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Title: Toward Recreation of Microstructure in Additively Manufactured Materials

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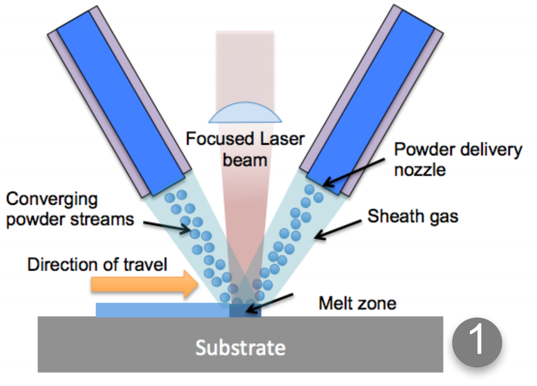
TOWARD … ☺

RECREATION OF MICROSTRUCTURE IN ADDITIVELY MANUFACTURED MATERIALS

Robert Foster, Scott Vander Wiel, Curt Bronkhorst, Veronica Livescu

International Conference on Plasticity, Damage, and Fracture
8 January 2018

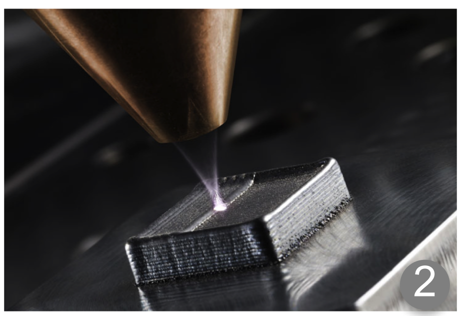
Additive Manufacturing by Laser Powder Forming

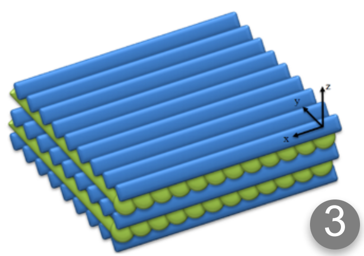


Tremendous design flexibility but …

process
complexity

unpredictable
performance





Hatch patterns

Need physical models to predict performance from material structure at micro- and meso-scale

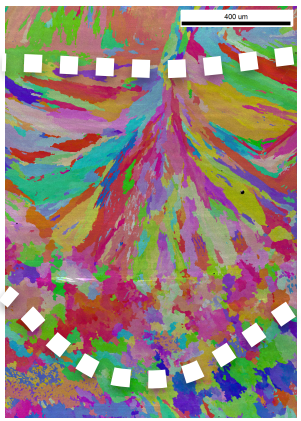
Complex microstructures are created within weld bead cross sections.

Image Credits:
1 www.studyblue.com 2. www.laseradditivesolutions.co.uk
3. www.additivemanufacturing.media 4. www.rtejournal.de/ausgabe11/3852

Physical models of weld beads need realistic initialization, so …

Goal: Generate Digital microstructures to match EBSD images

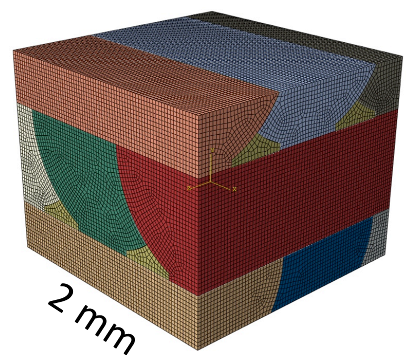
Model 3D grain shapes from 2D images …



1 mm

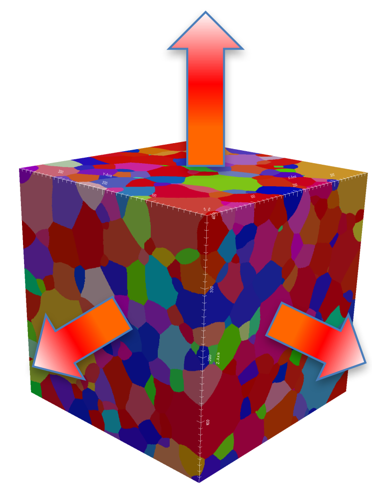
to populate

a computational weld bead mesh …



2 mm

and support material performance simulations.



Desired Results

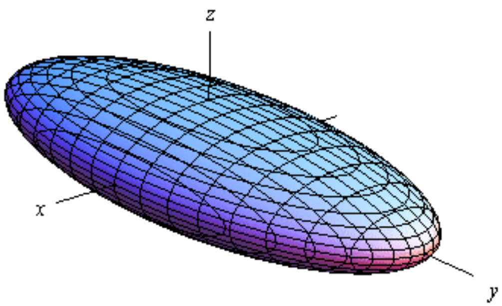
Example slice from 3D **ellipsoid growth model** (this one was hand-tuned)

Elliptical Growth Algorithm

Originally developed in Teferra and Graham-Brady (2016)[1]
Grains grow as ellipsoids until they interfere. Principal axes of grain j are given by columns of rotation matrix O_j (described in section below)

Growth velocities along principal axes are

$$\boldsymbol{v}_j = \left(v_{1j}, v_{2j}, v_{3j}\right)^T$$



Every spatial point $\boldsymbol{x}$ is assigned to the closest grain, as determined by travel times:

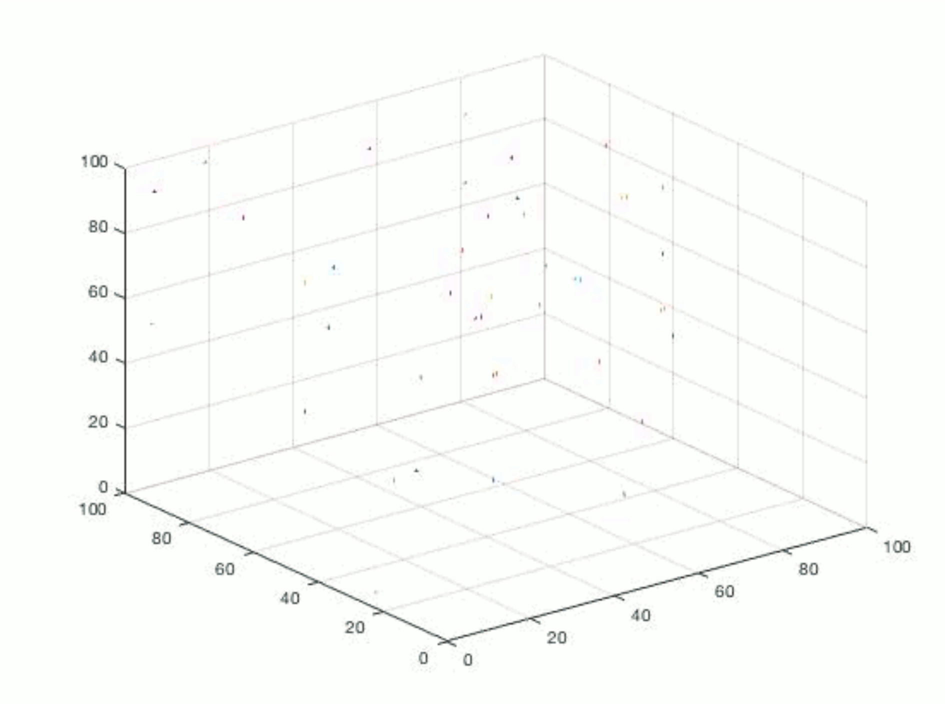
$$T\left(\boldsymbol{x} \to \boldsymbol{X}_j\right) = \left[\left(\boldsymbol{x} - \boldsymbol{X}_j\right)^T O_j^T \left(\mathrm{diag}\, \boldsymbol{v}_j^{-2}\right) O_j \left(\boldsymbol{x} - \boldsymbol{X}_j\right)\right]^{1/2}$$

Crystallographic orientations $(\phi_{1j}, \Phi_{2j}, \phi_{3j})$ (Euler angles) are drawn from orientation distribution function

1. Teferra, K. and Graham-Brady, L. *Tessellation growth models for polycrystalline microstructures.* Computational Materials Science 102 (May 2015) pp. 57 – 67

Elliptical Growth Algorithm

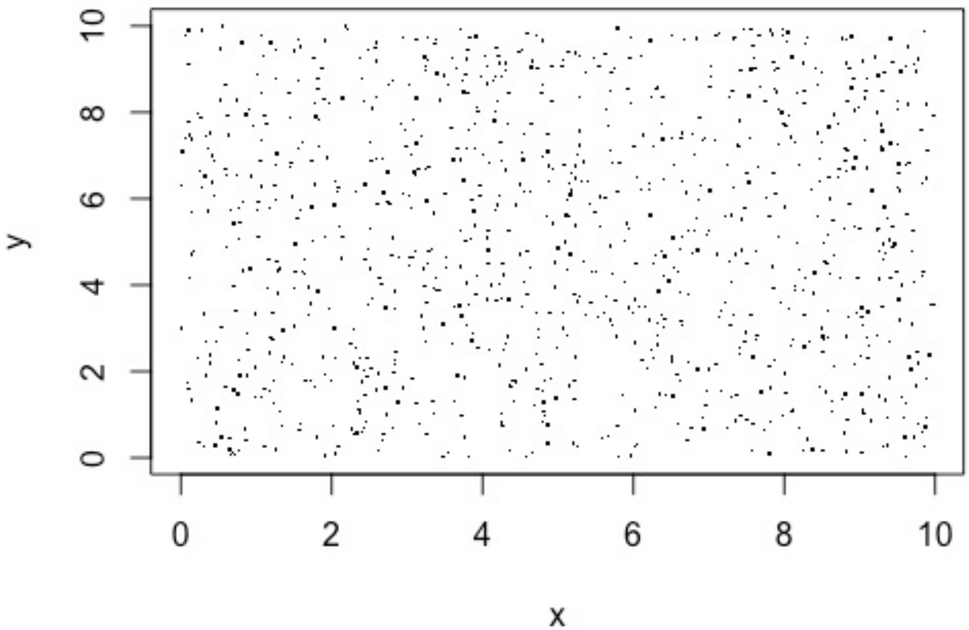
Computer algorithm: Allow grains to grow organically, stop when they interfere with each other.



If growth can be controlled by parameters, parameter values can be matched or chosen to recreate "real" orthogonally sectioned data sets.

Nucleation Site Generation

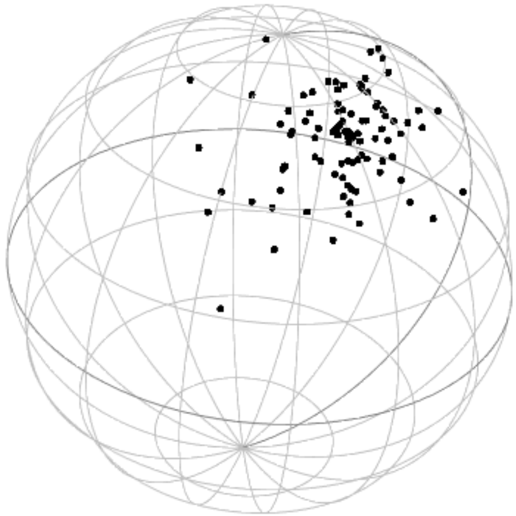
Matern's hard-core point process is used to generate points such that no two points are within distance *r* of each other.



Minimum distance used is *r = 0.2* - approximately matches real data sets.

Uniform Axis Random Spin (UARS)

Goal: Simulate rotations in SO(3) around a default orientation[2]



Polar coordinates θ and ϕ are simulated from a uniform distribution. An independent angle *r* is simulated from a circular symmetric distribution about zero.

$$U = (u_1 u_2 u_3)^T$$
$$= (\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta))^T$$

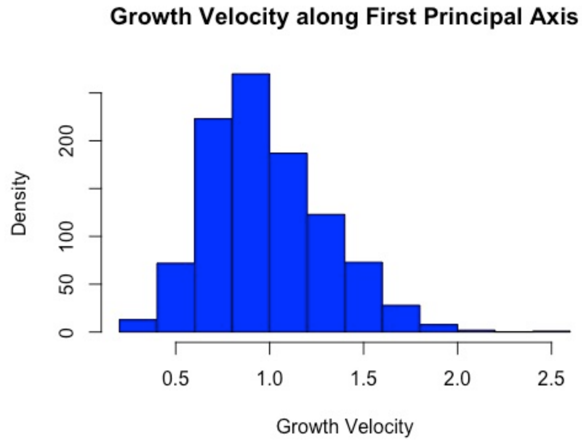
$$M(U,r) = UU^T + (I_{3x3} - UU^T)\cos(r) + \begin{pmatrix} 0 & -u_3 & u_2 \\ u_3 & 0 & -u_1 \\ -u_2 & u_1 & 0 \end{pmatrix} \sin(r)$$

$$O = S * M(U,r)$$

2. Bingham, M., Nordman, D. and Vardeman, S. Modeling and Inference for Measured Crystal Orientations and a Tractable Class of Symmetric Distributions for Rotations in Three Dimensions. Journal of the American Statistical Association 104 (488) (Dec. 2009), 1385 – 1397

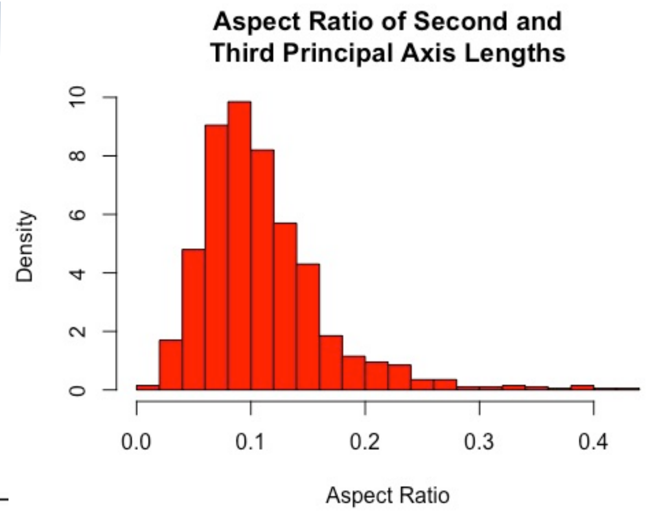
Growth Velocities and Aspect Ratios

Simulate growth velocities from gamma distributions…



With a given mean and concentration parameter (controlling how closely random velocities are around mean)…

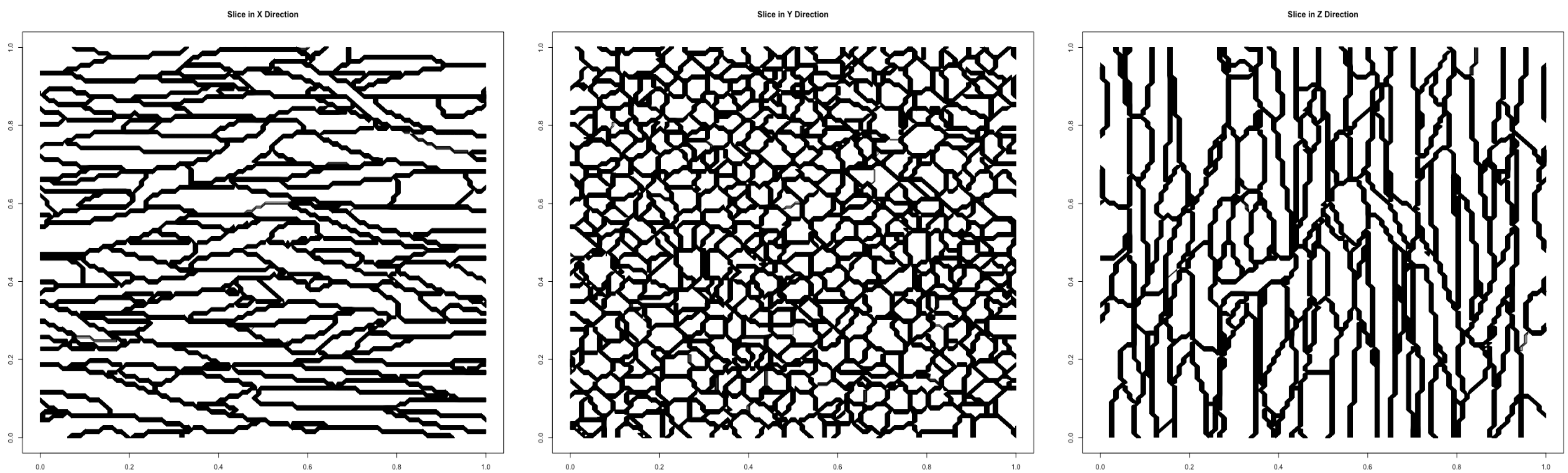
So that the distribution of aspect ratios has mean around desired quantity



Simulation Parameters Design

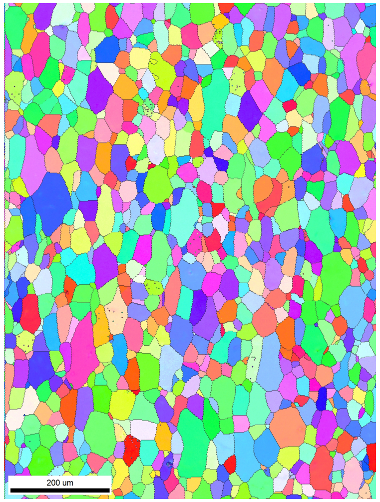
Five parameter design:

1. Default orientation S (rotation matrix, three degrees of freedom)
2. Angle concentration κ (concentration around rotation matrix)
3. Aspect ratio e_1 (major to secondary axis)
4. Aspect ratio e_2 (secondary to tertiary axis)
5. Ratio concentration s (concentration around desired aspect ratio)

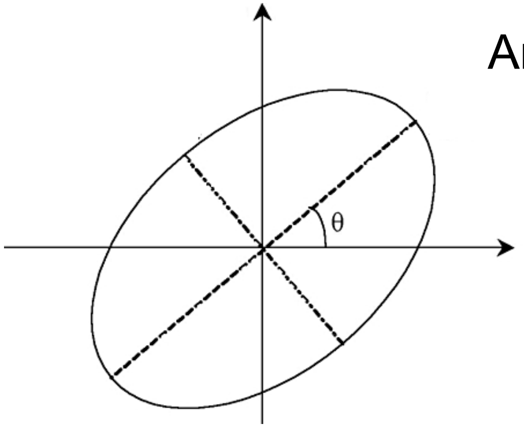


Orthogonally Sliced Data

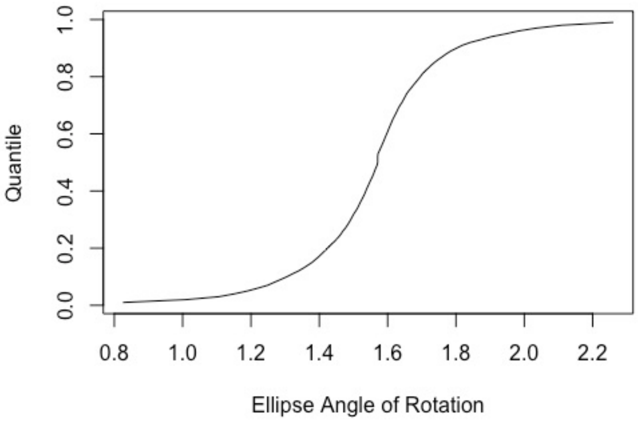
Data often given as orthogonally sliced EBSD images…



Assuming grains in slices are growths of ellipses, aspects can be quantified…

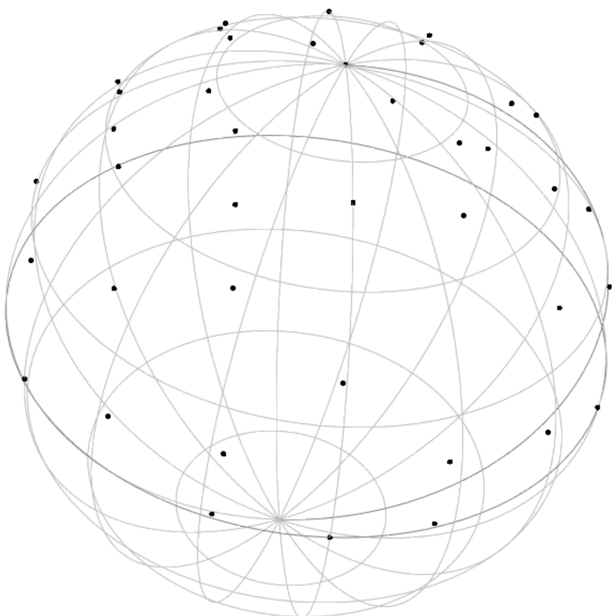


And distributions can be calculated…



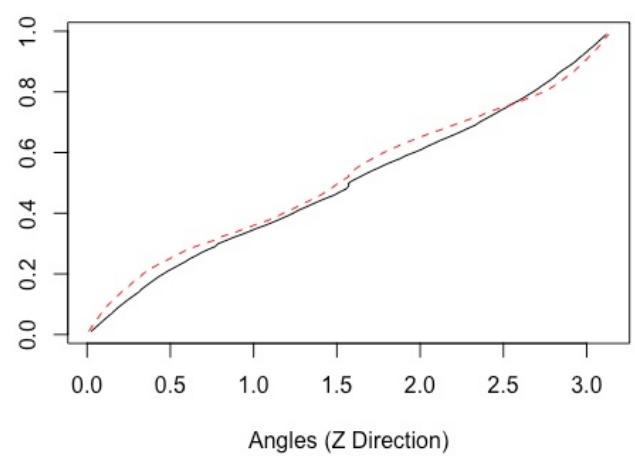
Growth parameters may be sought using only orthogonal slices by comparing distributions of slice summary quantities

Simulation Study

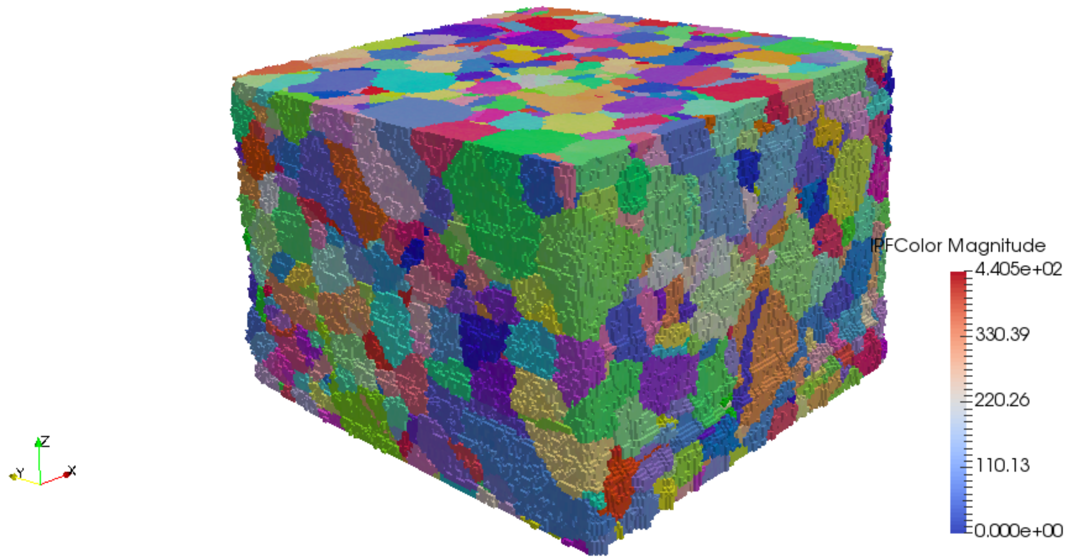


1. Set of 52 unique rotations that are sequentially space-filling in SO(3)
2. Sequence of 15 Aspect ratios e_1, e_2 equally spaced between 0.1 and 1
3. κ values of 0, 1, 5, and 10
4. *S* values of 1, 10, and 100 (log-scale 0, 1, and 2)

Distance = Maximum absolute difference between CDFs of measured quantities



IN100 Data Set



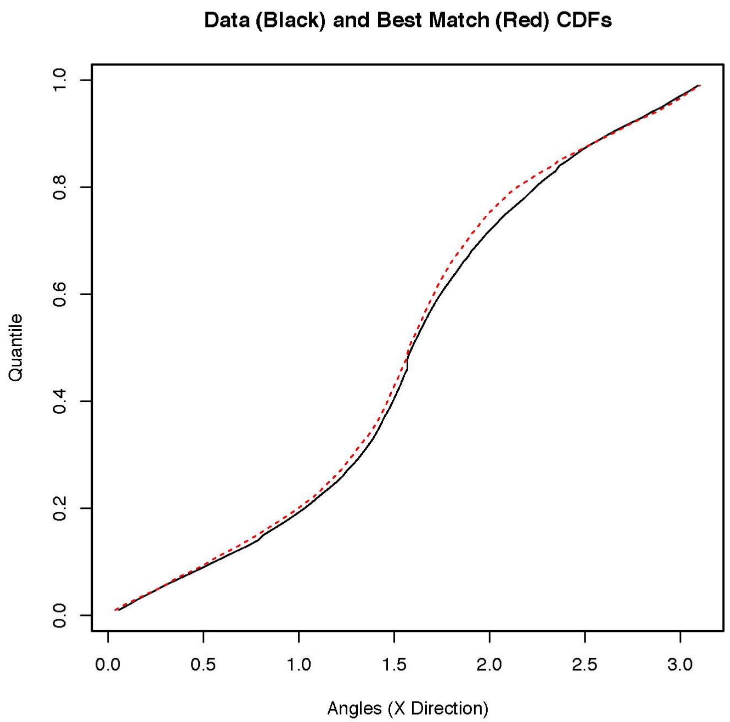
"The" IN100 data set given freely as example in Dream3D data package

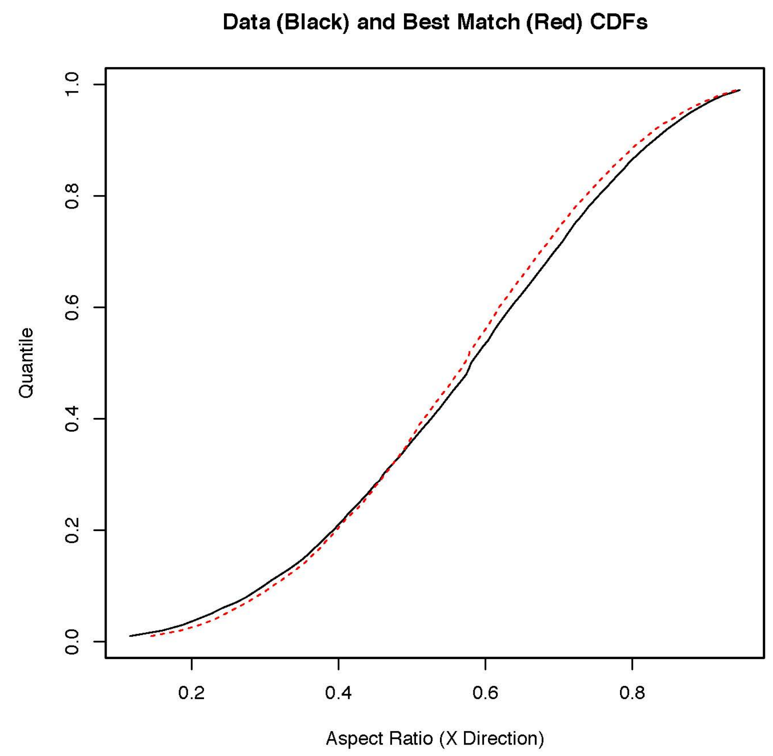
Grains not visibly elongated in a preferred direction, consistent morphology

Serial section of 170 slices approx. 30x30 microns and 250 nm apart allow for full recreation of microstructure

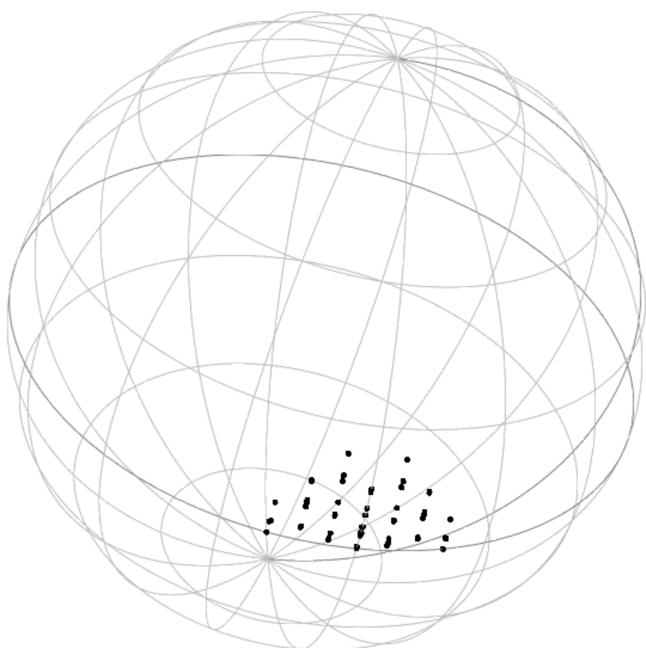
Analysis of IN100 Data Set

Best match identifies aspect ratios and angles well…





Focused Simulations

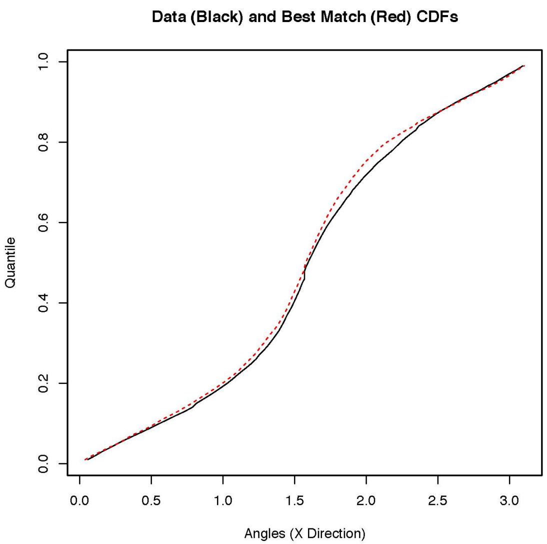


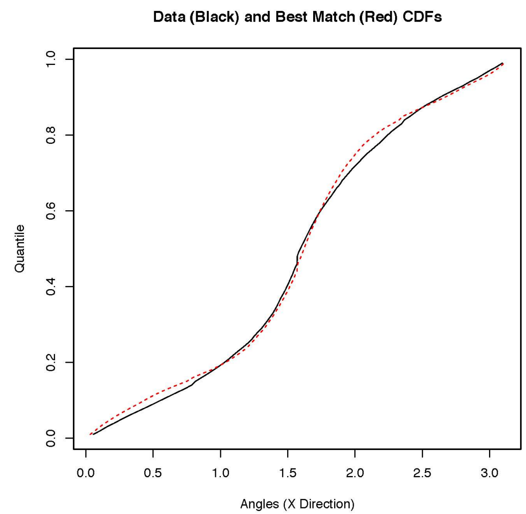
1. Set of 65 unique rotations that are close in SO(3) to best-fit match from general simulations
2. Sequence of 8 of aspect ratios e_1, e_2 equally space from 0.789 to 0.867
3. κ values of 5 and 10
4. *S* values of 10 and 100

Goal: Determine in improving resolution of simulations drastically improves fit

Analysis of IN100 Data Set

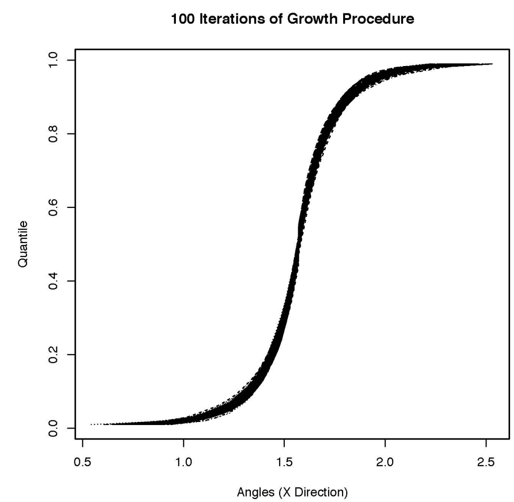
But improvement to fit is slight…





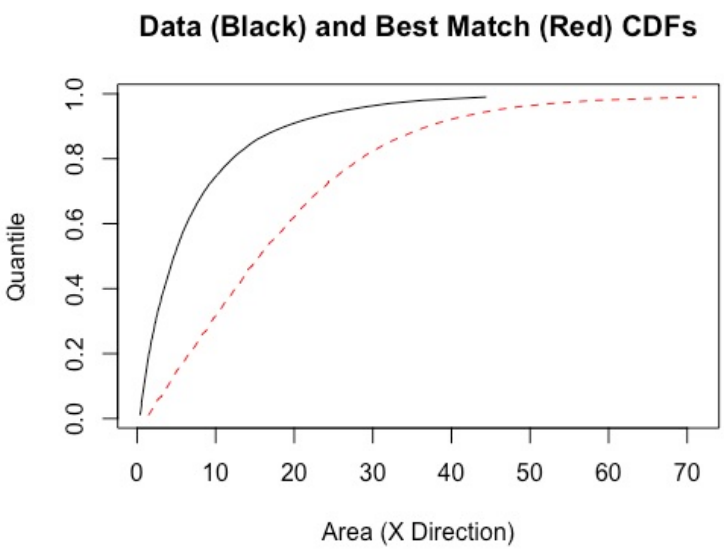
For equiaxed (or nearly so) grains, many sets of parameters may produce approx. the same output

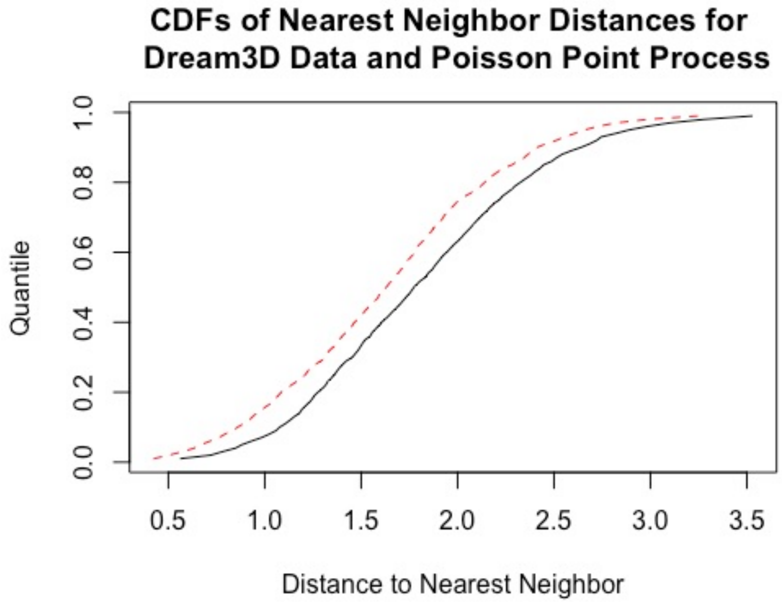
Randomness creates uncertainty in output, even for the same set of parameters…



Analysis of IN100 Data Set

Method is not capturing areas of orthogonal ellipses correctly…

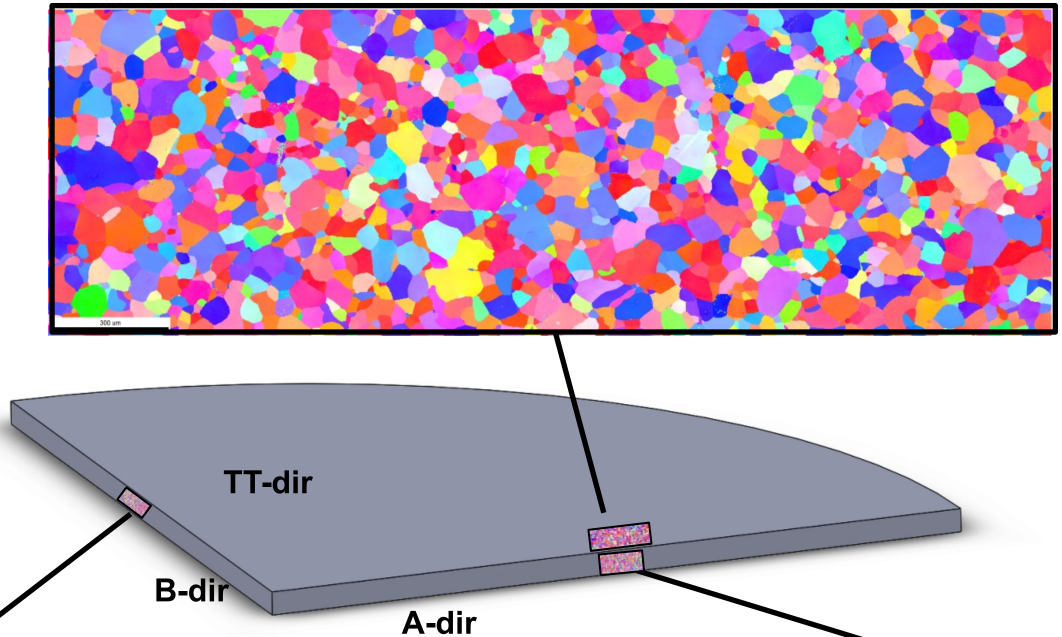




Hardcore Matern process not necessarily good fit to nucleation sites

Description of Tantalum Data Set

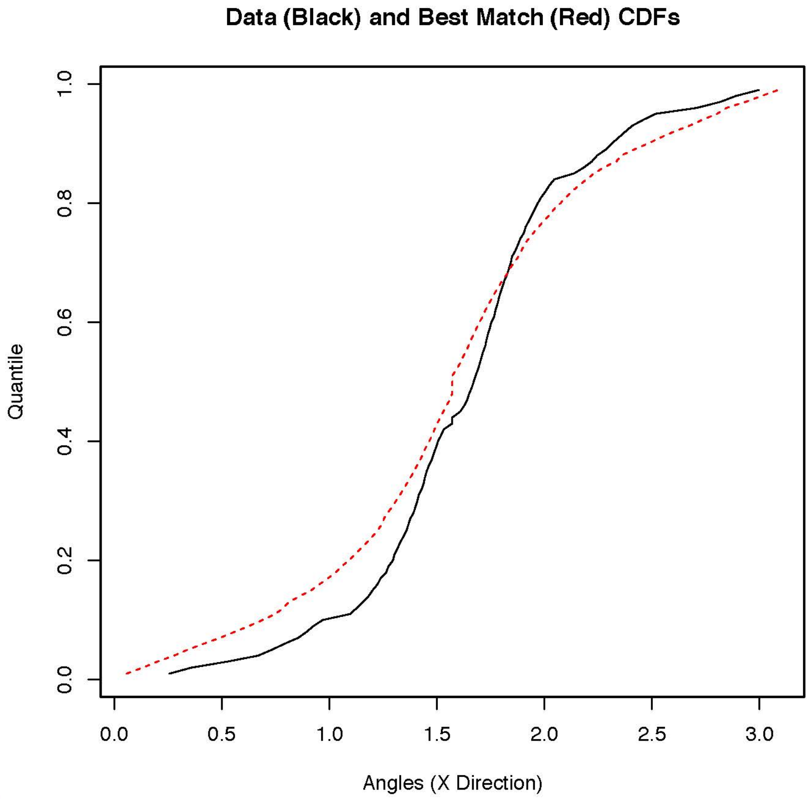
Tantallum Stack – grains slightly elongated along TT-direction

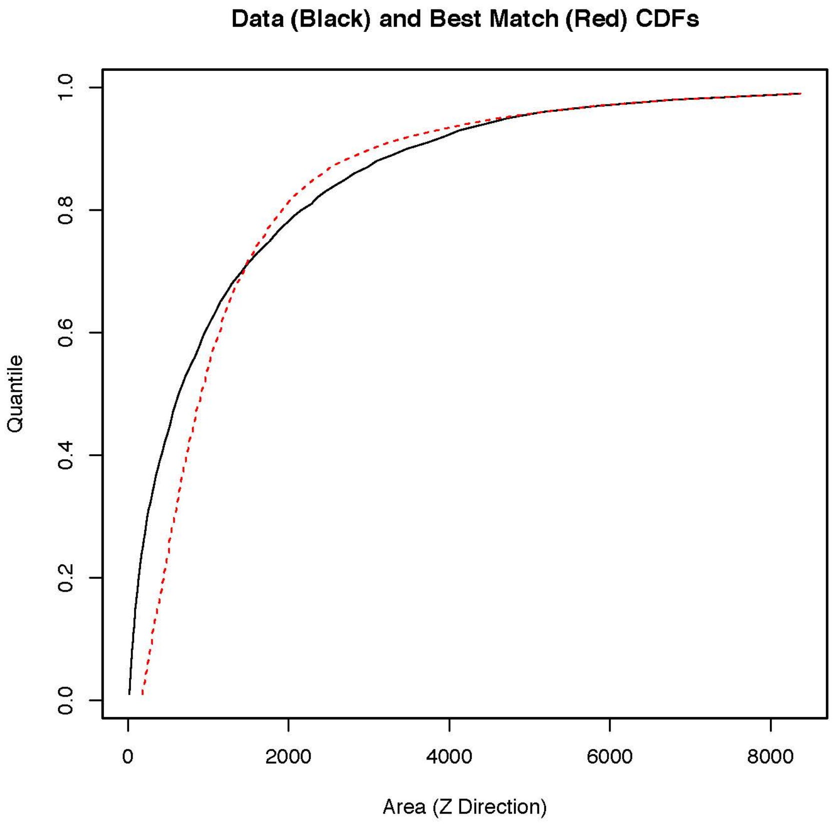


Six to ten slices available in each direction, only information is statistics o each slice...orientation is considered “unknown”

Analysis of Tantalum Data Set

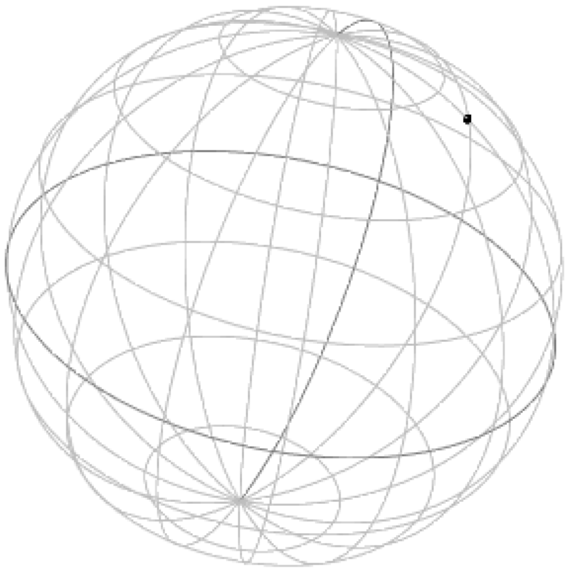
Areas and angles are fairly well determined, with respect to limited information…



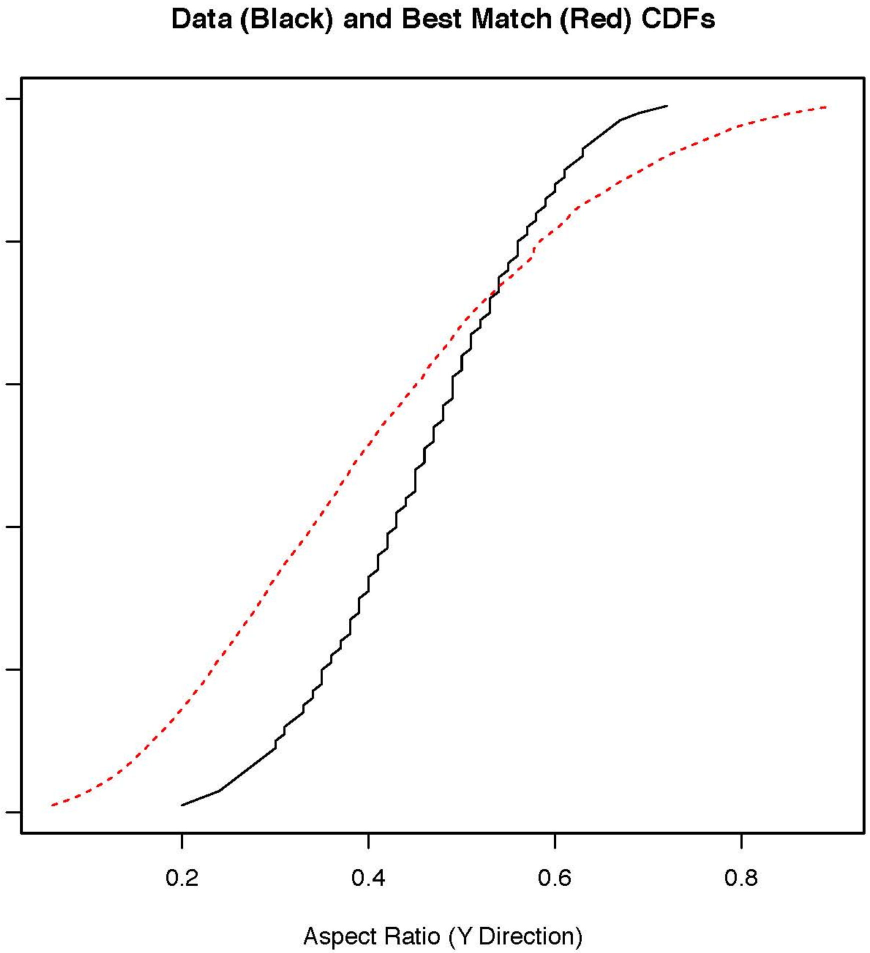


Analysis of Tantalum Data Set

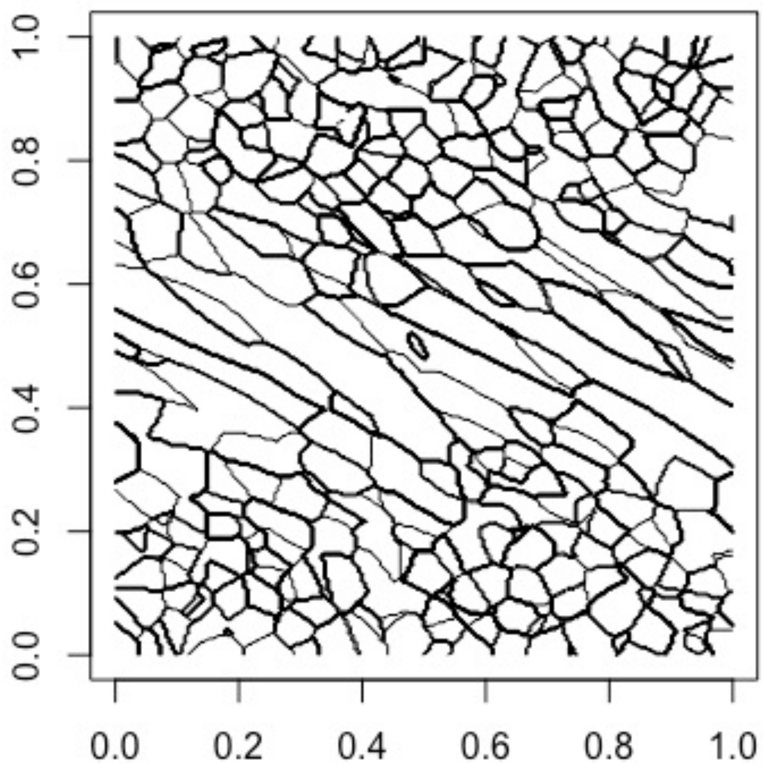
Default orientation identified well…



But aspect ratios are a problem…



Future Work



Control over rotation of grains in space allows for interesting microstructures….

Incorporate correlations between parameters into simulation process…

Use advanced statistical techniques to model output as a function of input rather than comparing simulations…

Ultimate goal is simulating microstructures from additively manufactured materials