SAND2023-07111C

Sandia National Laboratories

Exceptional service in the national interest

MODELING ADDITIVELY MANUFACTURED METALLIC MICROSTRUCTURES FOR DYNAMIC RESPONSE

Representing Microstructures on FE Meshes

John Mitchell

July 27 2023

17th U. S. National Congress on Computational Mechanics, Albuquerque, NM July 23-27, 2023

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

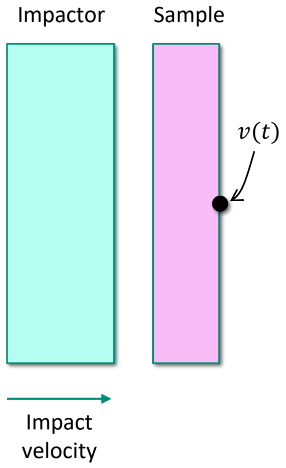
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly
artment of Energy's National Nuclear Security Administration under contract DE-NA0003525.

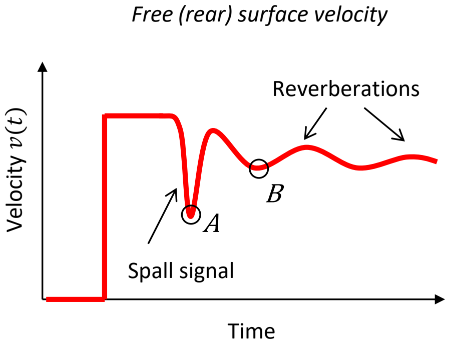
Request ID1715339

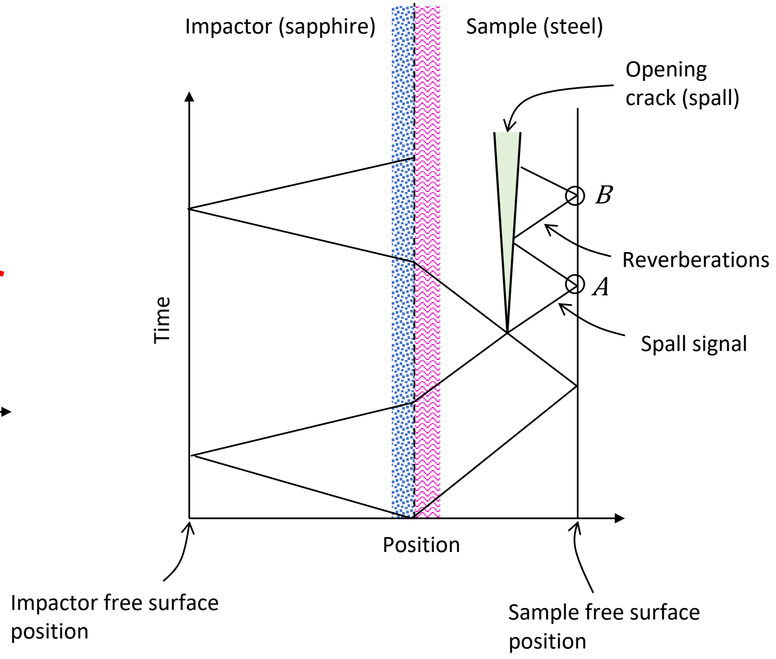
WORKFLOW TO ENABLE MICROSTRUCTURE AWARE SIMULATION OF SPALL DYNAMIC RESPONSE FOR AM STAINLESS STEEL

Challenges

- Complex microstructure morphologies arising from additive manufacturing process
- Material heterogeneity at test sample length scale
- Reconcile properties and morphologies on FE discretization
- Microstructure variability from build to build
- Spall dynamic response and failure is induced by tensile conditions not preexisting crack







ACKNOWLEDGMENTS: THANK YOU

spparks.github.io (open source kinetic Monte Carlo framework)

- Steve Plimpton, Aidan Thompson

Grain growth modeling and simulation

- Veena Tikare, Jon Madison, Theron Rodgers
- Reviewers of our submitted articles – thank you!

Thermal modeling

- Kyle Johnson

Microstructure analysis and analytics

- Andrew Castillo, Stephen Bond, Theron Rodgers

Project support, dynamic testing and modeling

- Paul Specht, Justin Brown, Stewart Silling, Edwin Chiu

Stitch IO development for spparks

- Jay Lofstead, Enze Chen

REFERENCE PAPERS

Journal of Peridynamics and Nonlocal Modeling
https://doi.org/10.1007/s42102-022-00093-2

ORIGINAL ARTICLES

Check for updates

Modeling Additively Manufactured Metallic Microstructures for Dynamic Response

John A. Mitchell[1] · Stewart A. Silling[1] · Edwin Chiu[1] · Stephen D. Bond[1] · Timothy Ruggles[1]

Received: 26 May 2022 / Accepted: 16 December 2022

REFERENCE PAPERS

PAPER • OPEN ACCESS

Parallel simulation via SPPARKS of on-lattice kinetic and Metropolis Monte Carlo models for materials processing

John A Mitchell[8,1], Fadi Abdeljawad[2], Corbett Battaile[1], Cristina Garcia-Cardona[3], Elizabeth A Holm[4], Eric R Homer[5], Jon Madison[1], Theron M Rodgers[1], Aidan P Thompson[1], Veena Tikare[6] + Show full author list

Published 9 May 2023 • © 2023 The Author(s). Published by IOP Publishing Ltd

Modelling and Simulation in Materials Science and Engineering, Volume 31, Number 5

Citation John A Mitchell *et al* 2023 *Modelling Simul. Mater. Sci. Eng.* **31** 055001

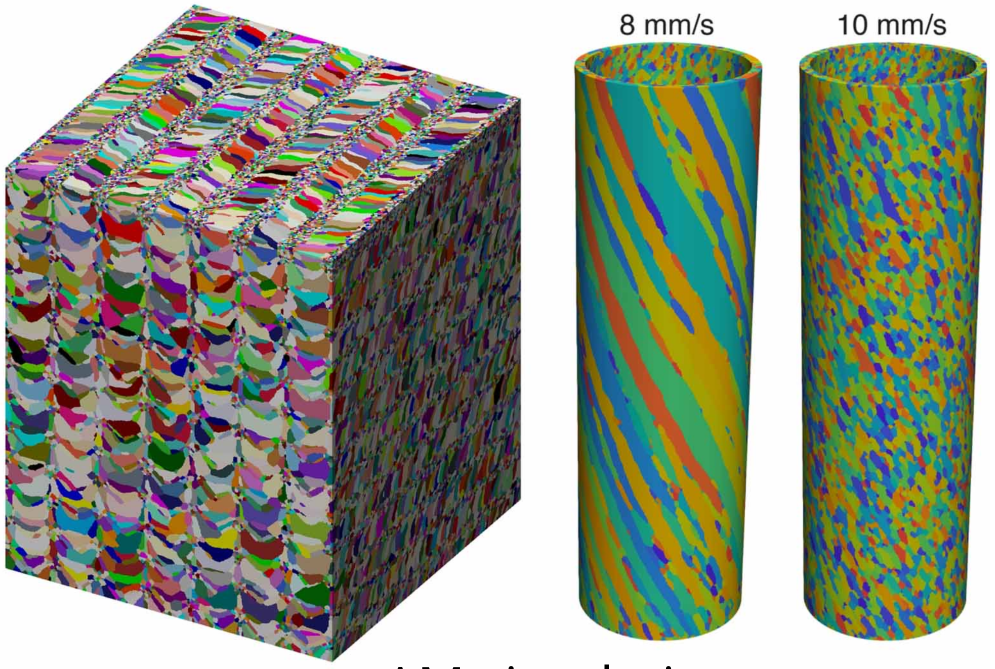
DOI 10.1088/1361-651X/accc4b

WHAT IS SPPARKS?

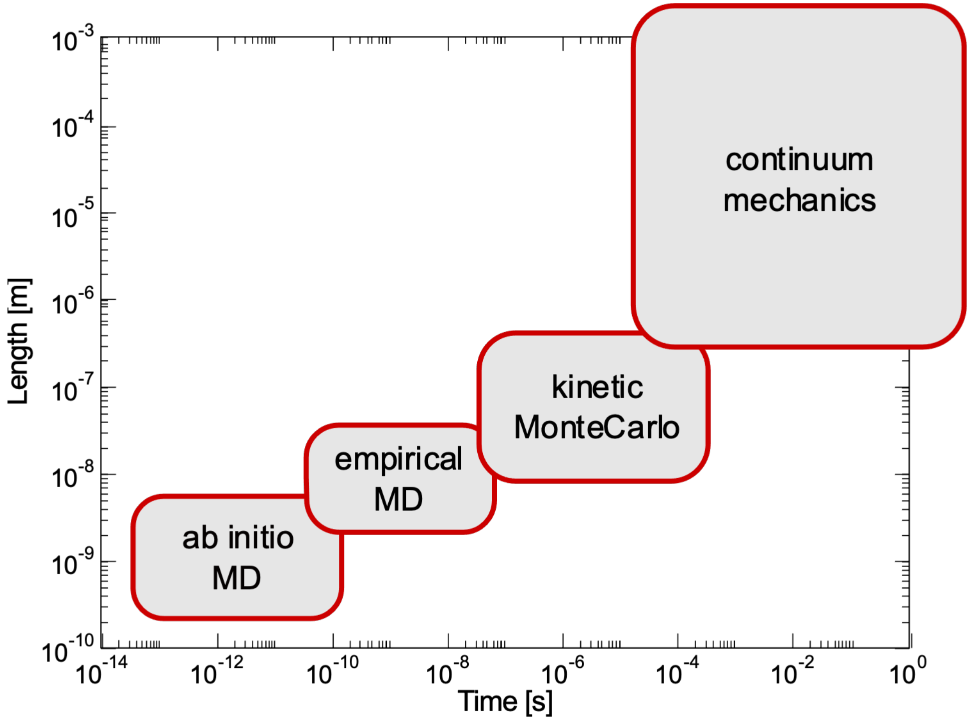
SPPARKS: Stochastic **P**arallel **PAR**ticle **K**inetic **S**imulator

Materials interact at the atomic scale, e.g. via mechanical, chemical, or electrical processes. However, response is often manifested and observed at the meso or continuum scales. Monte Carlo (MC) models are powerful computational tools for helping bridge these length and time scales.

- Stochastically evaluates and evolves ensembles of processes/events



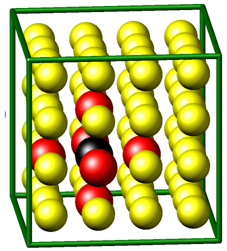
AM simulations

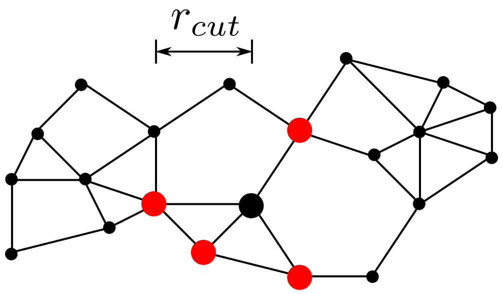


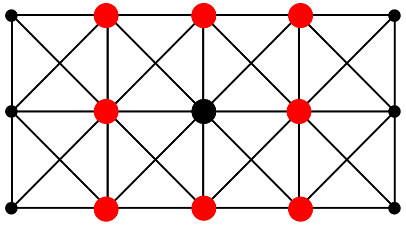
WHAT IS SPPARKS?

SPPARKS: Stochastic **P**arallel **PAR**ticle **K**inetic **S**imulator

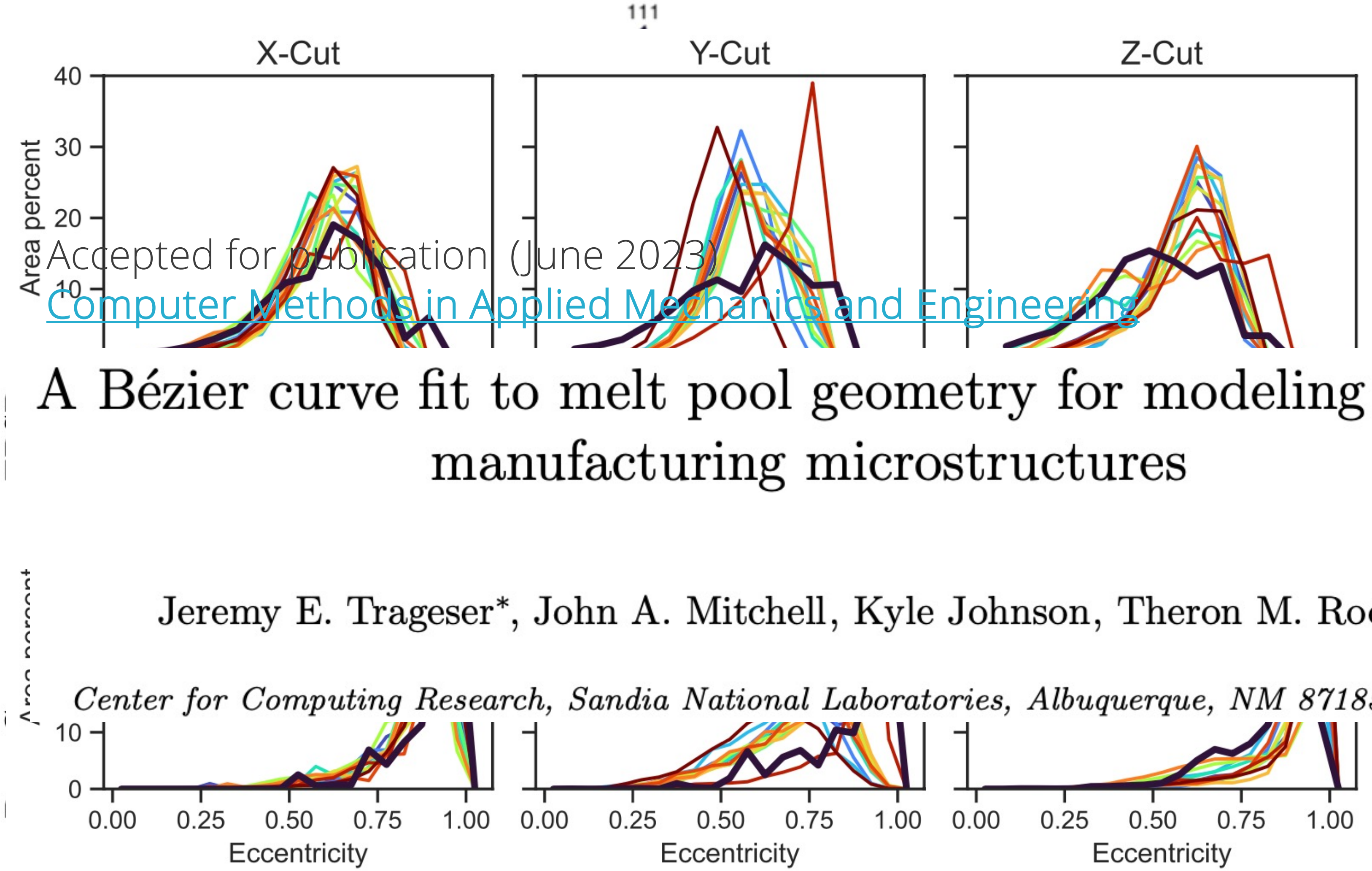
- spparks.github.io
- Parallel MC framework for simulating material processes
- Stochastically evaluates and evolves ensembles of processes/events
- C++, serial and parallel (using MPI)
- *2*- or *3D* simulations
- Extensibility to many material processes
- Suite of spatial lattices – lattice sites represent a ”glob” of material

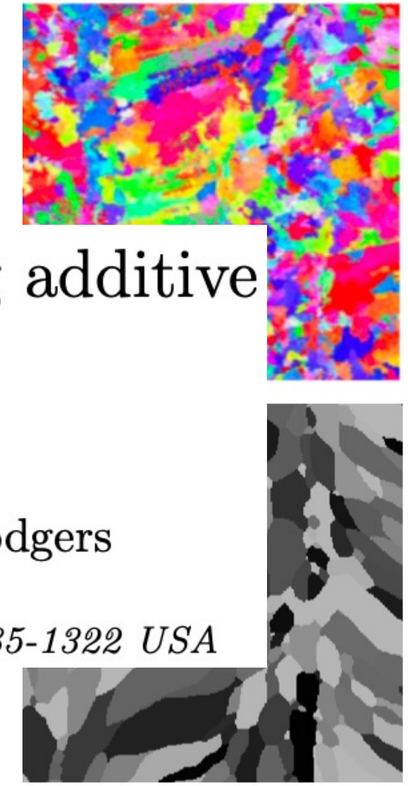






REFERENCE PAPERS





Accepted for publication (June 2023)
Computer Methods in Applied Mechanics and Engineering

A Bézier curve fit to melt pool geometry for modeling additive manufacturing microstructures

Jeremy E. Trageser*, John A. Mitchell, Kyle Johnson, Theron M. Rodgers

Center for Computing Research, Sandia National Laboratories, Albuquerque, NM 87185-1322 USA

Top row (EBSD) – color depicts grain orientations
Bottom row (SPPARKS) simulated morphologies

Thick black line (EBSD) data
Color lines are SPPARKS simulated

REPRESENTING MICROSTRUCTURES ON DISCRETIZATIONS USING TWO-POINT CORRELATIONS

Objectives

- Enable microstructure aware simulation for dynamic response of AM metallic materials
- Avoid vexing problem of meshing material details
- Provide a method for systematically representing grain morphologies at continuum scale
- Incorporate microstructure heterogeneity and AM material variability

REPRESENTING MICROSTRUCTURES ON DISCRETIZATIONS USING TWO-POINT CORRELATIONS

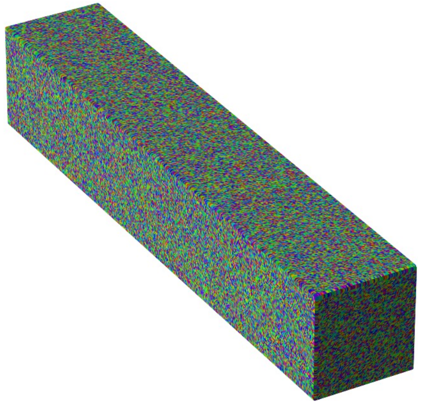
Approach

- Use SPPARKS to simulate AM microstructures for process
- Given FE discretization which be used for microstructure aware simulation
- Compute two-point spatial statistics at FE mesh element centroids
- Use spectral clustering to reconstruct microstructure on FE mesh

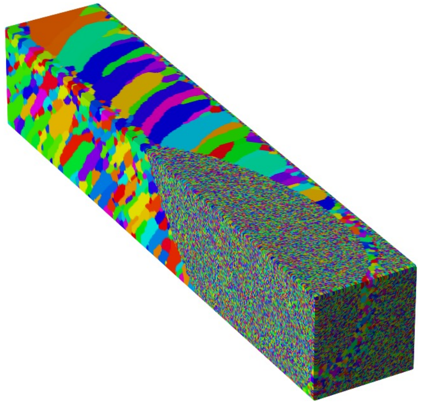
REPRESENTING MICROSTRUCTURES ON DISCRETIZATIONS USING TWO-POINT CORRELATIONS

Use SPPARKS to simulate AM microstructures for process

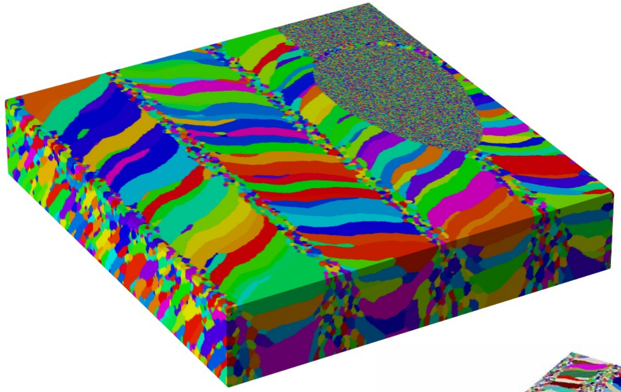
Initialize



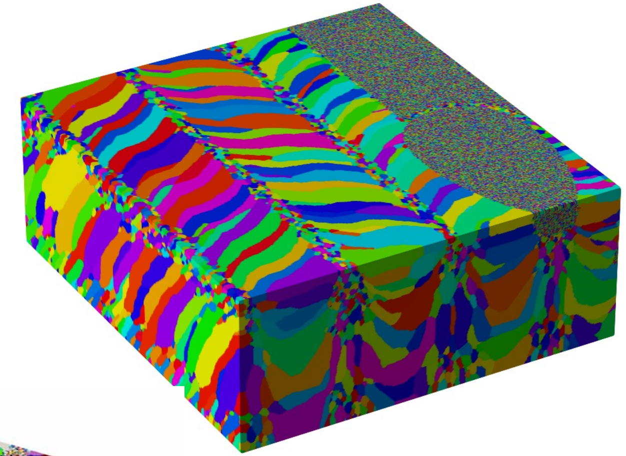
1st pass



1st layer



2nd layer

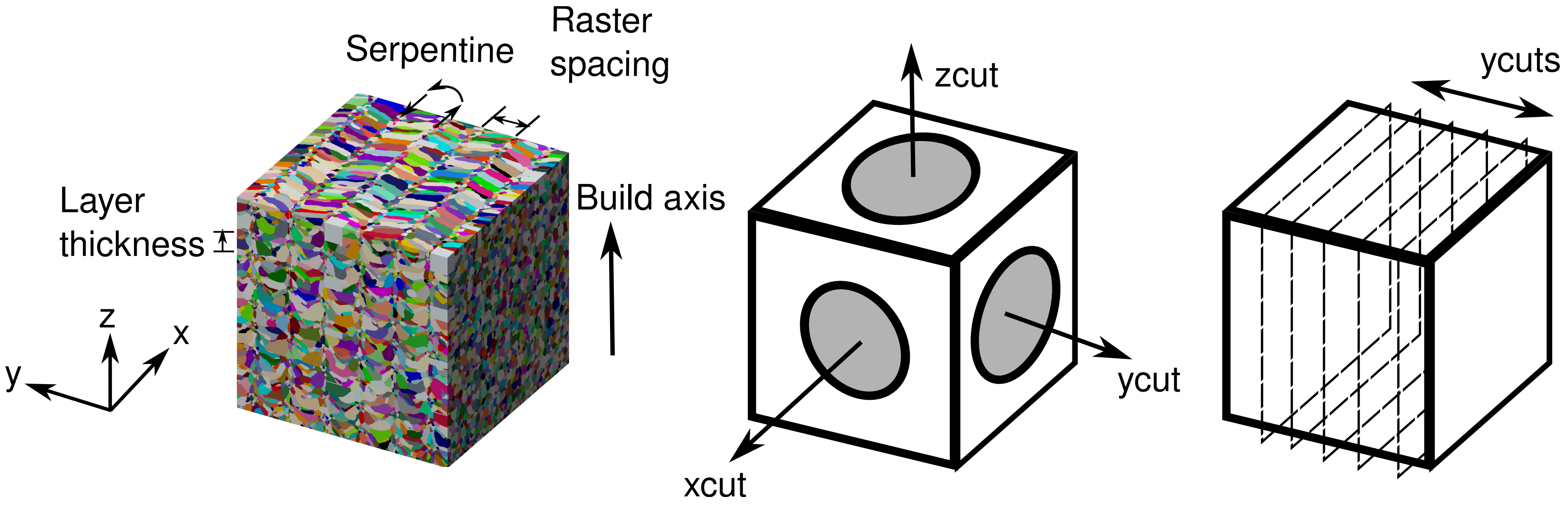


Simulate incrementally and use Stitch IO to combine (‘stitch’) domain together

REPRESENTING MICROSTRUCTURES ON DISCRETIZATIONS USING TWO-POINT CORRELATIONS

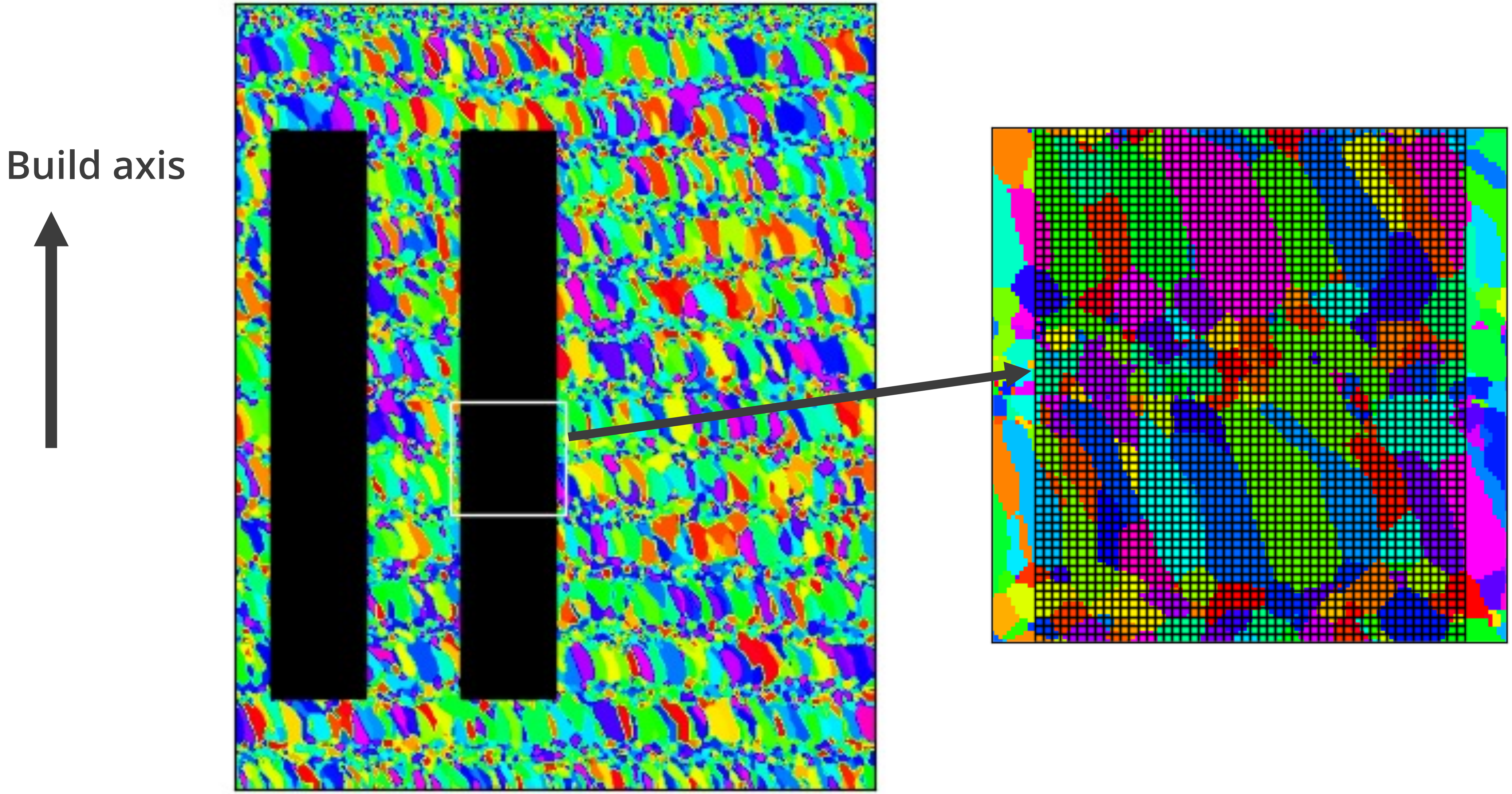
Compute two-point spatial statistics at FE mesh element centroids

Take 2d slices



Collecting data

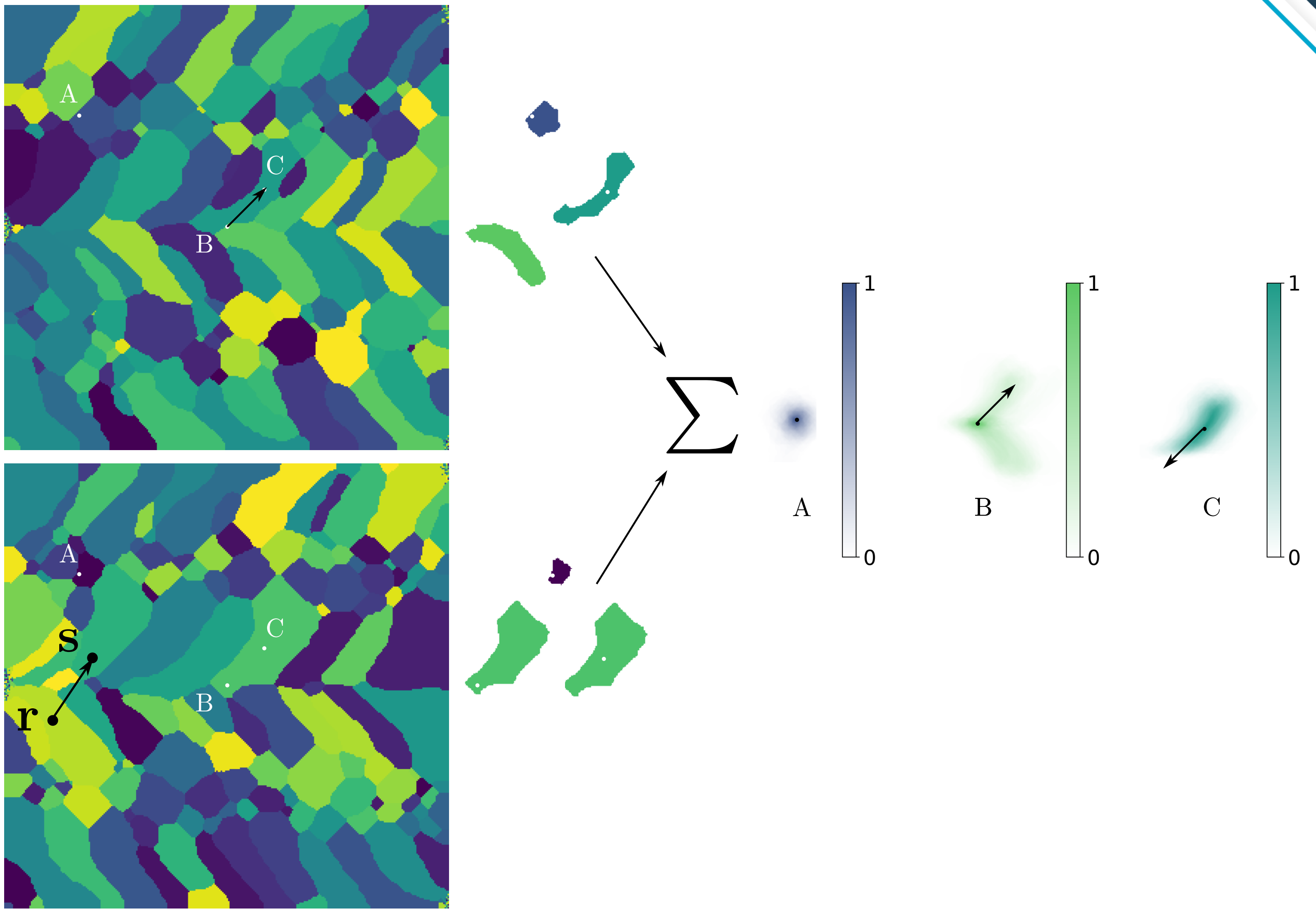
YCUT – each 2D FE overlays provide data set



REPRESENTING MICROSTRUCTURES ON DISCRETIZATIONS USING TWO-POINT CORRELATIONS

Compute two-point spatial statistics

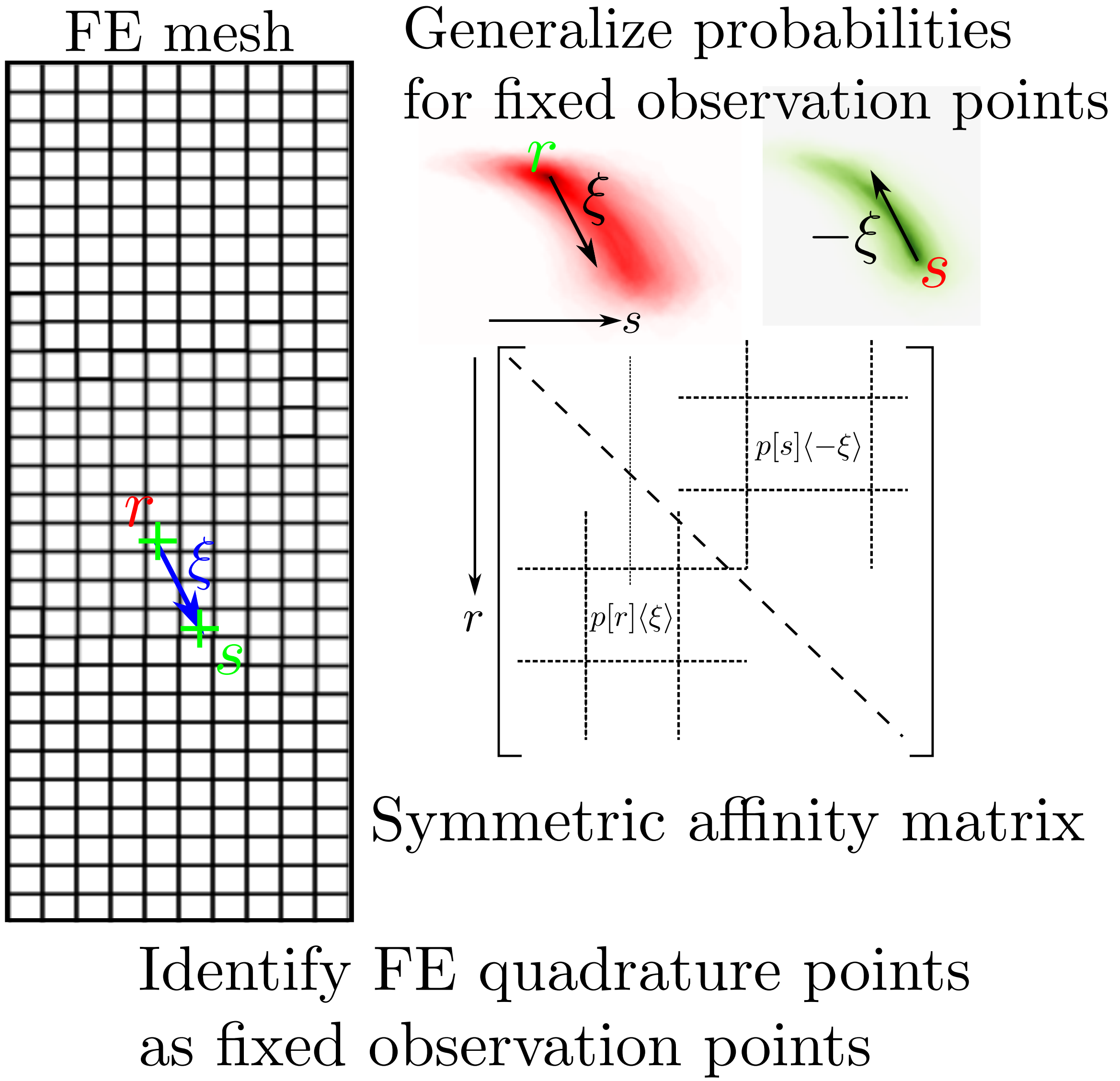
- **Fixed points**
- **FE centroids**
- **Average probabilities**



REPRESENTING MICROSTRUCTURES ON DISCRETIZATIONS USING TWO-POINT CORRELATIONS

Compute two-point spatial statistics

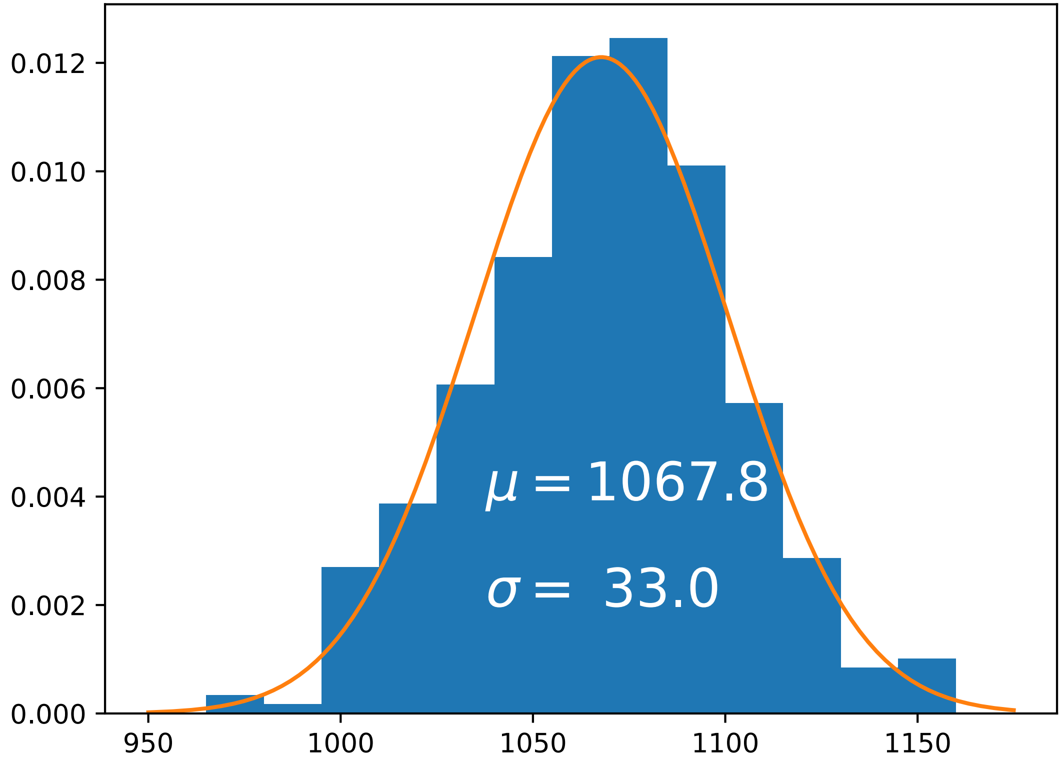
- Fixed points
- FE centroids
- Average probabilities



REPRESENTING MICROSTRUCTURES ON DISCRETIZATIONS USING TWO-POINT CORRELATIONS

Spectral clustering via Scikit-Learn

- **Reconstruct representation microstructure on FE mesh**
  - **Represents build and process variability**
  - **Average representation**
  - **Input n**

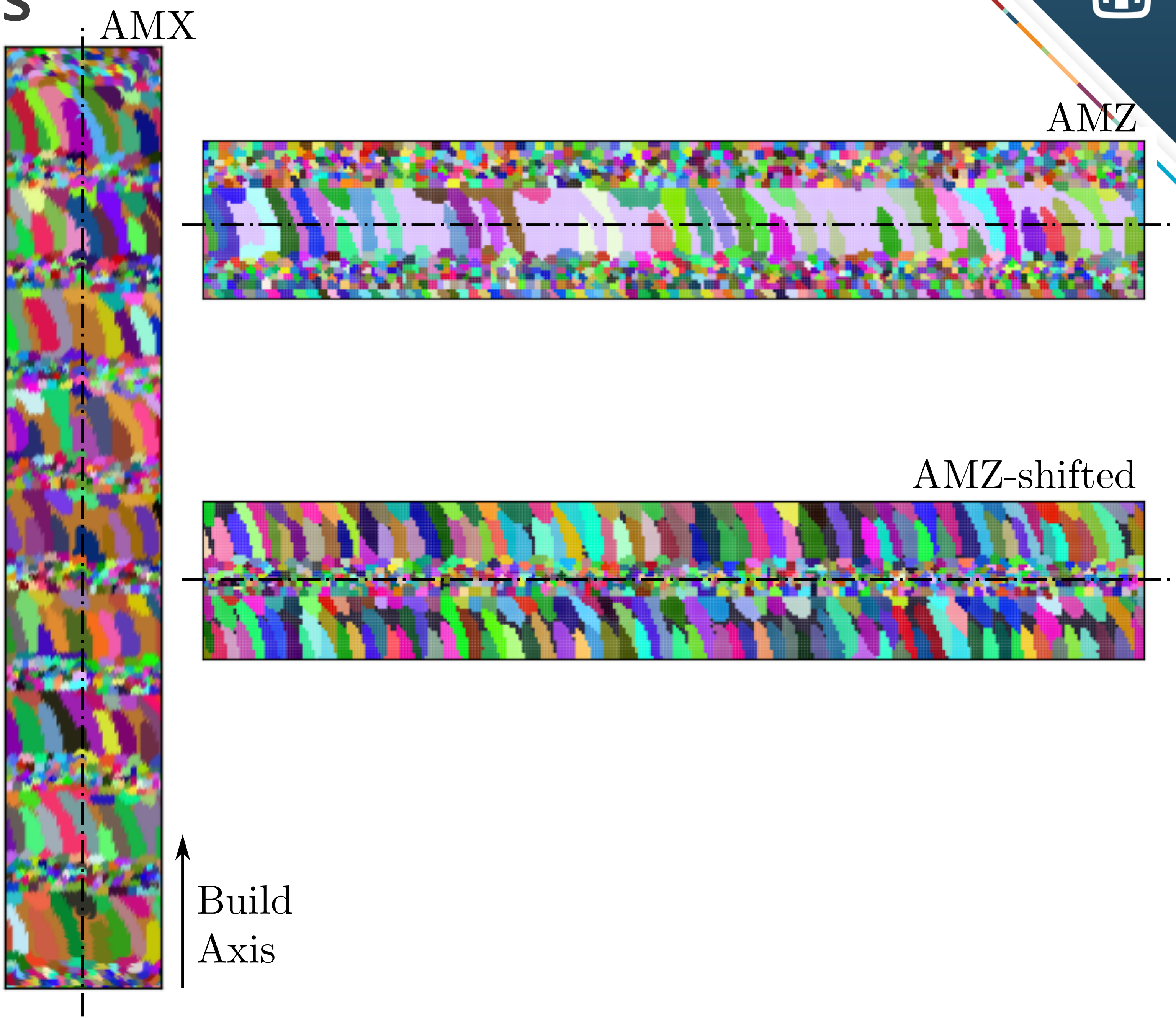


Number of unique grains ids associated with observation points for each sample forms a distribution across all data sets

Discretization examples

Spectral clustering methods

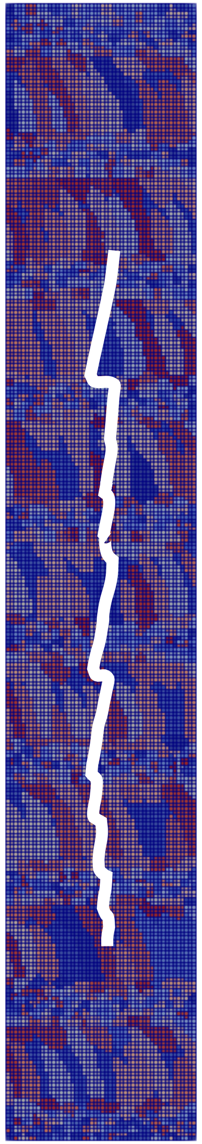
- "kmeans"
- "discretize"



Discretization examples -- spall cases

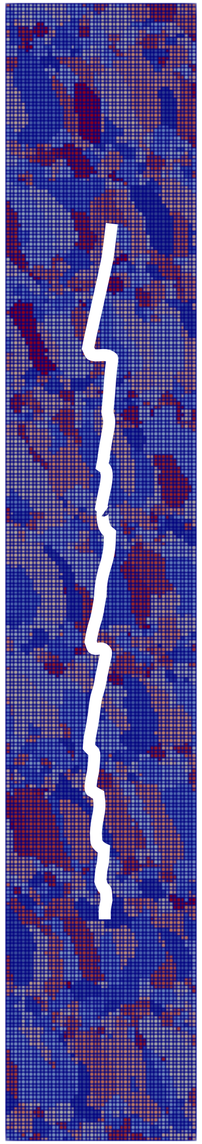
Build axis

kmeans



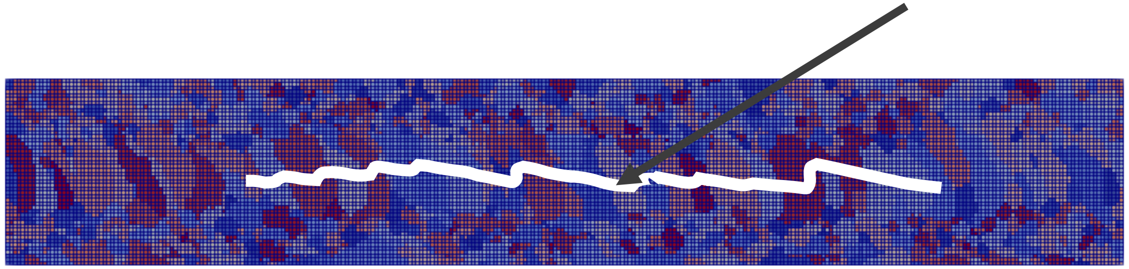
XCUT

imprint

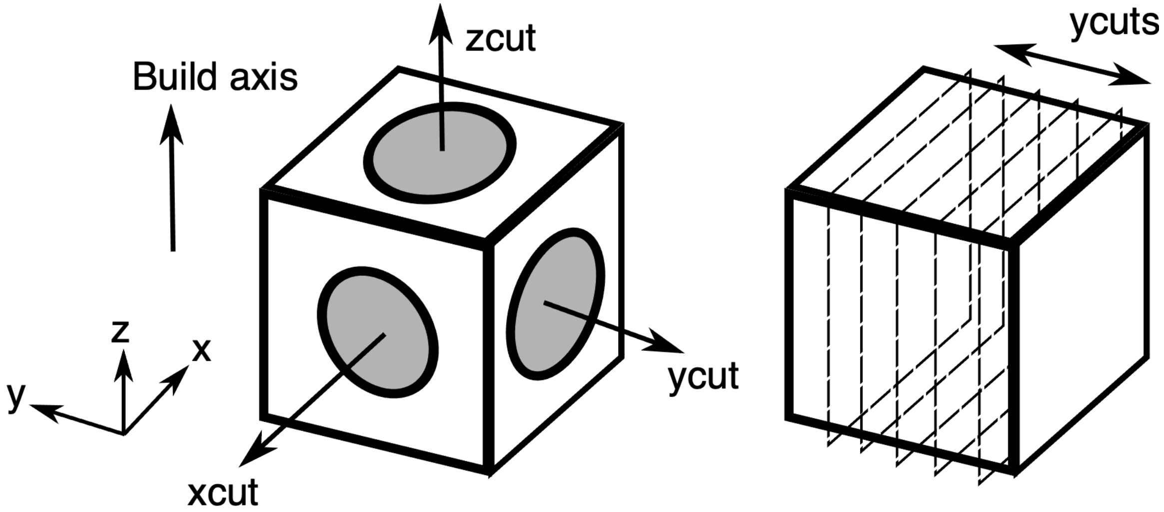


imprint

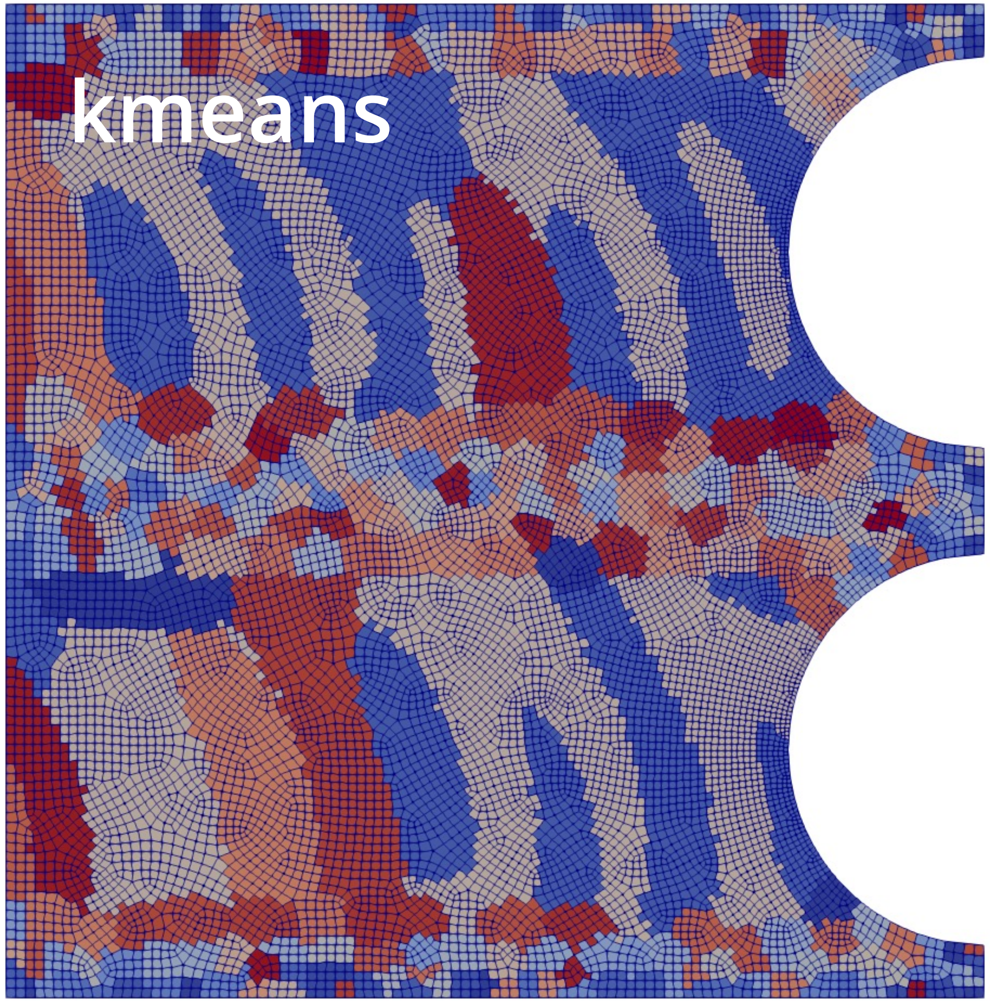
spall plane

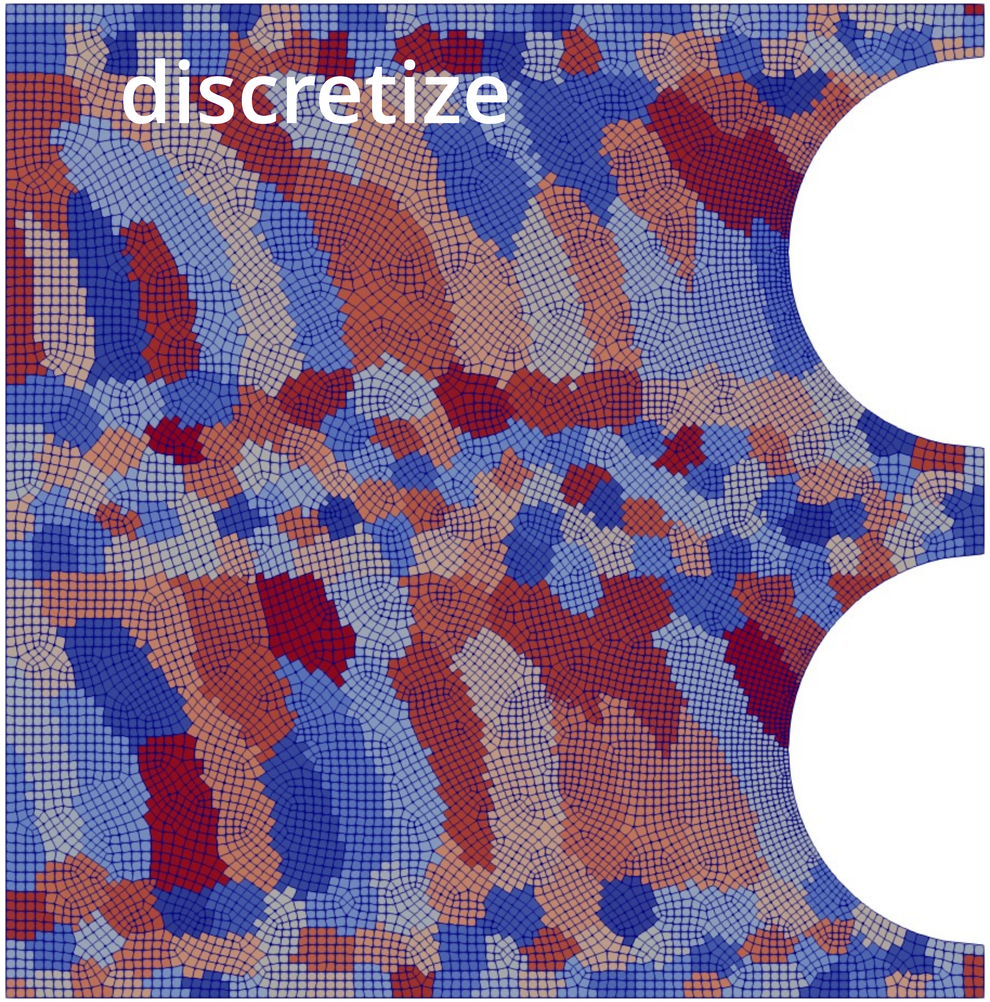


ZCUT

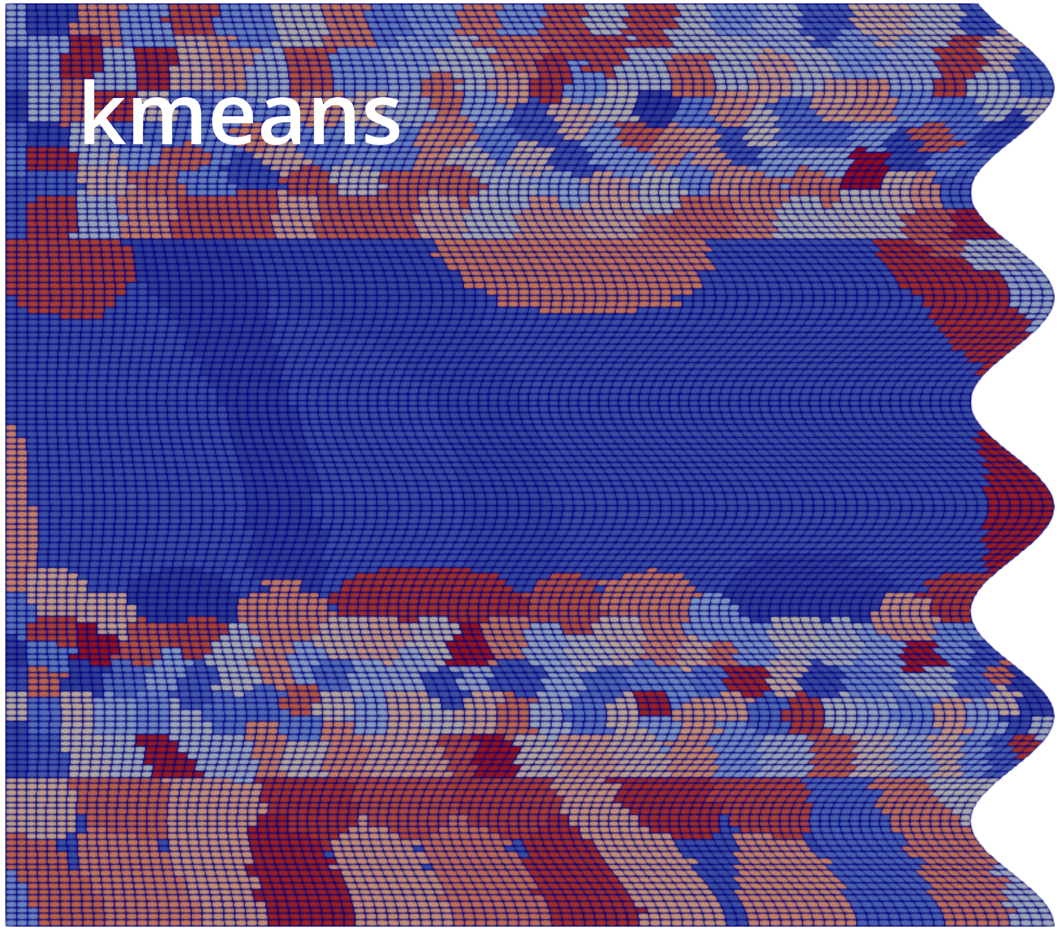


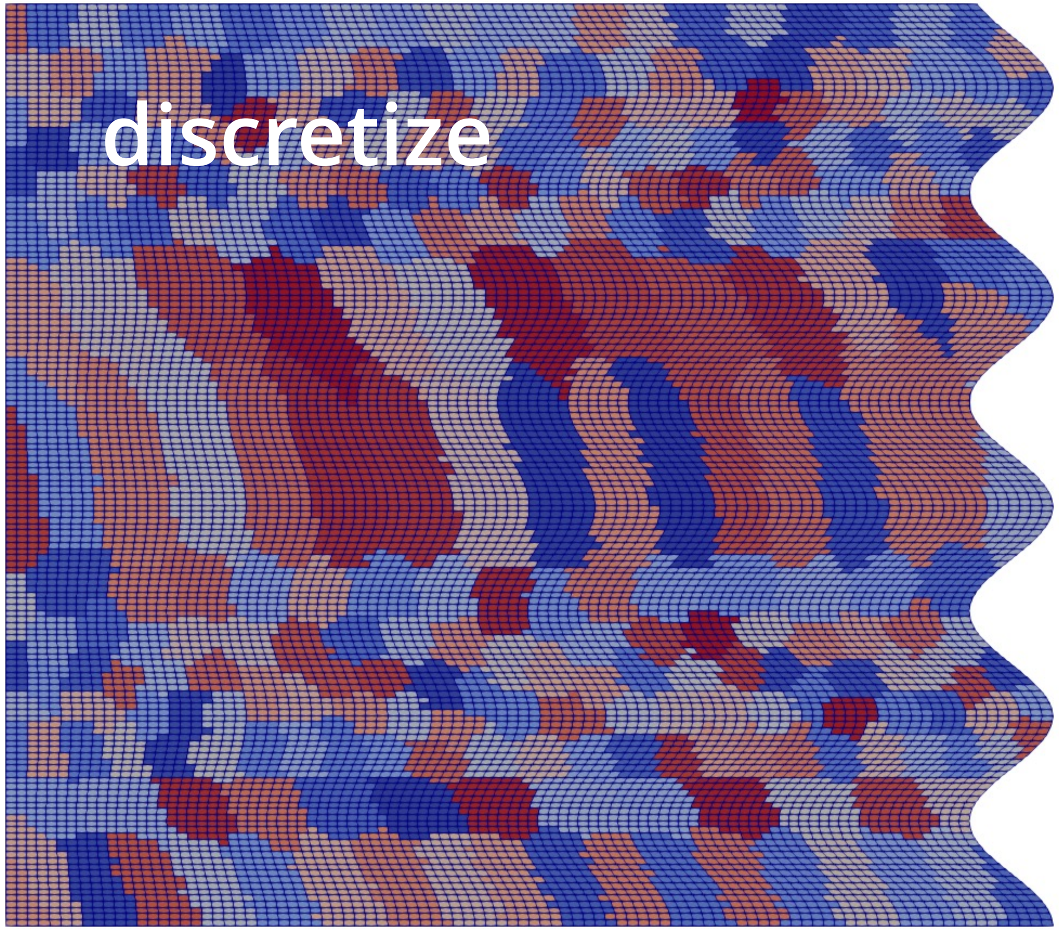
Discretization examples



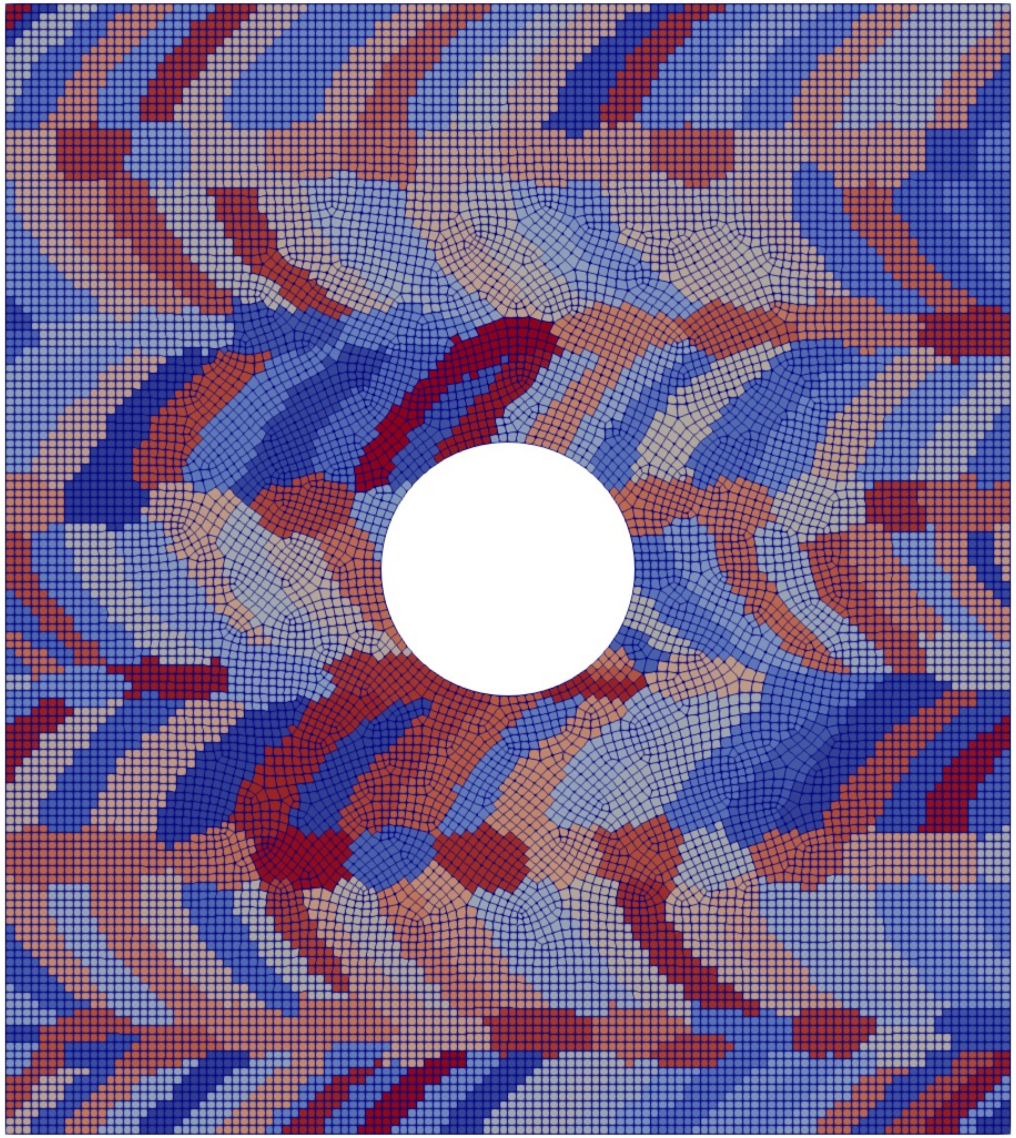


Discretization examples





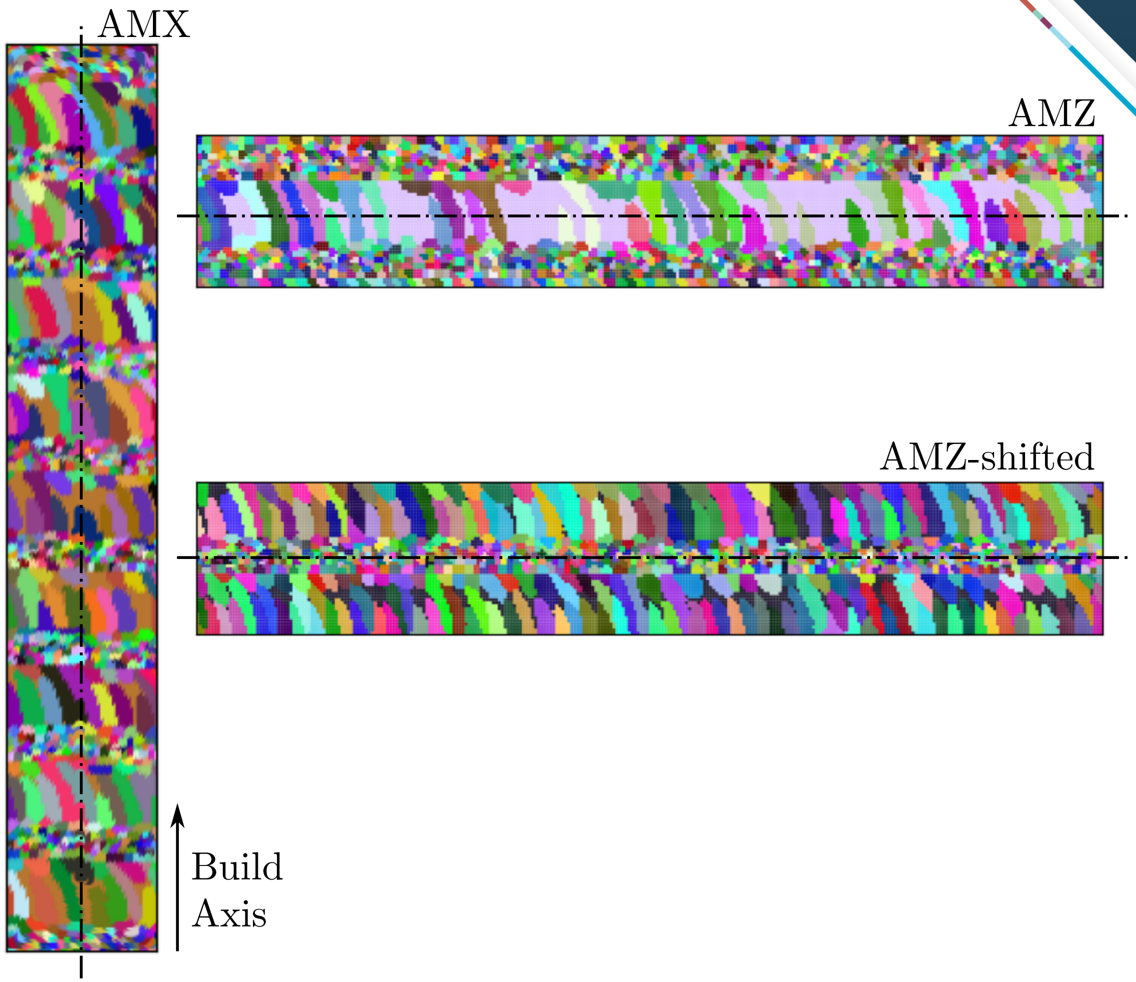
Discretization examples



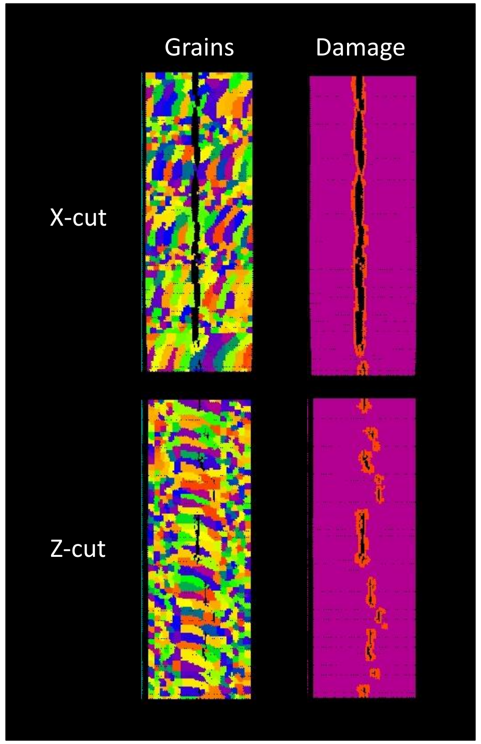
- Grains are like element blocks – collection of elements
- Each grain gets properties from a distribution

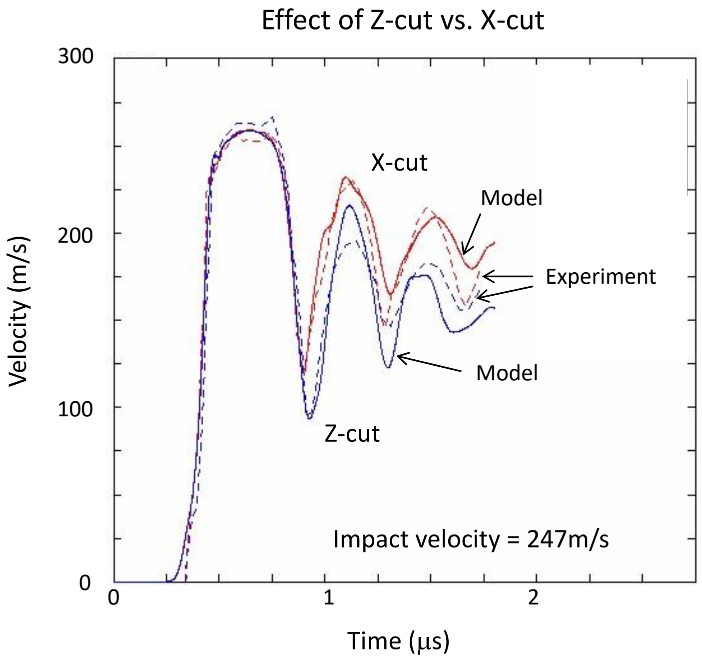
Spall kinetics (SK) model, simulations and testing (briefly)

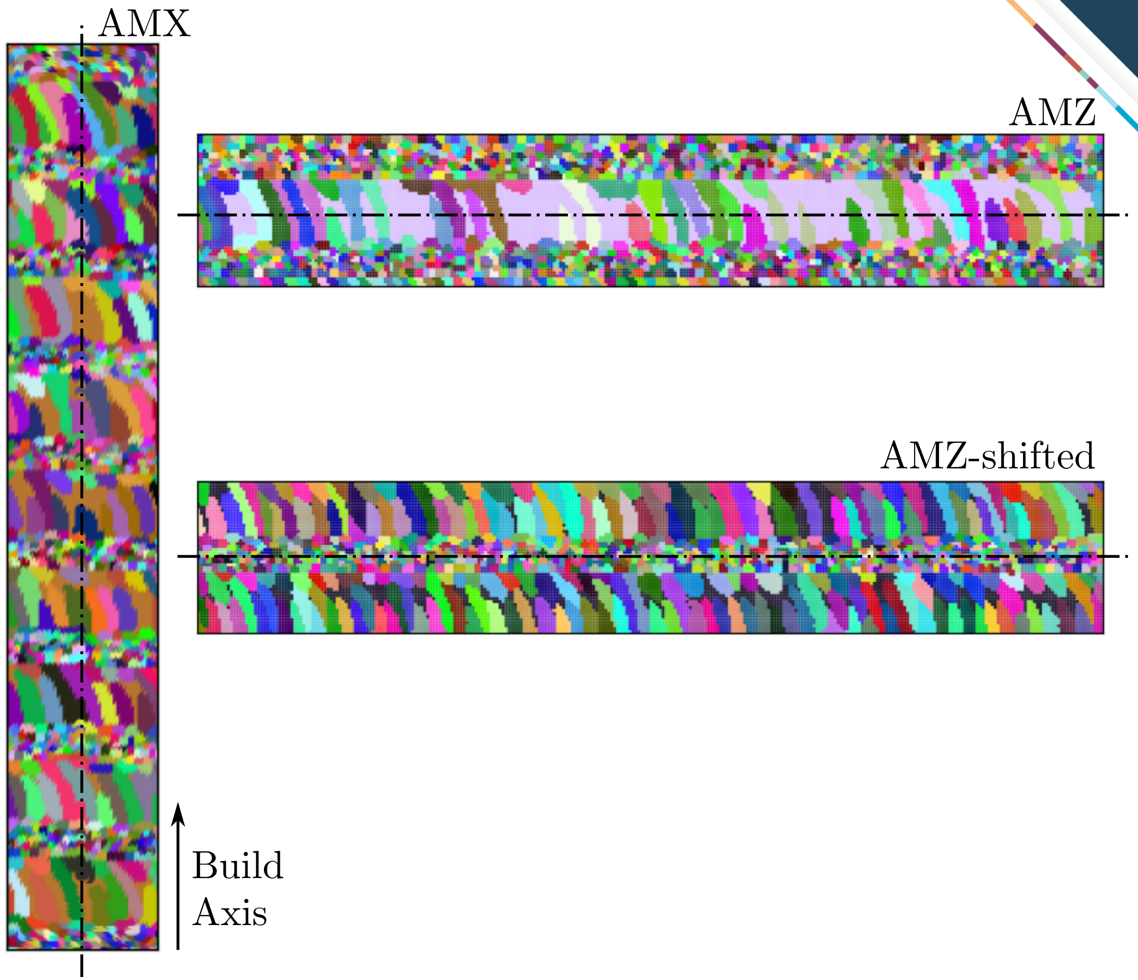
- **Isotropic elastic and plasticity parameters**
- **Elastic wave speed randomly assigned by grain**
- **SK Model**
  - Adjusts pressure from eos
    - Softens pressure leading up to spall
    - Slowly reduces pressure after spall
- **Spall response sensitive to SK model parameters**
  - Failure pressure at high loading rates
  - Grain size
  - Damage onset parameter
- **Spall response relatively insensitive to**
  - Plasticity model parameters
- **Microstructure effects decrease with increasing impact velocity**



Spall simulations and testing [1,2] (briefly)







1. *Wise, etal., (2017) Comparative shock response of additively manufactured versus conventionally wrought 304L stainless steel., In: AIP Conference Proceedings, AIP Publishing, vol 1793 .*
2. *Specht PE, etal. Shortening the design and certification cycle for additively manufactured materials by improved mesoscale simulations and validation experiments: Fiscal year 2019 status report. Tech. Rep. SAND2019-12275, Sandia National Laboratories, Albuquerque, NM*

Future and Ongoing Work

- Strength modeling: texture, anisotropy
- mpi c/c++ implementation for spatial statistics calculations
- SPPARKS modeling of AM microstructures
  - HAZ modeling
  - Grain growth competition and sensitivity to temperature gradient
  - Multiphase materials
  - EBSD and texture mapping to spparks microstructures