Uncertainty quantification and sensitivity analysis in process-structure-property simulations for laser powder bed fusion additive manufacturing

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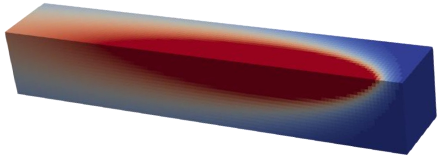
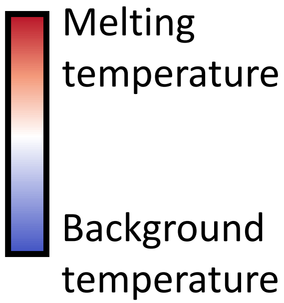
Outline

- Process-structure-property (PSP) model
  - Uncertainty quantification (UQ) challenges
- Multi-fidelity UQ for crystal plasticity
- Global sensitivity analysis (GSA) for process-structure model
  - Quantifying crystallographic texture
- Conclusions

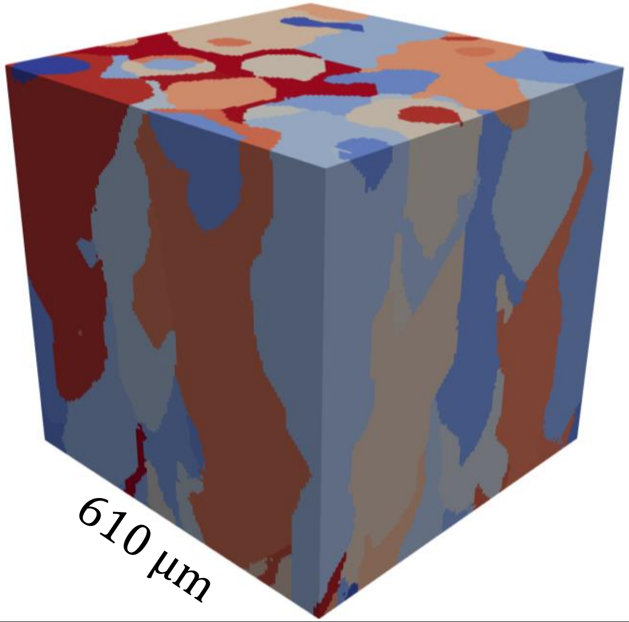
PSP model

1. Thermal model: melt pool, temperature field

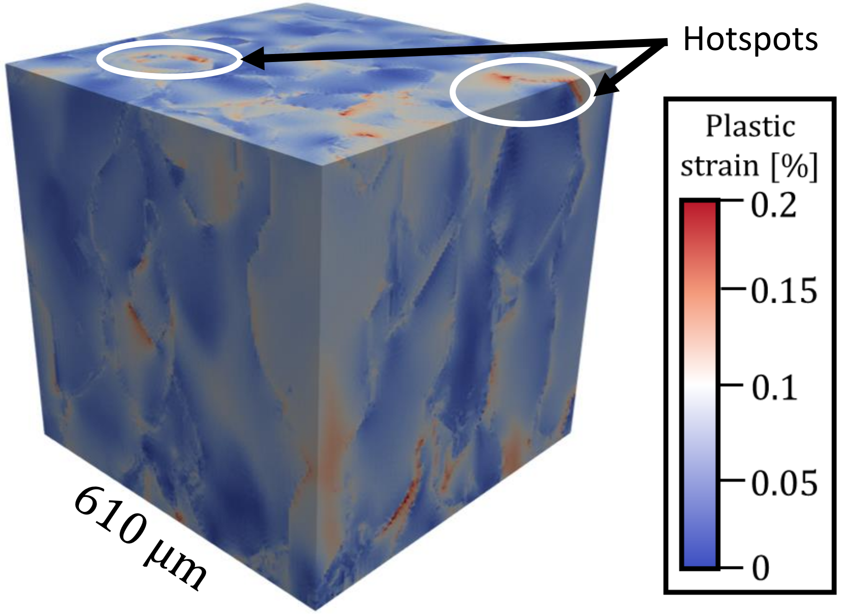




2. Process-structure model: solidification, texture, defects



3. Structure-property model: stress and strain fields, fatigue indicator parameters



- PSP simulations: understand how additive manufacturing (AM) process changes/variations influence mechanical behavior

J.D. Pribe, B. Richter, P.E. Leser, S.R. Yeratapally, G.R. Weber, A.R. Kitahara, E.H. Glaessgen, "A process-structure-property simulation framework for quantifying uncertainty in additive manufacturing: Application to fatigue in Ti-6Al-4V", *Integr Mater Manuf Innov* 12 (2023) 231–250. https://doi.org/10.1007/s40192-023-00303-9.

PSP model

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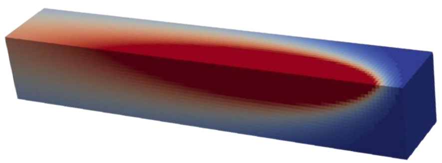
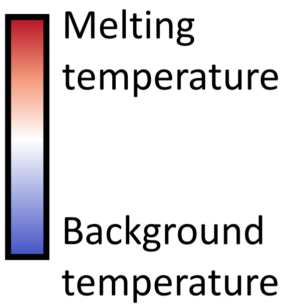
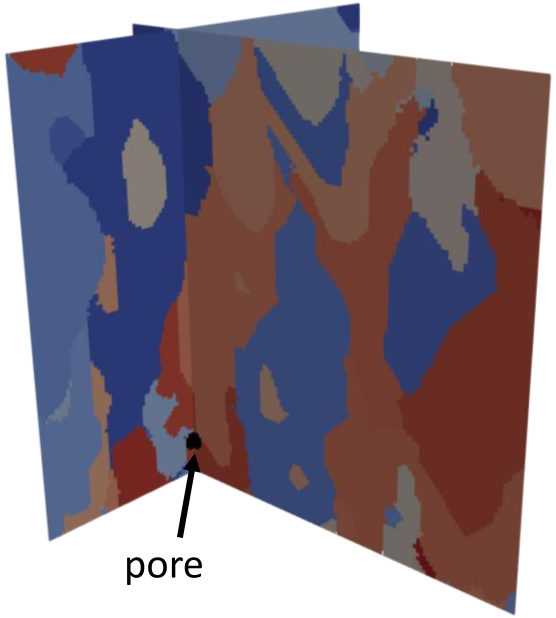




- PSP simulations: understand how additive manufacturing (AM) process changes/variations influence mechanical behavior
- Materials with and without defects (here: pores)
- Need calibration, validation, and UQ to build confidence in models for use in qualification and certification processes

2. Process-structure model: solidification, texture, defects



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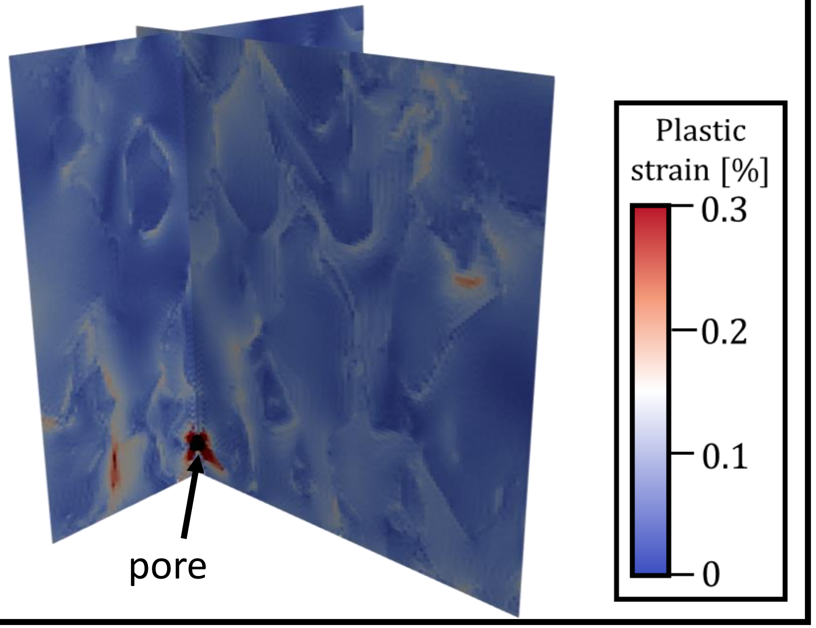

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PSP model with UQ

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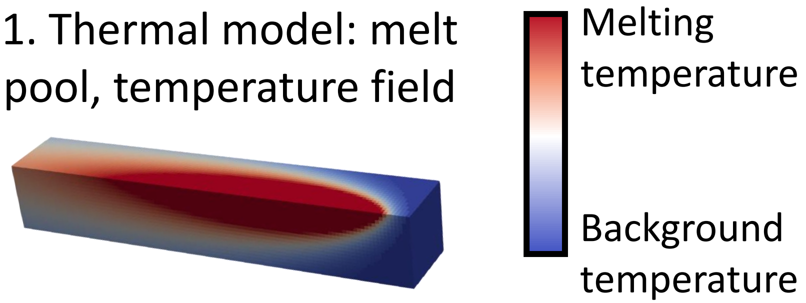
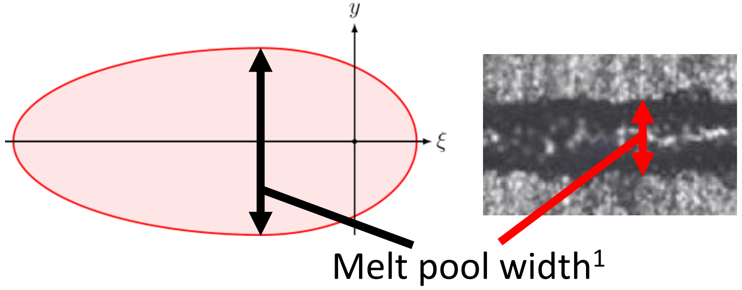
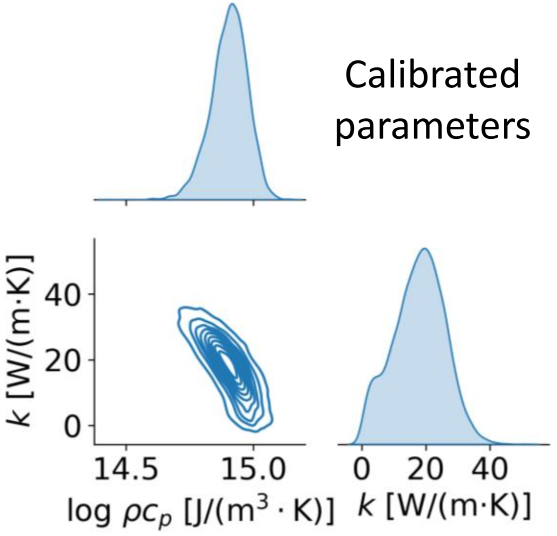


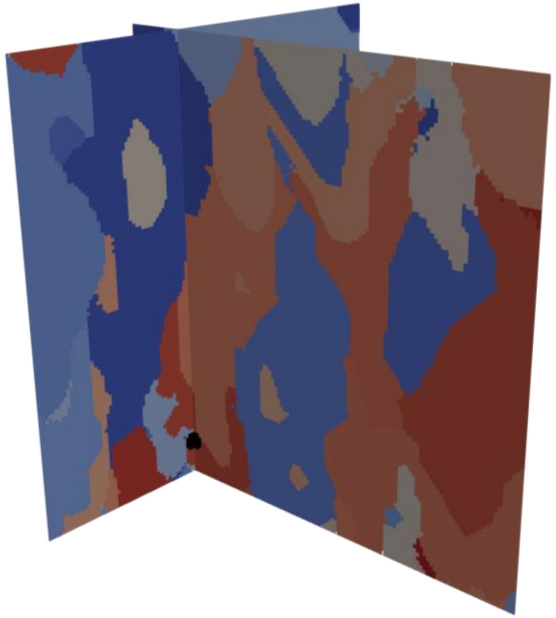
Probabilistic calibration





Repeat simulations

2. Process-structure model: solidification, texture, defects



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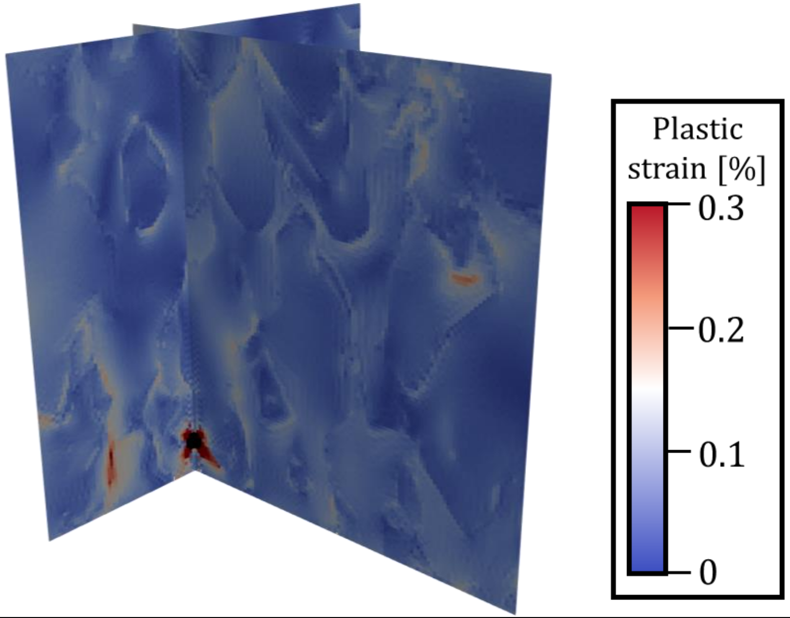

[1]Image of melt pool cropped from Fig. 4 in P. Bidare, R.R.J. Maier, R.J. Beck, J.D. Shephard, A.J. Moore, An open-architecture metal powder bed fusion system for in-situ process measurements, Addit Manuf 16 (2017) 177–185. Used under CC BY 4.0 ([https://creativecommons.org/ licenses/by/4.0/](https://creativecommons.org/licenses/by/4.0/)). © 2017 The Authors. Published by Elsevier B.V.

PSP model with UQ

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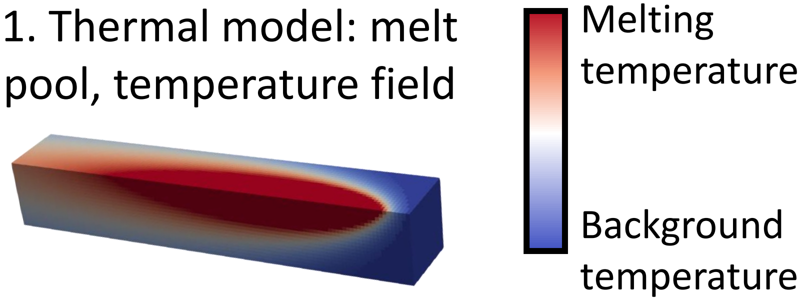

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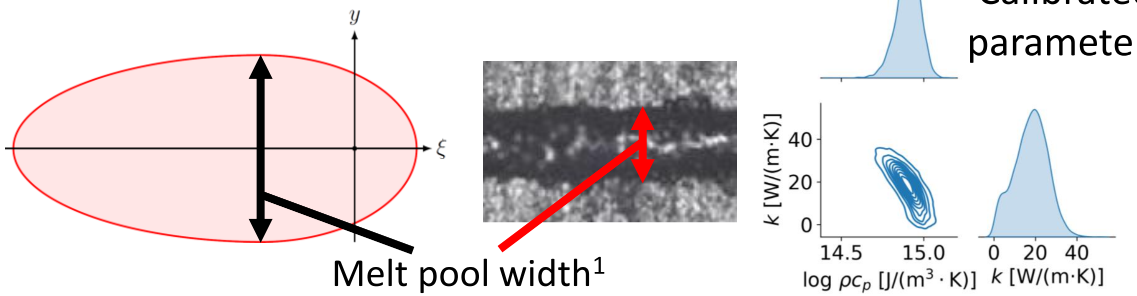

Repeat simulations

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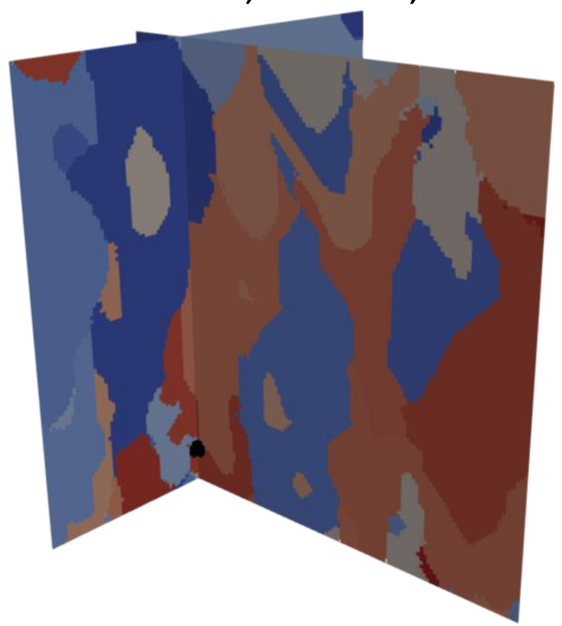

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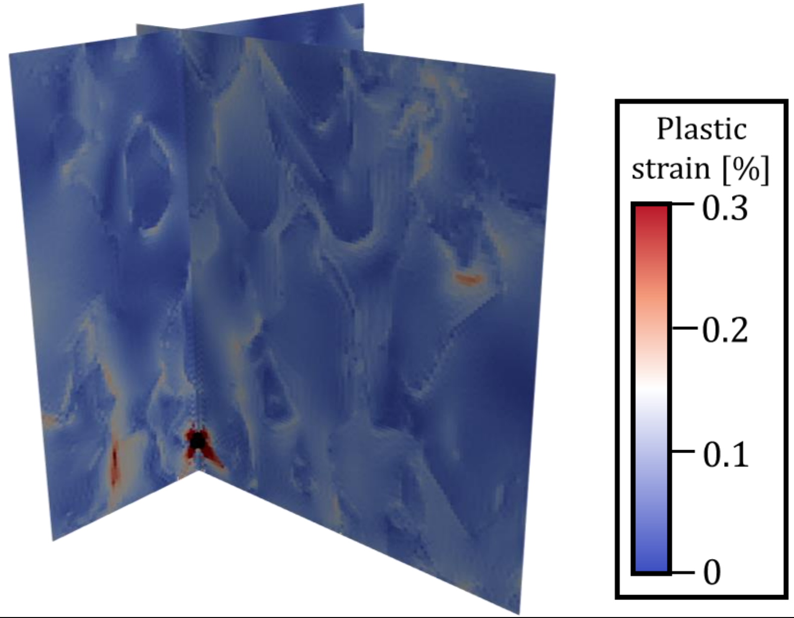
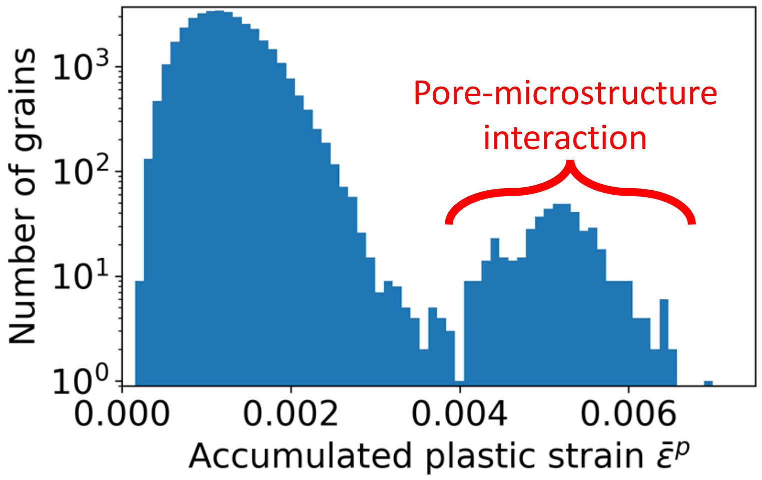


Fatigue indicator parameter statistics and extreme values



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UQ challenges for PSP models

- Expensive high-fidelity models (simulations take minutes, hours, days, …)
  - Uncertainty propagation with brute-force Monte Carlo is difficult
  - Probabilistic calibration may be intractable

- Numerous input parameters
  - Range from measurable properties to fitting parameters
  - Need to understand how uncertainty in these parameters affects predictions

UQ challenges for PSP models

- Expensive high-fidelity models (simulations take minutes, hours, days, …)
  - **Uncertainty propagation with brute-force Monte Carlo is difficult → multi-fidelity UQ**
  - Probabilistic calibration may be intractable

- Numerous input parameters
  - Range from measurable properties to fitting parameters
  - **Need to understand how uncertainty in these parameters affects predictions → GSA**

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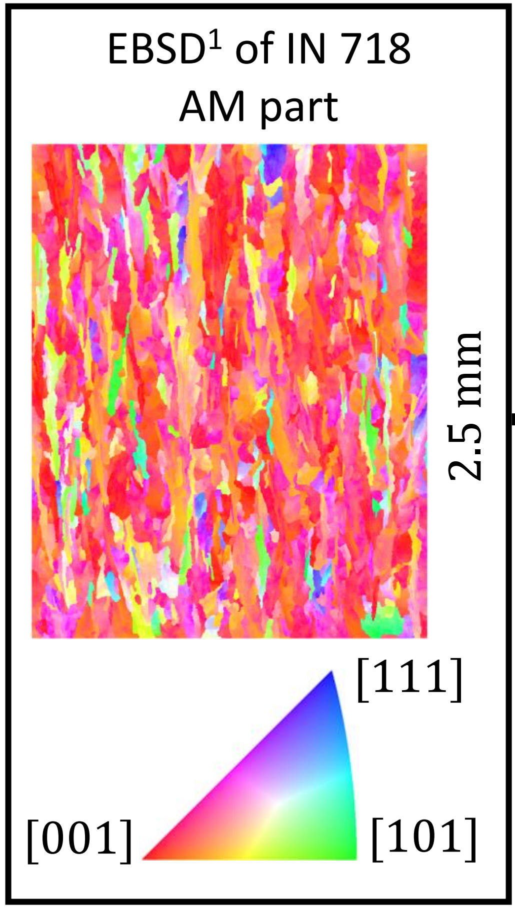
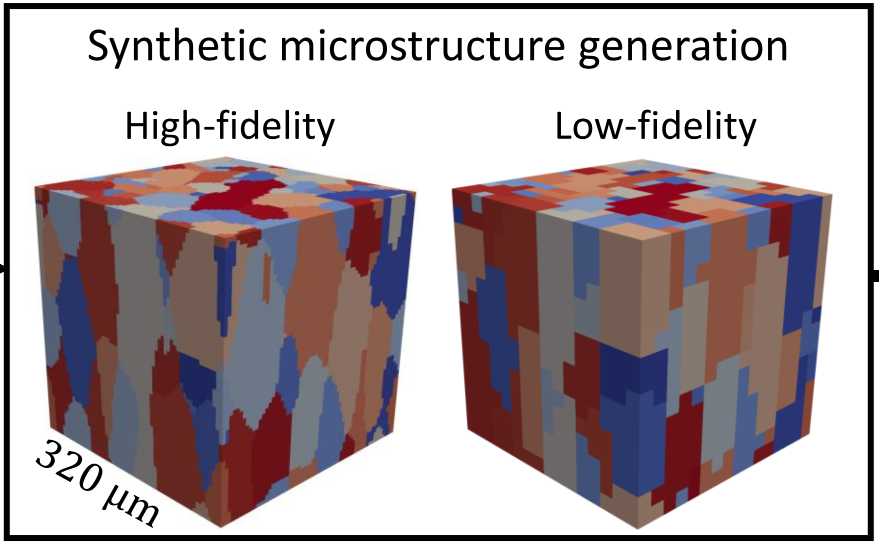
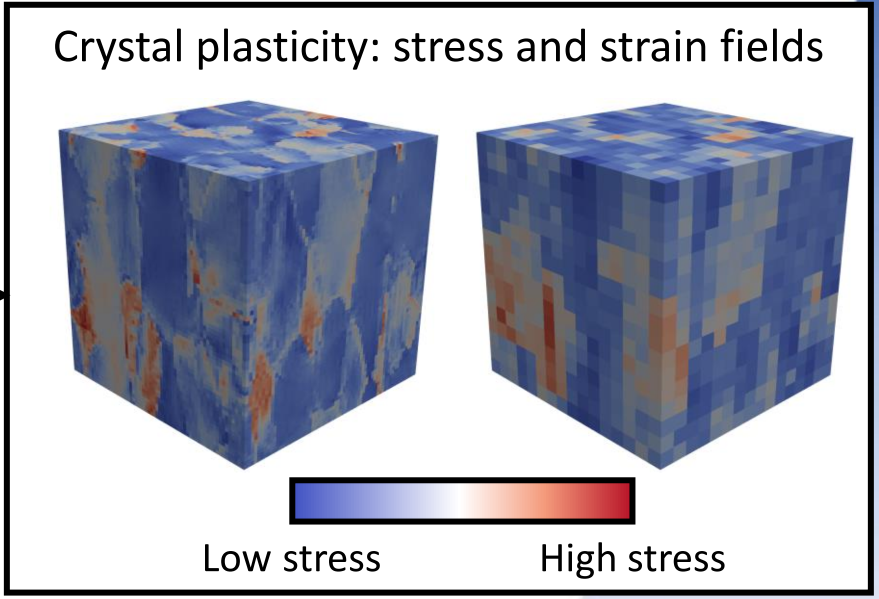
Multi-fidelity UQ for crystal plasticity

Goal: use multi-fidelity methods to estimate crystal plasticity quantities of interest (QoIs) more efficiently





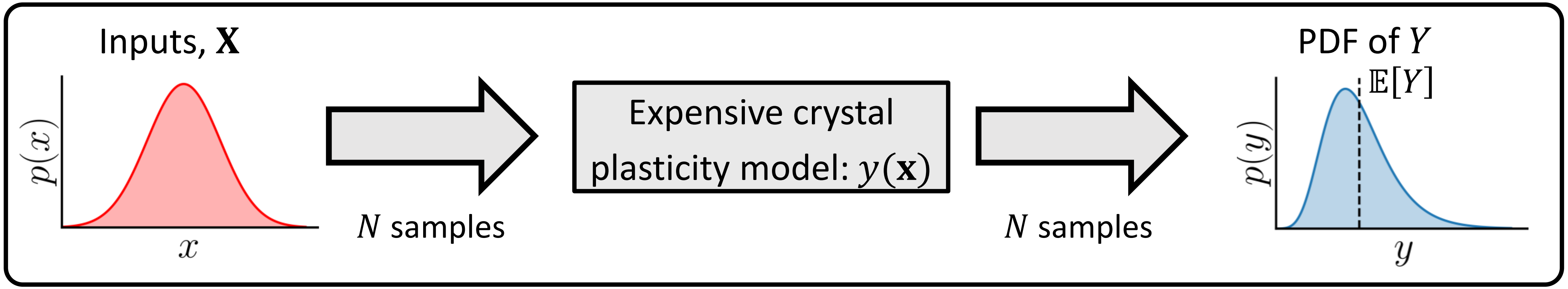


J.D. Pribe et al., "Multi-model Monte Carlo estimation for crystal plasticity structure-property simulations of additively manufactured metals", under minor revisions for *Computational Materials Science*

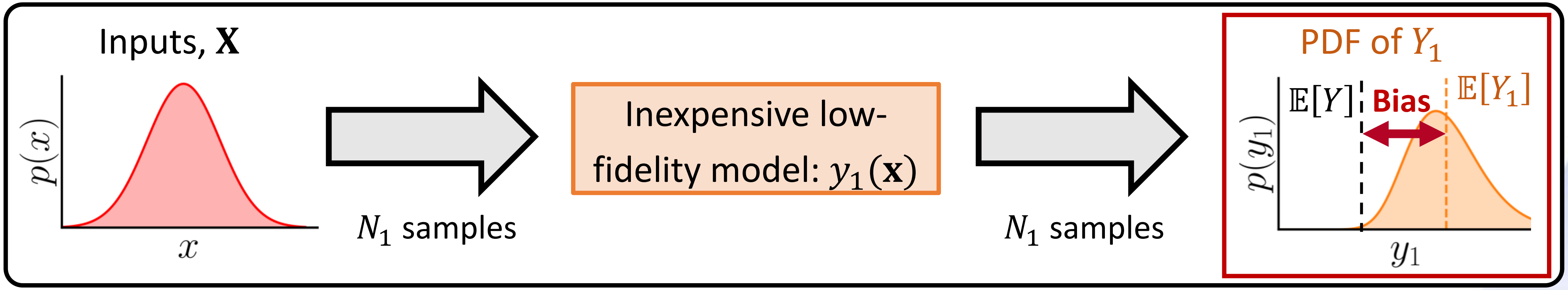
[1]Electron backscatter diffraction

Monte Carlo estimation

Problem: estimate the expected value, $\mathbb{E}[Y]$, for a QoI, Y



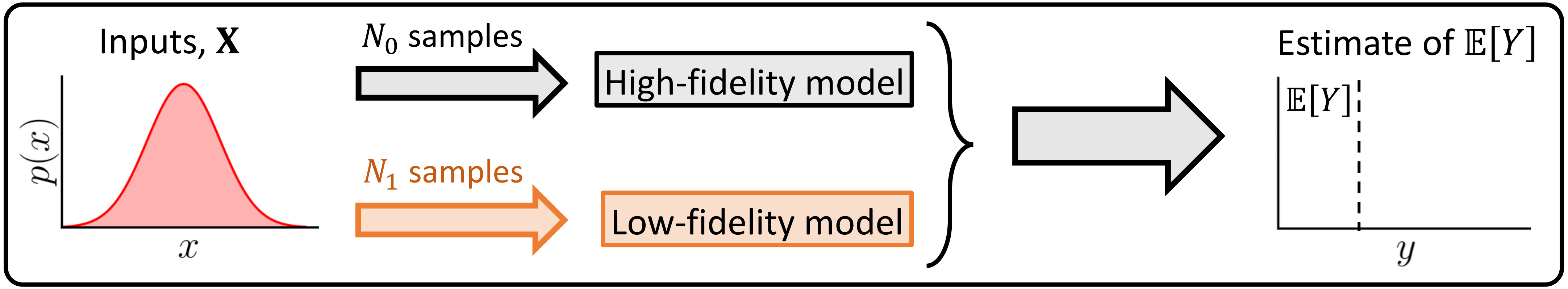
Monte Carlo estimate of $\mathbb{E}[Y]$: $\hat{Y}(\mathbf{x}) = \frac{1}{N}\sum_{i=1}^{N} y\left(\mathbf{x}^{(i)}\right)$ Slow convergence: $\mathbb{V}\mathrm{ar}\left[\hat{Y}\right] \propto 1/N$



Monte Carlo estimate of $\mathbb{E}[Y]$: $\hat{Y}_1(\mathbf{x}) = \frac{1}{N_1}\sum_{i=1}^{N_1} y_1\left(\mathbf{x}^{(i)}\right)$ Fast, but generally biased

Multi-fidelity approach

Problem: estimate the expected value, $\mathbb{E}[Y]$, for a QoI, Y



Multi-model Monte Carlo estimator[1]: $\tilde{Y}_{MM} = \hat{Y}(\mathbf{x_0}) + \alpha_1 \left(\hat{Y}_1(\mathbf{x}_1^+) - \hat{Y}_1(\mathbf{x}_1^-) \right)$

High-fidelity with sample set $\mathbf{x_0}$

Low-fidelity with two different sample sets ($\mathbf{x}_1^+$ and $\mathbf{x}_1^-$)

- Unbiased $\left(\mathbb{E}[\tilde{Y}_{MM}] = \mathbb{E}[\hat{Y}]\right)$
- Optimize **sample allocation,** $\{\mathbf{x_0}, \mathbf{x}_1^+, \mathbf{x}_1^-\}$**,** to **minimize cost** given a **target variance**
    - Equivalently: **minimize variance** given a **target cost or budget**

[1]Based on approximate control variates approaches: A.A. Gorodetsky et al., J Comput Phys. 408 (2020) 109257. https://doi.org/10.1016/j.jcp.2020.109257.

Multi-fidelity approach

- **Low cost** and **high correlation with high-fidelity model** are desirable
- Can extend to **any number of low-fidelity models and QoIs**

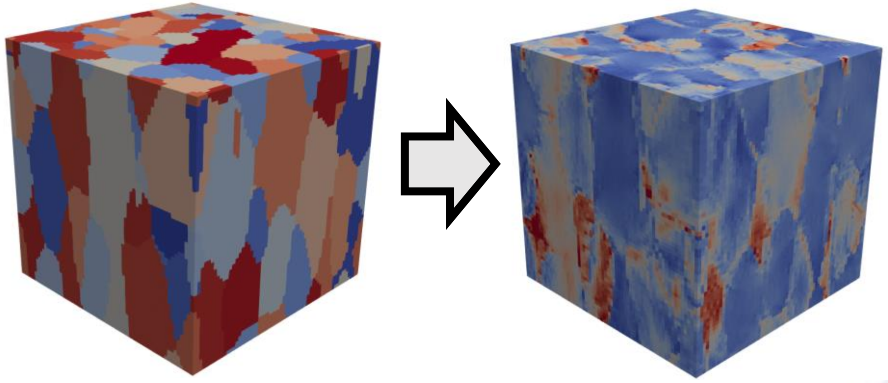
$$\tilde{Y}_{MM} = \hat{Y}(\mathbf{x_0}) + \sum_{j=1}^{M} \alpha_j \left(\hat{Y}_j(\mathbf{x_j^+}) - \hat{Y}_j(\mathbf{x_j^-}) \right)$$

M: number of low-fidelity models

- Application: propagating microstructure uncertainty through crystal plasticity models
  - Define high- and low-fidelity models and QoIs
  - Estimate correlations between models
  - Predict variance reduction

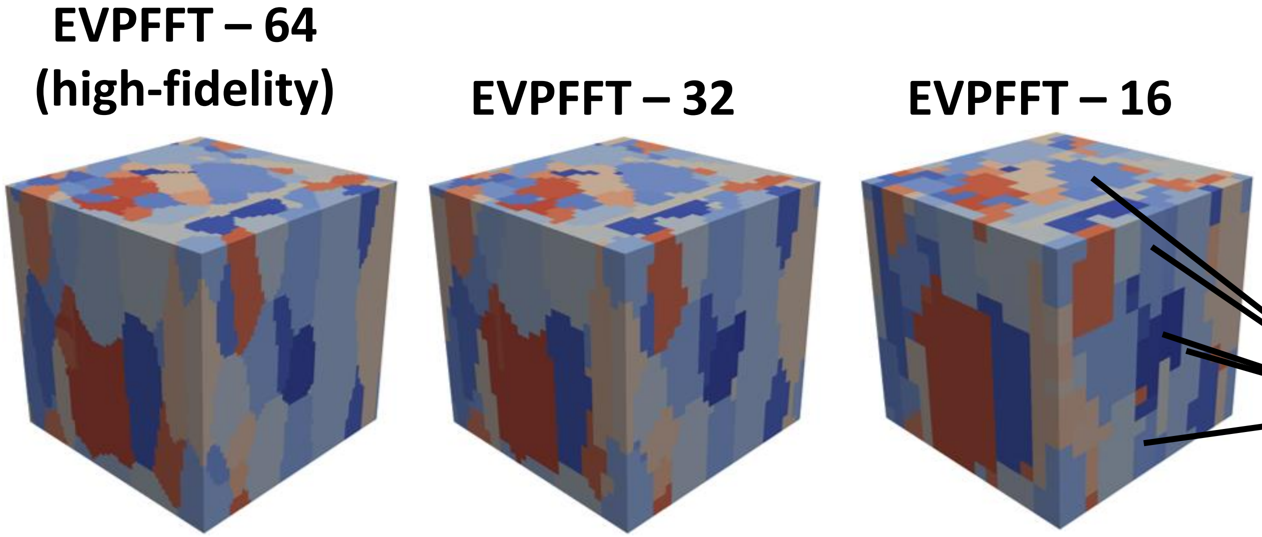
Microstructure

Stress and strain fields



Multi-fidelity UQ: Models

Three-dimensional full-field simulations



Model names refer to resolution (EVPFFT – 64 has $64 \times 64 \times 64$ voxel resolution with 5-µm voxel size)

EVPFFT: elasto-viscoplastic fast Fourier transform model[1]

- Calculate stress and strain for **all voxels**
- Generate low-fidelity models by coarsening the discretization

Extract grain-average quantities (size, aspect ratio, crystallographic orientation)

VPSC[2]: self-consistent homogenization-based formulation

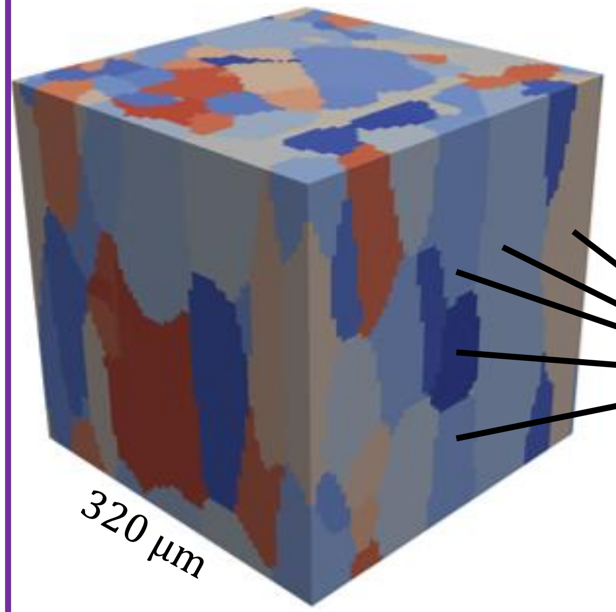
- Solve for **grain-average** stresses and strains
- Different linearization schemes → three models: **VPSC-affine, VPSC-FC, VPSC-tangent**

[1]R.A. Lebensohn et al., Int J Plast. 32–33 (2012) 59–69. https://doi.org/10.1016/j.ijplas.2011.12.005.
[2]Viscoplastic self-consistent; R.A. Lebensohn, C.N. Tomé, Acta Metall et Mater. 41 (1993) 2611–2624. https://doi.org/10.1016/0956-7151(93)90130-K.

Multi-fidelity UQ: QoIs

QoIs: key aspects of micromechanical behavior

Example microstructure



Aggregate yield strength (YS)

"mean QoIs"

Grain-scale QoIs (one value per grain)
- Equivalent stress, $\boldsymbol{\bar{\sigma}_g}$
- Shear strain, $\boldsymbol{\gamma_g}$
- Fatemi-Socie parameter (related to crack initiation), $\boldsymbol{FS_g}$

Mean across all grains

$\mathrm{mean}(\bar{\sigma}_g)$
$\mathrm{mean}(\gamma_g)$
$\mathrm{mean}(FS_g)$

Max across all grains

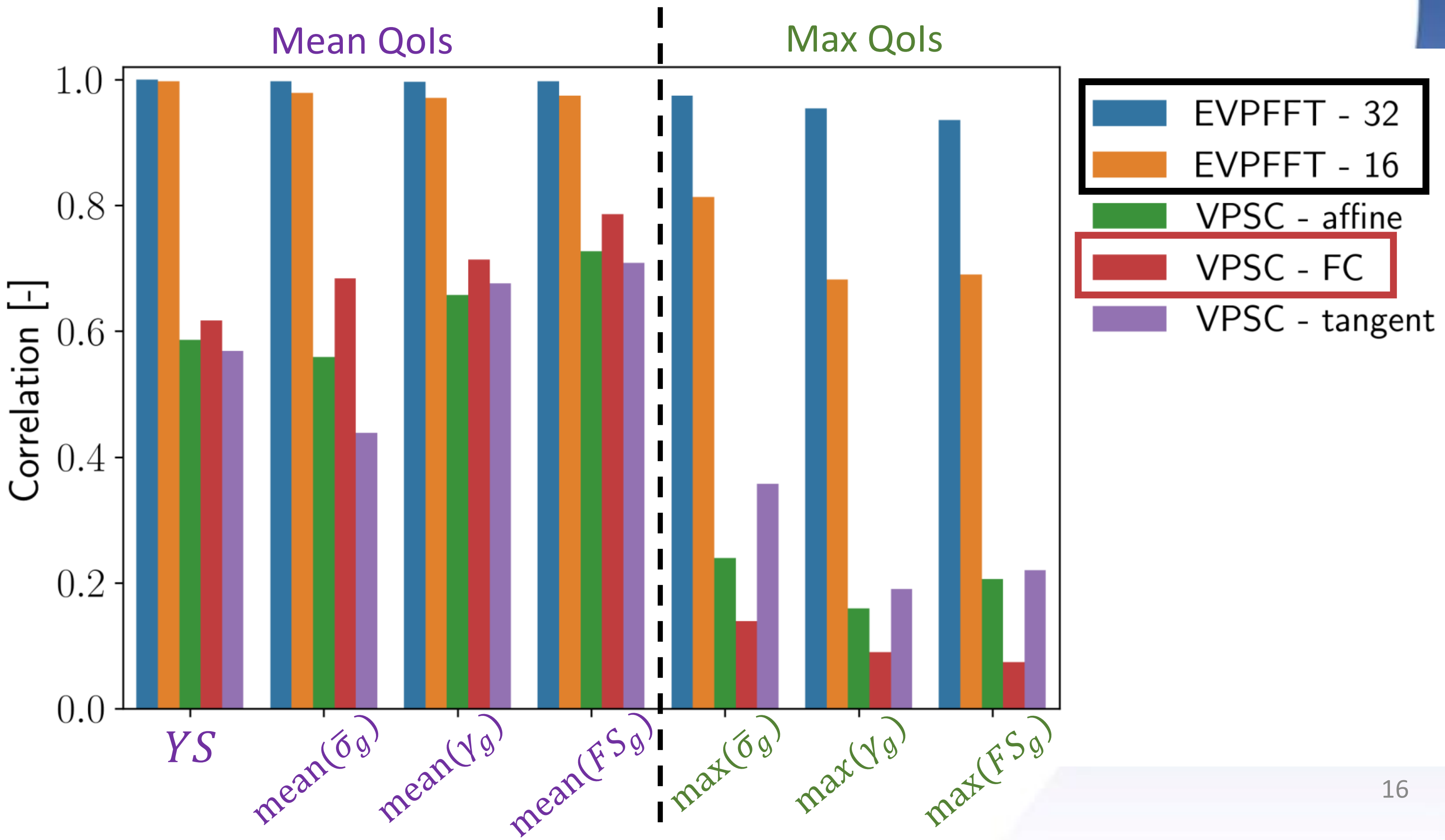
$\max(\bar{\sigma}_g)$
$\max(\gamma_g)$
$\max(FS_g)$

"max QoIs"

Multi-fidelity UQ: Model correlations

- Coarse full-field models
  - Better correlation than homogenized models
  - Higher correlation for mean QoIs; then drop off for max QoIs
- Homogenized models
  - VPSC-FC is best VPSC model for all mean QoIs; unclear which are most useful overall

Correlation with high-fidelity model (EVPFFT-64) for each QoI



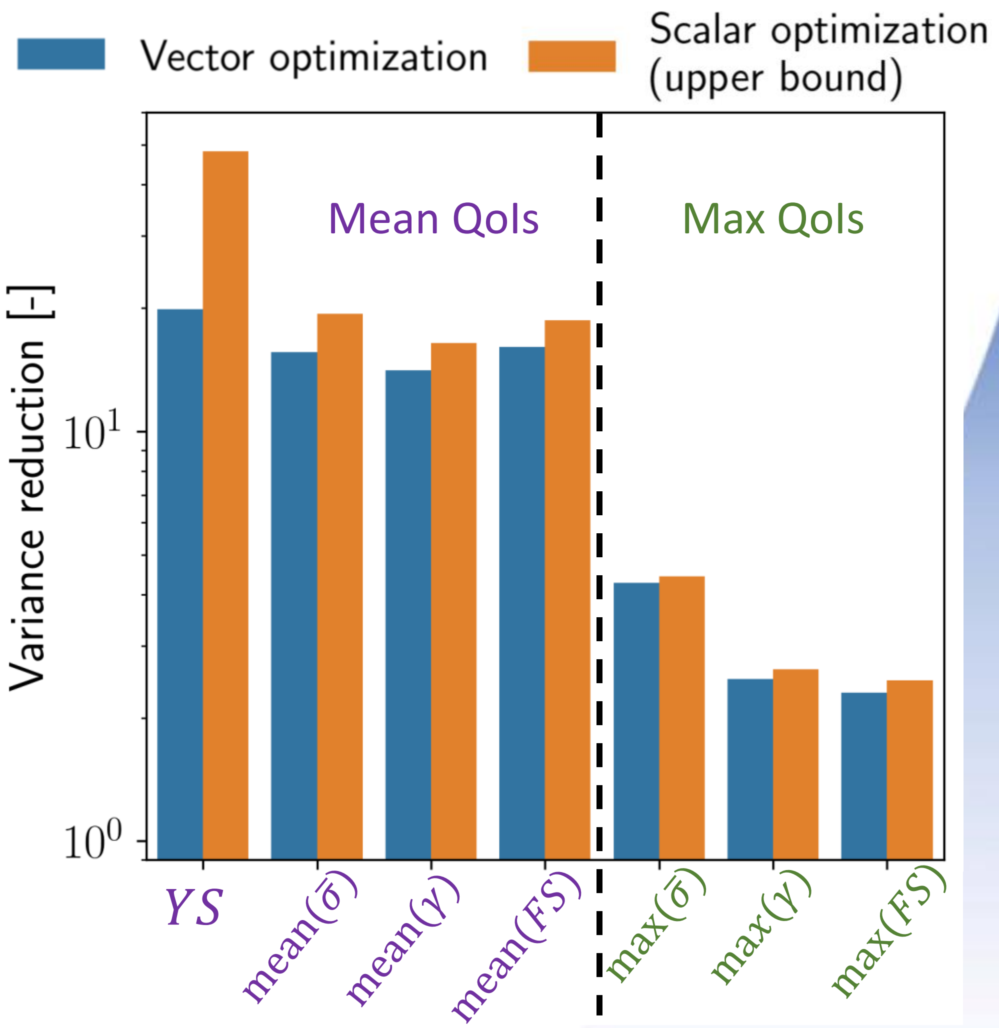
Multi-fidelity UQ: Variance reduction

- Scalar optimization: upper bound; optimize separately for each individual QoI
- Vector optimization: optimize for all QoIs at once

- $\sim 10\times$ variance reduction for mean QoIs; much less for max QoIs
- Vector optimization does not reach upper bound
  - Different optimal sample allocations for mean QoIs and max QoIs

J.D. Pribe et al., "Multi-model Monte Carlo estimation for crystal plasticity structure-property simulations of additively manufactured metals", under minor revisions for *Computational Materials Science*

Variance reduction relative to standard MC for a budget of 100 high-fidelity runs



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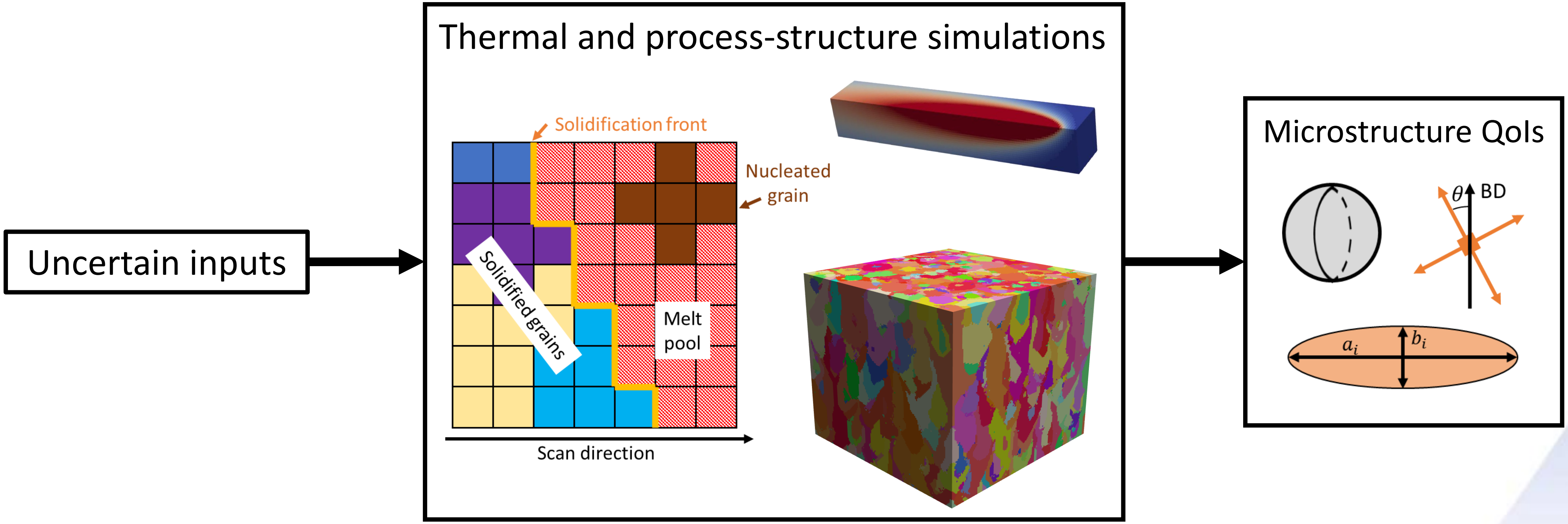
GSA for process-structure model

- Goal: identify most important material and process inputs for microstructure QoIs
  - Laser powder bed fusion IN 718
- Requirements: sensitivity measure, model definition, inputs and QoIs



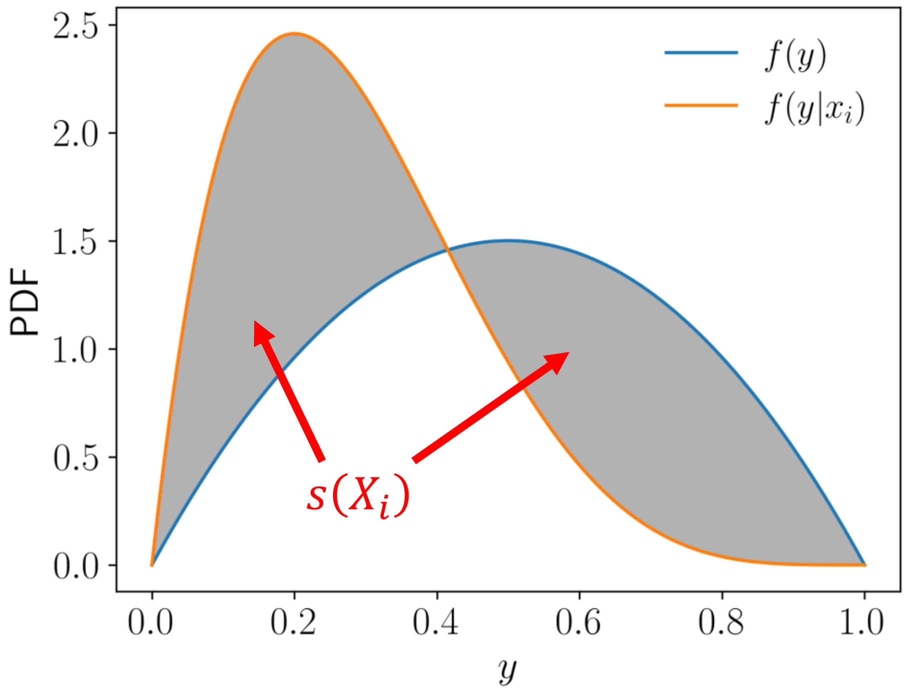
GSA: Sensitivity measures

- GSA relates uncertainty in a QoI (Y) to uncertainty in inputs (X_i)
- Variance-based GSA: partition QoI variance
  - First-order Sobol index: expected reduction in QoI variance if input X_i is fixed
- Moment-independent GSA: consider full distributions of inputs and QoI
  - Example: δ measure[1]

$$\delta_i = \frac{1}{2}\mathbb{E}[s(X_i)]$$
$$= \frac{1}{2}\mathbb{E}\left[\int |f(y) - f(y|x_i)|\, dy\right]$$

Area between marginal and conditional distributions of the QoI

δ measure example



[1]E. Borgonovo, Reliab Eng Syst 92 (2007) 771–784. https://doi.org/10.1016/j.ress.2006.04.015.
Computed using SALib: https://salib.readthedocs.io/en/latest/

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Area between marginal and conditional distributions of the QoI

Properties of δ:

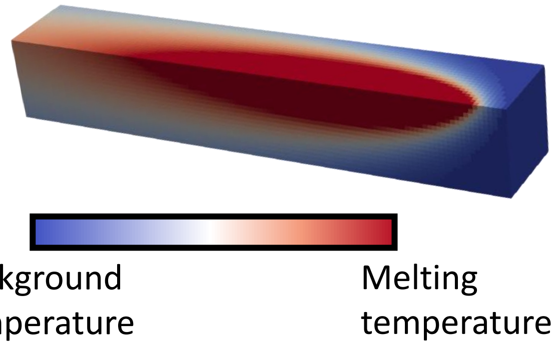
- Quantifies expected shift in QoI distribution when an input is fixed
- $0 \leq \delta_i \leq 1$
- $\delta_i = 0$: parameter X_i does not influence the output
- $\delta_i = 1$: parameter X_i is perfectly correlated with the QoI

[1]E. Borgonovo, Reliab Eng Syst 92 (2007) 771–784. https://doi.org/10.1016/j.ress.2006.04.015.
Computed using SALib: https://salib.readthedocs.io/en/latest/

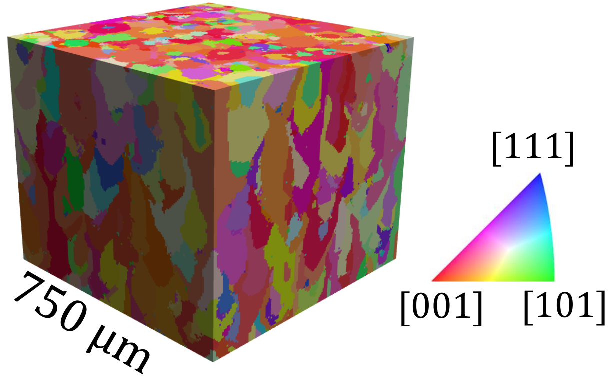
GSA: Model

- Kinetic Monte Carlo[1,2] with analytical temperature field (Rosenthal equation)
- Solidification through nucleation and epitaxial growth

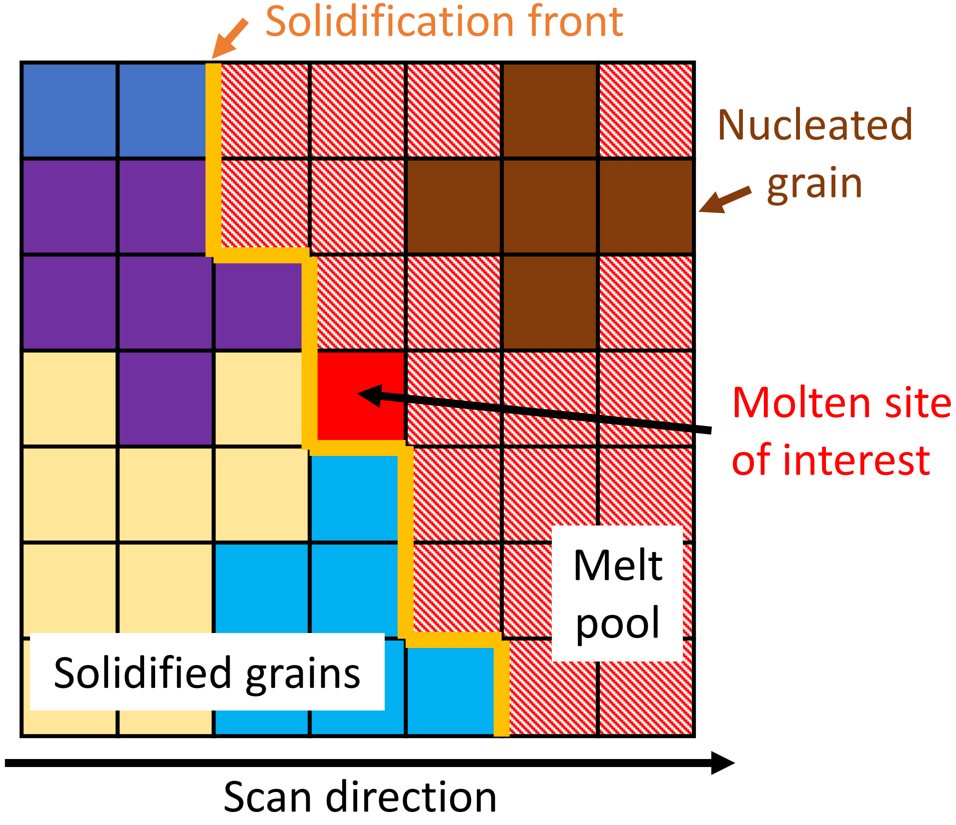
Melt pool from Rosenthal equation



Example microstructure



Nucleation and epitaxial growth



Solidification velocity:
$v = a\Delta T^m$

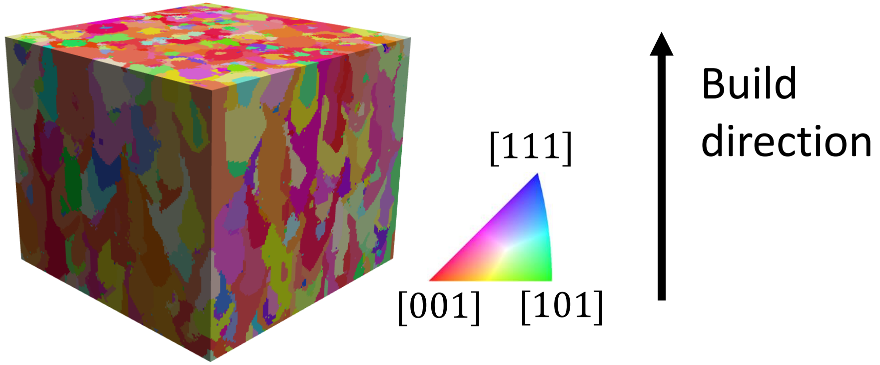
Undercooling

Weighting accounts for texture development

[1]Stochastic Parallel Particle Kinetic Simulator (SPPARKS): https://spparks.github.io/ [2]T.M. Rodgers et al., Addit Manuf. 41 (2021) 101953. https://doi.org/10.1016/j.addma.2021.101953.

GSA: QoIs

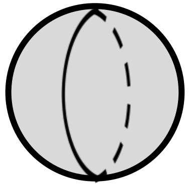
Example inverse pole figure with respect to build direction



- Mean grain size
- Weighted mean sphericity

$$\Phi_i = \frac{\pi^{1/3}(6V_i)^{2/3}}{A_i}$$

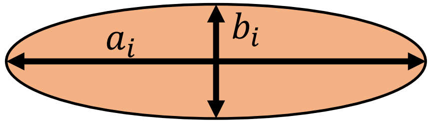
V_i: grain volume
A_i: grain surface area



- Weighted mean aspect ratio

$$R_i = \frac{b_i}{a_i}$$

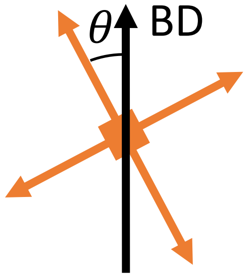
a_i, b_i: two largest semiaxis lengths of equivalent ellipsoid, $a_i \geq b_i$



- Weighted mean texture strength

$$\theta_i = \min_j \arccos\left(\mathbf{d}_\mathbf{i}^{(\mathbf{j})} \cdot \mathbf{BD}\right)$$

$\mathbf{d}_\mathbf{i}^{(\mathbf{j})}$: j^{th} <001> direction for grain i
$\mathbf{BD}$: build direction



GSA: Inputs

- Material
  - Effective thermophysical properties: ρc_p and k
  - $\boxed{\text{Nuclei density: } N_0}$
  - Solidification exponent: m
- Material + process
  - $\boxed{\text{Emissivity/absorptivity: } \epsilon}$
  - Depth scaling: η_z
- Process
  - Background temperature: $T_{\mathrm{substrate}}$
- Sources of distributions
  - Calibration
  - Literature data
  - Estimated from experiments

Nuclei density from parameter study with similar model[1]: $\log N_0 \sim \mathcal{U}(13{,}15)$ (N_0 in m^{-3})

Absorptivity from range in literature[2]: $\epsilon \sim \mathcal{U}(0.38{,}0.51)$

Fixed inputs: power, laser speed, hatch spacing from AM Bench 2022[3]

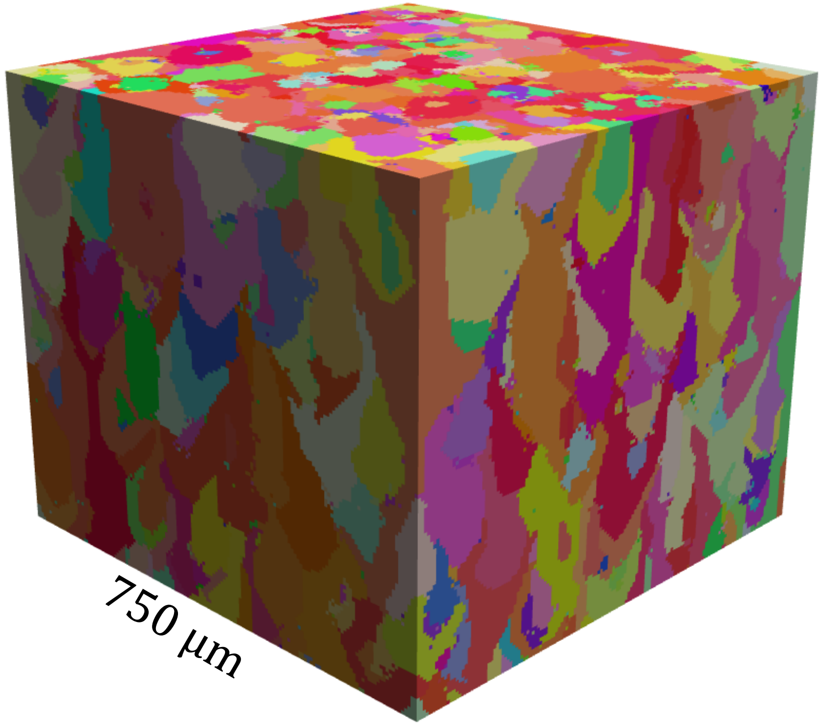
[1]T.M. Rodgers et al., Addit Manuf. 41 (2021) 101953. https://doi.org/10.1016/j.addma.2021.101953.
[2]P. Promoppatum et al., Engineering 3 (2017) 685–694. https://doi.org/10.1016/J.ENG.2017.05.023.
[3]L.E. Levine et al., Integr Mater Manuf Innov 13 (2024) 380–395. https://doi.org/10.1007/s40192-024-00361-7.

GSA: Results

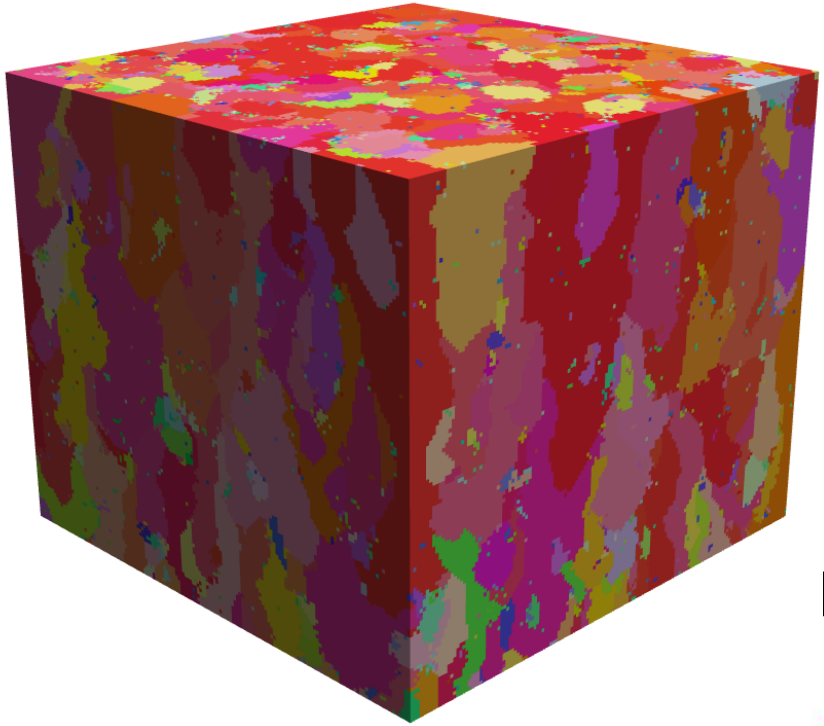
Nuclei density dominates visual features of the microstructure

Inverse pole figure maps with respect to the build direction

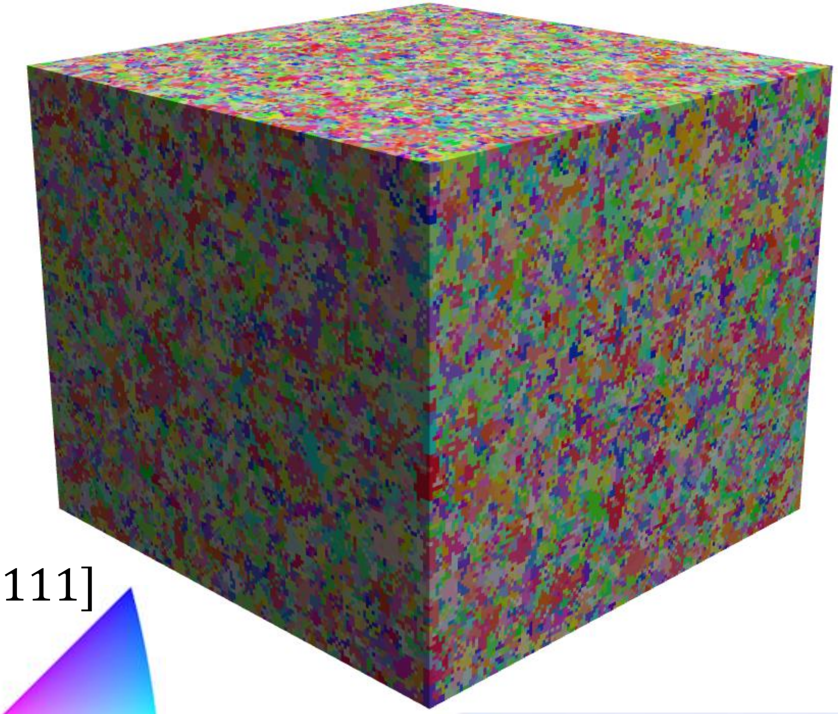
$N_0 \approx 10^{13}/\text{m}^3$



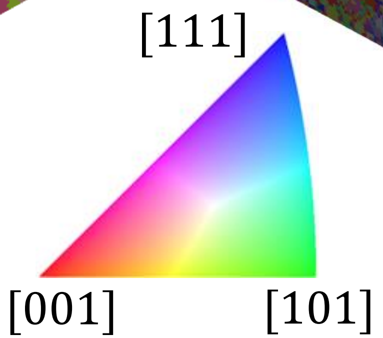
$N_0 \approx 10^{14}/\text{m}^3$



$N_0 \approx 10^{15}/\text{m}^3$



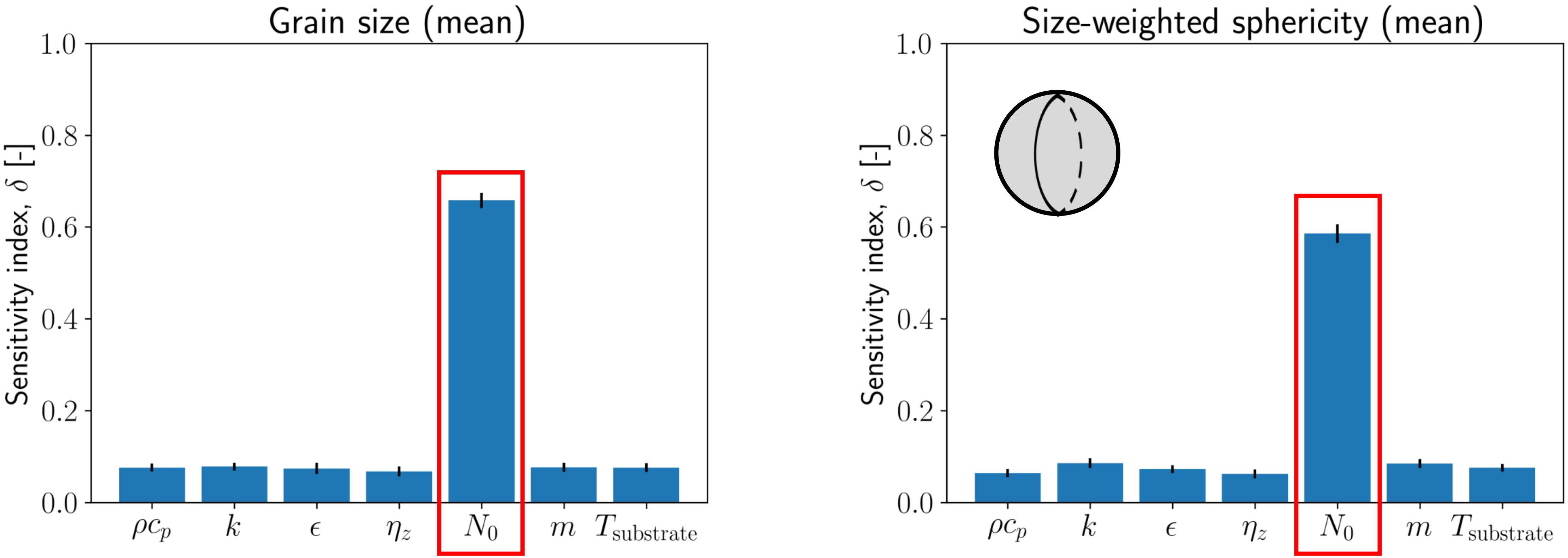
…but it is not the whole story, particularly with texture



GSA: Results

Consistent with visual observations, grain size and sphericity are most sensitive to nuclei density: increasing N_0 $\longrightarrow$ more small, round grains

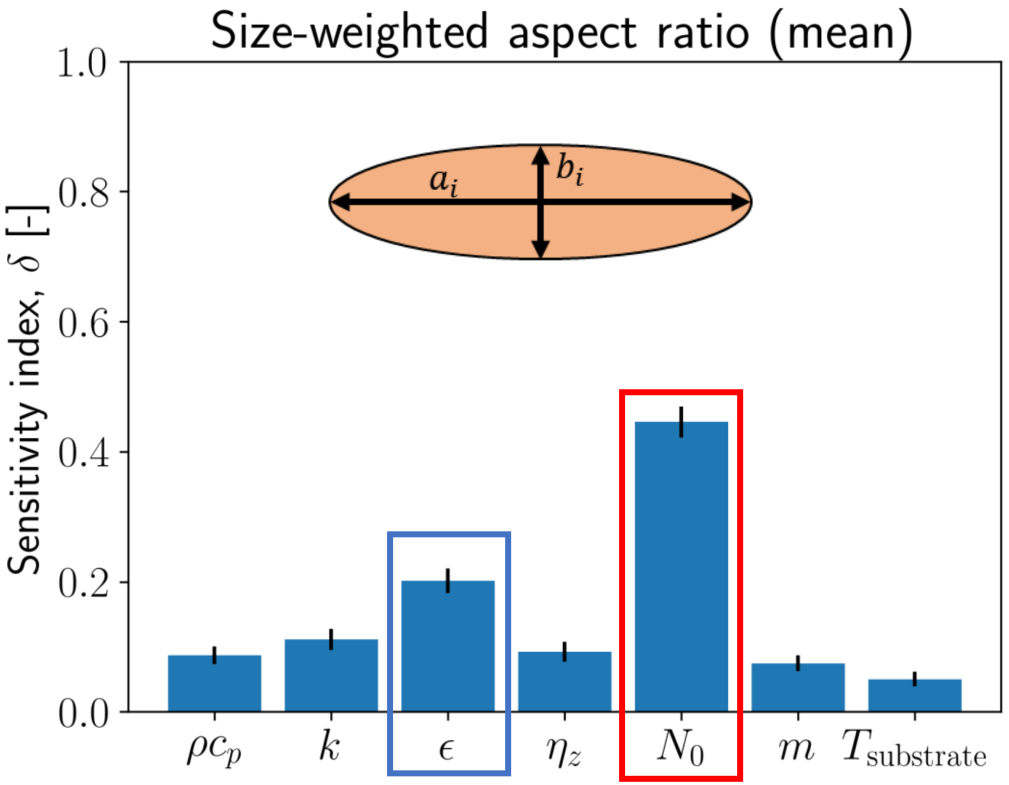
Comparison of sensitivity indices for each input parameter

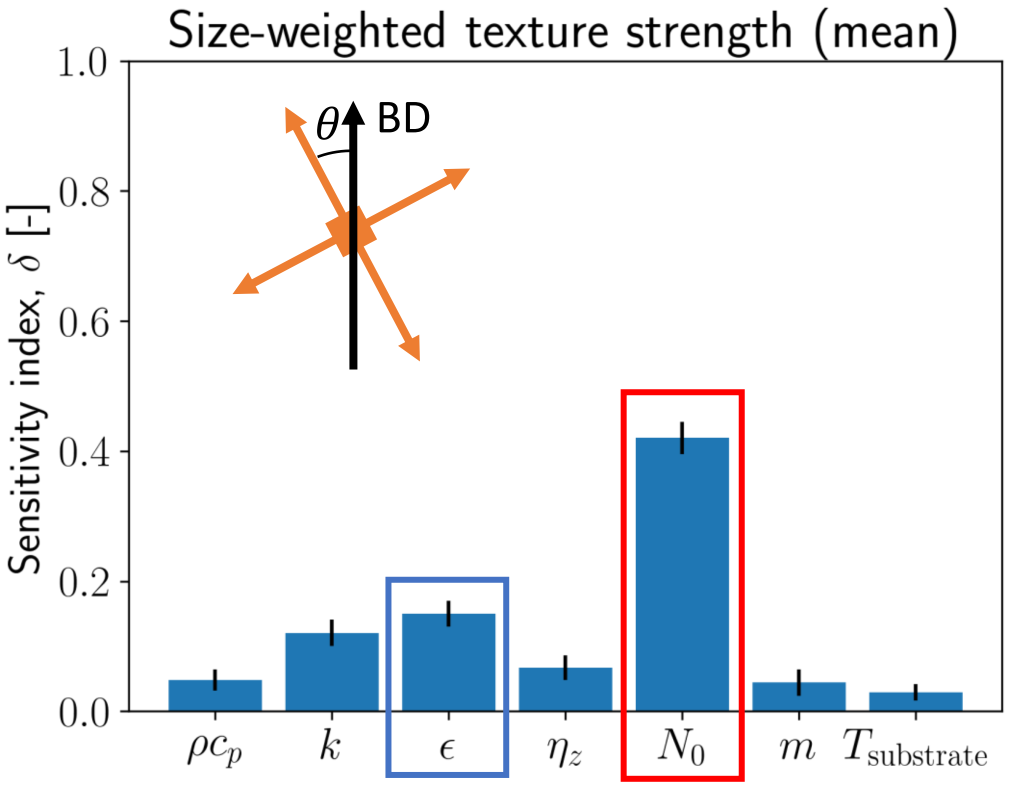


GSA: Results

- Nuclei density still dominates, but emissivity becomes more important for aspect ratio and texture
- Try using principal component analysis (PCA) to get more texture information

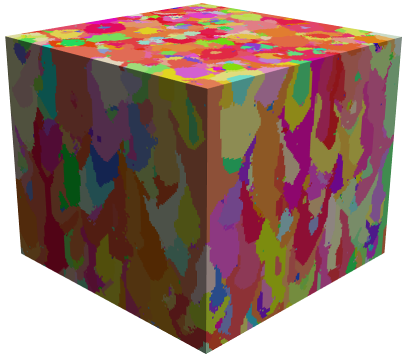
Comparison of sensitivity indices for each input parameter





Crystallographic texture PCA

- Challenge: orientation distribution functions (ODFs) are very high dimensional
- Hypothesis:
  - PCA captures key features of the orientation distribution function (ODF)
  - Most important PC(s) are interpretable → effects can be visualized in pole figures
  - Sensitivity indices for most important PC(s) capture inputs that most strongly affect the texture



Extract Euler angles and size of each grain

Find ODF coefficients using generalized spherical harmonics (MTEX[1])

Repeat for all simulated microstructures

ODF coefficients

samples

ODF principal components

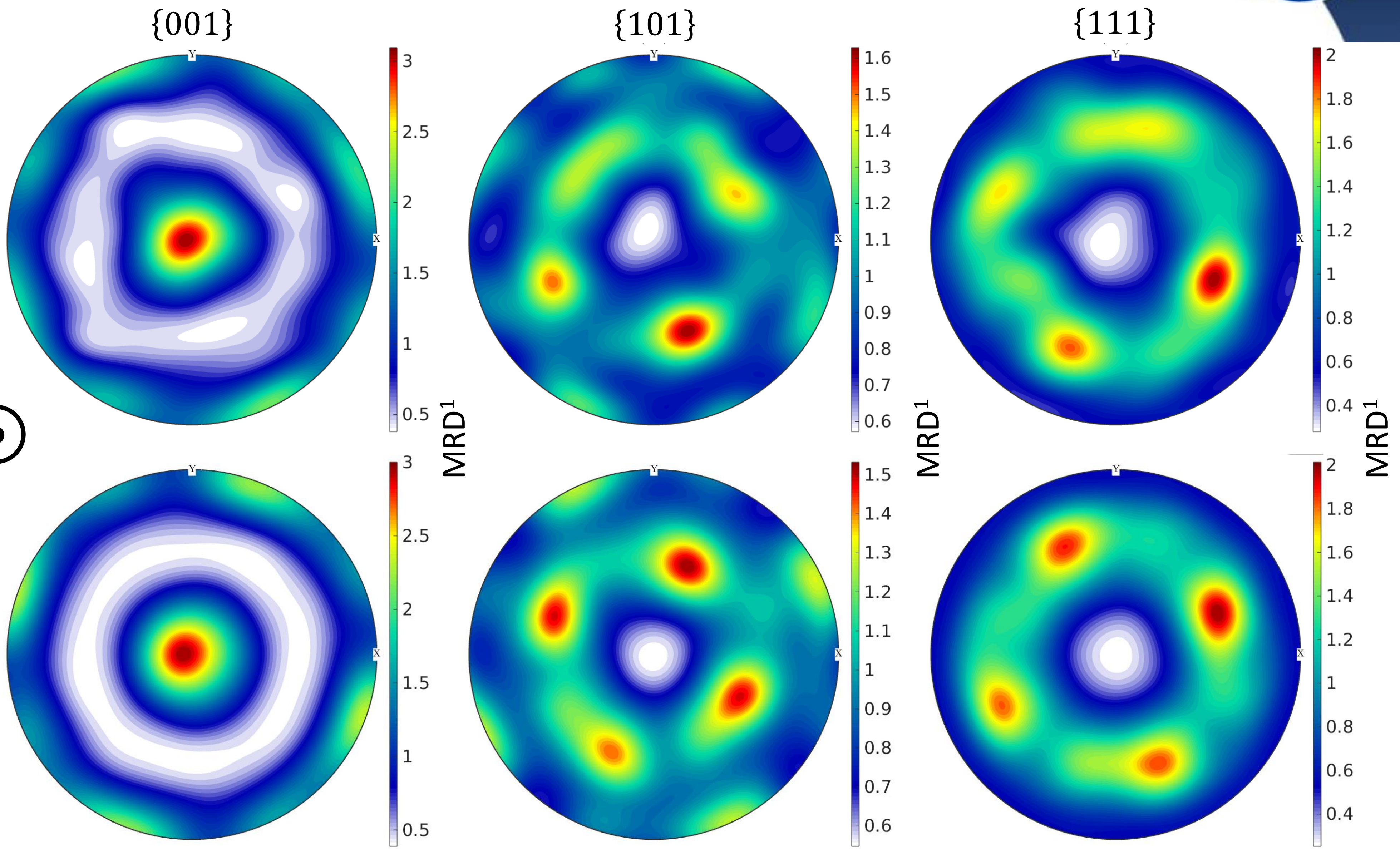
[1]https://mtex-toolbox.github.io/

Crystallographic texture PCA

Actual pole figures

BD

Reconstruction (first 10 PCs – about 70% variance explained)



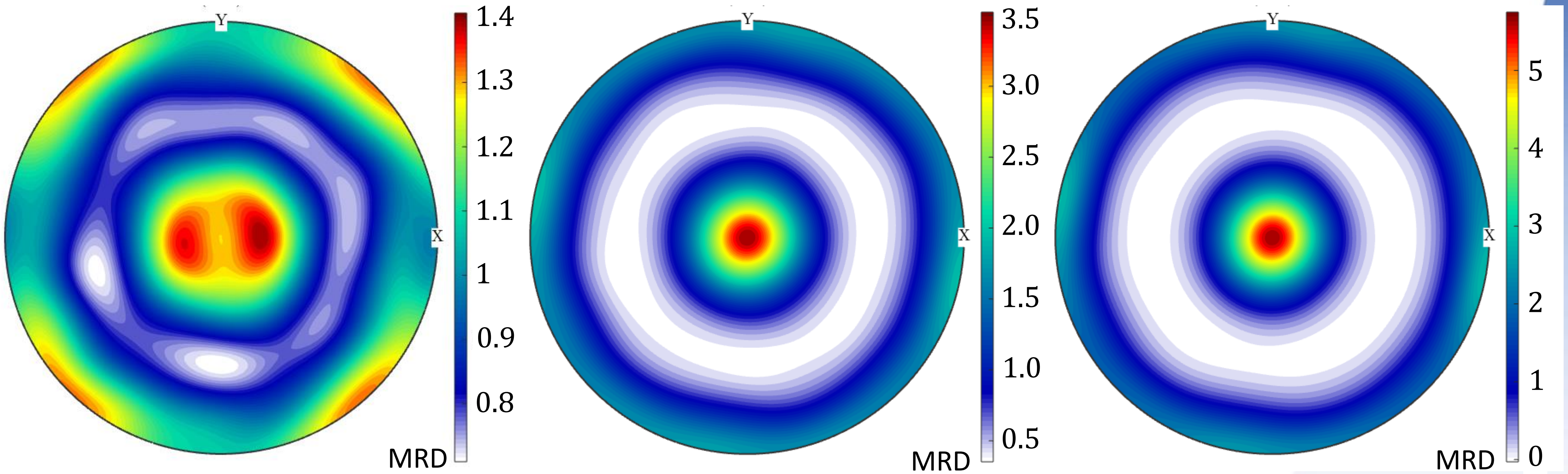
[1]MRD: multiples of random density

Crystallographic texture PCA

First PC also captures texture strength (alignment of {001} poles with BD)

Reconstructed {001} pole figures

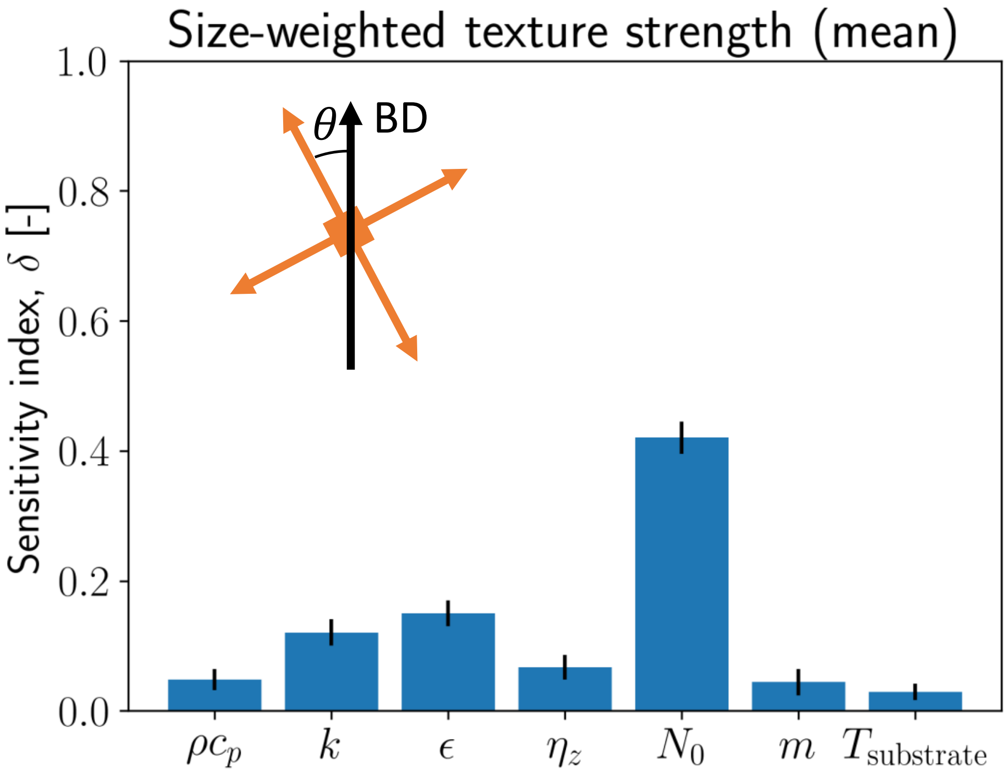
Increasing first PC

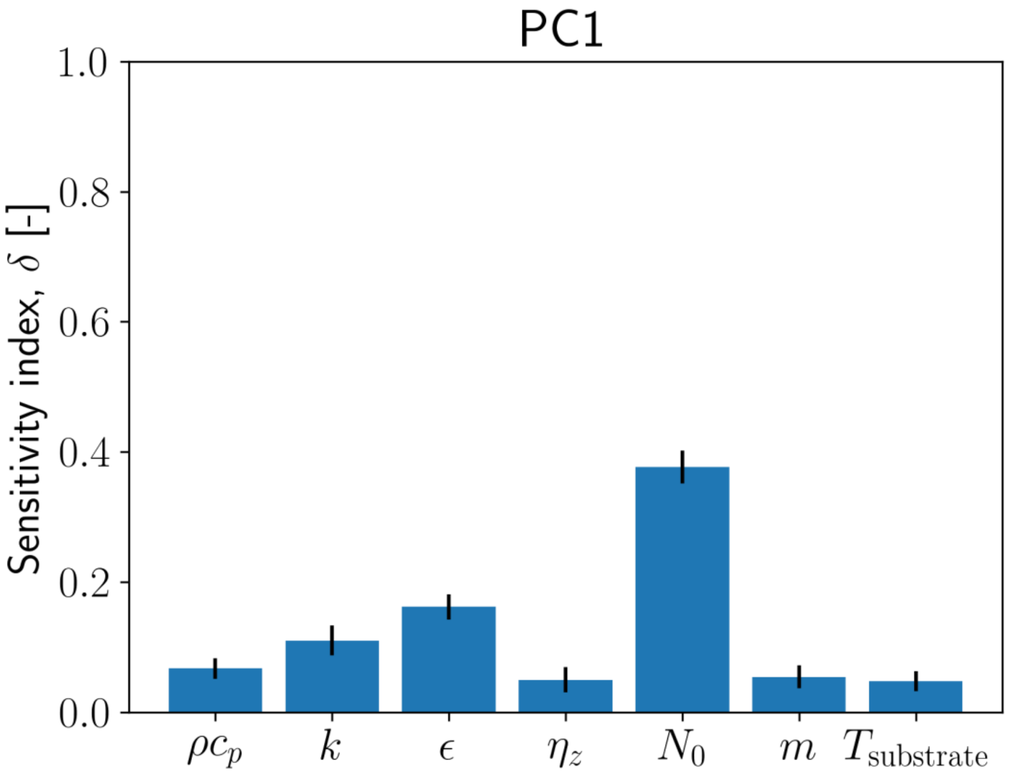


Crystallographic texture PCA

Texture strength and first PC (PC1) have similar sensitivity results

Comparison of sensitivity indices for each input parameter



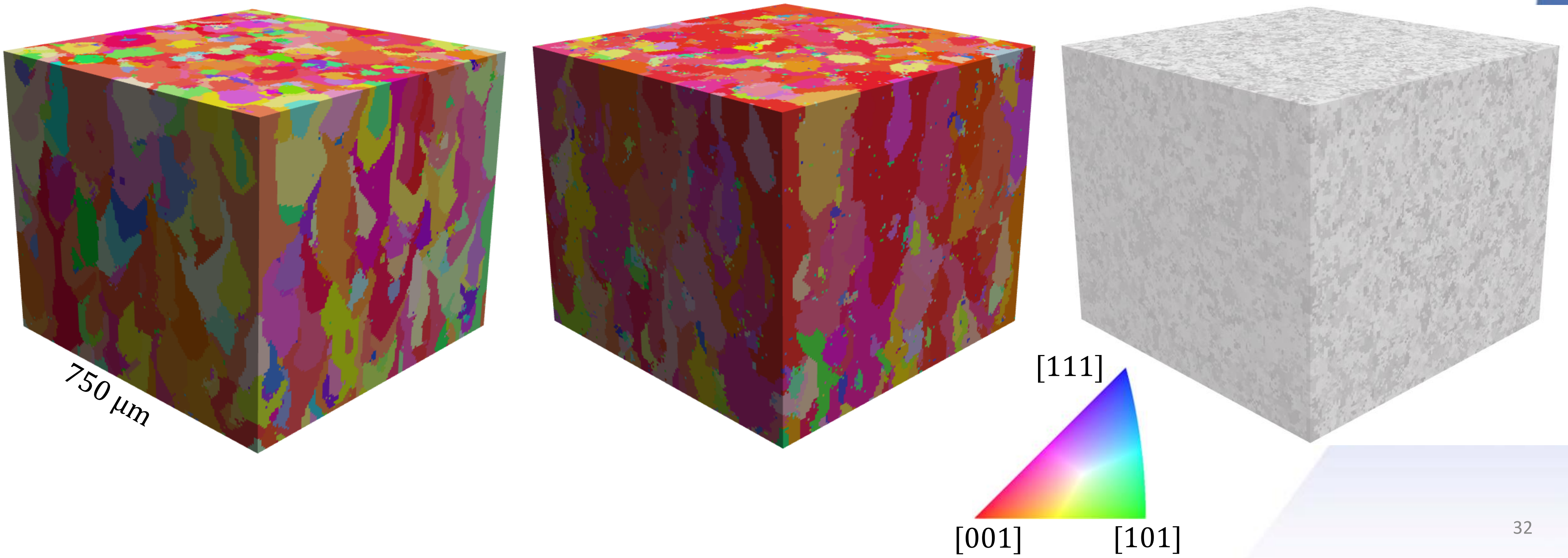


GSA: Results

Upper bound on N_0 is very conservative → what if it is reduced by an order of magnitude?

Inverse pole figure maps with respect to the build direction

$N_0 \approx 10^{13}/\mathrm{m}^3$ $N_0 \approx 10^{14}/\mathrm{m}^3$ $N_0 \approx 10^{15}/\mathrm{m}^3$

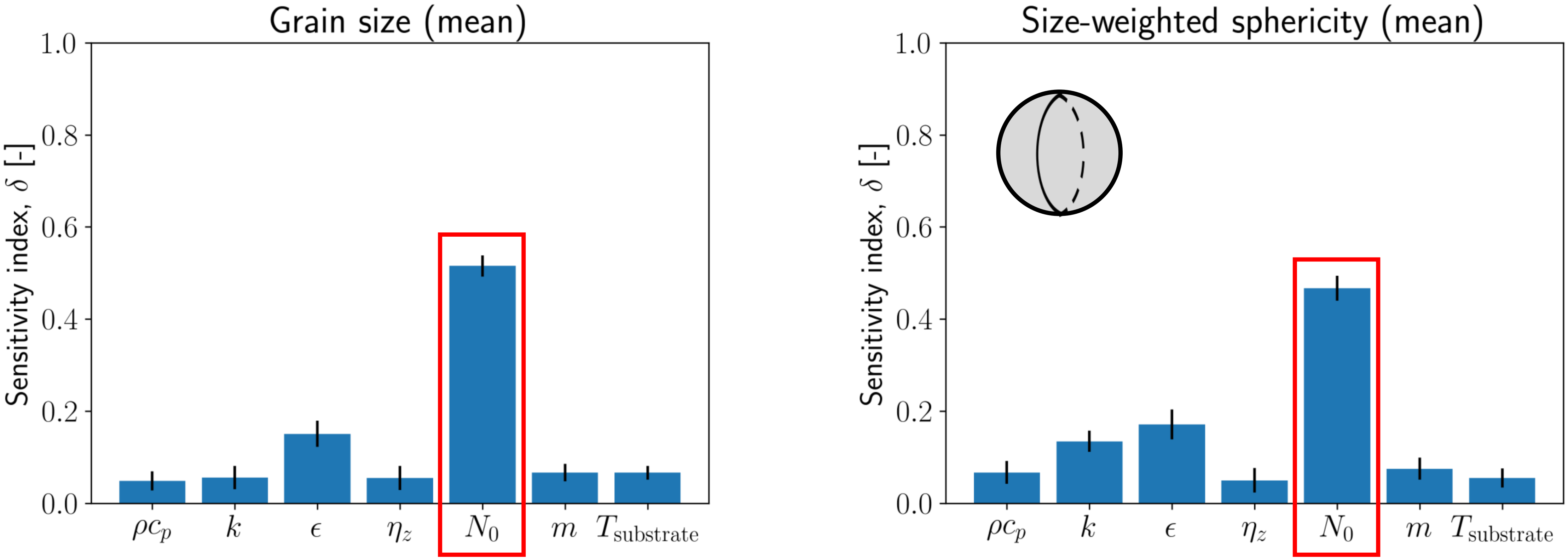


GSA: Results

Grain size and sphericity still most sensitive to nuclei density

- Epitaxially-growing grains are generally large and non-spherical

Comparison of sensitivity indices for each input parameter

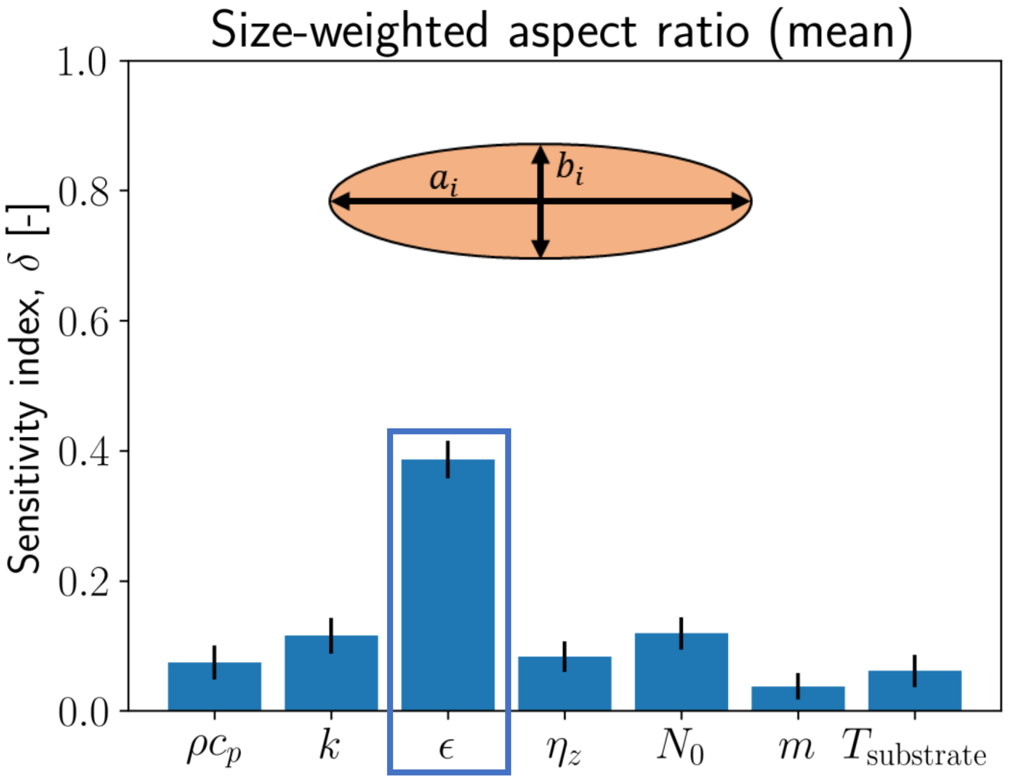


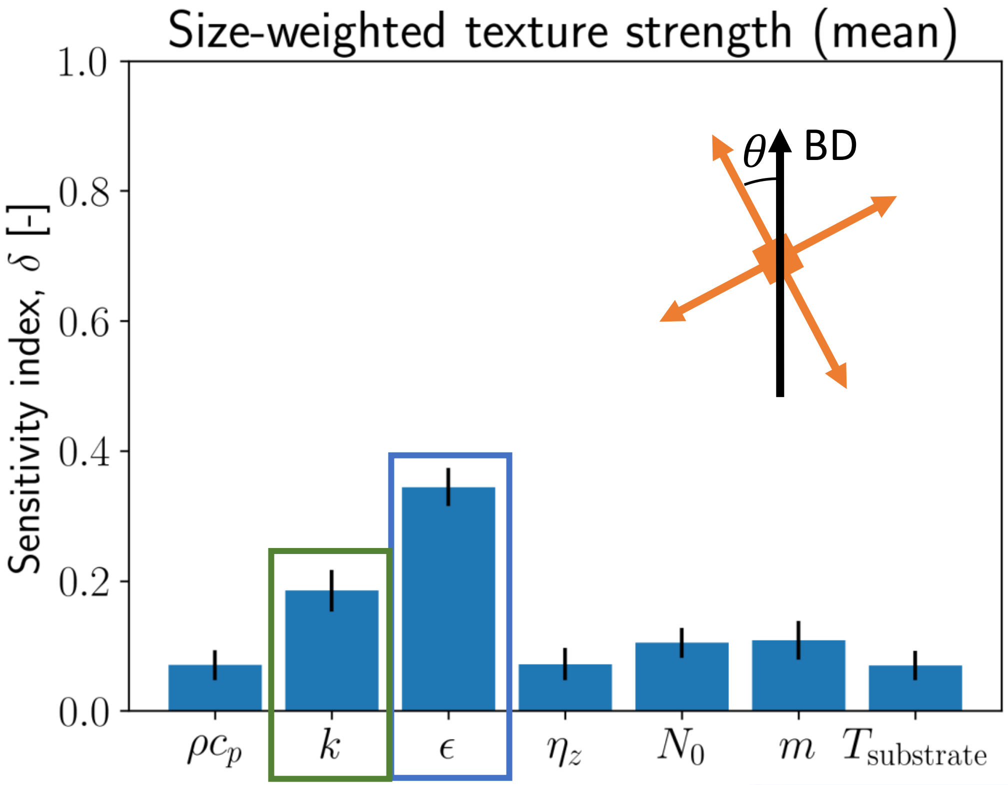
GSA: Results

Emissivity dominates for aspect ratio and texture

- Change in absorbed power → changes in melt pool size
- Conductivity influences melt pool length

Comparison of sensitivity indices for each input parameter





Conclusions

- PSP models link material and AM process to mechanical behavior
- Challenges: calibrating and validating expensive, high-fidelity models
- Multi-fidelity methods can accelerate crystal plasticity simulations
  - Optimized sample allocation across a variety of models
  - May need better low-fidelity models for predicting hotspots
- GSA can identify important input parameters to calibrate or control
  - Important to calibrate or at least bound nuclei density
  - PCA is promising for quantifying texture for GSA but needs more analysis
  - May need better solidification models to capture texture development
- Future: Probabilistic validation metrics accounting for model and data uncertainty

Acknowledgements

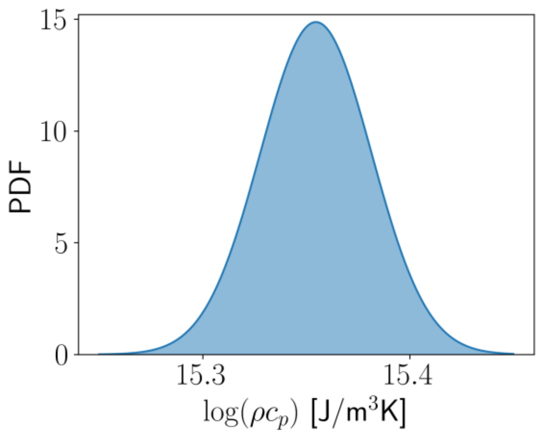
- This work was supported by the NASA Aeronautics Research Mission Directorate (ARMD) Transformational Tools and Technologies (TTT) project

- The authors also thank:
  - Ricardo Lebensohn from Los Alamos National Laboratory for sharing the EVPFFT code
  - Wes Tayon and Bryan Koscielny for completing the EBSD scans for the multi-fidelity models

- MXMCPy – Multi-model Monte Carlo in Python: https://github.com/nasa/MXMCPy

- Contact information: joshua.pribe@nasa.gov

GSA: Input parameters

<table>
<tr><th>Para-meter</th><th>Volumetric heat capacity: ρc_p</th><th>Thermal conductivity: k</th><th>Nuclei density: N_0</th><th>Solidification exponent: m</th></tr>
<tr><td>Data source</td><td>Calibration</td><td>Room temperature to liquid range</td><td>Literature</td><td>Fits to literature and CET</td></tr>
<tr><td>PDF</td>
<td>
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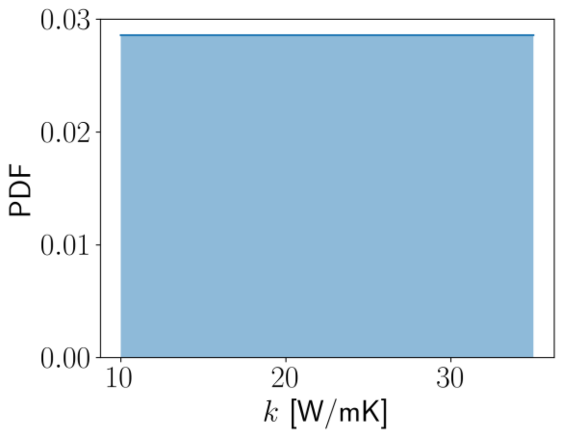
<td>
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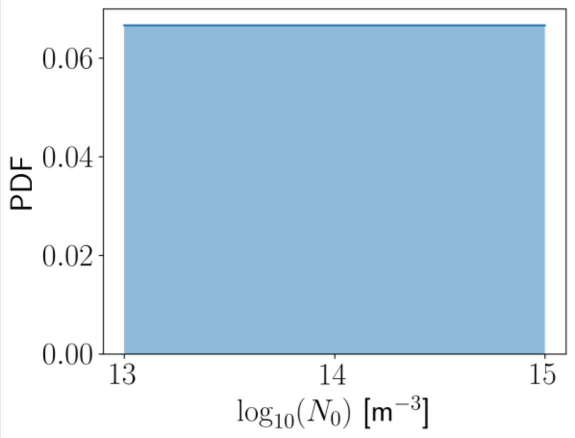
<td>
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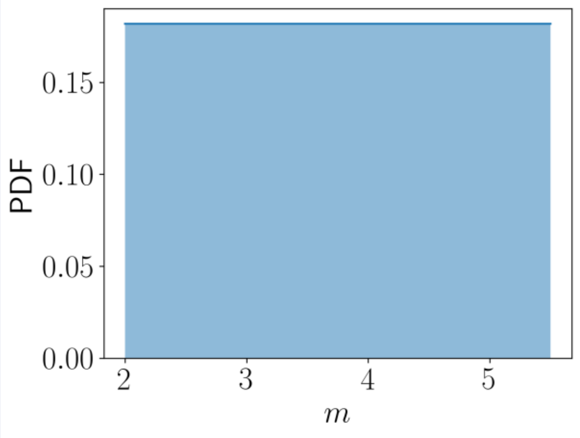
<td>
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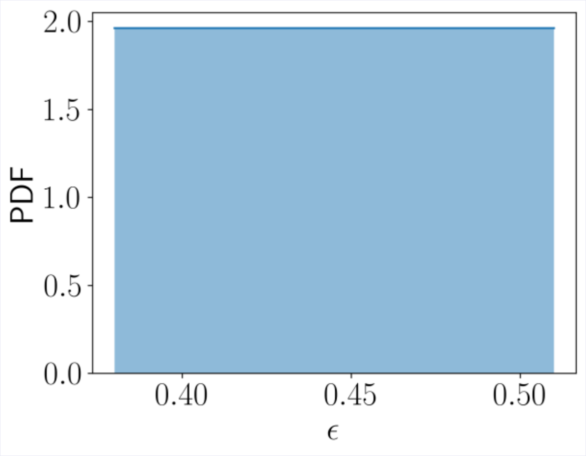
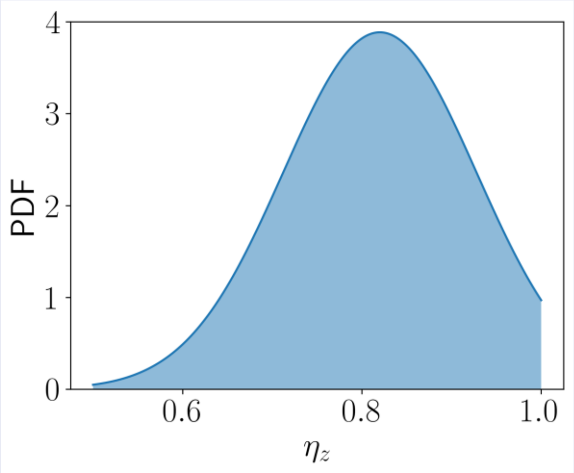
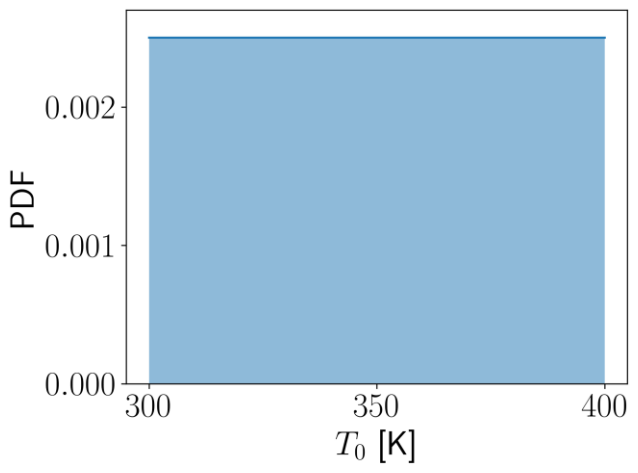
<tr><td>Notes</td><td></td><td>Calibration did not reduce bounds from this range</td><td>Wide range used partly for verification (see [1])</td><td>Analytical fit for prefactor (a) given m value</td></tr>
</table>

[1] T.M. Rodgers et al., Addit Manuf 41 (2021) 101953. https://doi.org/10.1016/j.addma.2021.101953.

GSA: Input parameters

Para-meter	Emissivity: ϵ	Depth scaling: η_z	Background temperature: $T_{substrate}$
Data source	Literature range[1]	Fit to melt pool width versus depth data for IN 718	Based on temperature rise over regions of interest in AM-Bench
PDF			
Notes		$\eta_z = \text{mean}(W/_{2D})$ Truncated to avoid very large/ small melt pools	Could consider wider range

[1]P. Promoppatum et al., Engineering 3 (2017) 685–694. https://doi.org/10.1016/J.ENG.2017.05.023.