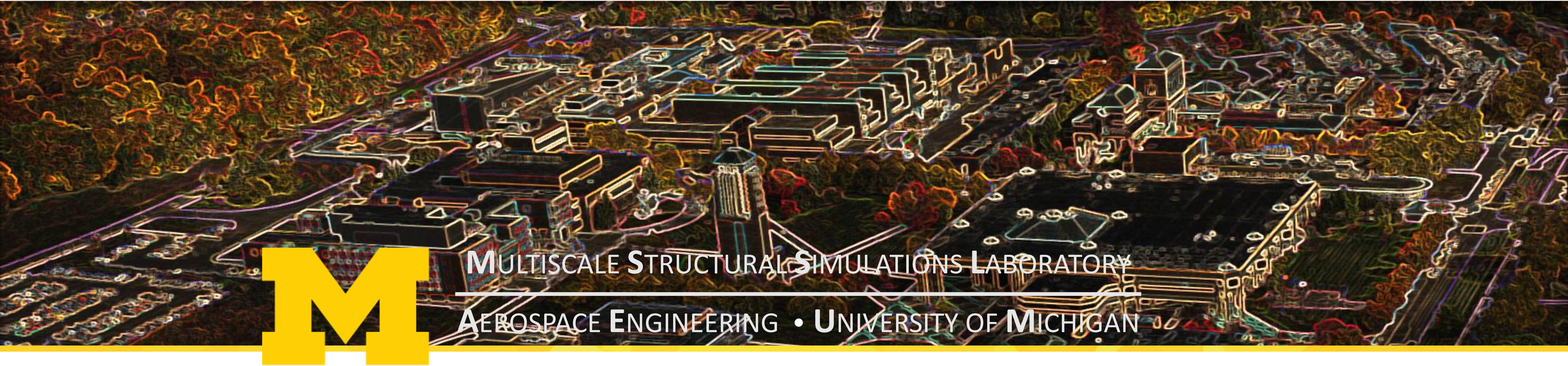

Generation of 3D Microstructures From 2D Surface Images Using Markov Random Fields

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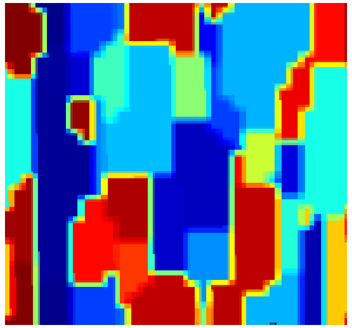
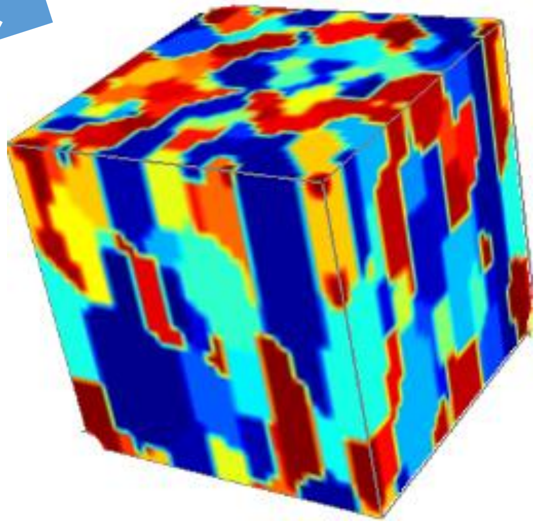
Overview

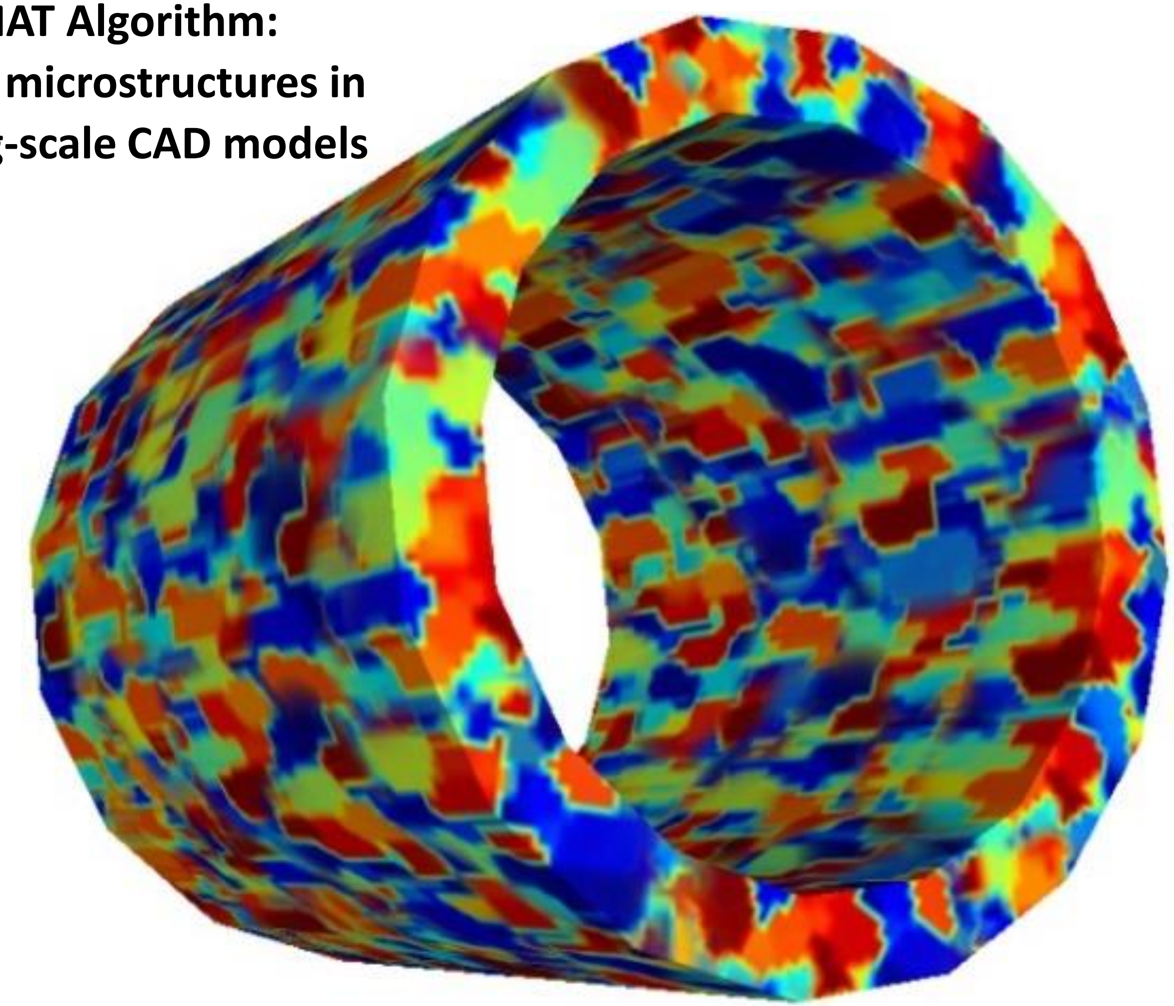
2D Micrograph



Markov Random Field Algorithm:
3D reconstruction from
orthogonal surface images



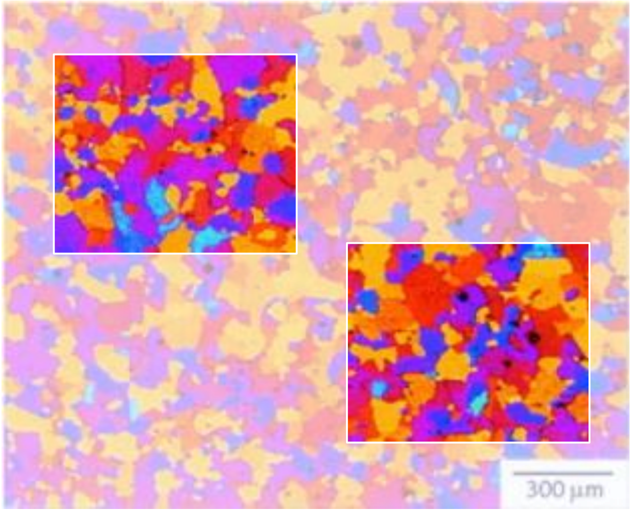
LEGOMAT Algorithm:
embedding microstructures in
engineering-scale CAD models

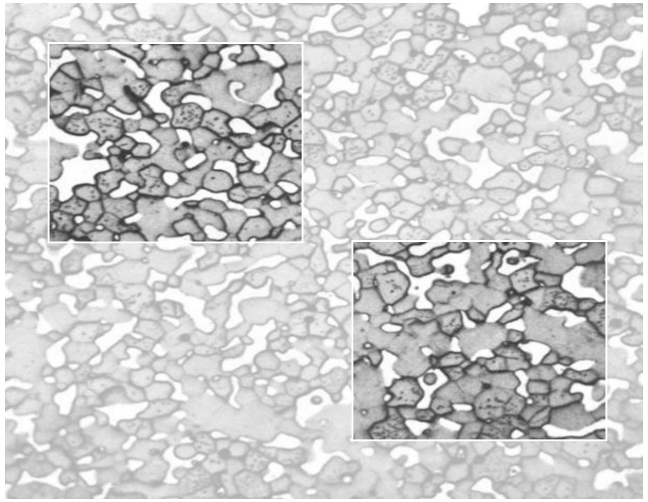


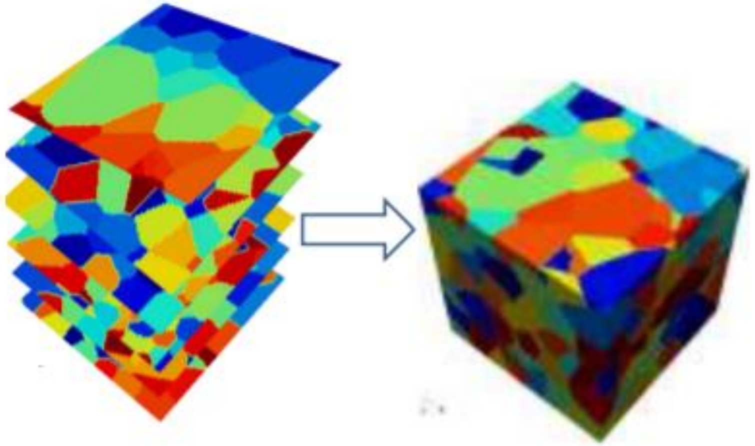
LEGOMAT: Locally-Extracted Globally-Organized Markovian Material Models

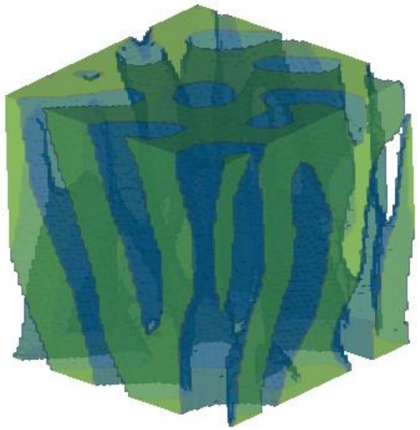
Background

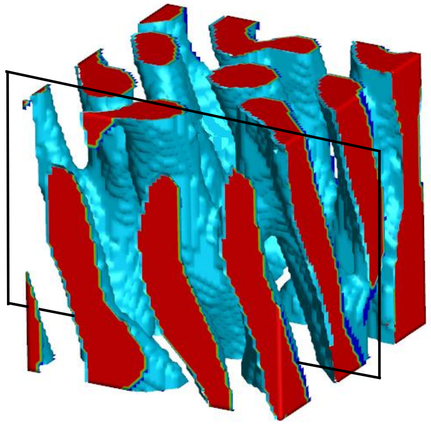
- Explore the notion of **stationary probability distribution** i.e. *Markov Random Fields (MRF)*:
  - Different windows on a 2D microstructure ‘look-alike’
  - Different sections on a 3D microstructure ‘look-alike’
- Reconstruction of 3D synthetic microstructural models from orthogonal 2D images taken along x-, y-, and z- directions
- *Applications*:
  - Generation of large-scale models with full-field microstructural features
  - Analysis of Process-Structure-Property relationships







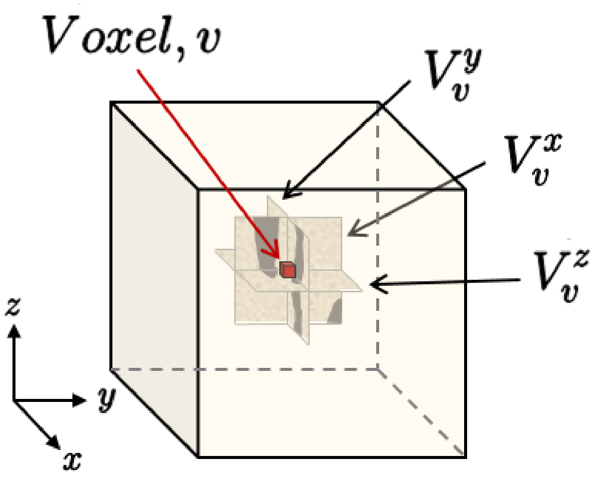




3D Reconstruction Formulation

- The 3D microstructure is to be synthesized by solving an L_2 minimization of the cost function:
  - Where $\boldsymbol{\omega}^{i}_{\boldsymbol{v},\boldsymbol{u}}$, $\boldsymbol{V}^{i}_{\boldsymbol{v},\boldsymbol{u}}$, and $\boldsymbol{S}^{i}_{\boldsymbol{v},\boldsymbol{u}}$ denote the weight, color of voxel u in the neighborhood of $\boldsymbol{V}^{i}_{\boldsymbol{v}}$, and color of pixel u in the neighborhood of $\boldsymbol{S}^{i}_{\boldsymbol{v}}$, respectively

$$E(\boldsymbol{V}) = \sum_{i\in\{x,y,z\}} \sum_{v} \sum_{u} \omega^{i}_{v,u} \| \boldsymbol{V}^{i}_{v,u} - \boldsymbol{S}^{i}_{v,u} \|^2$$

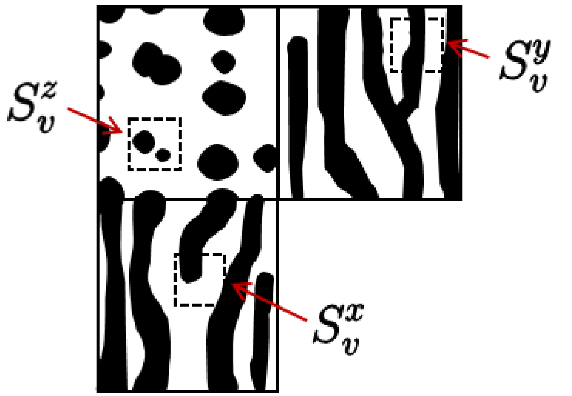


- Each iteration for the optimization problem is carried out in two steps:
  - *<u>Minimization Step</u>:* Minimize the *cost function* w.r.t. the set of input neighborhoods, $\boldsymbol{S}_{\boldsymbol{v}}$. Here, the **best-matching neighborhood** of voxel v, say along x-plane, is selected by solving the following:

$$\boldsymbol{S}^{x}_{v} = \arg \min_{\boldsymbol{S}^{x,w}} \sum_{u} \omega^{x}_{v,u} \| \boldsymbol{V}^{x}_{v,u} - \boldsymbol{S}^{x,w}_{u} \|^2$$

  - *<u>Expectation Step</u>*: Minimize the *cost function* w.r.t. $\boldsymbol{V}_{\boldsymbol{v}}$. In this step a **unique value** for the voxel v is found:

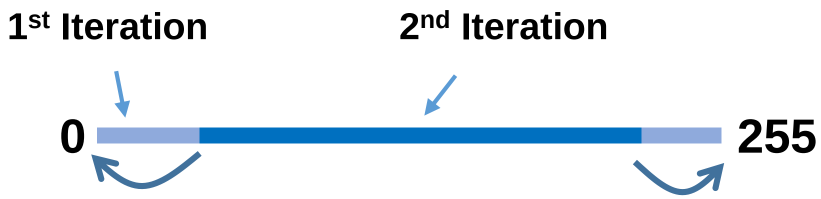
$$\boldsymbol{V}_{v} = \Big(\sum_{i\in\{x,y,z\}} \sum_{u} \omega^{i}_{u,v} \boldsymbol{S}^{i}_{u,v} \Big) \Big/ \Big(\sum_{i\in\{x,y,z\}} \sum_{u} \omega^{i}_{u,v} \Big)$$



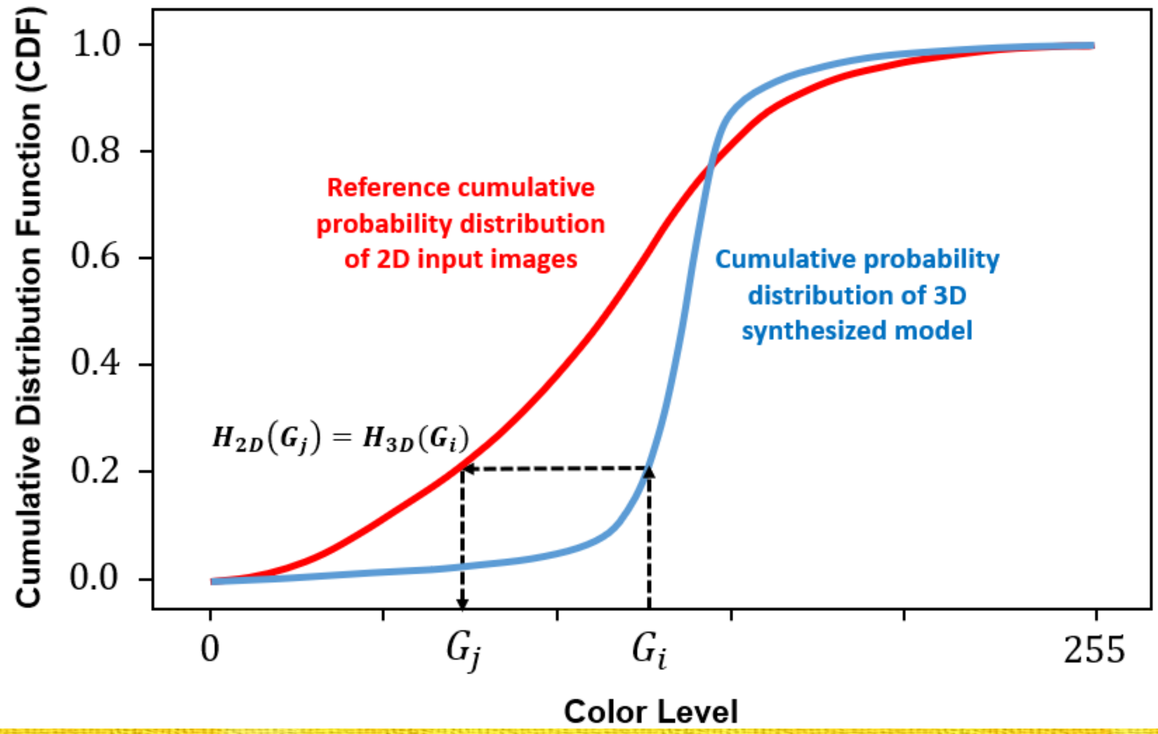
Javaheri et al., *Computer-Aided Design*, 120 (2020)

Histogram Matching

- The averaging tends to shrink the Red-Green-Blue (RGB) color levels. To solve this issue, **histogram matching** is performed after every iteration such that color levels are stretched back properly



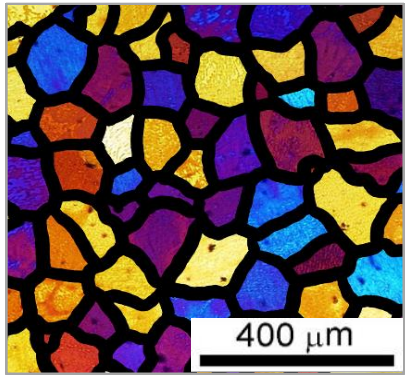
- Histogram matching modifies the MRF algorithm's color density such that its overall **cumulative distribution function (CDF)** matches with the input images
- This process is applied after every iteration for each color channel (RGB) separately



Histogram Matching

- The reference 2D micrograph shows an Al-Mg-Fe-Si alloy containing less than 1 wt. % of each solute that was obtained through cross-polarized light microscopy

Courtesy of Univ. of Cambridge



Reference Image

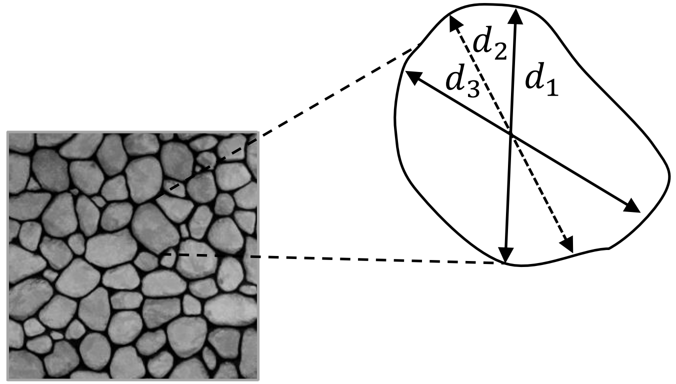
Al-Mg-Fe-Si alloy (cross-polarized light microscopy)

Without histogram matching, the color space shrinks, phase information is lost

With histogram matching, the color space remains consistent with input image

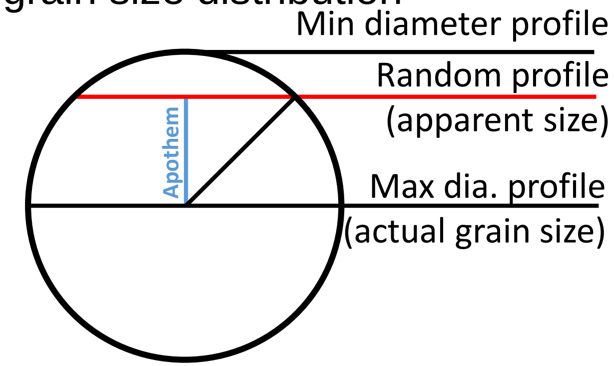
Grain Size Distribution

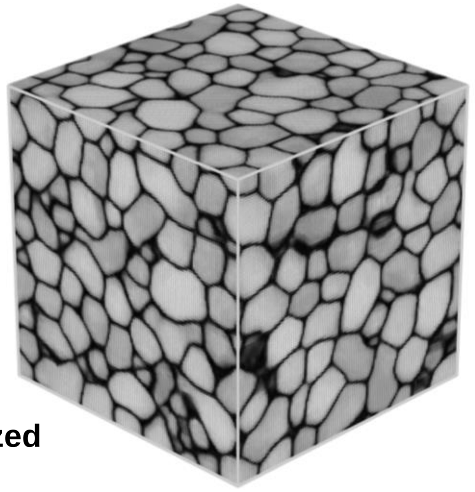
- Saltykov method was used for estimation of 3D grain size distribution from 2D sectional images:
  - Where R is the 3D grain size, r_1 and r_2 are lower and upper limits of the subinterval for 2D grain size, P is the probability to cut the section within the defined interval, Δ is the bin size, and $F(R)$ is 3D grain size distribution



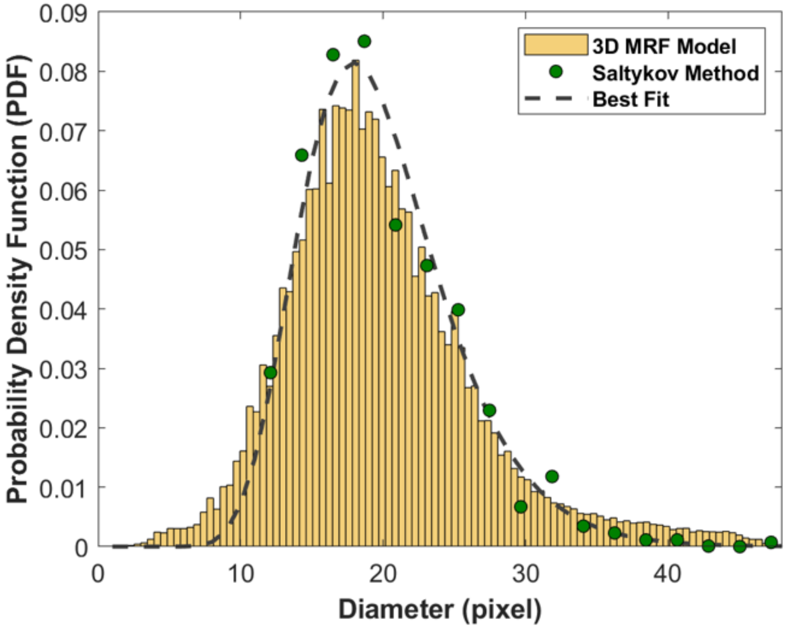
Experimental

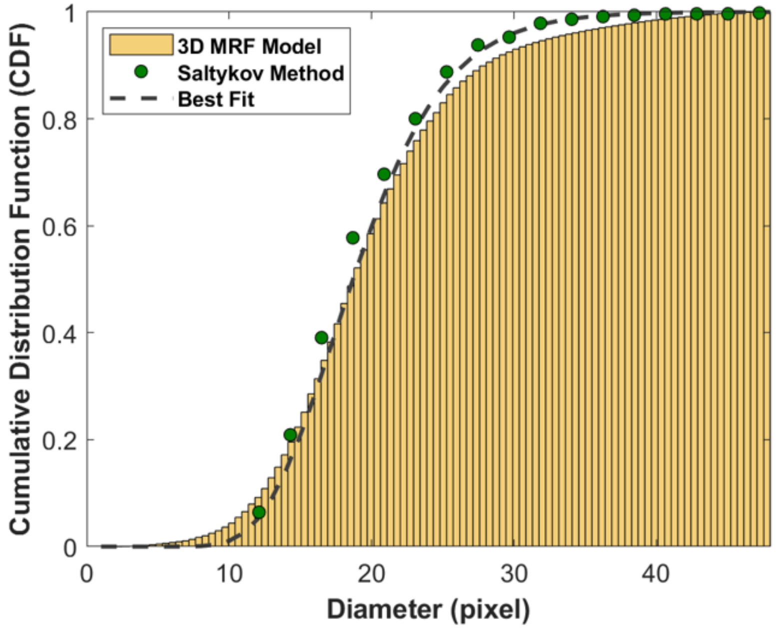
$$P(r_1 < r < r_2) = 2\Delta \sum_{i=1}^{n} \left(\sqrt{R_i^2 - r_1^2} - \sqrt{R_i^2 - r_2^2} \right) F(R_i)$$





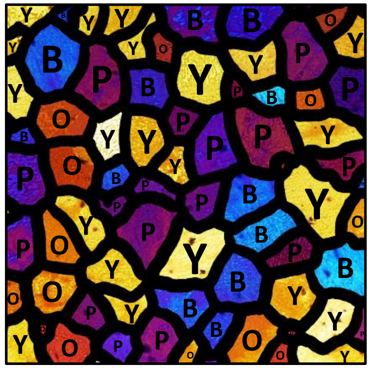
MRF Synthesized



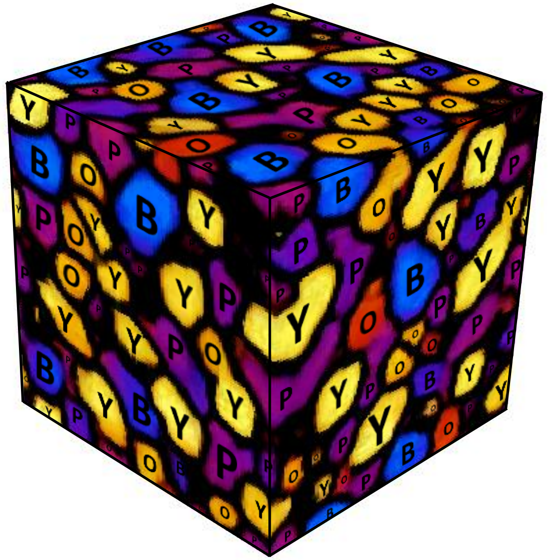


Javaheri et al., *Computer-Aided Design*, 120 (2020)

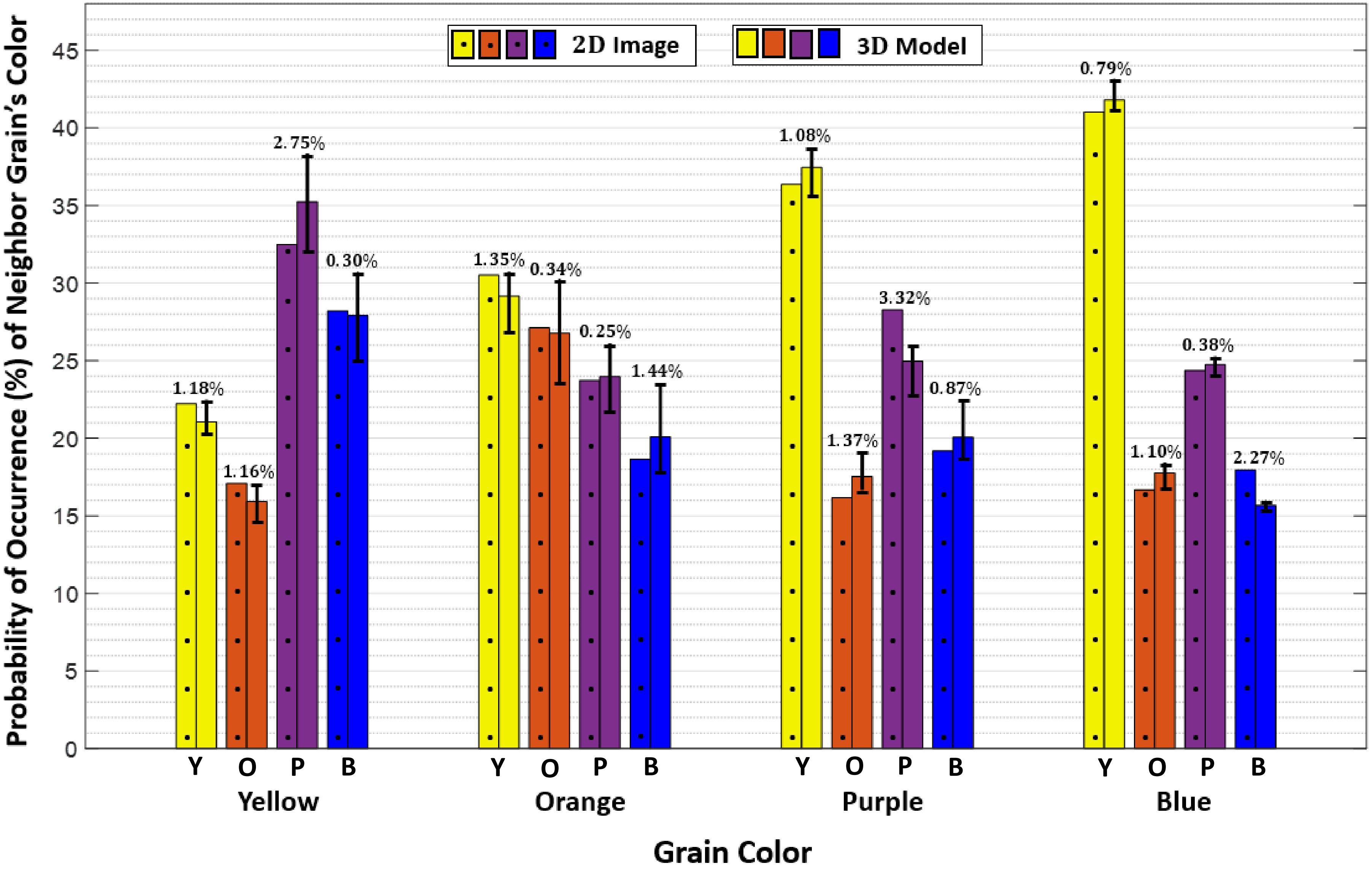
Nearest Neighbor Correlation



2D Image

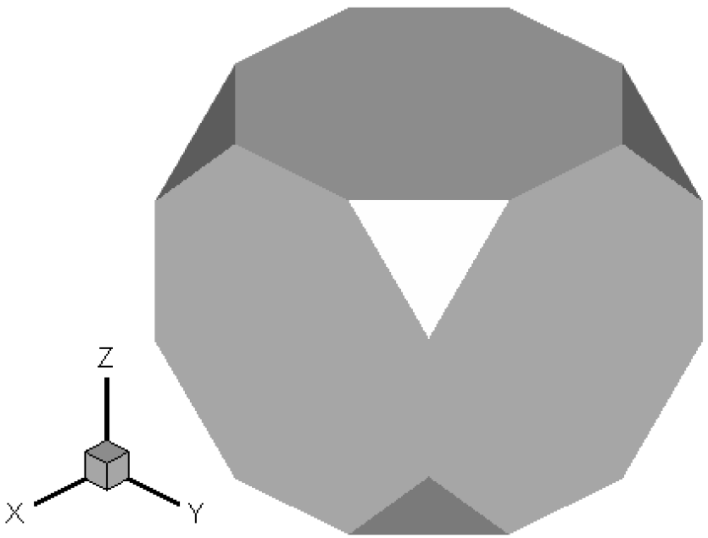


MRF Reconstruction

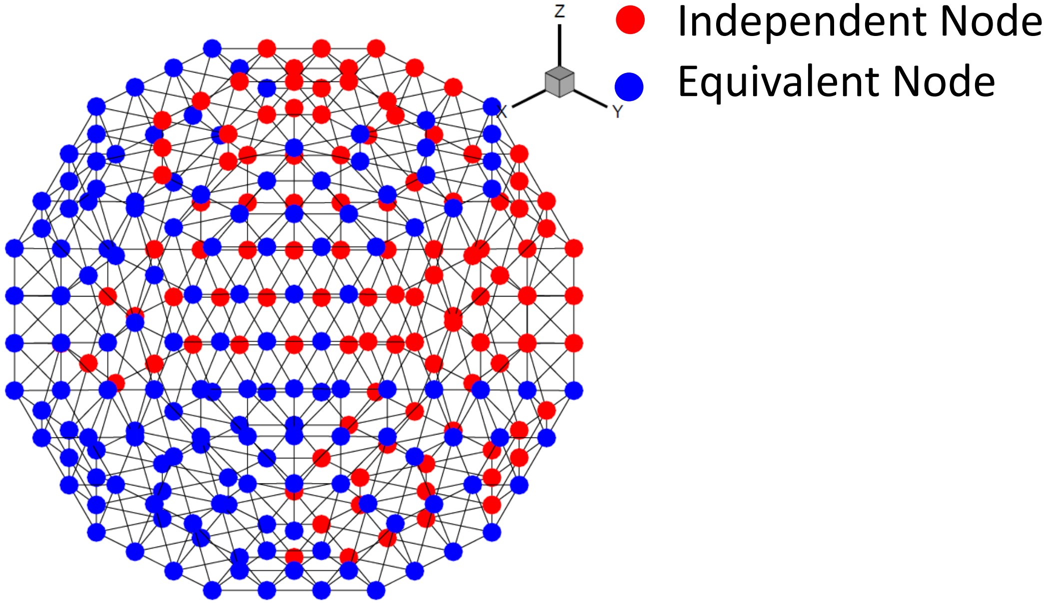


Modeling Crystal Orientation

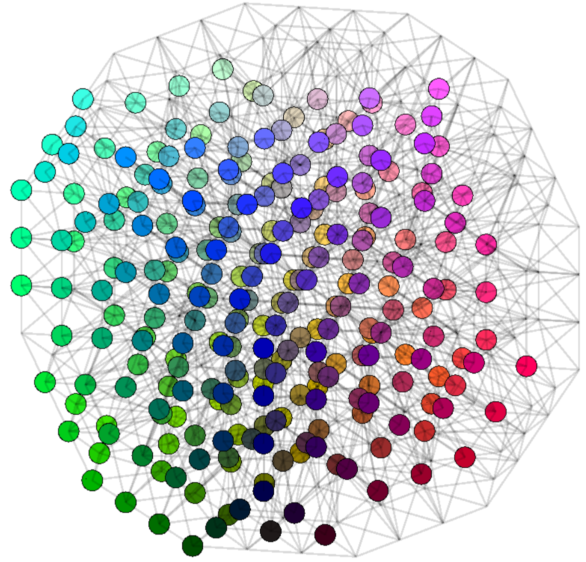
- Orientations are colored according to the **nearest nodes** in the orientation space (Rodrigues space)
- Nearest node may not be independent, so a symmetry map is performed
- Number of colors in an Electron Backscatter Diffraction (EBSD) image controlled by the discretization of the fundamental region



FCC fundamental Rodrigues space

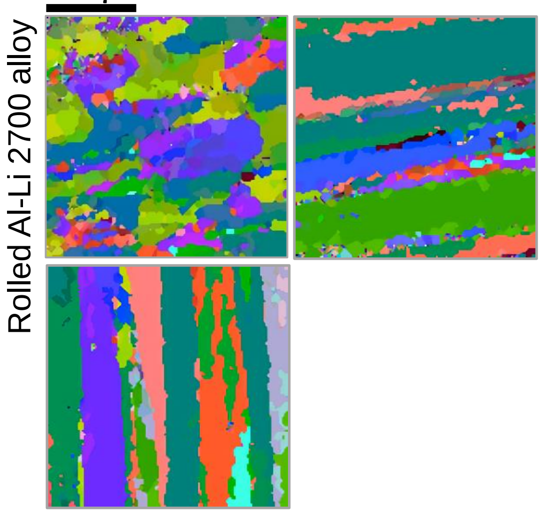


399 nodes, 254 independent nodes

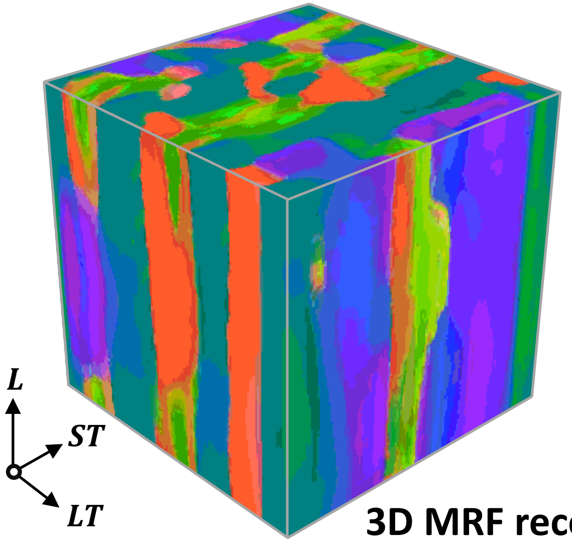


A colormap based on distances in fundamental region

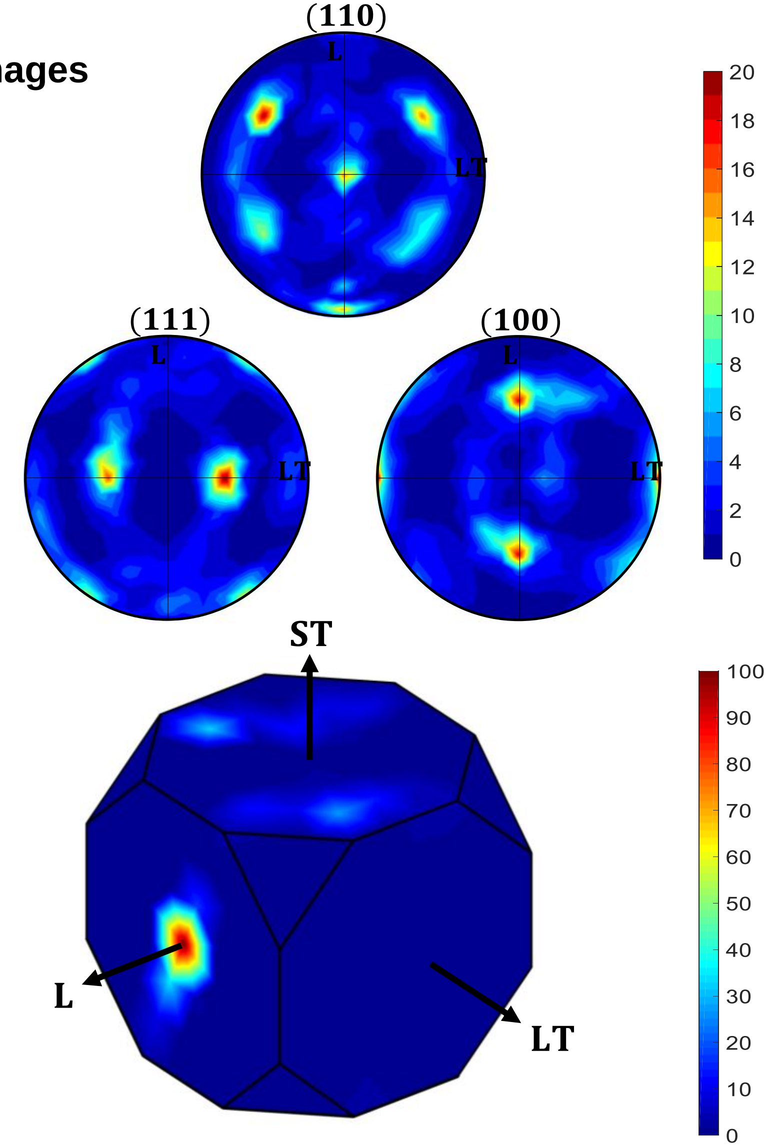
Orientation Distribution

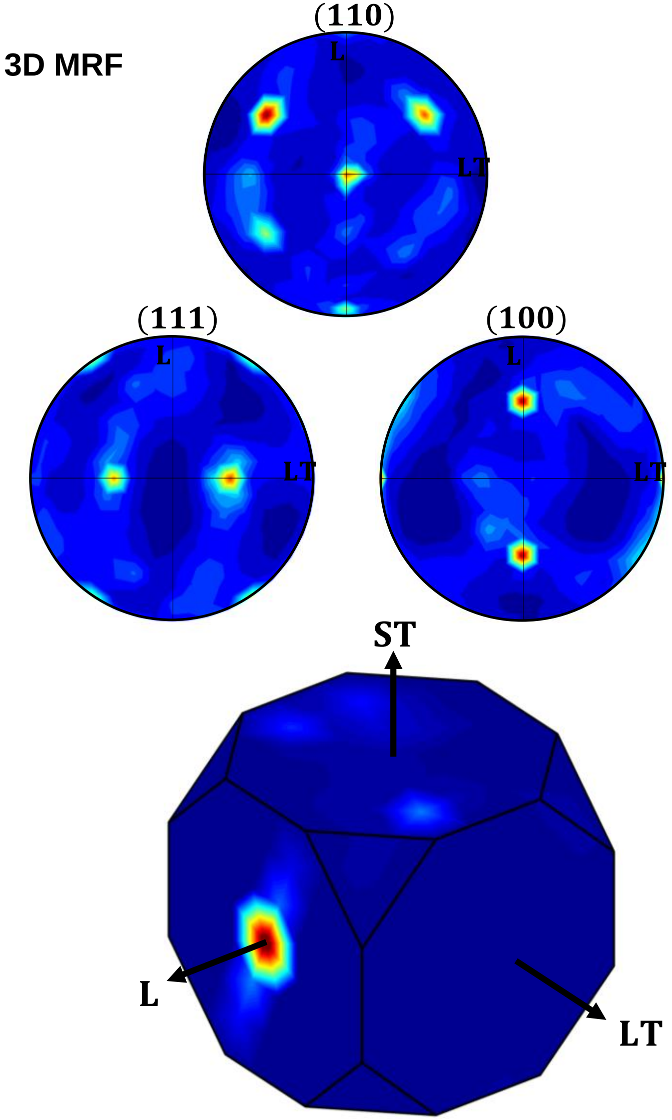


2D planar images



3D MRF reconstruction

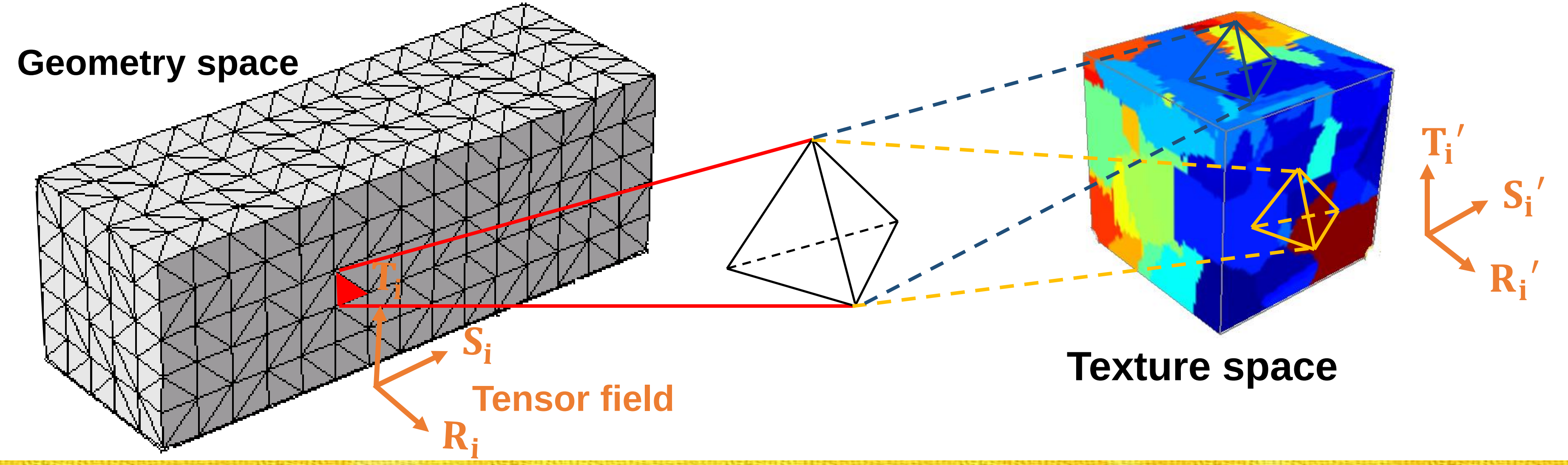




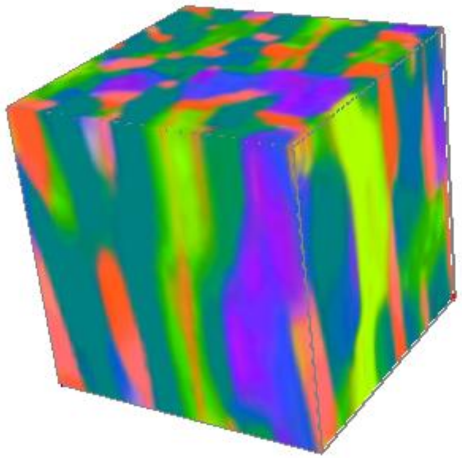
Javaheri et al., *Computer-Aided Design*, 120 (2020)

LEGOMAT Technique

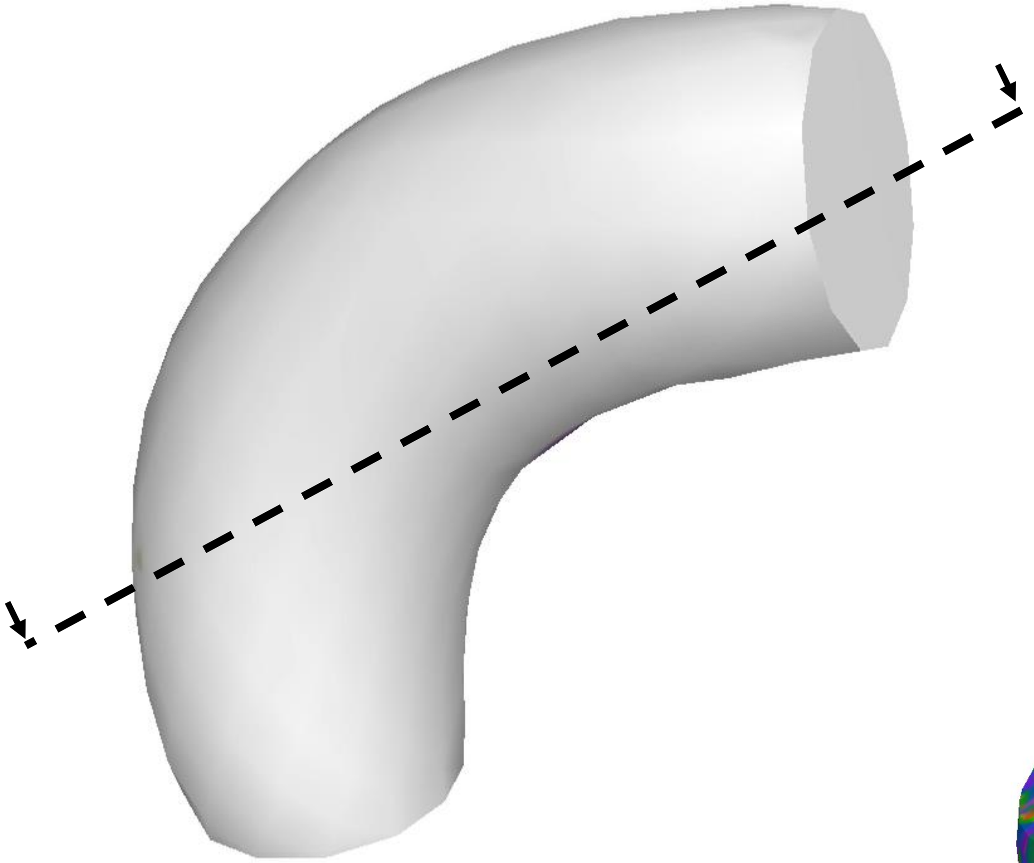
- **Patch-Based** MRF algorithm:
  - Discretization of the geometry space via tetrahedral elements
  - Mapping the geometry space to microstructural domain by associating nodes in the geometry to nodes in the textural mesh
  - Patches merge together seamlessly through optimization of the boundary patches
- *Approach:*
  - User defines the **scale and direction** of patches to control grain size
  - Warp microstructure according to geometry to control anisotropy directions



Controlled Axial Orientation

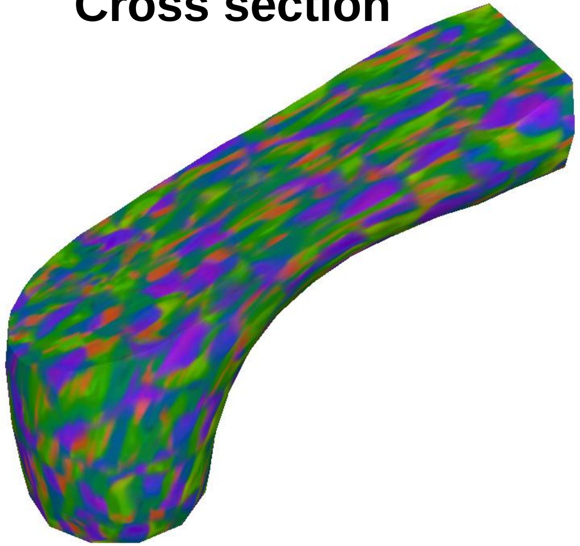


MRF reconstructed unit cell

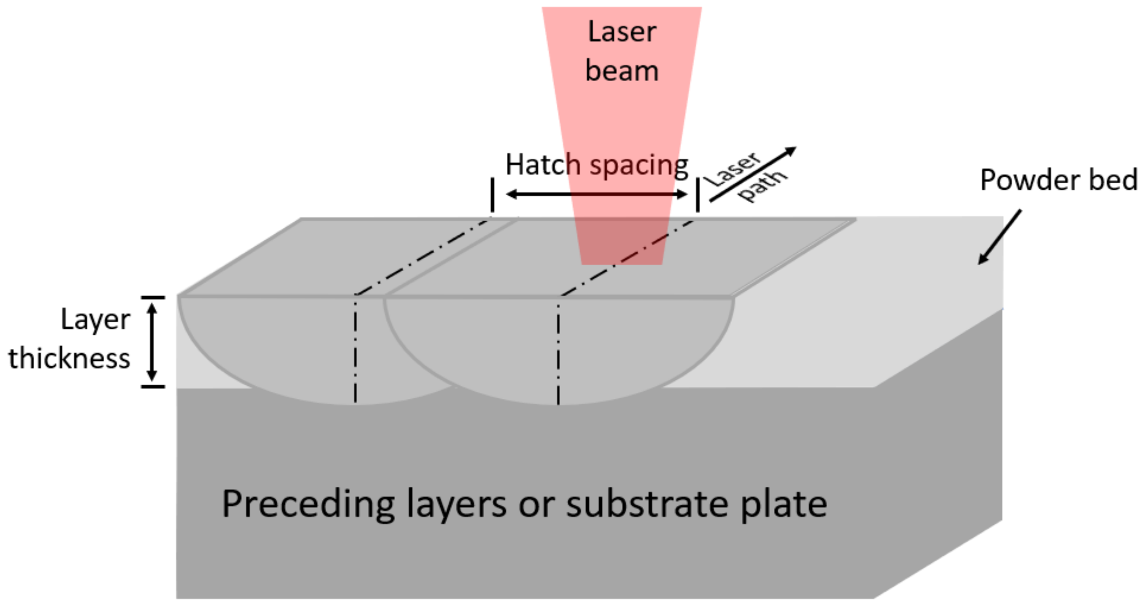


Synthesized model with full-field microstructural information

Cross section



Additive Manufacturing (AM)



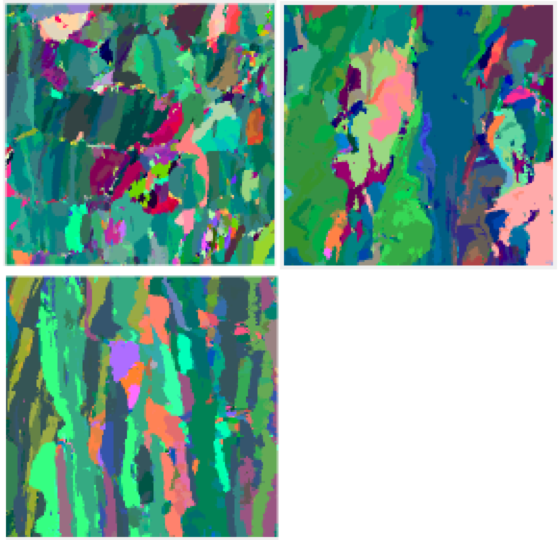
- Process: Selective Laser Melting (SLM)
- Material: 316 L stainless steel

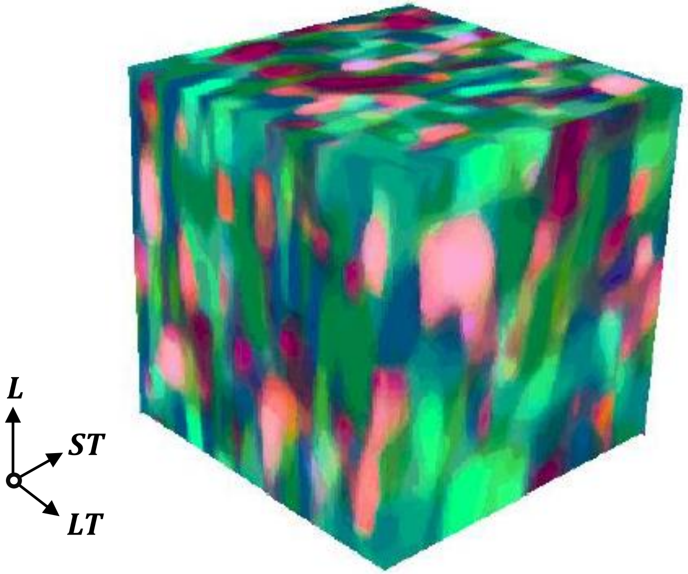
- Process Parameters:
  - Effective laser power: $200\ W$
  - Layer thickness: $30\ \mu m$
  - Scan velocity: $800\ \frac{mm}{s}$
  - Hatch spacing: $120\ \mu m$
  - Zigzag scans

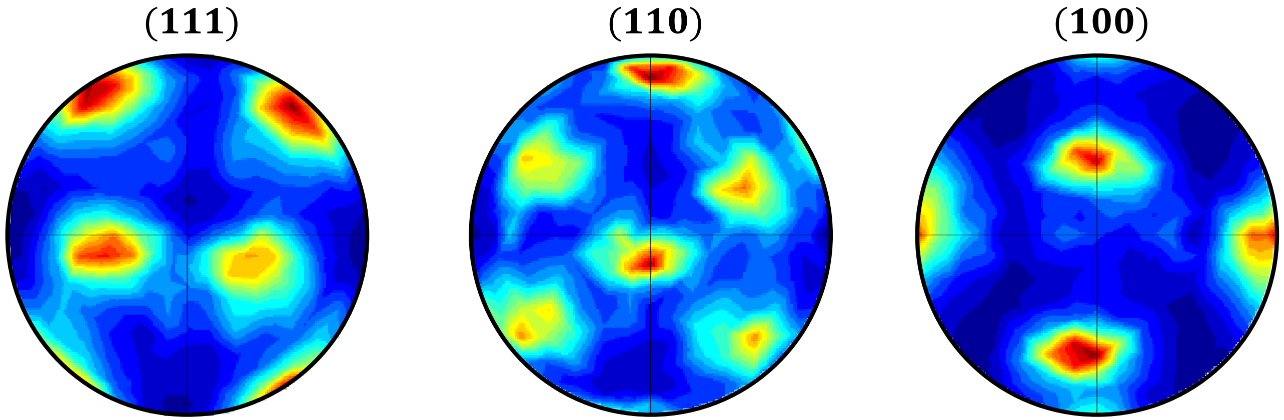
3 orthogonal EBSD images:

Courtesy of M. T. Andani (Univ. of Michigan)

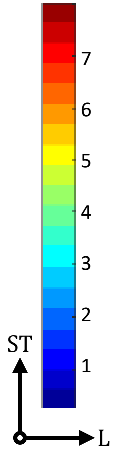
EBSD Reconstruction of AM

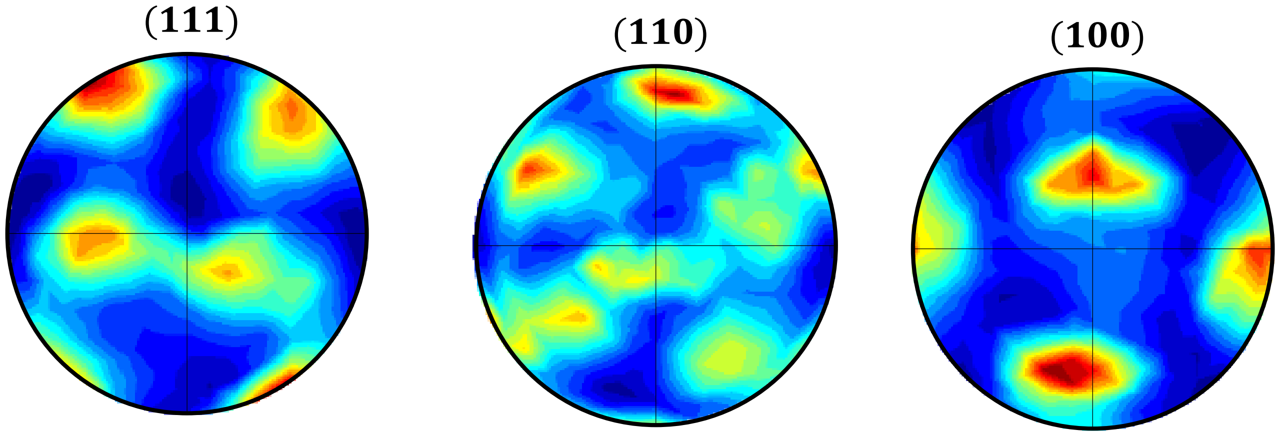






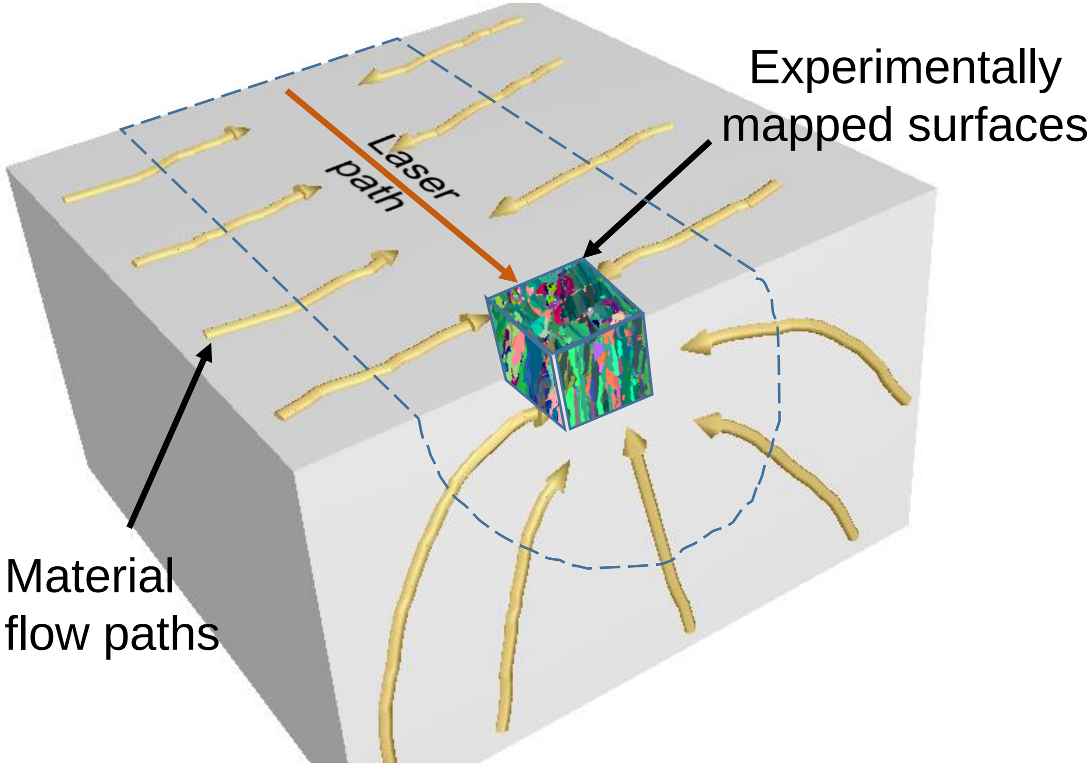
Texture (experiment)

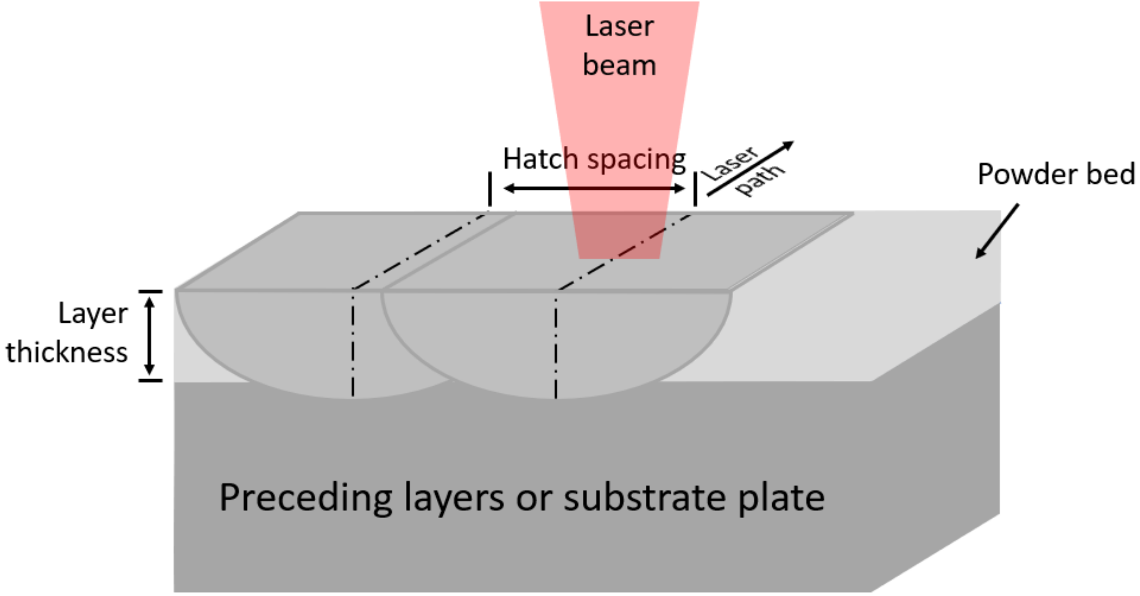




Texture (MRF reconstruction)

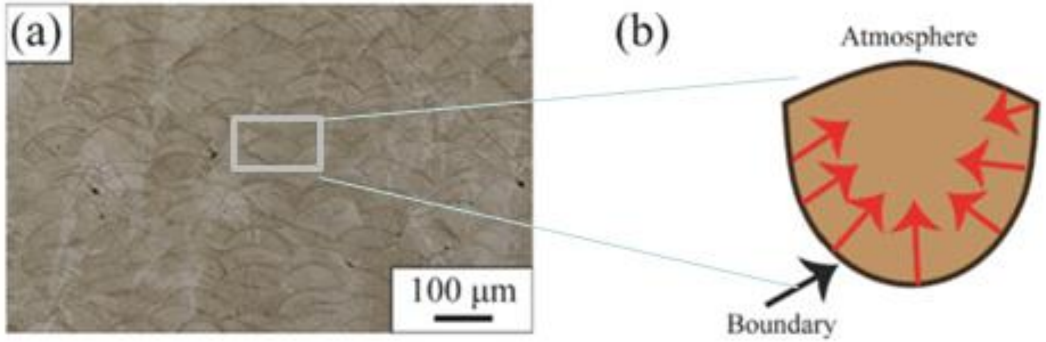
EBSD Reconstruction of AM



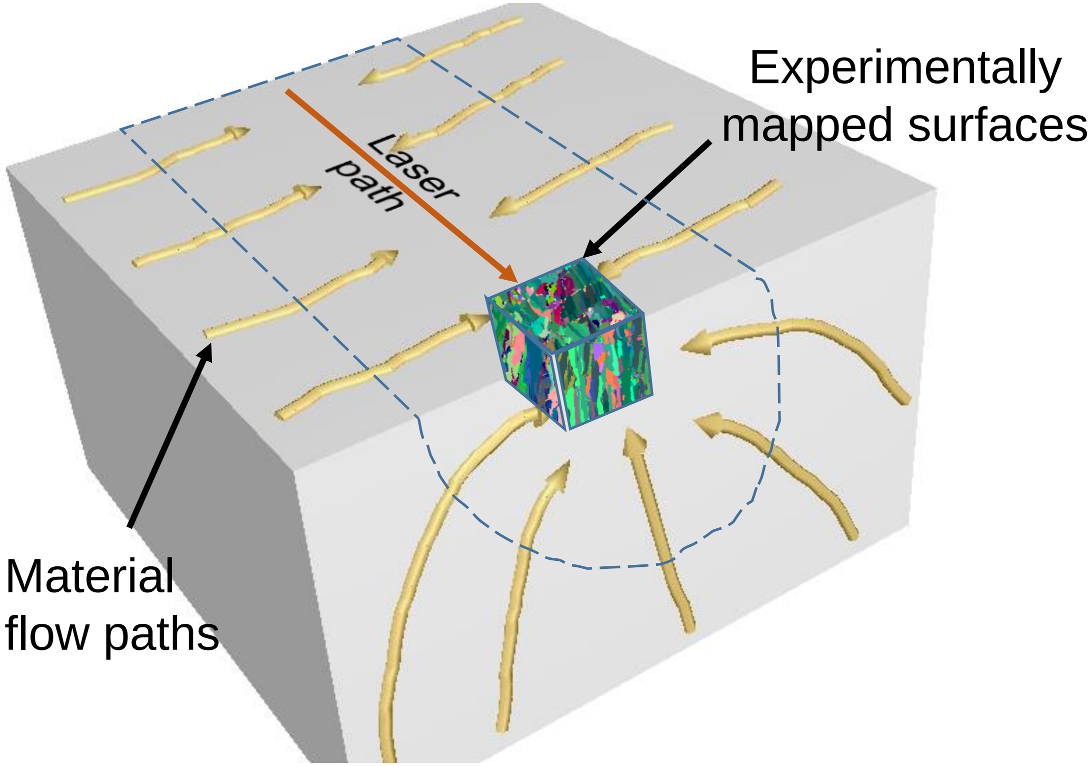


Rodgers, Madison, and Tikare, CMS 2017

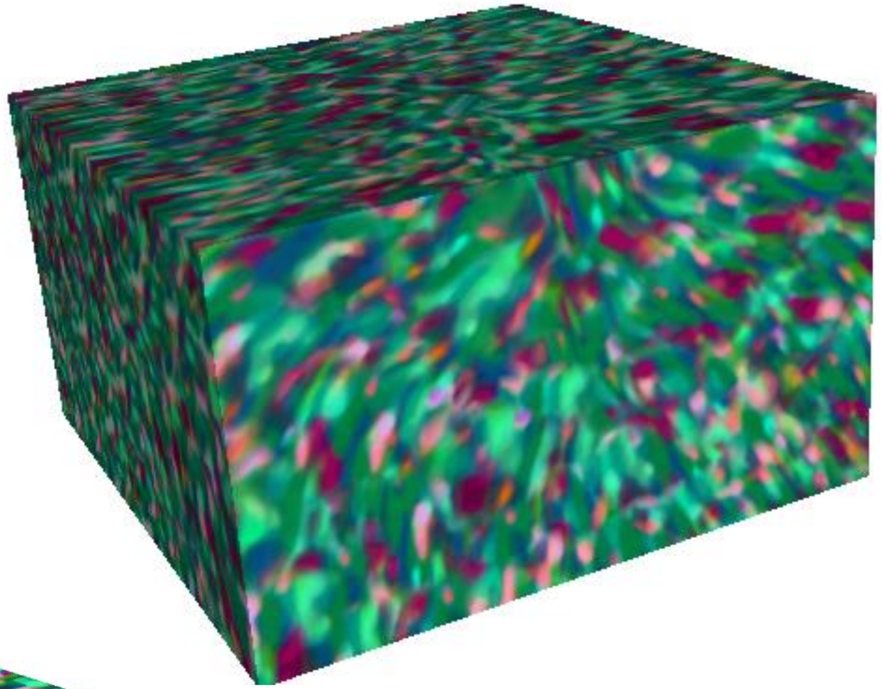
Andani et al., Materials & Design,137, 2018

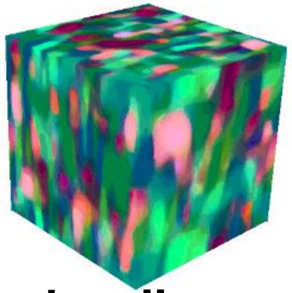


EBSD Reconstruction of AM



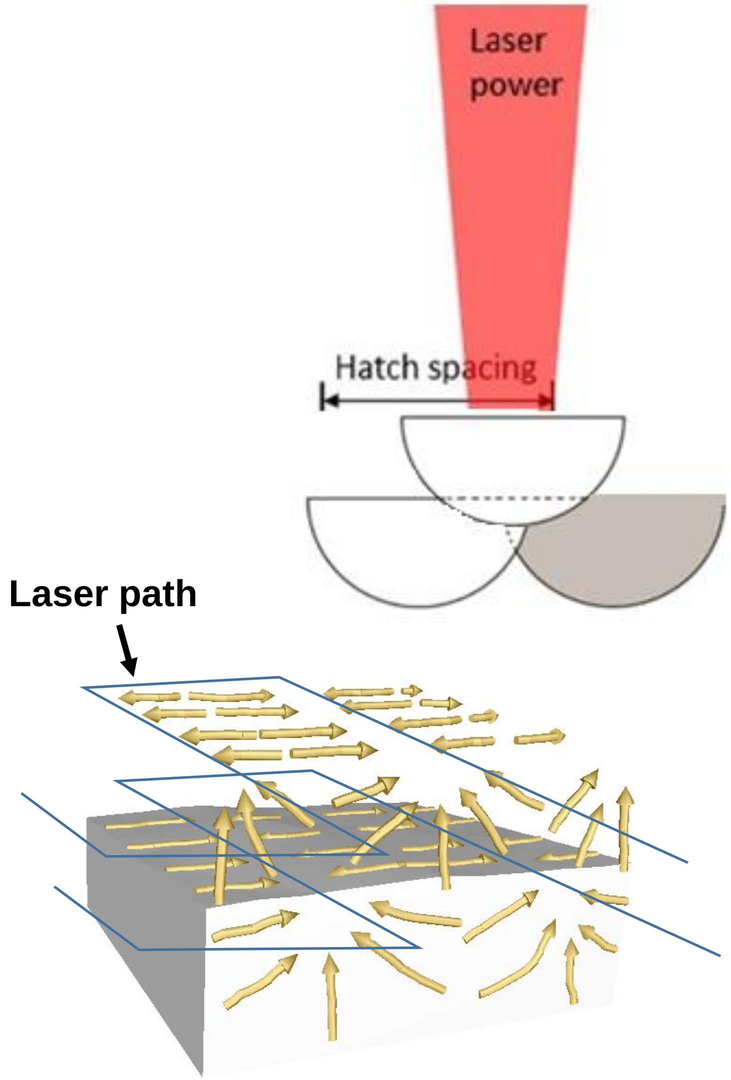
LEGOMAT reconstruction with user-specified flow paths

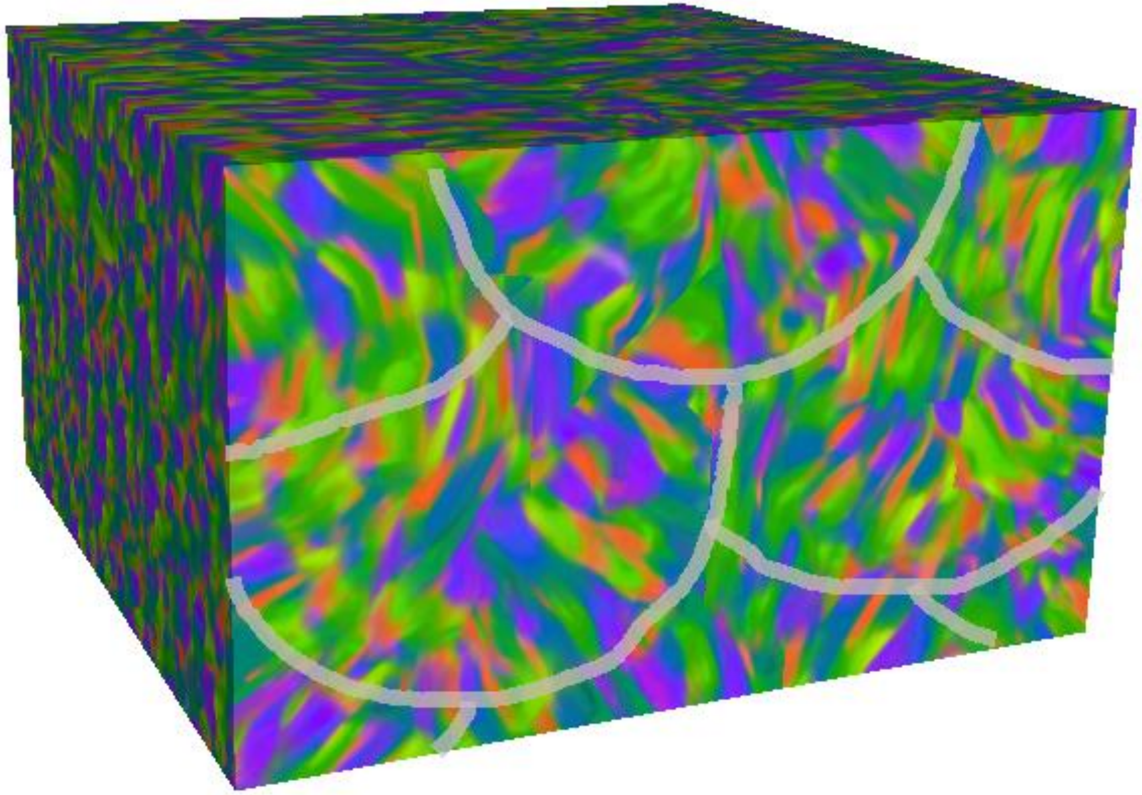




MRF unit cell

EBSD Reconstruction of AM





Simulation of large-scale AM microstructure based on laser path and processing variables

LEGOMAT for Additive Manufacturing

Method	Computational Cost	Benefits	Challenges
Phase-field	Extremely high	Physics-based	Small scale prediction
Cellular Automata	High	Texture prediction	Accuracy depends on cell size
Kinetic Monte Carlo (e.g., SPPARKS)	Intermediate	Allows large-scale prediction	Texture prediction
LEGOMAT	Real-time	Allows large-scale prediction	Experimental data-dependent & must be coupled to thermal models

Summary

- An MRF approach for reconstruction of diverse 3D microstructures from 2D experimental imaging was presented
- Verification of grain size distribution (via stereological formula), crystal orientations (e.g., ODFs and pole figures), and neighborhood correlations
- LEGOMAT for microstructure embedding
  - Combining flow fields with MRF for real-time description of microstructure distribution
- Future work:
  – Input laser paths directly in LEGOMAT and learn thermal fields from simulations
  – Adaptive microstructure selection based on laser parameters using machine learning in LEGOMAT

Thank You

Questions can be directed to imanajv@umich.edu