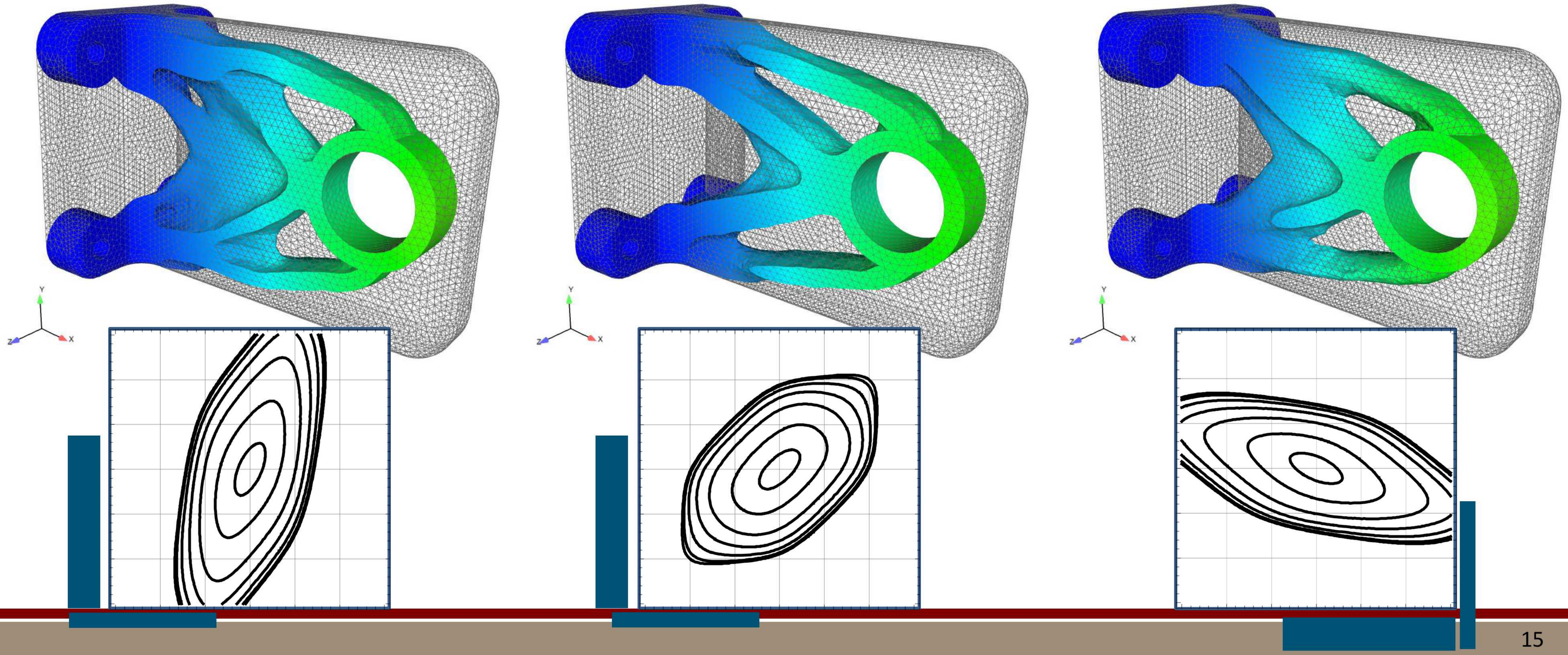
Mechanical and thermal load cases. 2 GPUs.

elements: 187k
dofs: 110k
iterations: 26
Run time: 28s



Example: Material-aware compliance minimization

V_f: 0.25

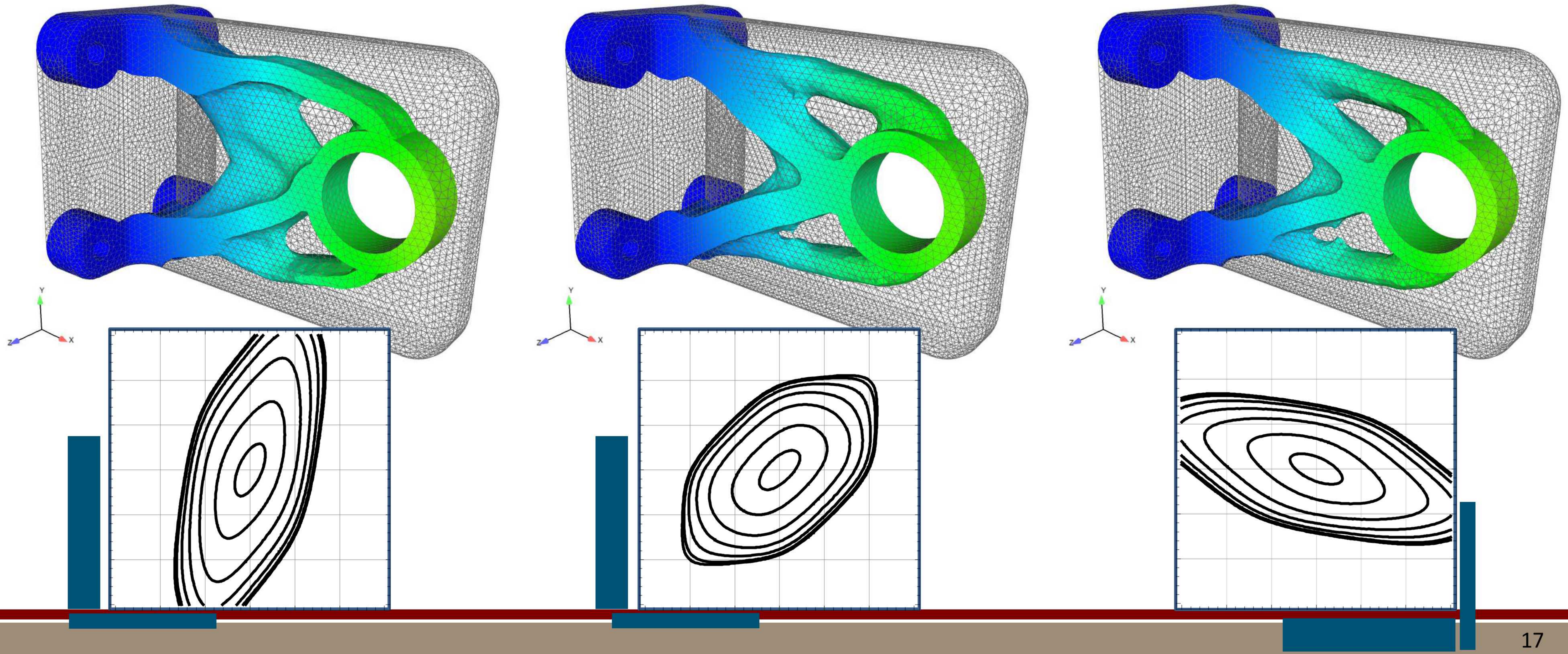


REMARK

In AM, it is common to see anisotropy in the build direction. Therefore, the desired bulk properties might influence choice of build direction.

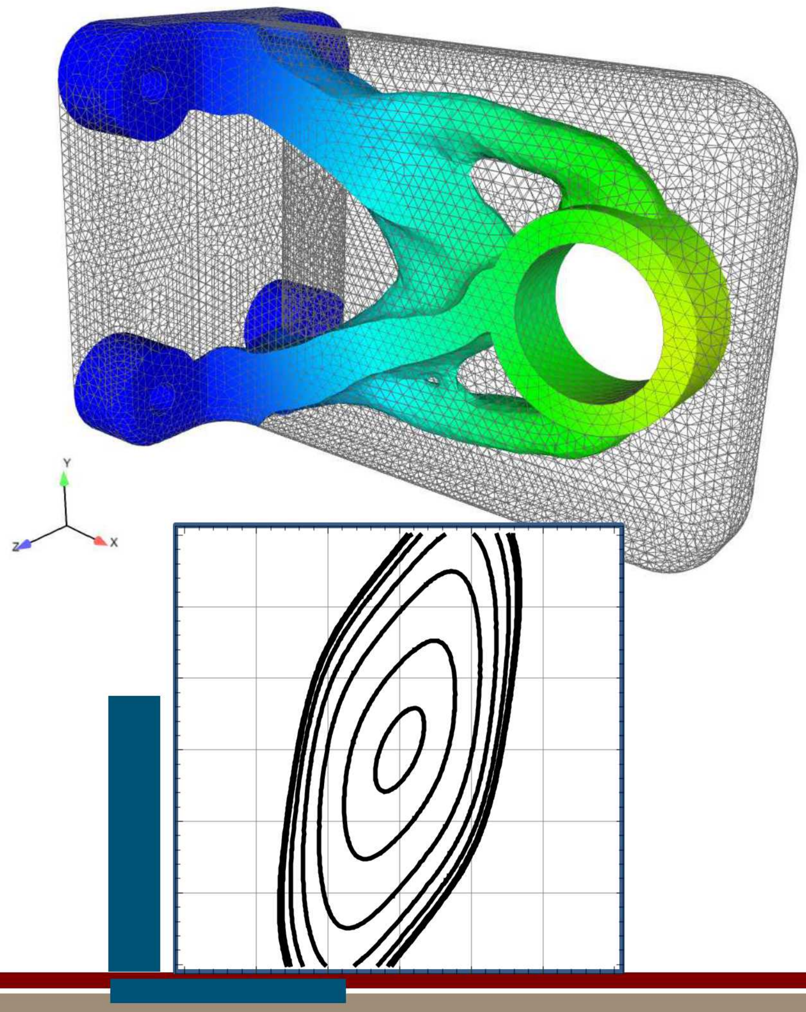
Example: Material-aware compliance minimization

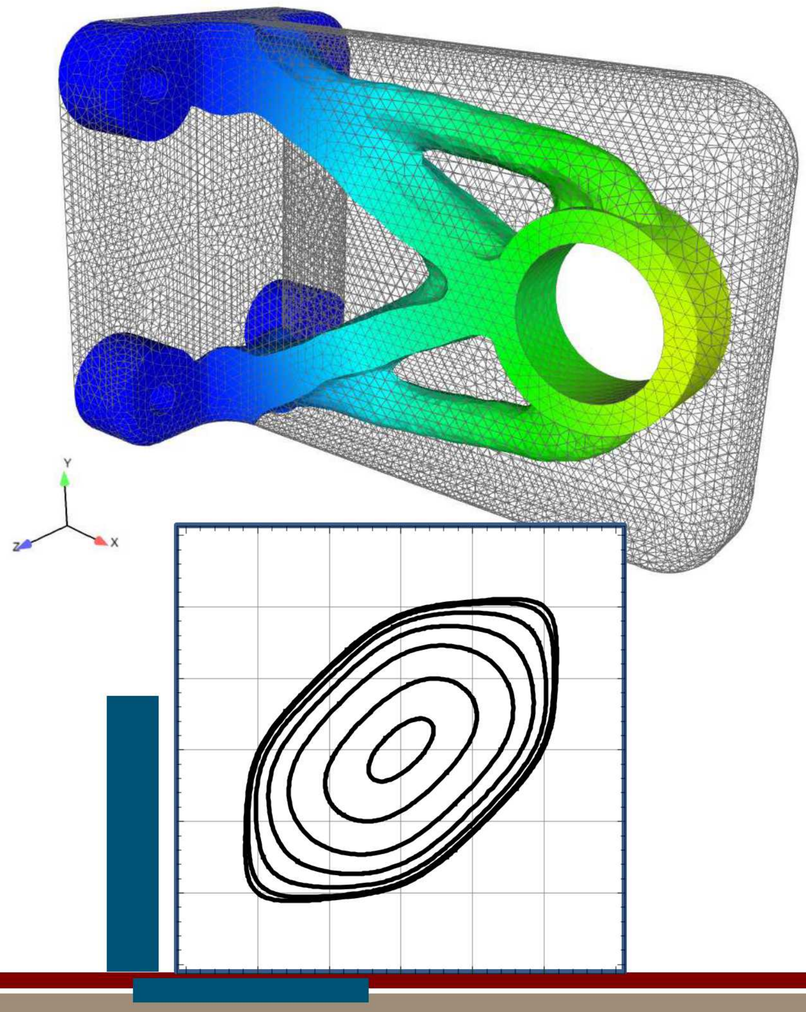
Vf: 0.20

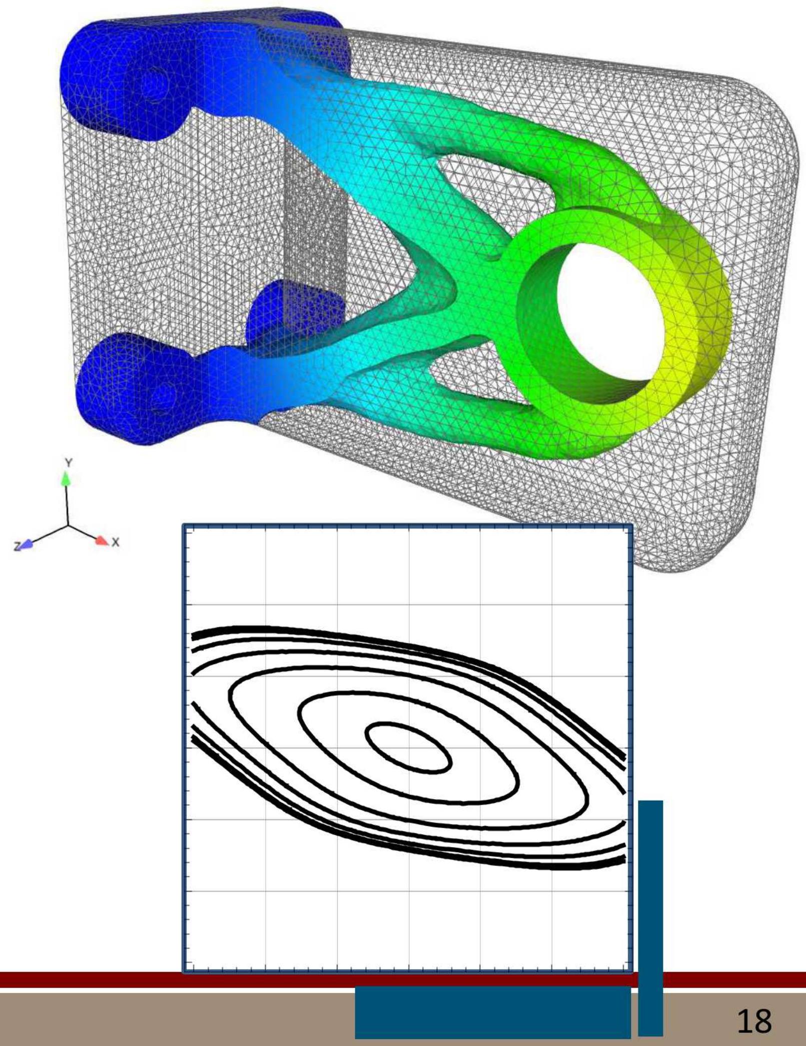


Example: Material-aware compliance minimization

V_f: 0.15

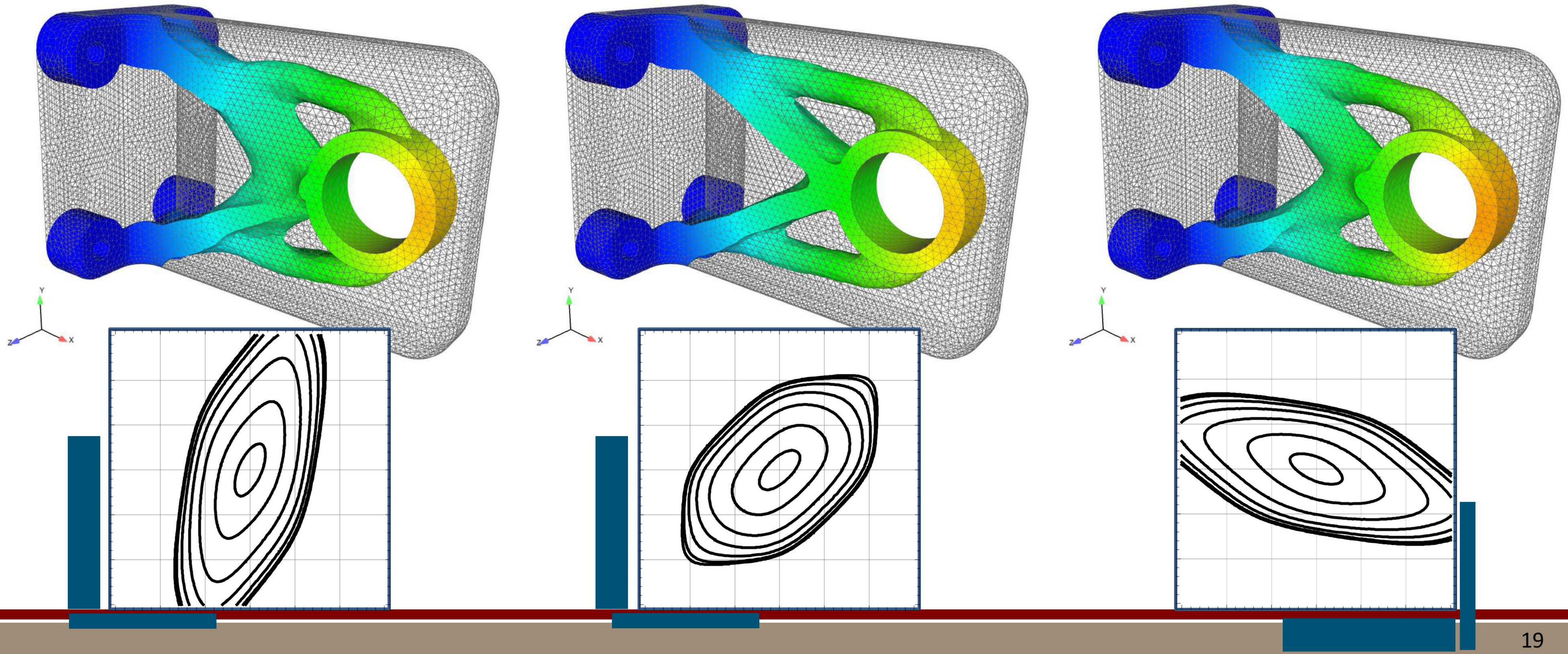


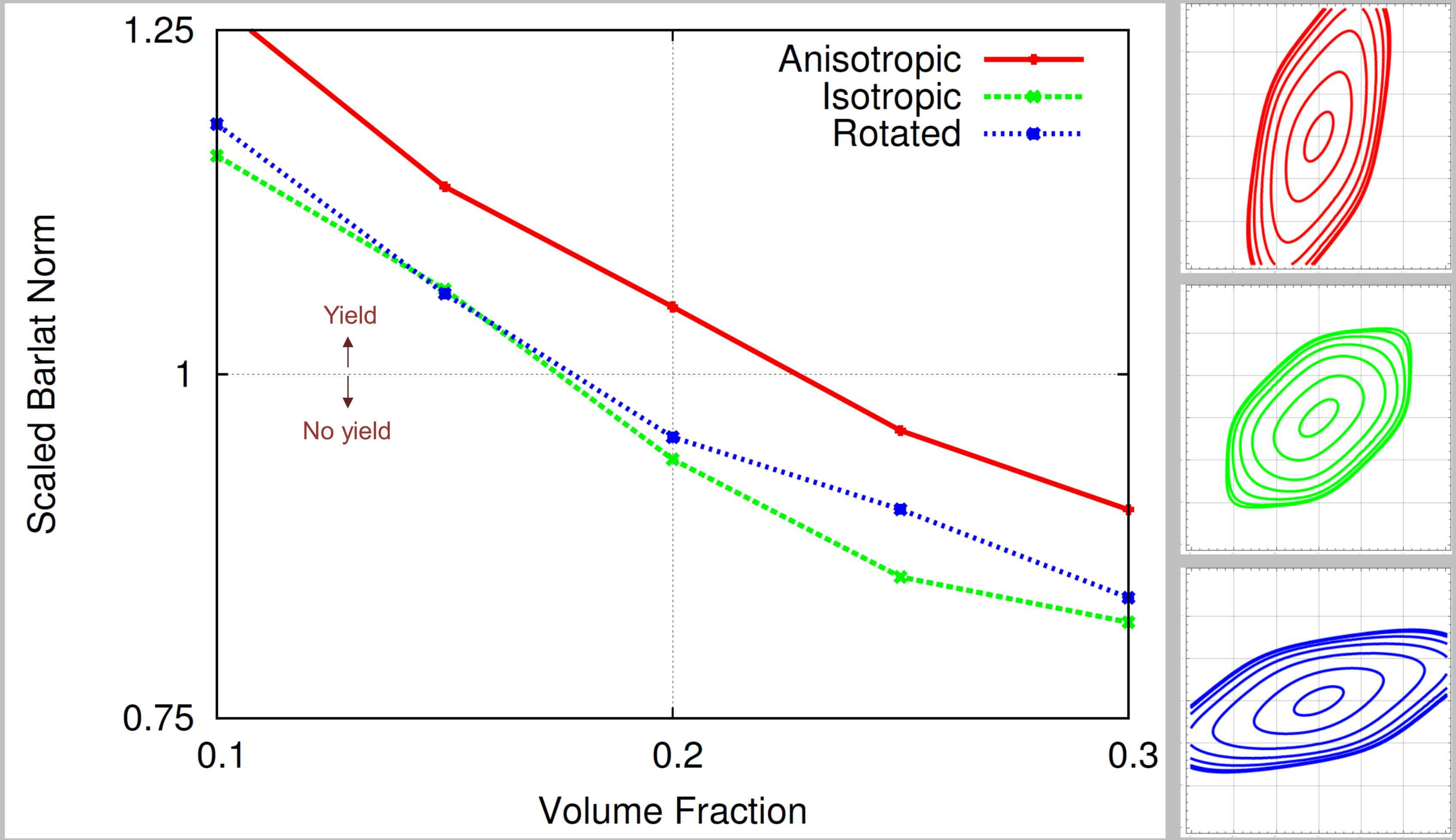




Example: Material-aware compliance minimization

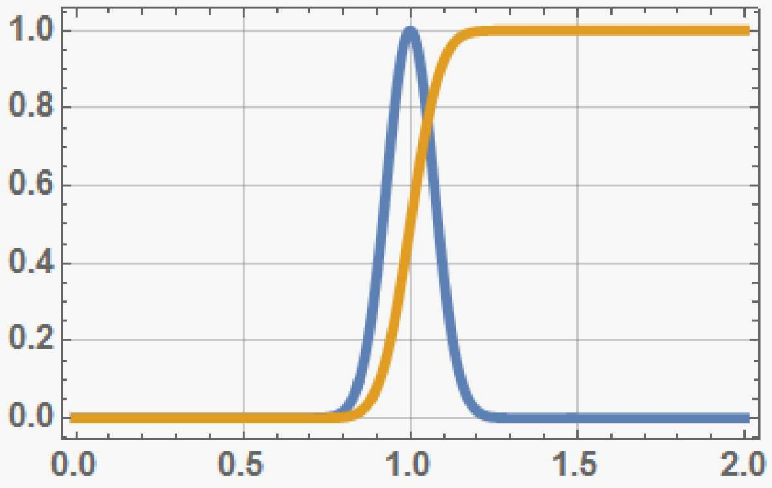
V_f: 0.10



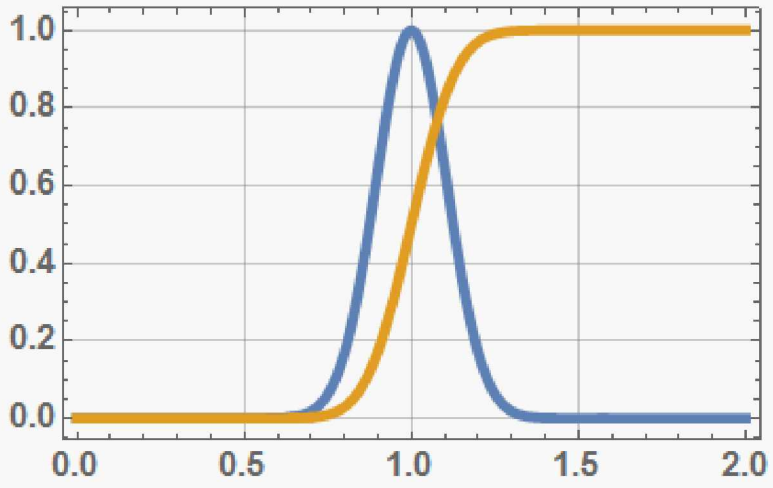

1.25
1
0.75
0.1
0.2
0.3
Scaled Barlat Norm
Volume Fraction
Anisotropic
Isotropic
Rotated
Yield
No yield

What if Yield Stress is Uncertain?

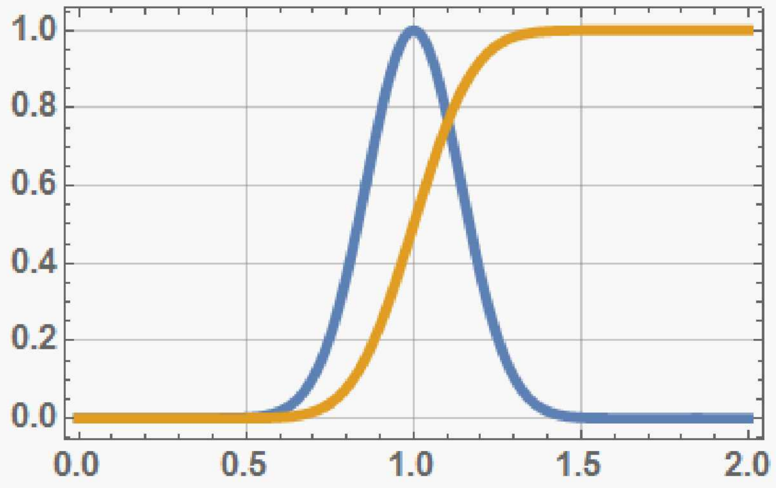
Standard Deviation: 0.1



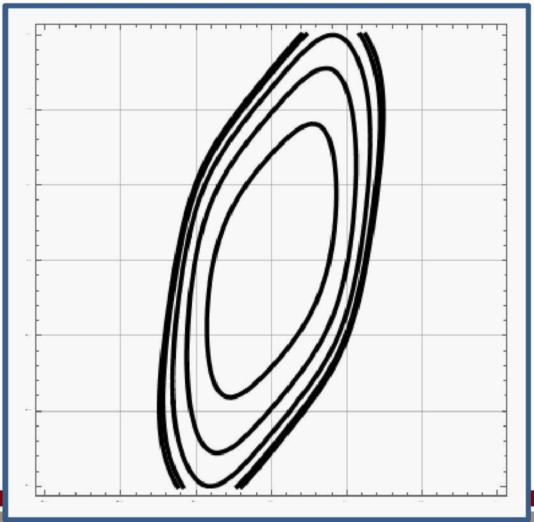
Standard Deviation: 0.15



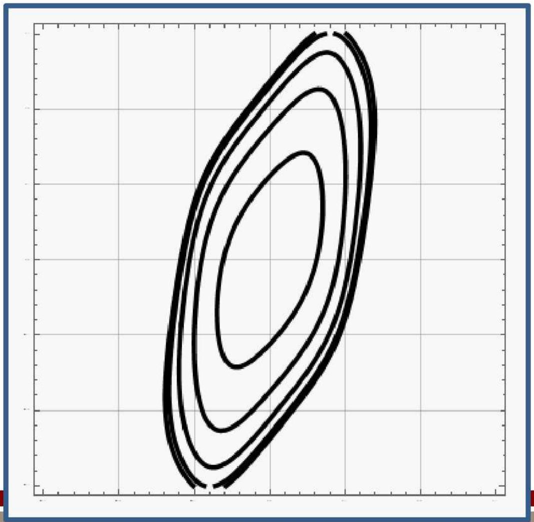
Standard Deviation: 0.2



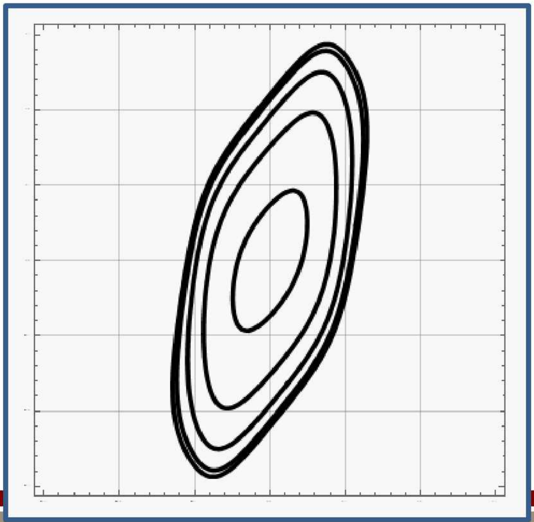
95% Confidence: 0.884

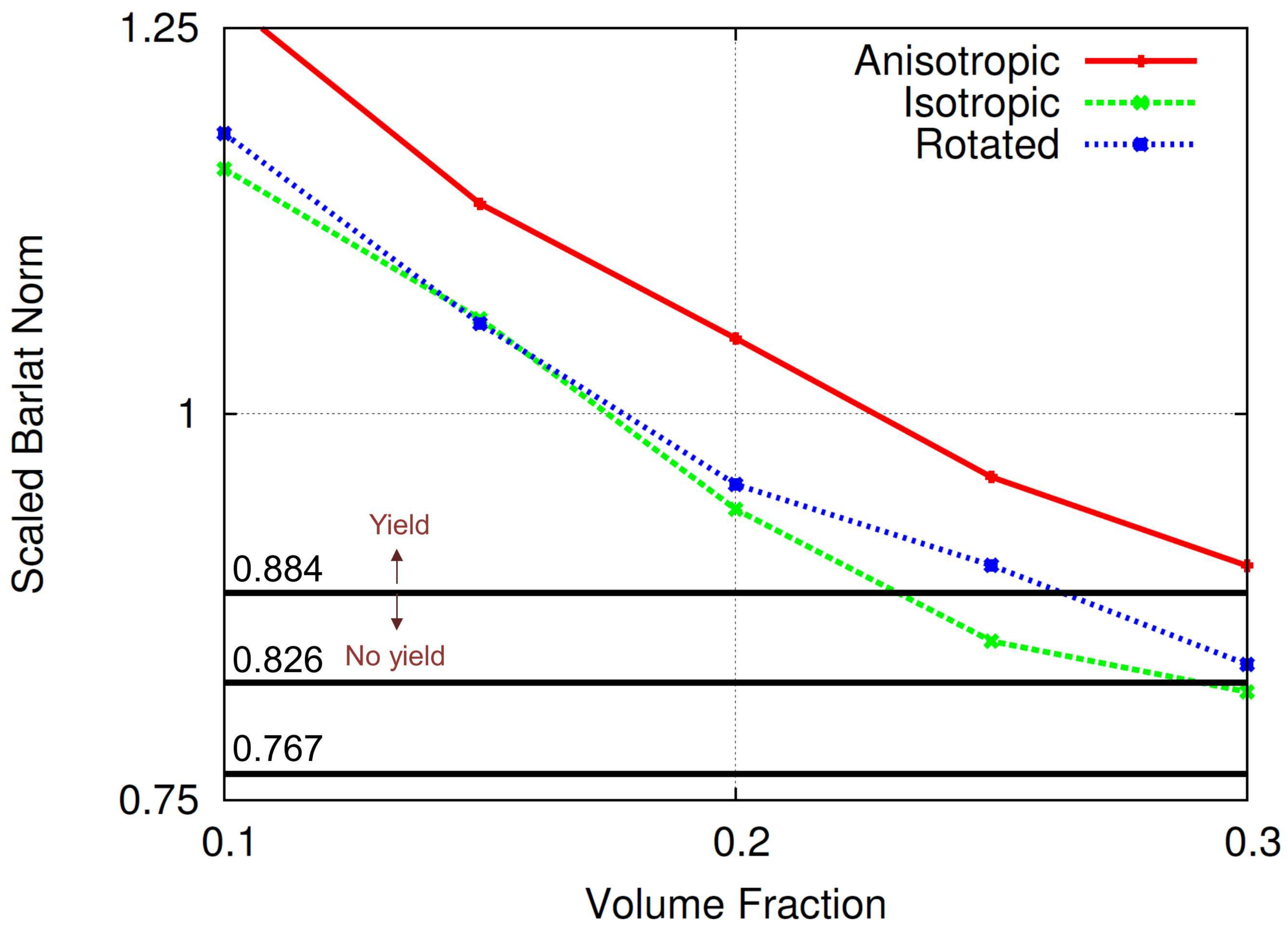


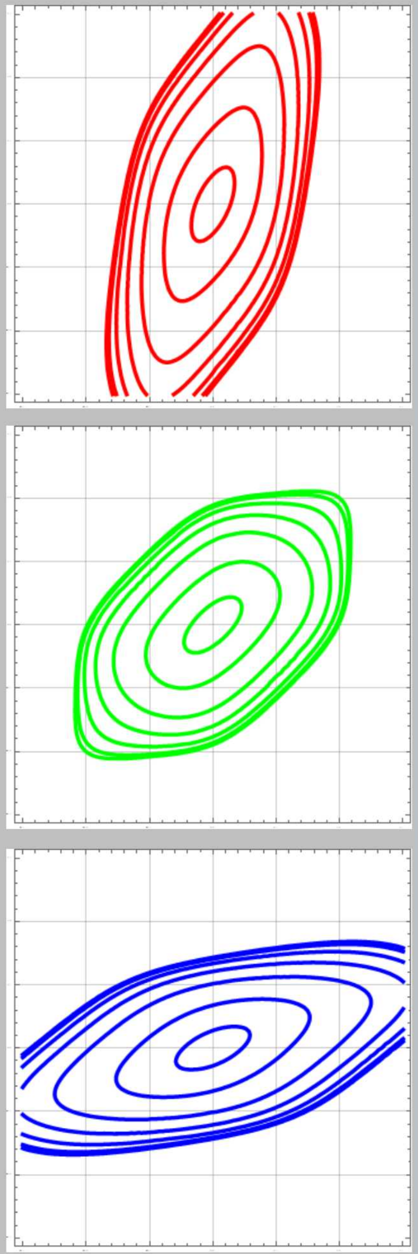
95% Confidence: 0.826



95% Confidence: 0.767




1.25
1
0.75
0.1
0.2
0.3
Scaled Barlat Norm
Volume Fraction
Anisotropic
Isotropic
Rotated
Yield
No yield
0.884
0.826
0.767



Incorporating Uncertainty

- **Probabilistic optimization**
  - Risk measures
  - Buffered probabilities
- **Material-aware optimization**
  - Continuum material anisotropy
  - Microstructure anisotropy due to additive manufacturing

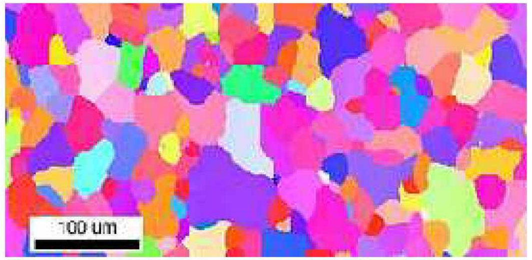
Additive Manufacturing for Metals

What are the issues?

Additive Manufacturing & Engineering Design

Caveat: not exhaustive

Wrought 304L stainless steel microstructure



AM 304L stainless steel microstructure

AM materials exhibit spatial heterogeneity

- Heterogeneous textures and morphologies at various length scales
- Residual stresses

Measurements indicate higher variability than wrought materials

- Yield stress, ductility, ultimate stress, rate effects

Challenges traditional deterministic modeling and design approaches

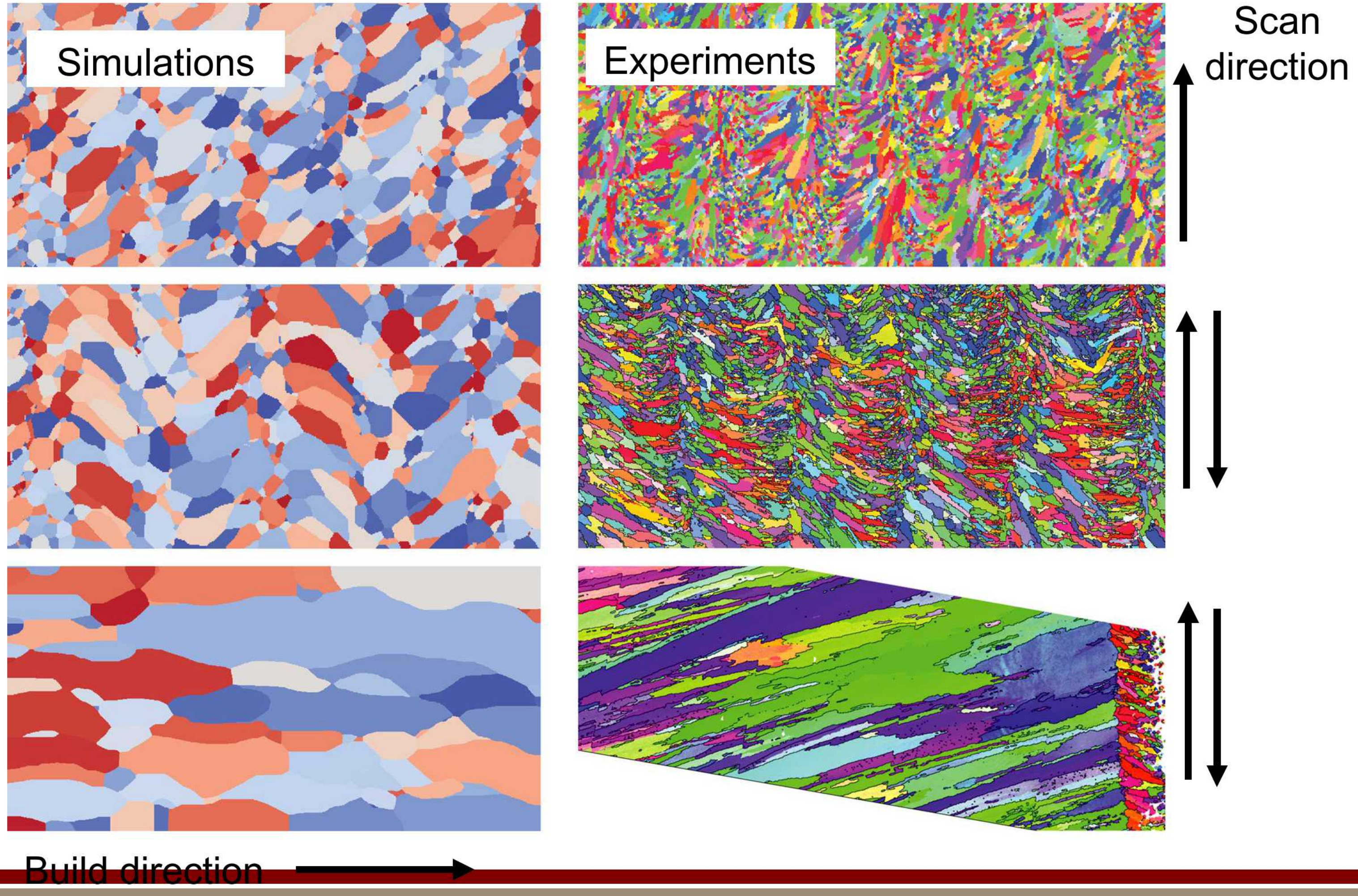
- Spatial heterogeneity and length scales

WHY IS A MICROSTRUCTURE SIMULATOR IMPORTANT?

Microstructural variations within and between different components control variation in engineering properties

Simulation of microstructural evolution during fabrication will inform:

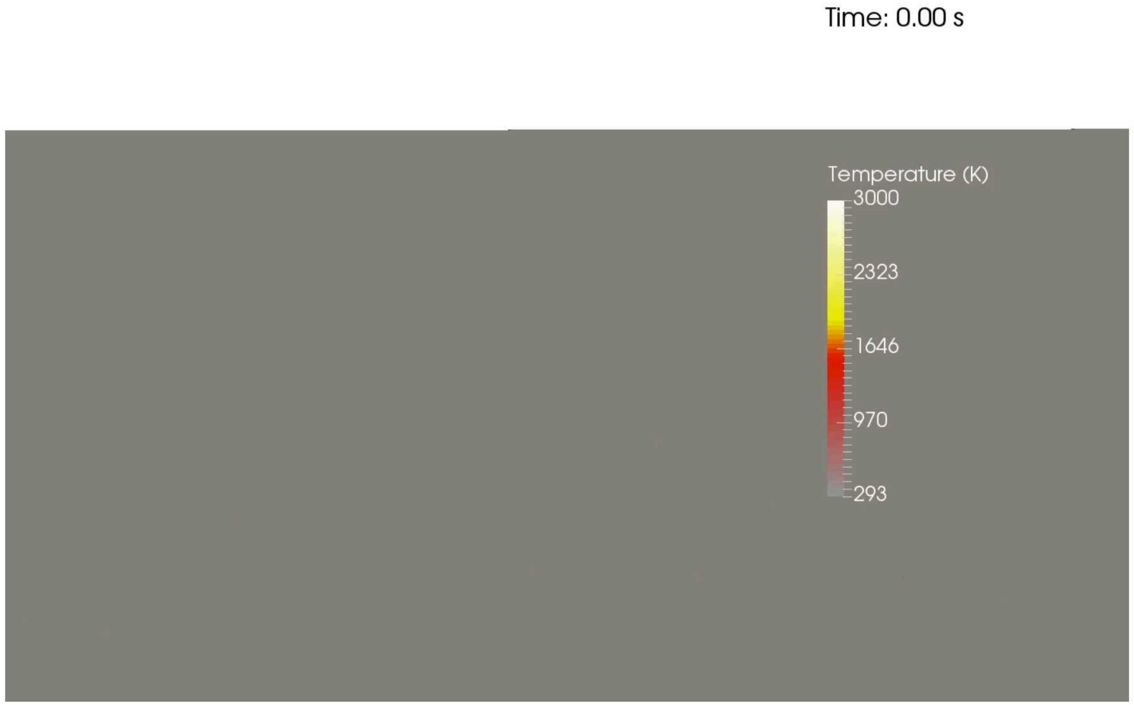
- Design of process variables
- Uncertainty quantification in final components produced



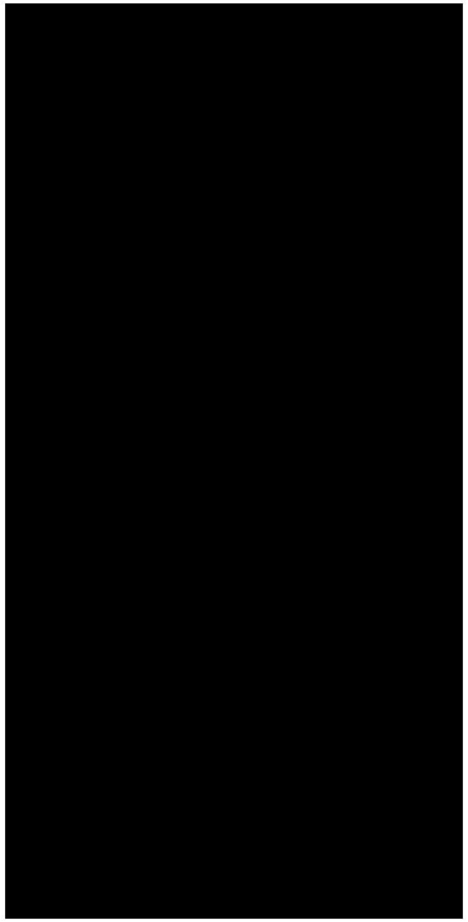
SPPARKS: Stochastic Parallel PARticle Kinetic Simulator
spparks.sandia.gov

PROCESS PARAMETERS – MICROSTRUCTURE – PERFORMANCE

Process determines structure



Sierra FEA Thermal Model

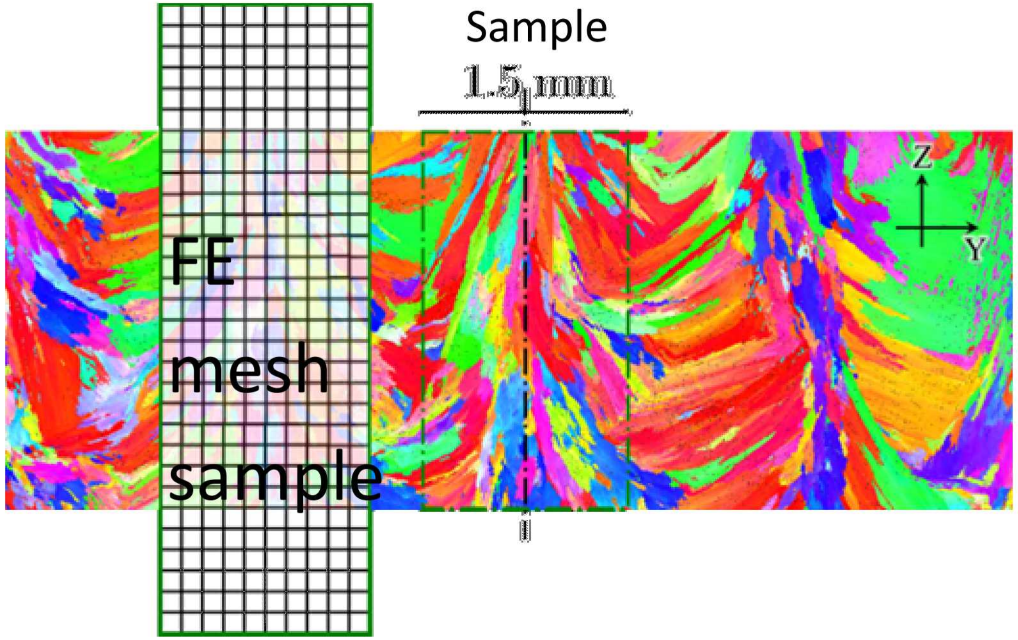


SPPARKS
MC Model

Coupling with SIERRA thermal models

How to model this heterogeneity and variability?

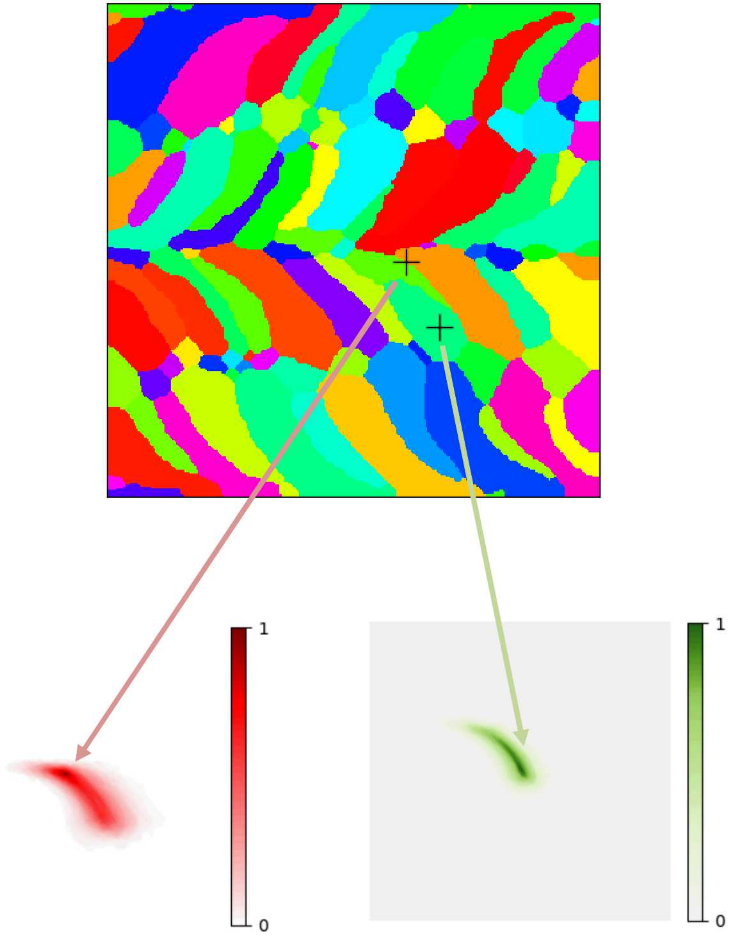
Approach: *Upscale microstructural effects*



- ❑ Avoids vexing problem of meshing material details
- ❑ *Systematically represents properties on coarse continuum model*
- ❑ Respects length scale and microstructure morphologies
- ❑ Reflects microstructure heterogeneity and variability

Upscaling Approach

- **Use synthetic microstructures via SPPARKS model of AM process**



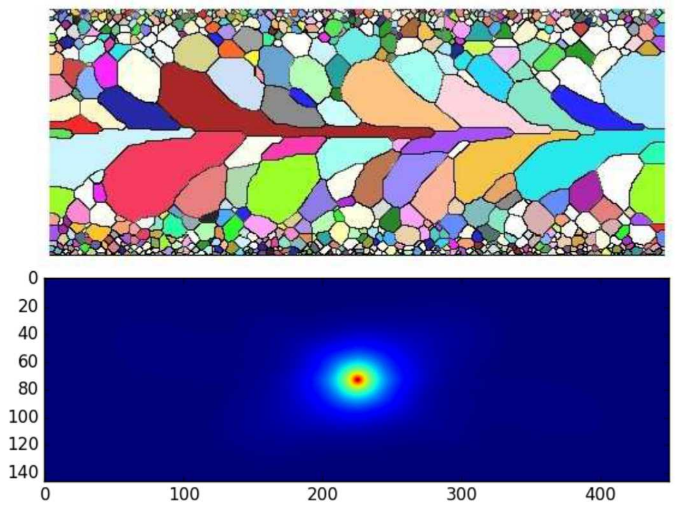
Spatial probability surrounding locations are part of grain +

- **Compute spatial statistics for FE quadrature points**

  (for 150 SPPARKS simulations)

- **Apply cluster algorithms from machine learning**

Comparison to current state-of-the-art

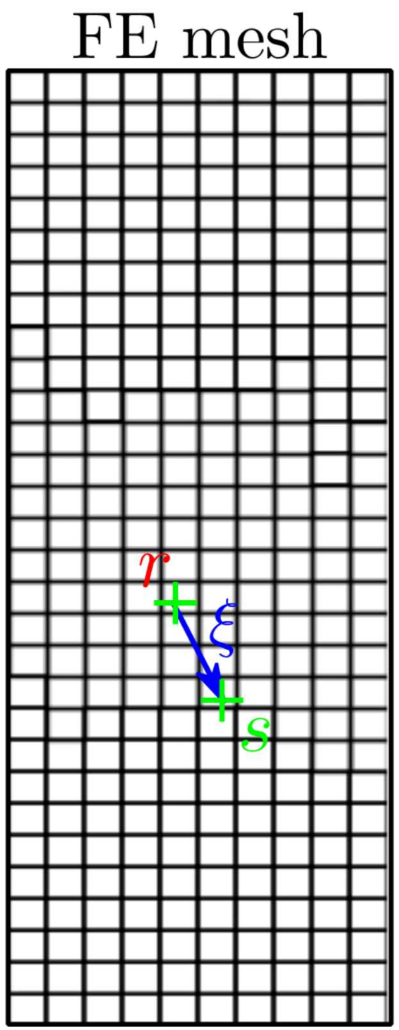


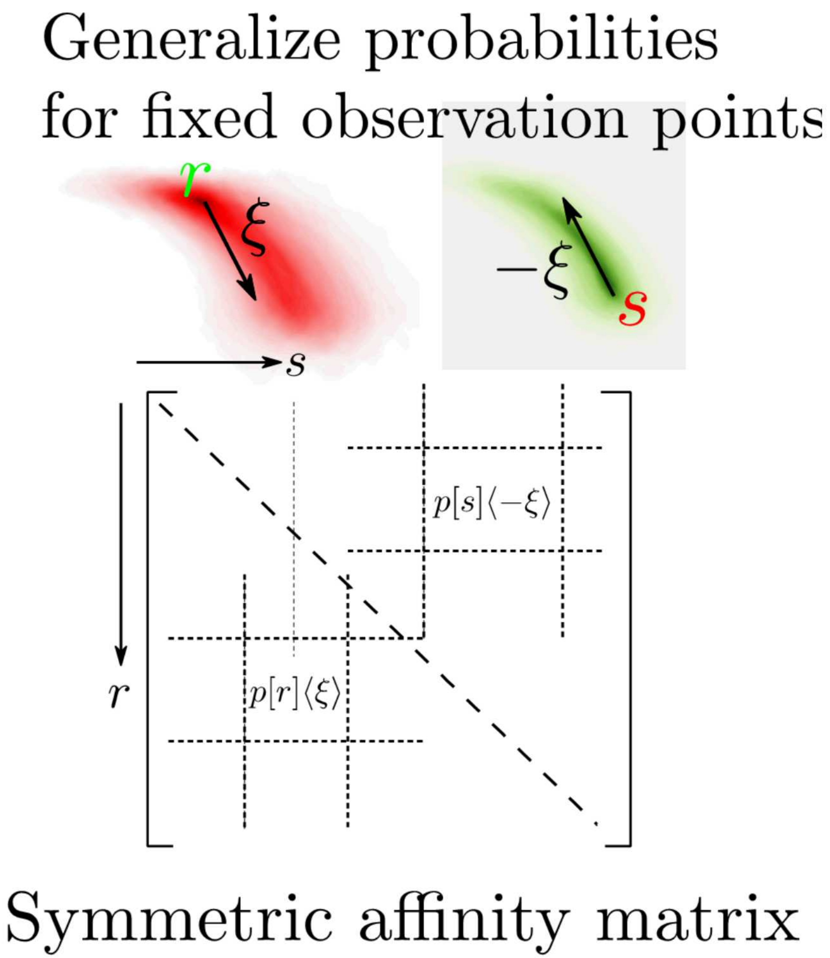
Sample Microstructure

Global S2: *Spatial heterogeneity lost*

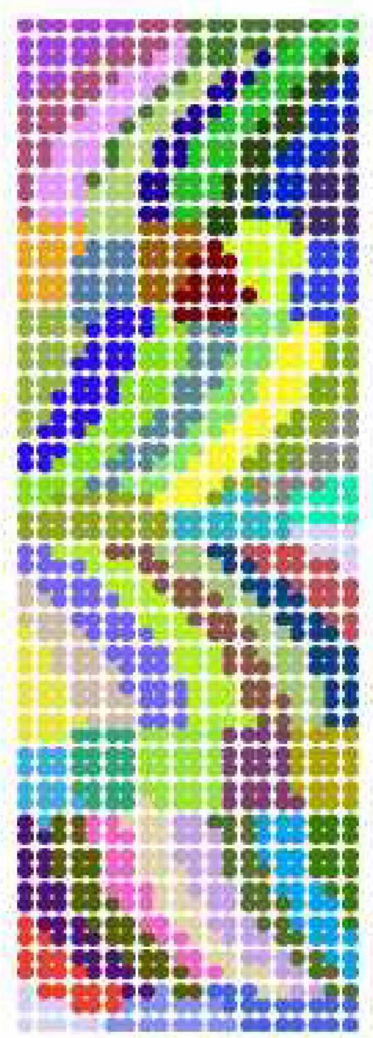
Computing spatial statistics

Identify FE quadrature points as fixed observation points



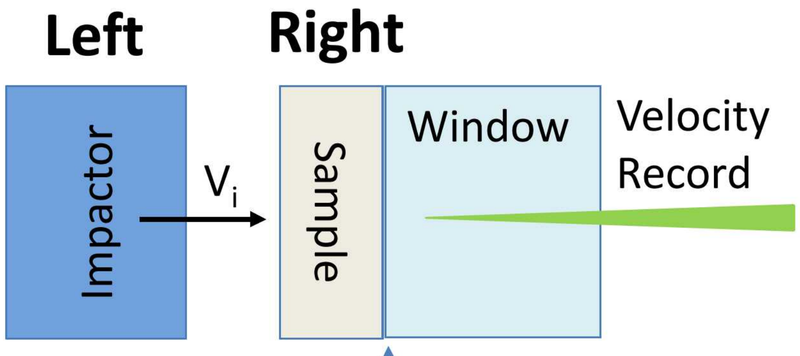


ML Clustering



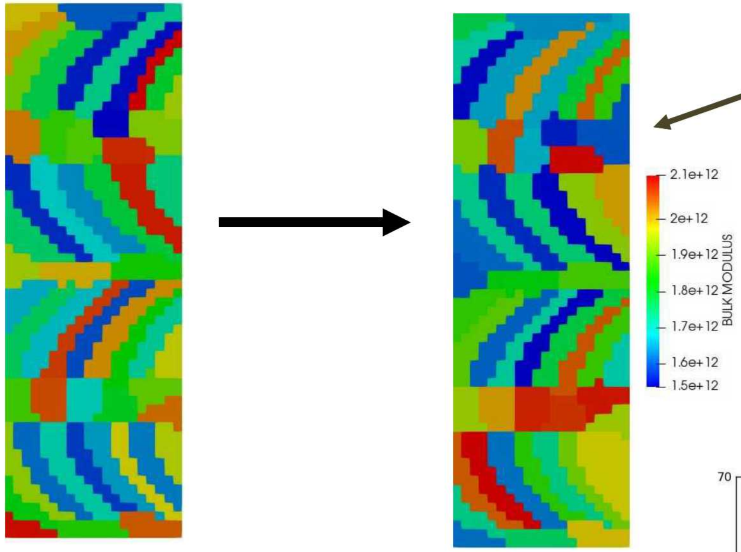
RESULT: Upscaled “mean” microstructure

Example: Sandia’s ALEGRA Shock Physics Code



Gas gun experiment schematic

***QoI:** Velocity*

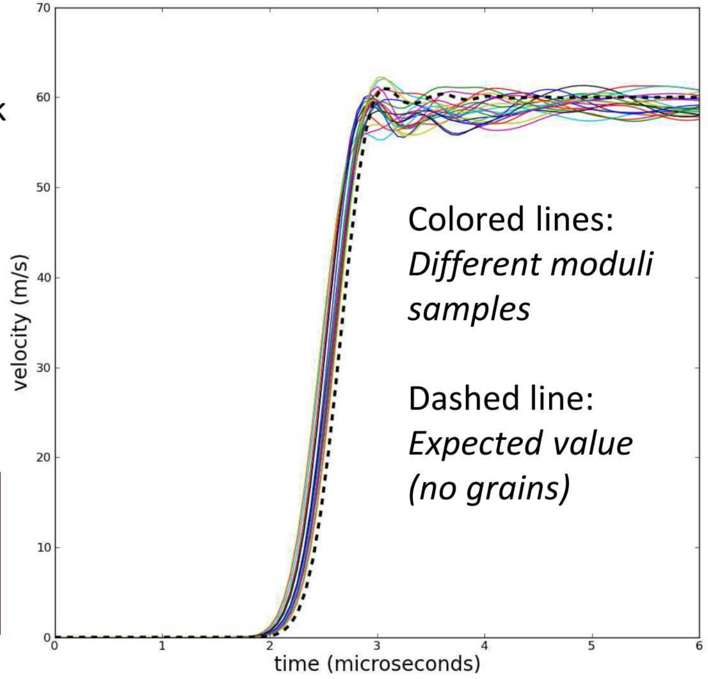


Upscaled mean micro-structure of “Sample”

Distribution of bulk modulus

Bulk modulus: *Assign each grain a random value from assumed uniform distribution*

Velocity vs. Time



Simplified computational model represents gas gun experiment

- Two materials (**Left** & **Right**) just touching at impact
- **Left** has initial velocity, **Right** at rest

Challenge: How do we generalize these ideas for enabling *control of the microstructure* & *performance prediction* of the bulk material?

Summary

- **Context:** **New designs and materials enabled by** ***additive manufacturing***
- **New risk measures for topology optimization**
  - Buffered probabilities
- **Importance of accounting for** ***AM-induced material anisotropy and variability*** **in design and analysis**
- **Introduced an approach for upscaling the heterogeneous and variable AM microstructure**
  - Leverages SPPARKS stochastic simulator of microstructural evolution

Discussion Topics

Broader challenges and potential new directions

1. **New science of materials**
   a) Can we “discover” new materials with desired (and revolutionary) performance properties?
2. **Reproducibility and certifiability**
   a) Can we reproduce such materials in a predictable and cost-effective way?
   b) Can we confidently “certify” that a particular material will perform as intended in a given application?
3. **New models and algorithms**
   a) Beyond AM process control -- how do we model the extremely heterogeneous and variable materials at all length scales?
   b) How do we obtain and assimilate potentially *voluminous, uncertain data* into our models?
   c) Digital twins?
4. **How do we package our results for human decision-making?**
   a) Influencing engineering designs, risk and failure analyses, research funding, etc.