Process-Structure-Properties Simulations for Predicting Fatigue Indicator Parameters of Additive Manufactured Ti-6Al-4V with Quantified Uncertainty

Joshua D. Pribe[1], Saikumar R. Yeratapally[1], Brodan Richter[2],
Patrick E. Leser[2], George Weber[2], Edward H. Glaessgen[2]

[1]National Institute of Aerospace
[2]NASA Langley Research Center

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Outline

- Motivation and objectives
- Process-structure: Physically-based Monte Carlo
  - Thermal model and solidification
  - Example microstructures
- Structure-properties: Crystal plasticity
  - Model formulation
  - Micromechanical fields and fatigue indicator parameters
- Fatigue indicator parameter distributions and uncertainty quantification
- Concluding remarks

Motivation

- Challenge using laser powder bed fusion additive manufacturing (AM) for flight hardware (Ti-6Al-4V): need to ensure acceptable fatigue performance
  - Influenced by build conditions, defects, microstructure, texture, etc.
- Process-structure-properties (PSP) simulations: understand how the design space maps to quantities of interest relevant for fatigue
- Need uncertainty quantification (UQ), verification, and validation to build confidence in AM processes and models[1]
  - Requires enough simulations or experiments to build up statistics on a quantity of interest

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[1] S. Mahadevan et al., ASCE-ASME J Risk and Uncert in Engrg Sys Part B Mech Engrg. 8 (2022) 010801. https://doi.org/10.1115/1.4053184.

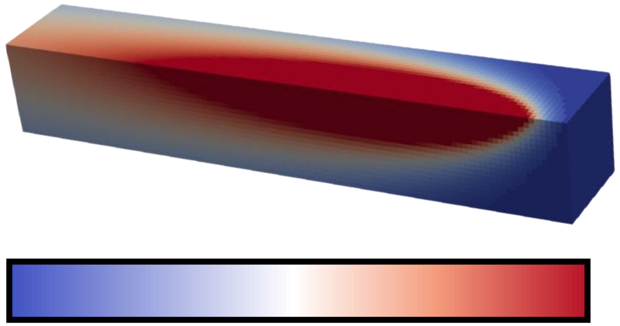
Objectives

- Build a PSP framework capable of simulating many AM-generated microstructures
- Predict distributions of fatigue indicator parameters in the simulated microstructures
- Understand the influence of microstructural randomness, process parameters, and build defects (porosity) on the fatigue indicator parameters

Process-structure: Physically-based Monte Carlo

- **S**tochastic **P**arallel **Par**ticle **K**inetic **S**imulator (SPPARKS)[1]
  - Kinetic Monte Carlo framework from Sandia National Laboratories https://spparks.github.io/
  - Initially used for microstructural evolution (e.g., annealing, recrystallization)
- Application to AM: Physically-based Monte Carlo (PBMC)[2,3]
  - Thermal model → temperature field → melt pool

Melt pool from analytical thermal model (Rosenthal equation)



$$T = T_0 + \frac{Q}{2\pi r k}\exp\left(-\frac{v(\xi + r)}{2\alpha}\right)$$

T: temperature
T_0: background temperature
Q: absorbed power
v: scan speed
r: distance from point source
ξ: local scan direction coordinate
k: thermal conductivity
α: thermal diffusivity

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[1] This is not an endorsement by the National Aeronautics and Space Administration (NASA)

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

[3] J.G. Pauza et al., Modelling Simul Mater Sci Eng. 29 (2021) 055019. https://doi.org/10.1088/1361-651X/ac03a6.

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  - Solidification → epitaxial grain growth, columnar grains

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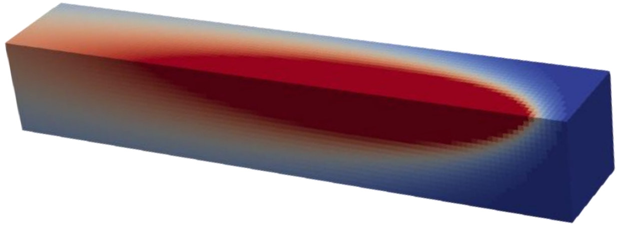
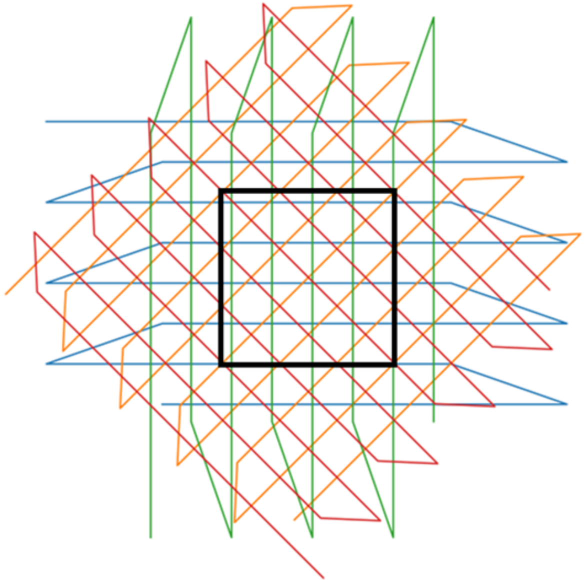
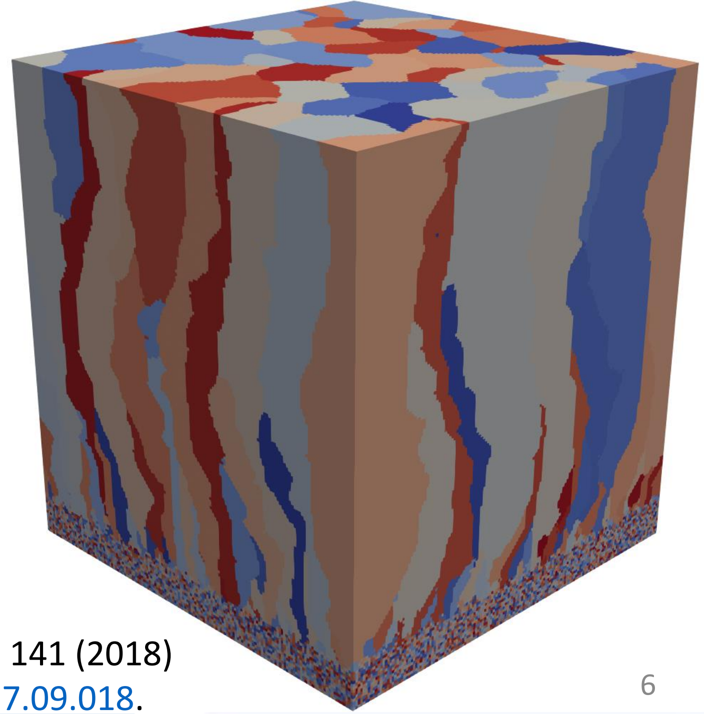


Scan strategy (schematic)



Example microstructure



Ti-6Al-4V build parameters from O. Zinovieva et al., 141 (2018) 207–220. https://doi.org/10.1016/j.commatsci.2017.09.018.

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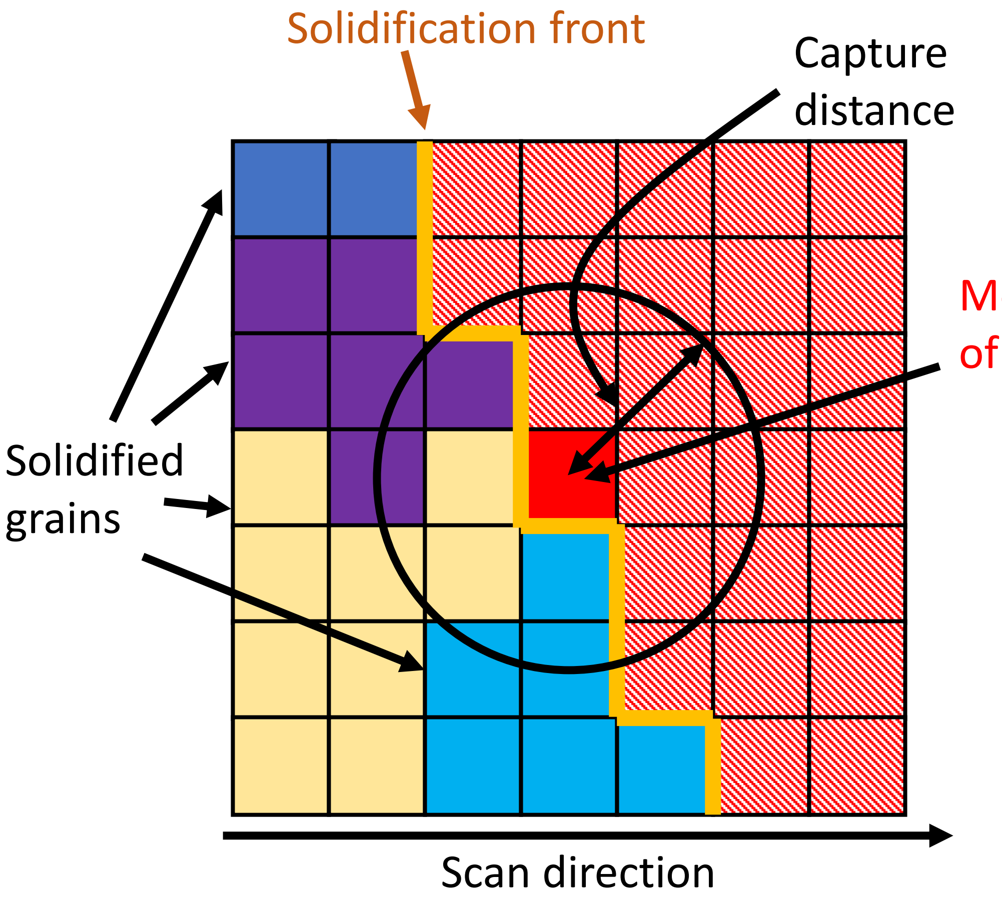
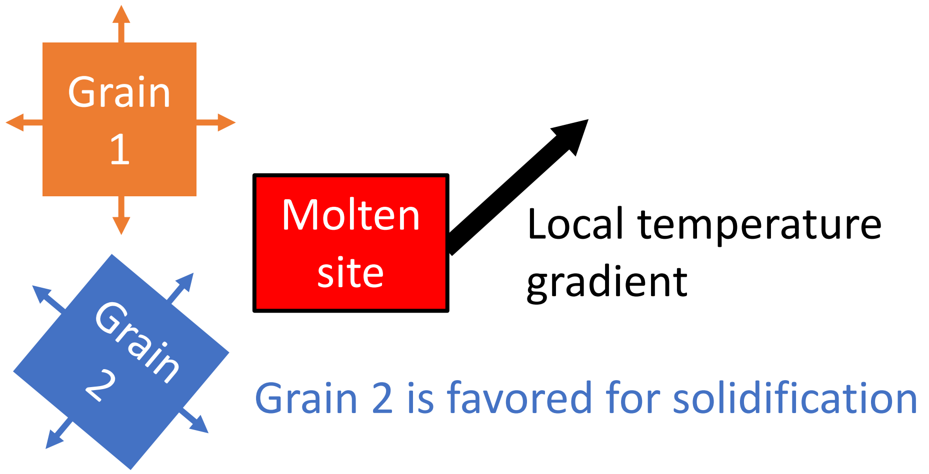
Process-structure: Physically-based Monte Carlo

Solidification: select probabilistically from eligible grains[1]

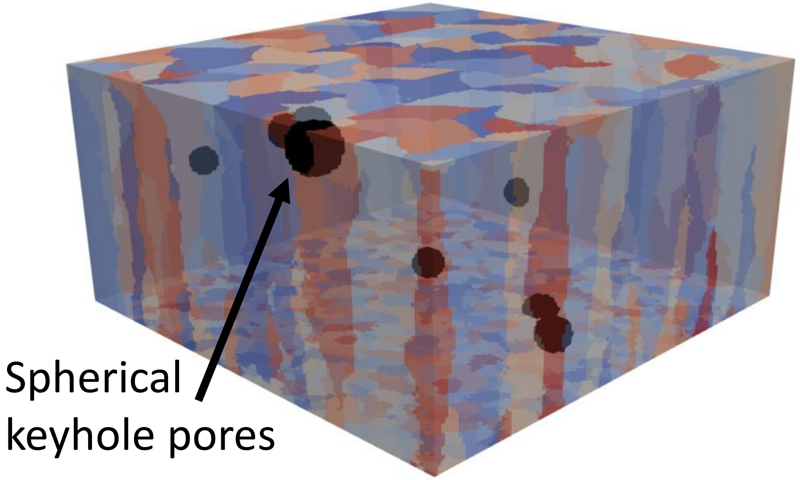


Weighted by alignment of <001> crystal directions with thermal gradient



Grain 2 is favored for solidification

Stochastic insertion of keyhole porosity



Assumptions

- Steady-state temperature field
- Neglect grain nucleation

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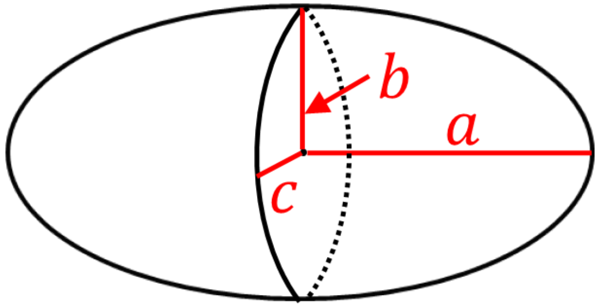
[1] Adapted from T. M. Rodgers et al., Addit Manuf. 41 (2021) 101953. https://doi.org/10.1016/j.addma.2021.101953.

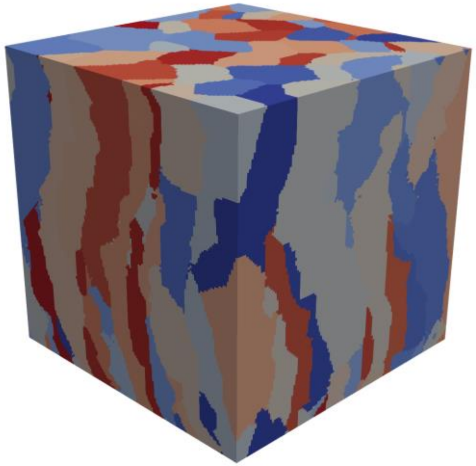
Microstructures: Equivalent ellipsoids

Aspect ratios for equivalent ellipsoids support observed dominance of columnar grains

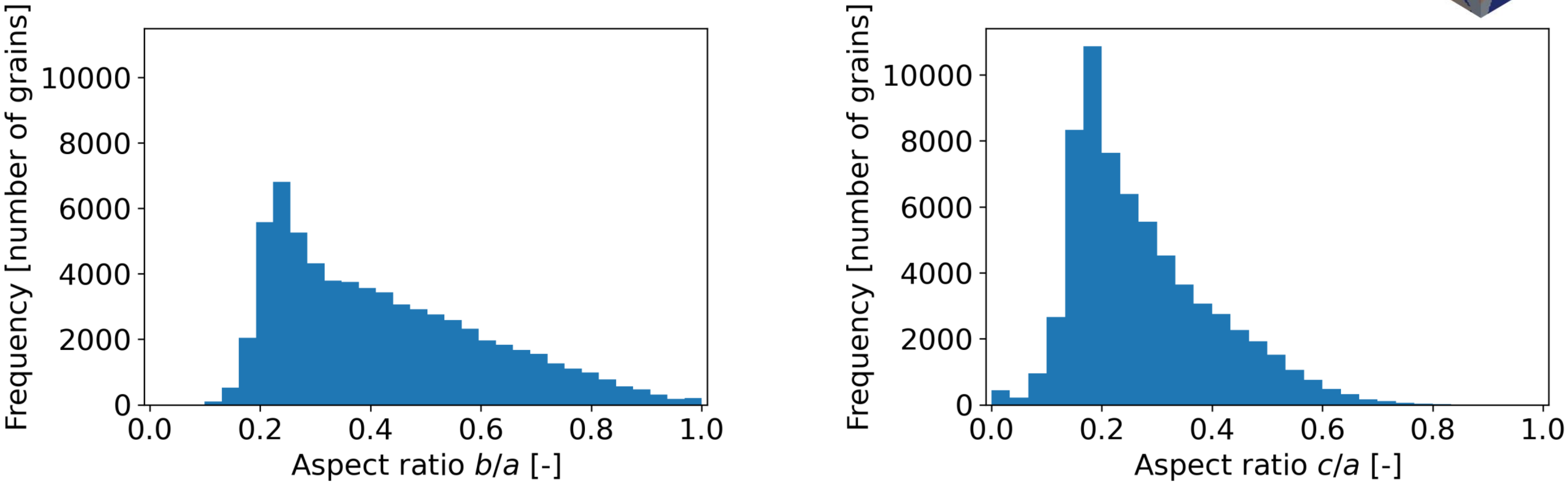
Equivalent ellipsoid dimensions



Example micro-structure



Aspect ratios for all grains across 200 simulations



Structure-properties: Crystal plasticity

- **E**lasto-**V**isco**p**lastic **F**ast **F**ourier **T**ransform (EVP-FFT)[1]
- Advantages
  - Speed improvements over crystal plasticity finite element methods
  - Shares voxel-based microstructure representation with SPPARKS (no need for meshing)

Flow rule:

$$\dot{\boldsymbol{\varepsilon}}^p = \dot{\gamma}_0 \sum_{s=1}^{N_s} \boldsymbol{m}^s \left(\frac{|\boldsymbol{m}^s\!:\boldsymbol{\sigma}|}{\tau^s}\right)^n \operatorname{sgn}(\boldsymbol{m}^s\!:\boldsymbol{\sigma})$$

Voce hardening:

$$\tau^s = \tau_0 + (\tau_1 + \theta_1\Gamma)\left[1 - \exp\left(-\frac{\theta_0}{\tau_1}\Gamma\right)\right]$$

$$\Gamma = \sum_{s=1}^{N_s} \int \dot{\gamma}^s dt$$

Implicit time discretization:

$$\boldsymbol{\sigma} = \mathbf{C} : \left(\boldsymbol{\varepsilon}_{\boldsymbol{t+\Delta t}} - \boldsymbol{\varepsilon}_{\boldsymbol{t}}^{\boldsymbol{p}} - \dot{\boldsymbol{\varepsilon}}_{\boldsymbol{t+\Delta t}}^{\boldsymbol{p}} \Delta t\right)$$

$\dot{\gamma}_0$: reference strain rate
n: viscoplastic exponent
$\dot{\boldsymbol{\varepsilon}}^p$: plastic strain rate tensor
$\boldsymbol{\sigma}$: stress tensor
$\boldsymbol{m}^{\boldsymbol{s}}$: Schmid tensor for slip system *s*
τ^s: critical resolved shear stress for slip system *s*
$\dot{\gamma}^s$: plastic shear strain on slip system *s*
$\tau_0, \tau_1, \theta_0, \theta_1$: Voce hardening law parameters
Γ: accumulated slip on all slip systems
t, Δt: time, time step
$\mathbf{C}$: stiffness tensor
$\boldsymbol{\varepsilon}$: total strain tensor
$\boldsymbol{\varepsilon}^{\boldsymbol{p}}$: plastic strain tensor

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[1] R.A. Lebensohn et al., Int J Plast. 32–33 (2012) 59–69. https://doi.org/10.1016/j.ijplas.2011.12.005. This is not an endorsement by NASA.

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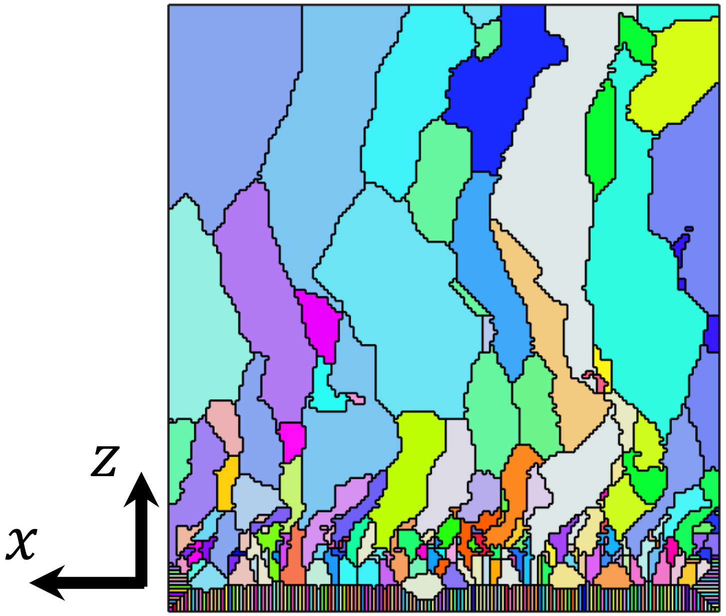
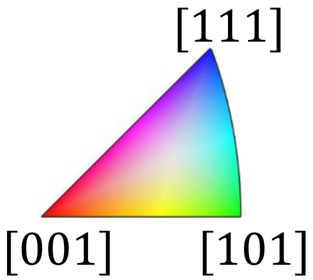
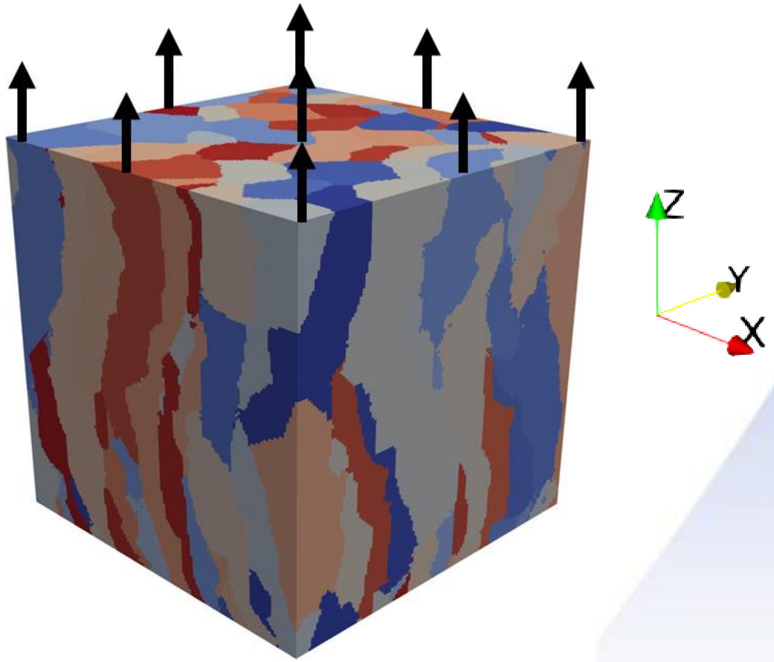
One of 12 possible α variants randomly selected for each grain



Prior β texture, z ref. direction



0.6% applied strain in build direction; periodic boundary conditions on sides of domain



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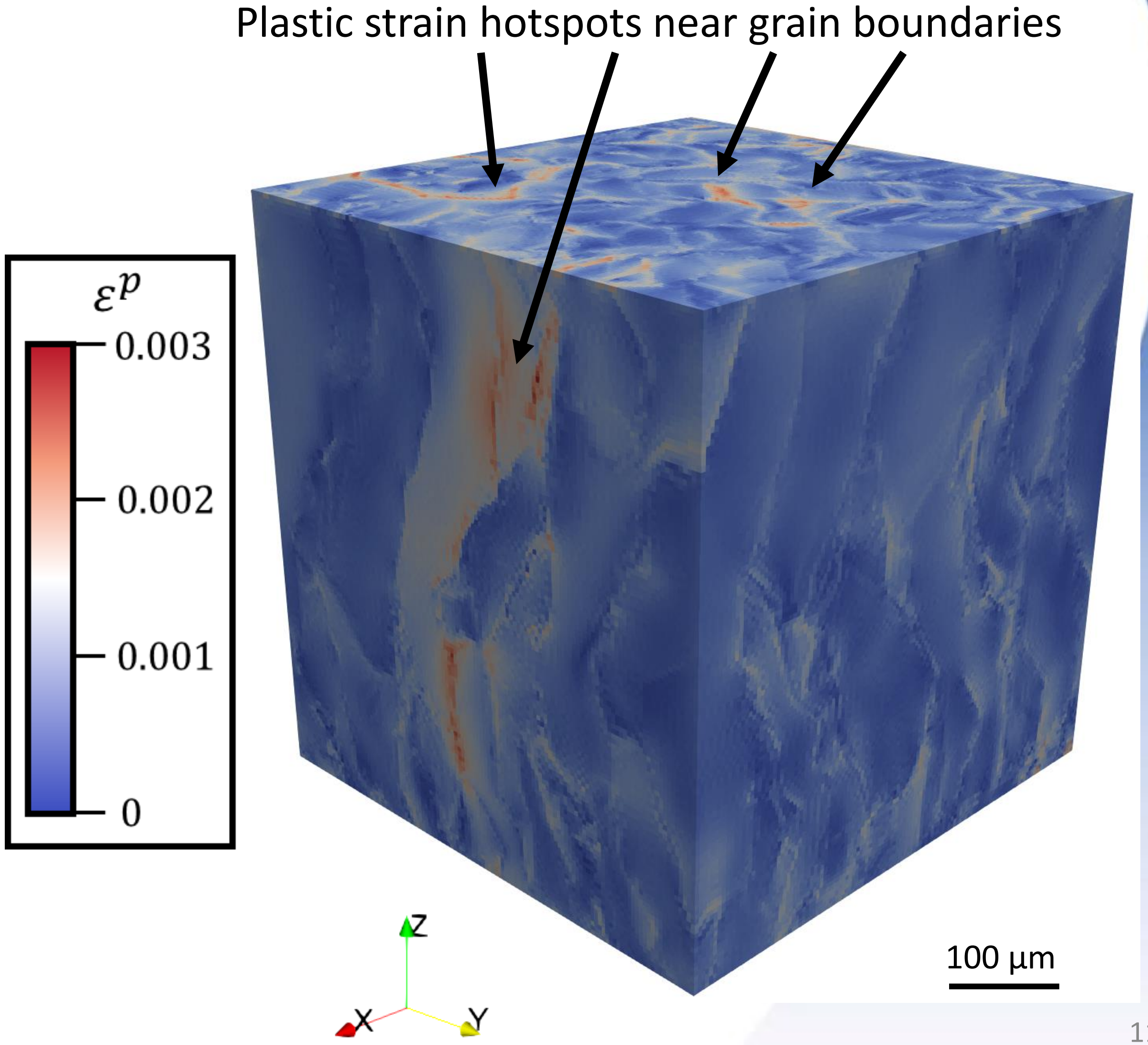
[1] R.A. Lebensohn et al., Int J Plast. 32–33 (2012) 59–69. https://doi.org/10.1016/j.ijplas.2011.12.005. This is not an endorsement by NASA.

Micromechanical fields

- Goal: distributions of fatigue indicator parameters (FIPs)
- Here: equivalent plastic strain

$$\varepsilon^p = \int \dot{\varepsilon}^p dt \qquad \dot{\varepsilon}^p = \sqrt{\frac{2}{3}\dot{\boldsymbol{\varepsilon}}^p : \dot{\boldsymbol{\varepsilon}}^p}$$

- Value assigned to each grain by volume averaging near hotspots
- Other possibilities: crystallographic parameters (e.g., slip-system-based Fatemi-Socie[1])



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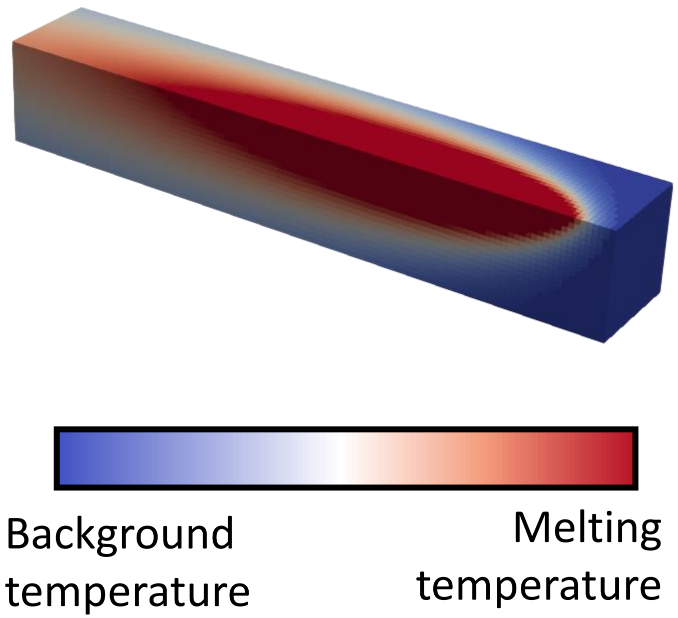
[1] V. Bennett, D.L. McDowell, Int J Fatigue. 25 (2003) 27–39. https://doi.org/10.1016/S0142-1123(02)00057-9.

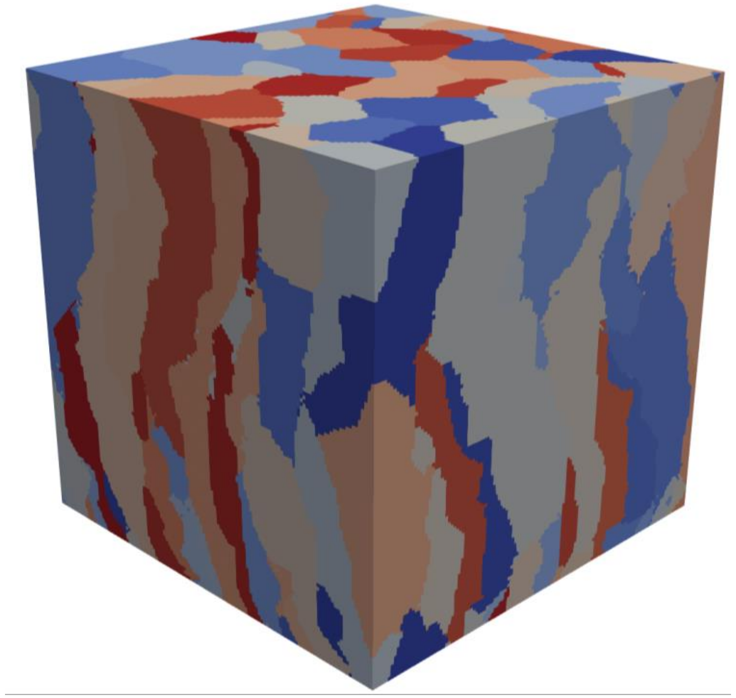
Summary of PSP framework

Multiple simulations → probability distributions of FIPs and UQ

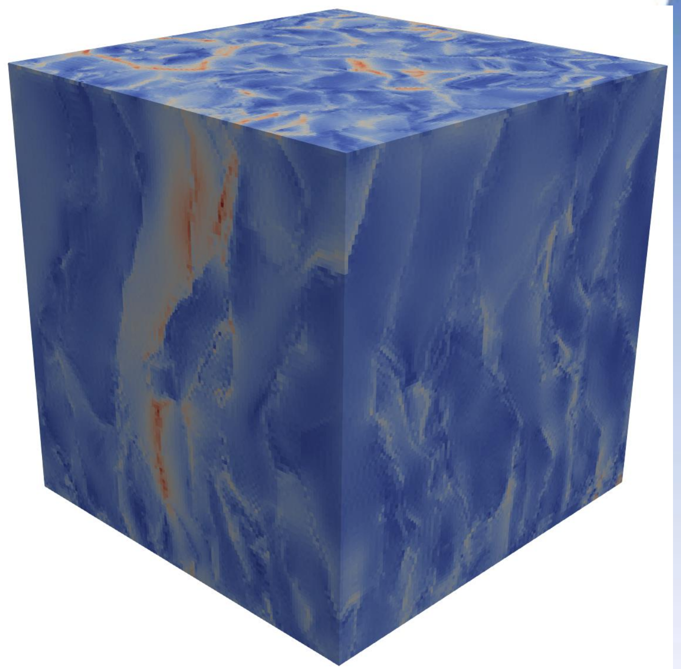
Analytical thermal model



Microstructures from PBMC



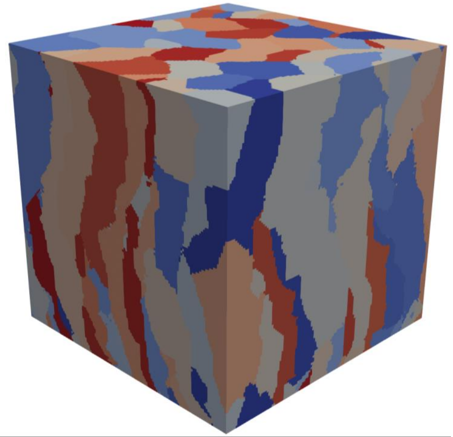
Micromechanical fields from crystal plasticity



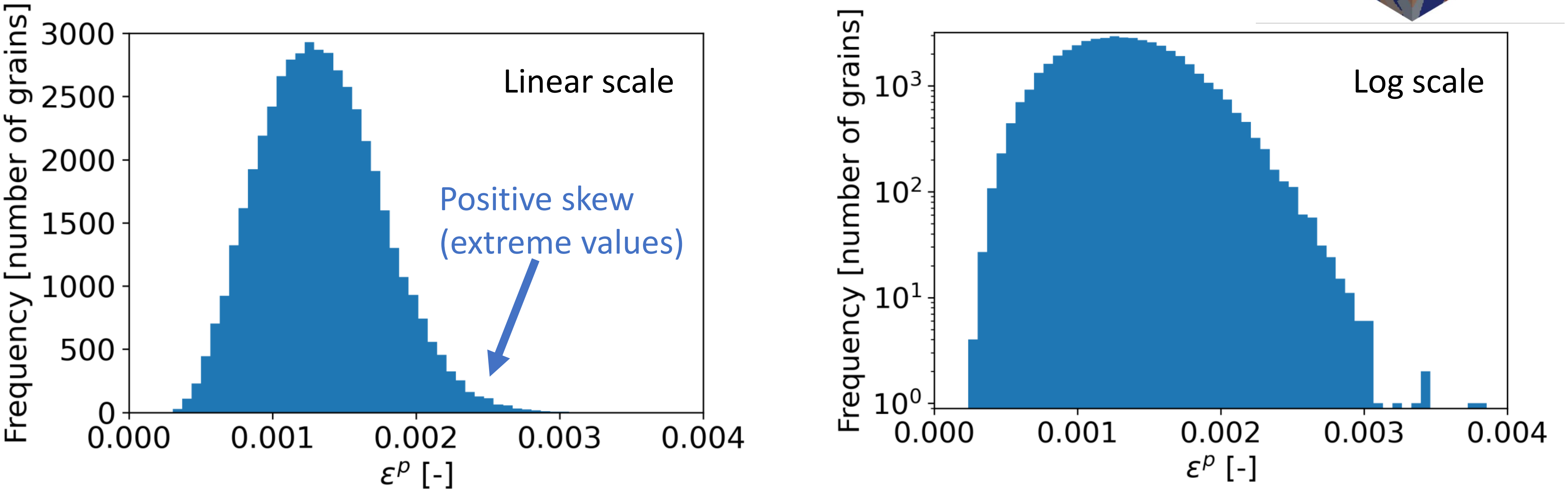
FIP distributions: No porosity

- 200 simulations with full PSP framework, no pores
- Fatigue is an extreme value phenomenon → consider upper tail of the distribution
- How does the distribution shift in the presence of pores?

Example microstructure

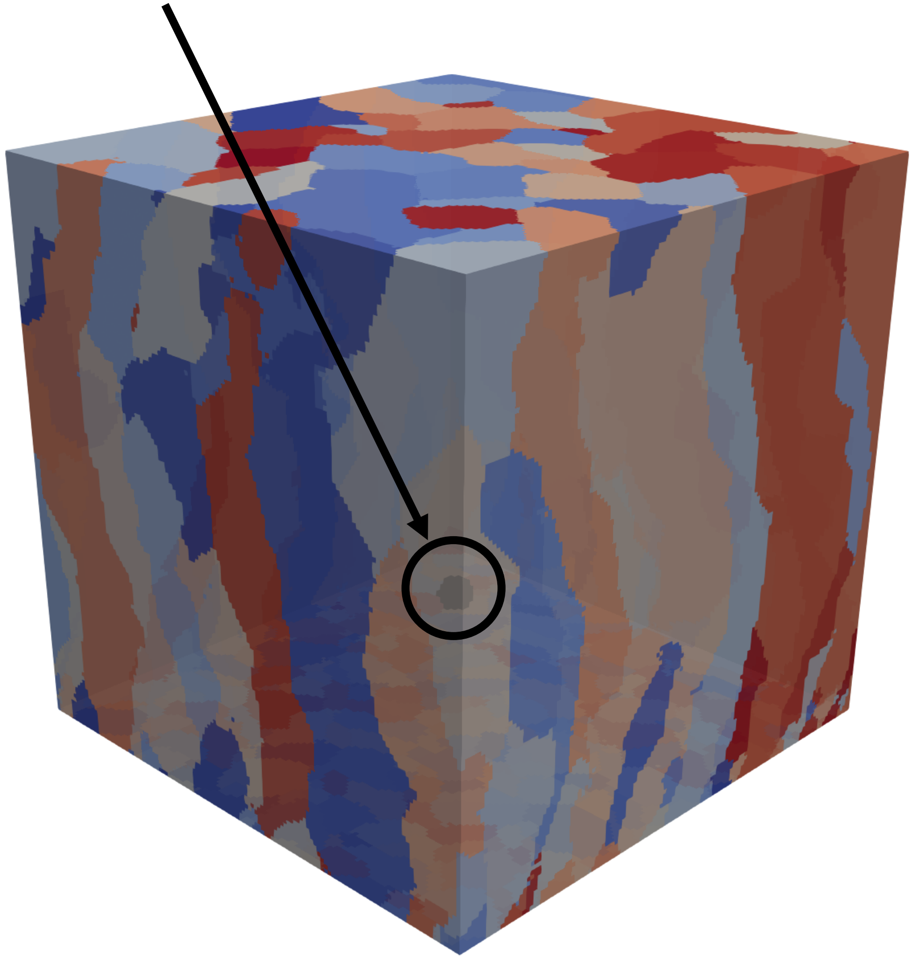


Equivalent plastic strain for all grains across 200 simulations



FIP distributions: Porosity vs. no porosity

- 200 simulations with average of one 30-µm keyhole pore per simulation

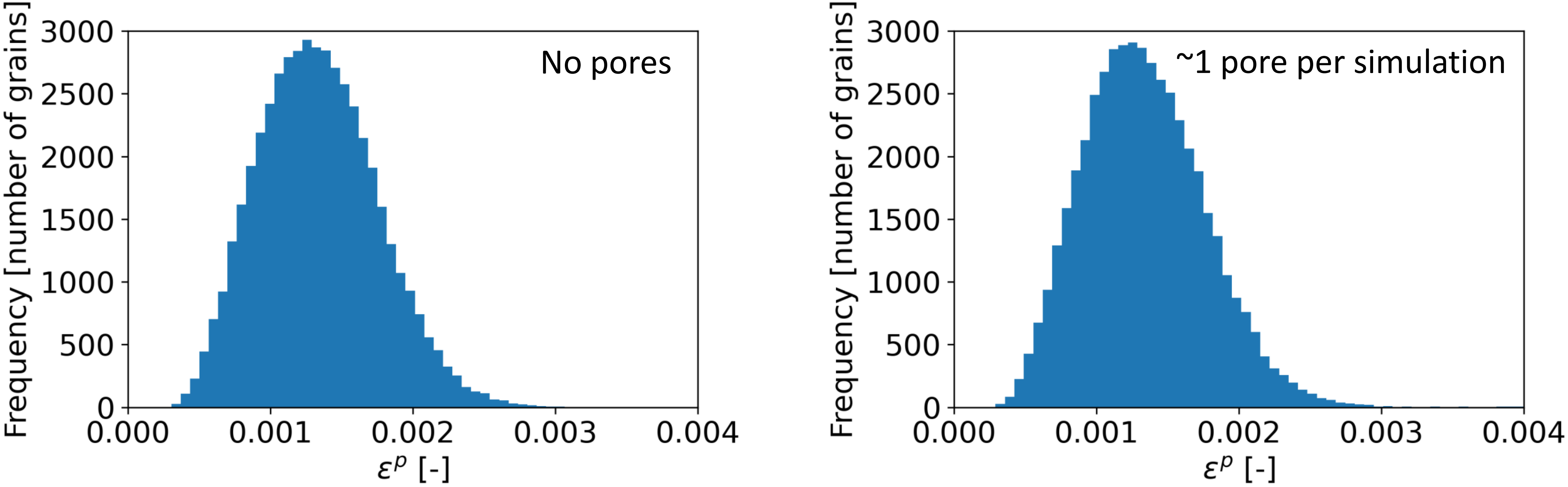


Example microstructure
with a keyhole pore

FIP distributions: Porosity vs. no porosity

- 200 simulations with average of one 30-µm keyhole pore per simulation
- Overall distribution of plastic strain is similar

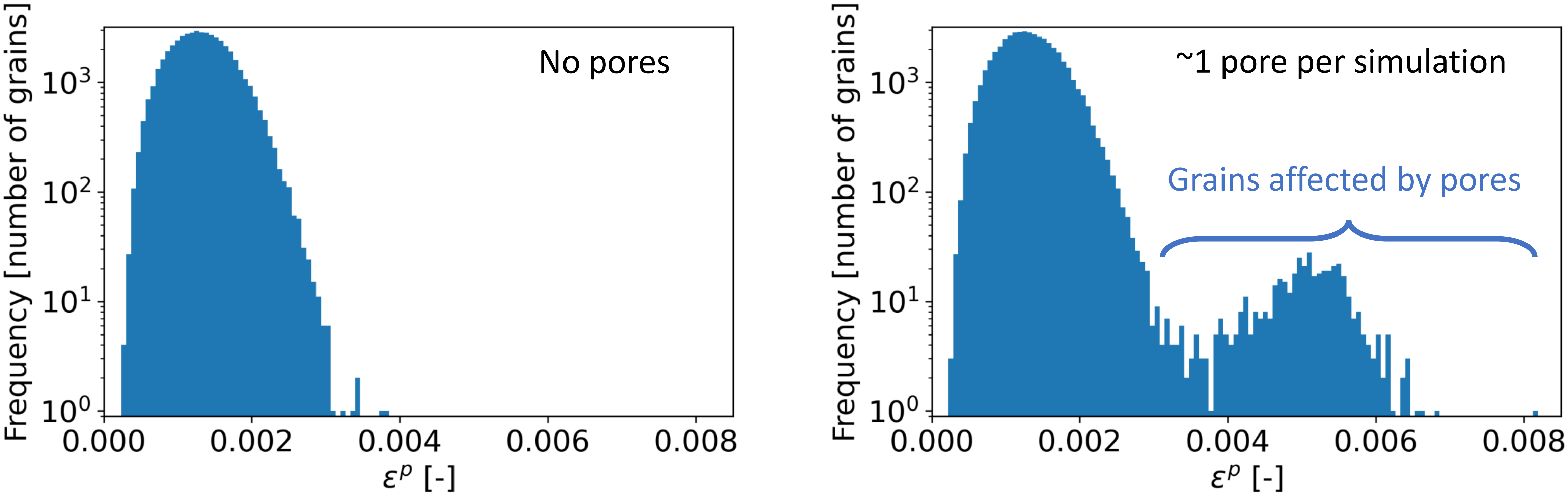
Equivalent plastic strain for all grains across 200 simulations, linear scale



FIP distributions: Porosity vs. no porosity

- 200 simulations with average of one 30-µm keyhole pore per simulation
- Overall distribution of plastic strain is similar
- But extreme values are shifted!

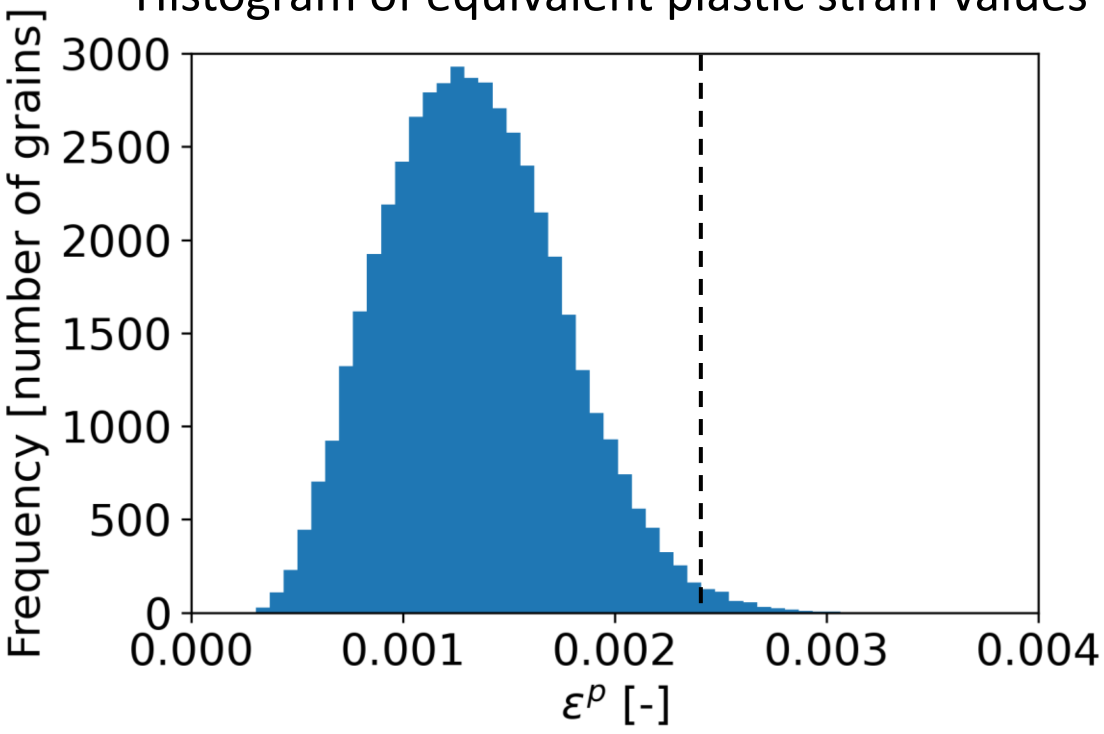
Equivalent plastic strain for all grains across 200 simulations, log scale



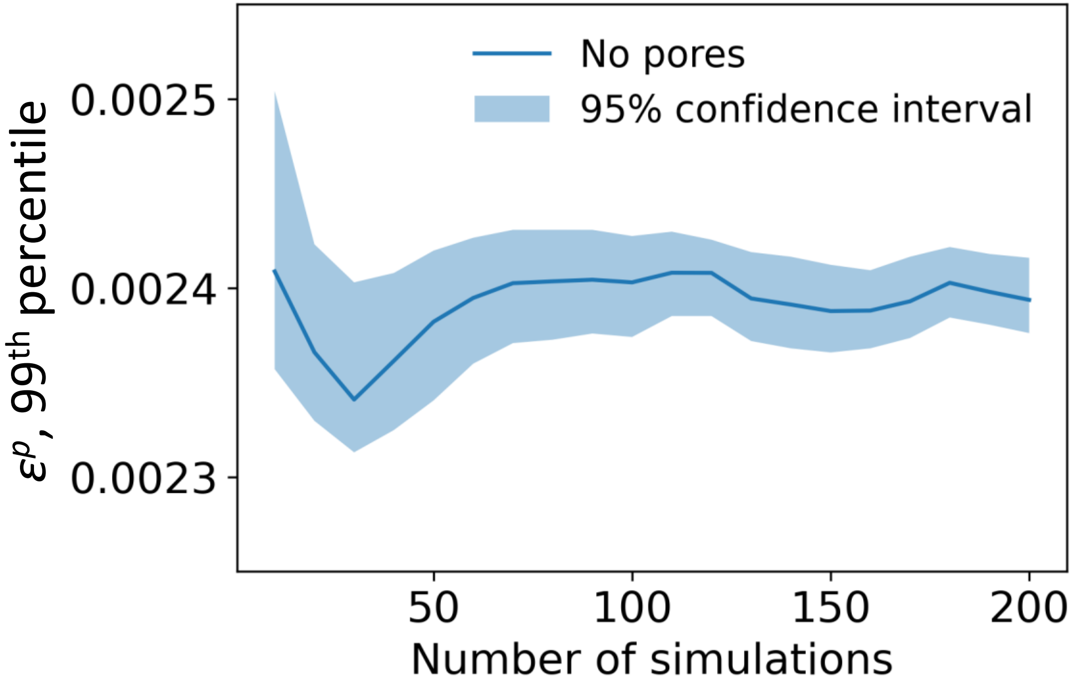
FIP: Extreme values, no porosity

- 99th percentile of equivalent plastic strain → extreme values of the FIP
- Uncertainty bounds (confidence interval) based on binomial distribution[1]

Histogram of equivalent plastic strain values



Sample-based estimate of equivalent plastic strain 99th percentile across all grains with increasing number of simulations



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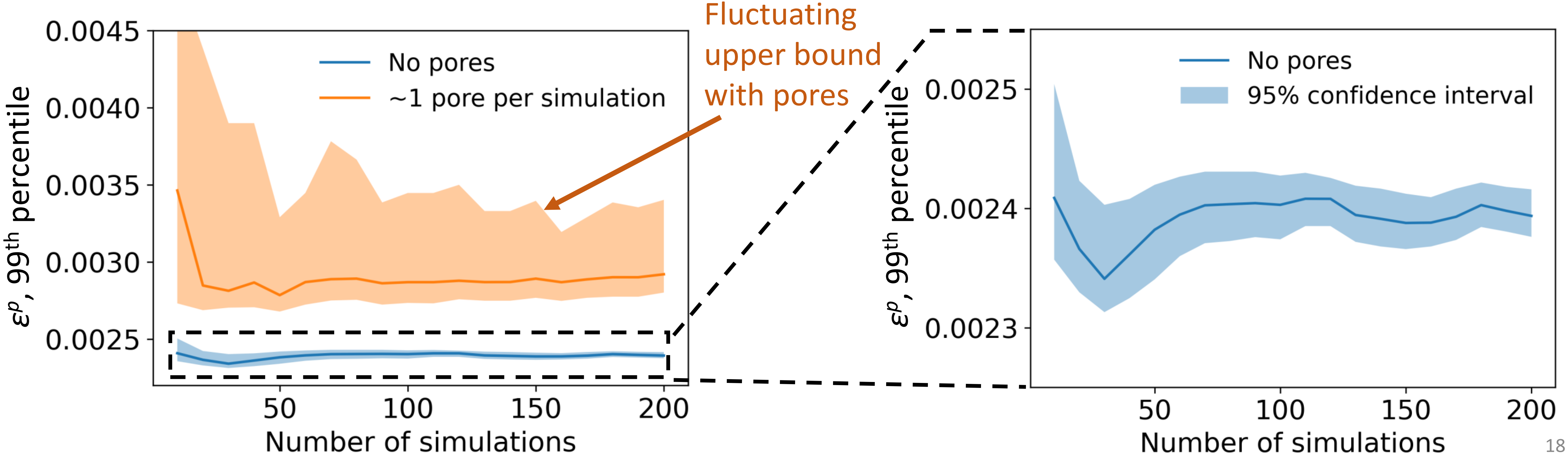
[1] A.B. Owen, *Monte Carlo Theory, Methods, and Examples*. 2013.

FIP: Extreme values, porosity vs. no porosity

99^{th} percentile for simulations with pores

- Stable lower bound but upper bound of 95% confidence interval fluctuates
- Points toward pore-microstructure interactions

Sample-based estimate of equivalent plastic strain 99^{th} percentile across all grains **without** and **with** porosity


Fluctuating upper bound with pores

Concluding remarks

- PSP framework can simulate many builds and determine distributions of quantities of interest relevant to fatigue (FIPs)
- We can quantify the influence of pores on the extreme values of FIP distributions
  - Small, isolated pores: minimal influence on overall distribution
  - Small pores + interaction with local microstructure → heavy tail of FIP distribution
- Ongoing work
  - Enhancements to each step in the framework (e.g., grain nucleation, columnar-equiaxed transition, α variant selection, FIP determination)
  - More advanced UQ (e.g., sensitivity analysis, multi-fidelity Monte Carlo, extreme value distributions)

Acknowledgements

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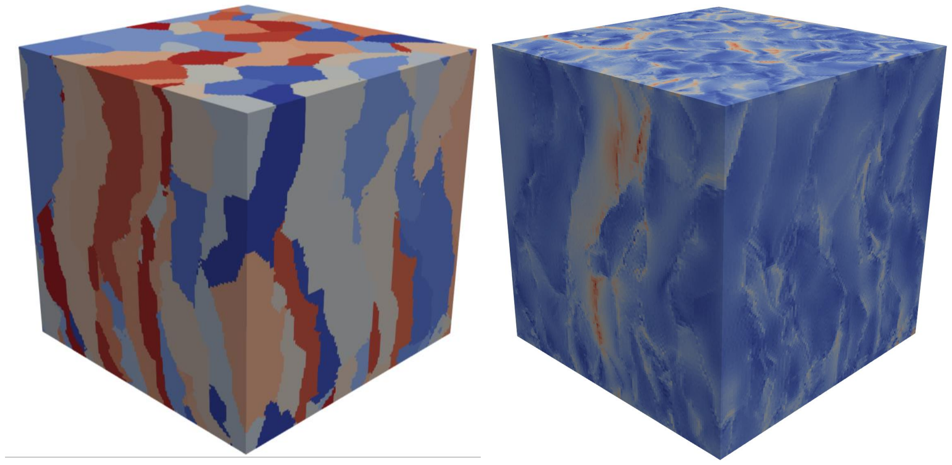
- We also thank Dr. Ricardo A. Lebensohn from Los Alamos National Laboratory for sharing the serial/distribution version of the EVP-FFT code

- Contact information: joshua.pribe@nasa.gov

Example microstructure and plastic strain contours



99th percentile of equivalent plastic strain across 200 simulations