Team TBD – IDETC Hackathon 2023

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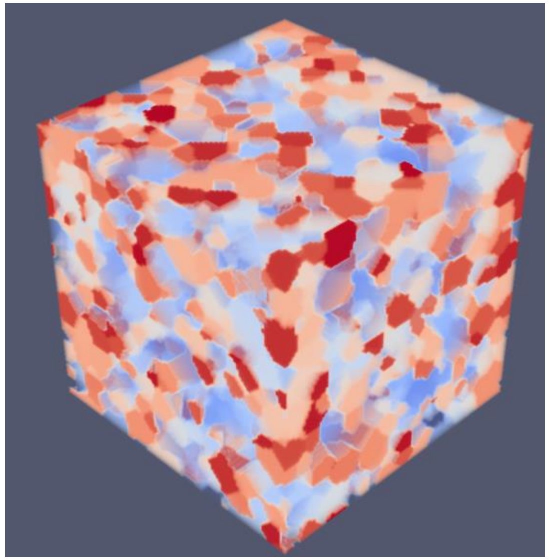
Problem 2: Exascale Material Design

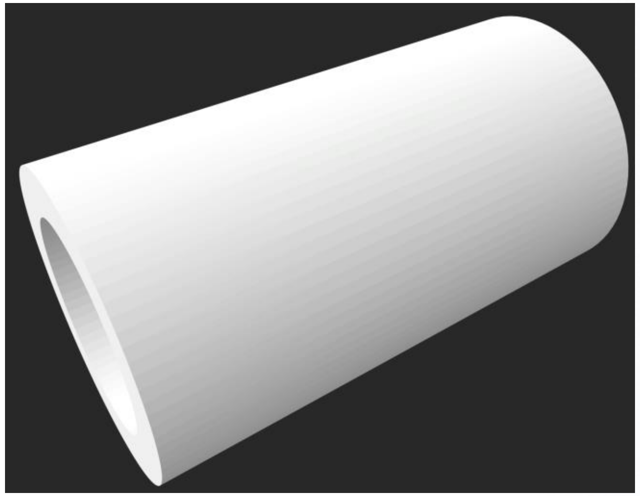
Introduction

- The main goal is to synthetize the texture of CAD models using microstructure data generated by SPPARKS.



Arbitrary Microstructure

+



Arbitrary CAD Model

Assumptions

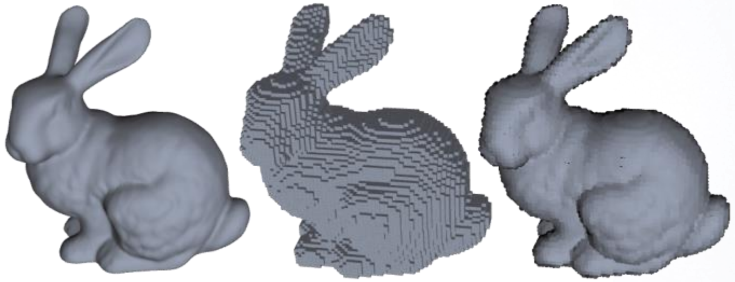
- SPPARKS provides us with 1000s of microstructures. We assumed we could use any number (including only one) of them to texturized the CAD file.

- The final texturized CAD file needs to be realistic. We assumed that the spin ID transitions within the model are smooth in all axes.

Smooth Boundary

- We assume that we can voxalize the CAD model in any way we want while using a resolution of at least 10 micrometers.

Canonical Stanford Bunny Model

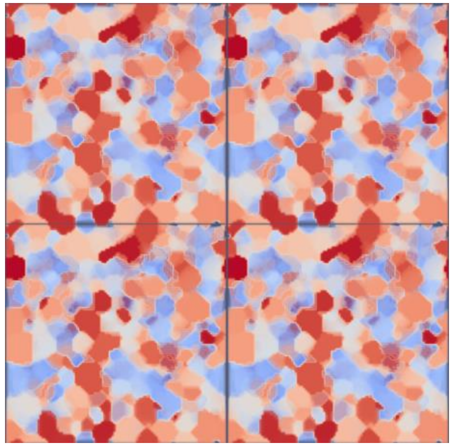


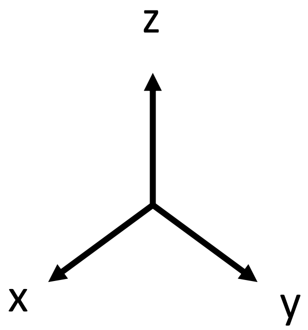
Methodology - Overview

- Given our assumptions, our main approach was to take advantage of the periodicity of the microstructures.

seed-001-potts_3d.50

Side profile connected in a tile-like fashion



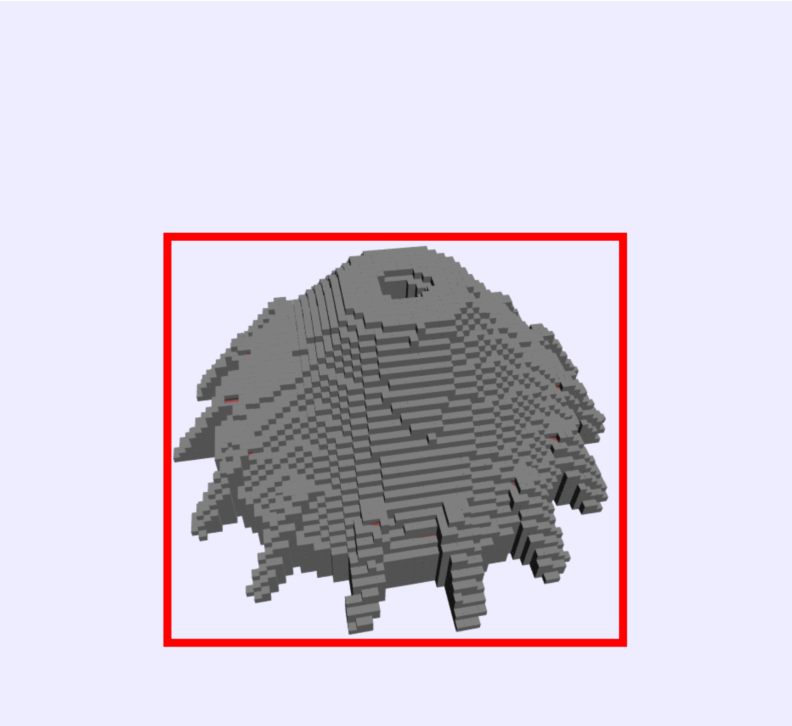


- Therefore, we can voxalize the original CAD model and populate it with one periodic microstructure at a time to generate different textures.

- To do that efficiently, we must perform some **rescaling** and **stacking** operations.

Methodology - STL Voxalization

- First, we start by voxalizing the CAD model.



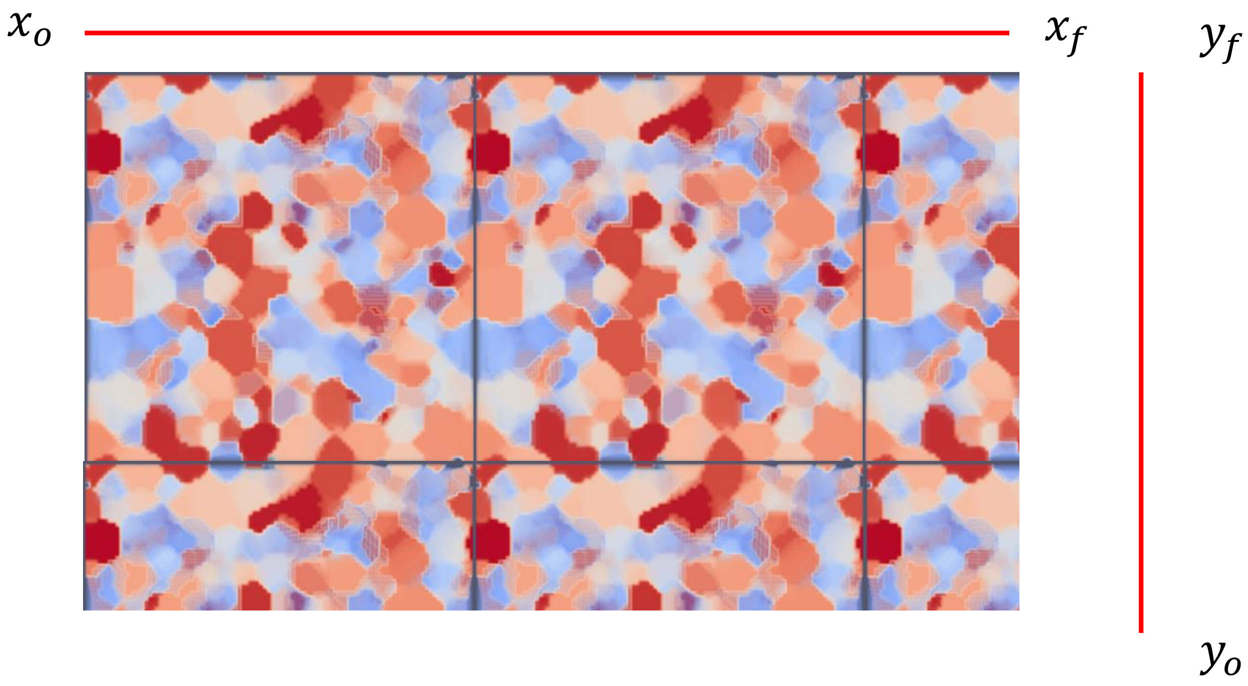
Bounding Box in 3 Dimensions

trimesh

$\longrightarrow [x_o, x_f, y_o, y_f, z_o, z_f]$

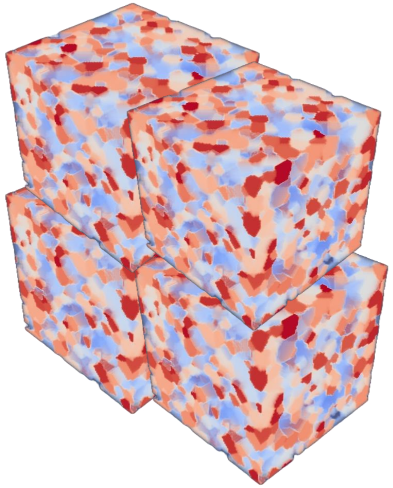
Methodology – Microstructure Rescaling

- Second, we use the bounding box information to rescale the microstructure while keeping it periodic.

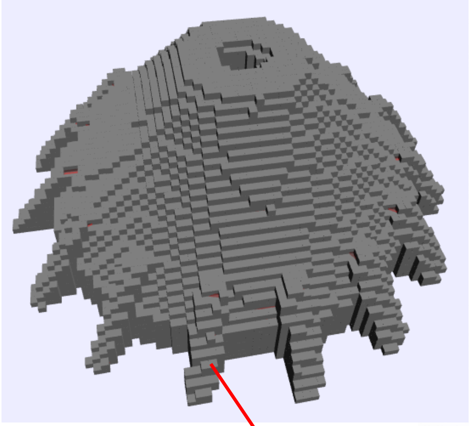


Methodology – Mapping STL and Microstructure

- Finally, we map them to the same frame of reference and perform a nearest neighbor calculation to match the spin IDs of each voxel.



Overlay →

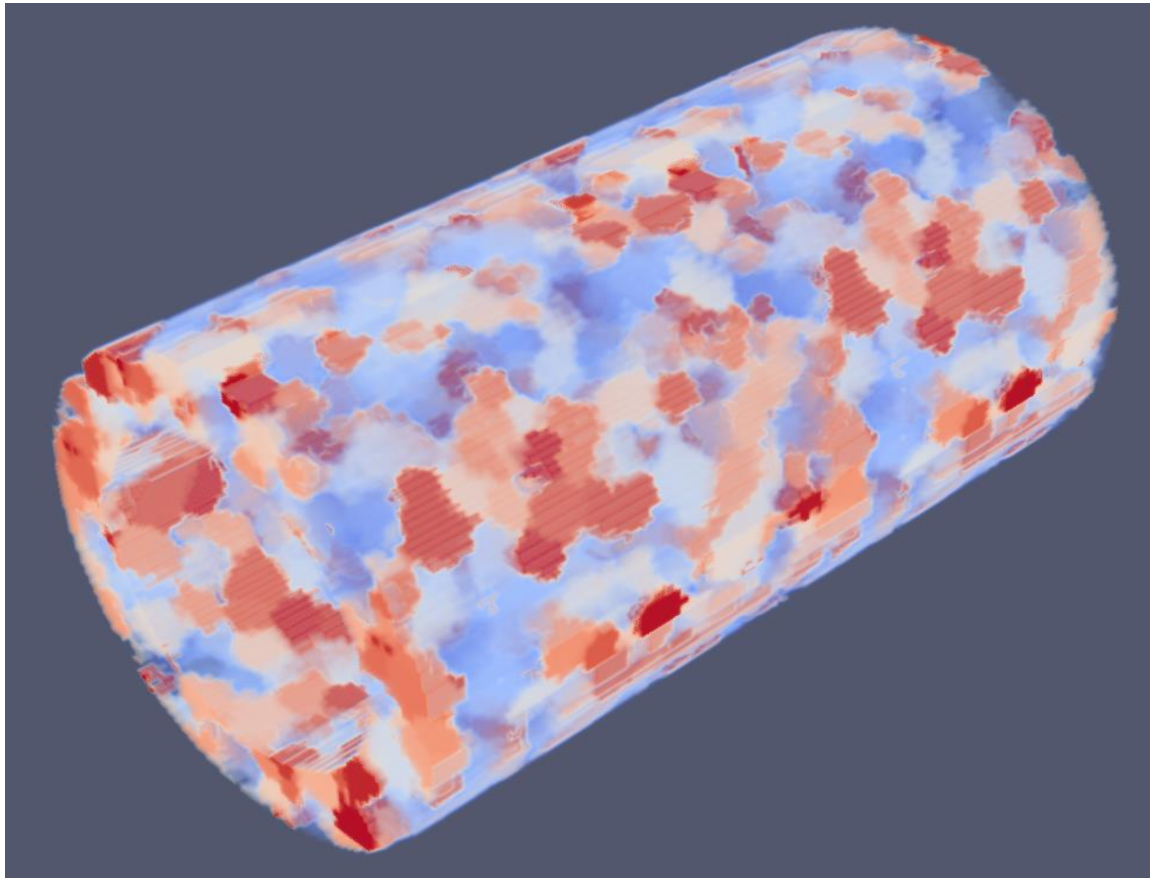


Build KD-tree using rescaled microstructure

O(n log(m))
n: voxels in STL
m: voxels in microstructure

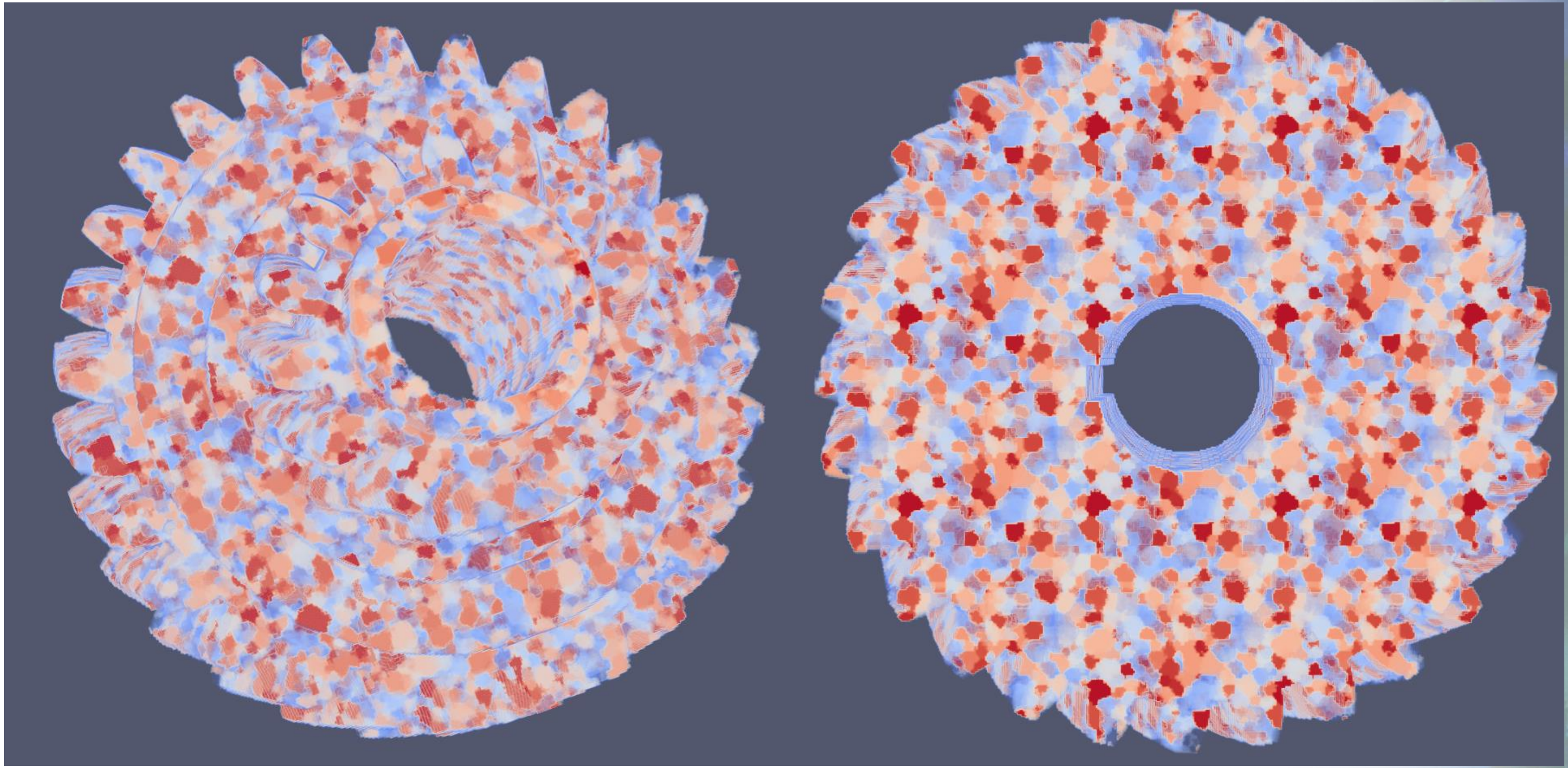
Assign each voxel a spin based on KD-tree

Results - Tube



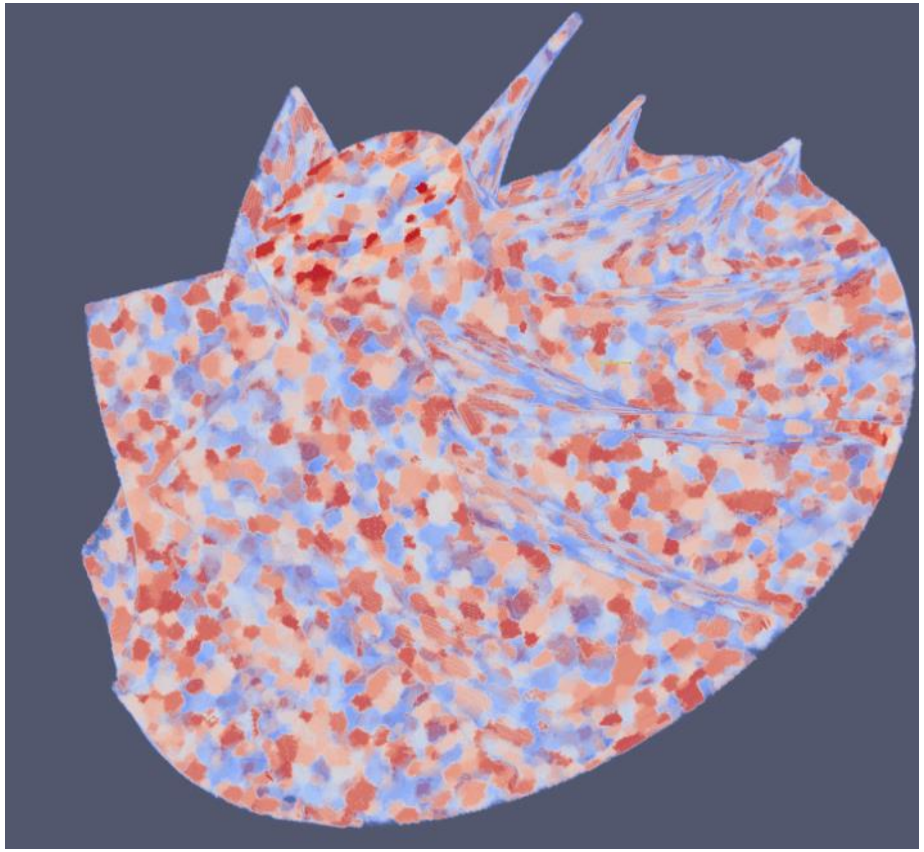
Average Runtime: 20s

Results - Helical Gear



Average Runtime: 165s

Results - Turbo Blade

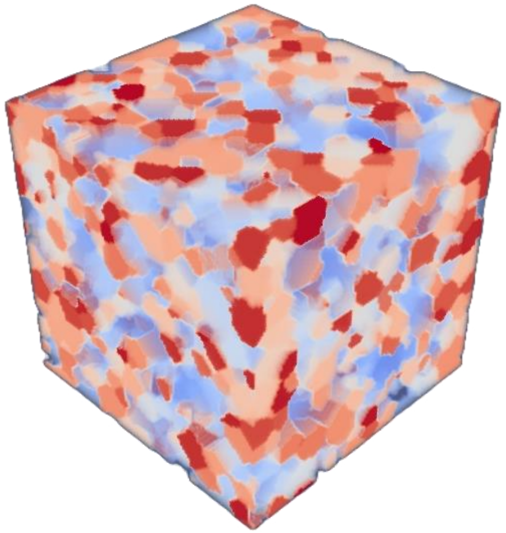


10 different textures

From 001 to 010 dataset

Future Work – Multiple Microstructures

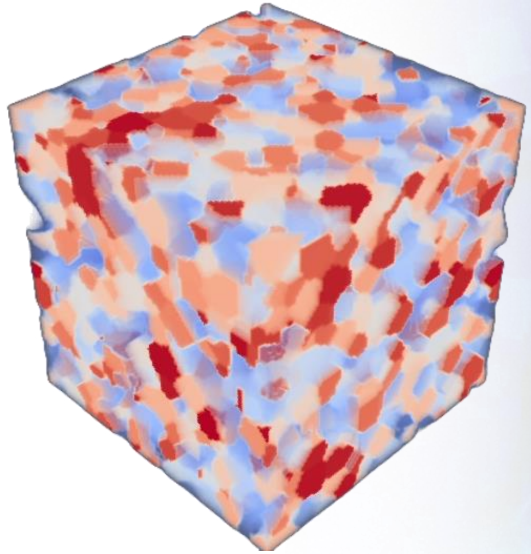
- If we disregard the need for periodicity, we can use multiple microstructures with a few tweaks in our algorithm.



Compare boundaries that

↔

can stack together



- We iterate over each voxel in the boundary and assign a similarity score based on their spin differences.

+X face of 001: $[s_2, s_3, s_4 \ldots, s_{1000}]$

Where generally: $s = \frac{1}{n}\sum|(v_{ijk} - u_{ijk})|$

Future Work – Multiple Microstructures

- We performed this analysis for microstructure 001 as a baseline:


```
295.4757
704
[330.0931, 347.3716, 330.5259, 330.2111, 338.3206, 329.6832, 334.3185, 316.593, 311.2766, 347.969, 334.1493, 356.7454, 342.6373, 316.6525, 310.8167, 322.1186, 361.8218, 347.6606, 327.6463,
327.33, 329.8603, 324.9495, 342.3685, 330.1674, 334.3827, 365.9009, 296.4379, 327.7374, 335.065, 340.3686, 306.7398, 348.3376, 334.1216, 320.1863, 318.0827, 335.1894, 315.1924, 317.1118,
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334.4227, 335.6847, 334.5145, 324.1243, 317.27, 342.6731, 352.6539, 337.3455, 319.7436, 315.9546, 323.8671, 319.3007, 318.6286, 302.8585, 320.9529, 318.0674, 345.7647, 334.3449, 337.6334,
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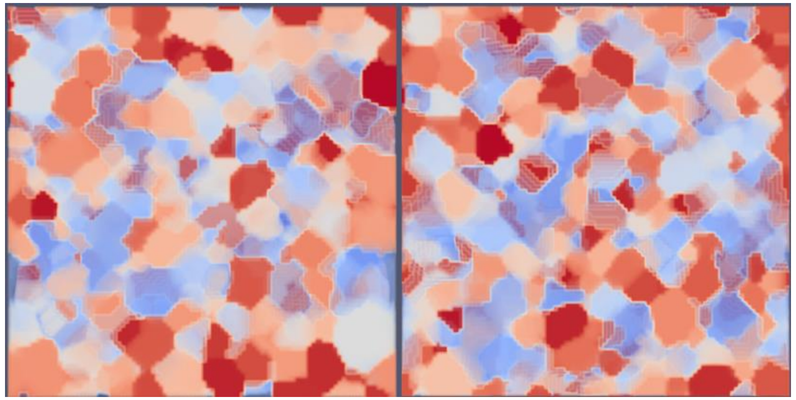
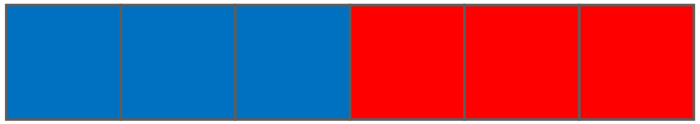


The closest match is 704

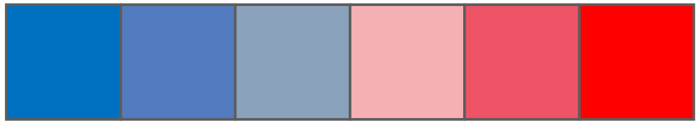
Future Work – Multiple Microstructures

- After we perform a similarity analysis, we can stack the microstructures that have the lowest differences.
- However, we can go further by assuming that we are allowed so slightly modify the boundaries of each microstructure.



Left side is 001 Right side is 704

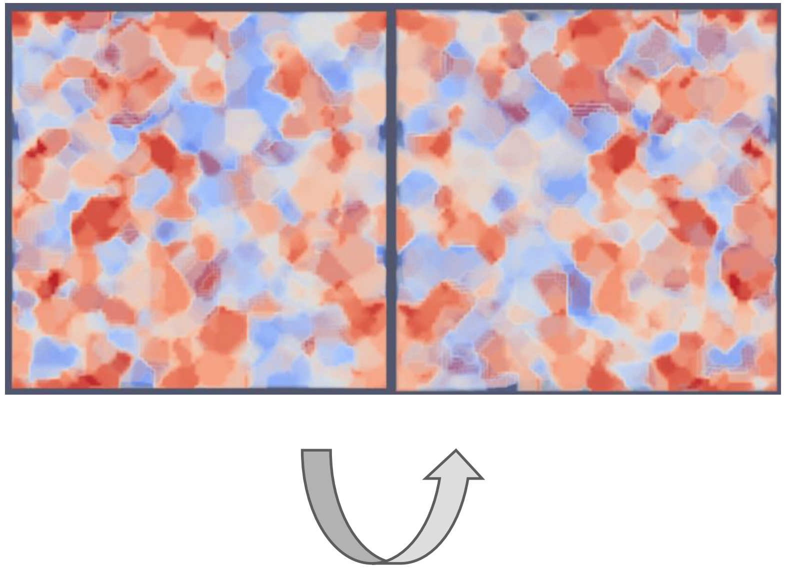
- By progressively averaging out the spin IDs we can ensure smooth transitions:



Left side is 001 Right side is 704

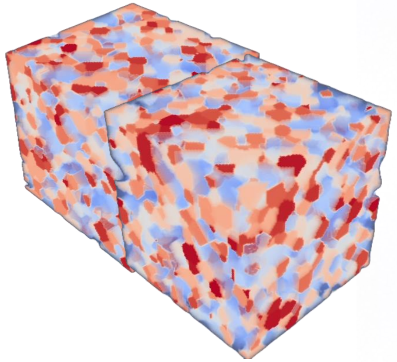
Future Work – Proof of Concept

- We show that this smooths out the transitions between different microstructures while keeping their interiors unique and faithful to the SPPARKS output.



Fold on itself and boundaries are matching

Robustness of algorithm is maintained but now without periodicity



Stacking process now based on similarity metrics

The University of Texas at Austin

SiDi lab

Thank you!

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