Process-Structure Linkages for Grain Boundary Pinning During Grain Growth

CSE 8803/ME 8883 Fall 2015

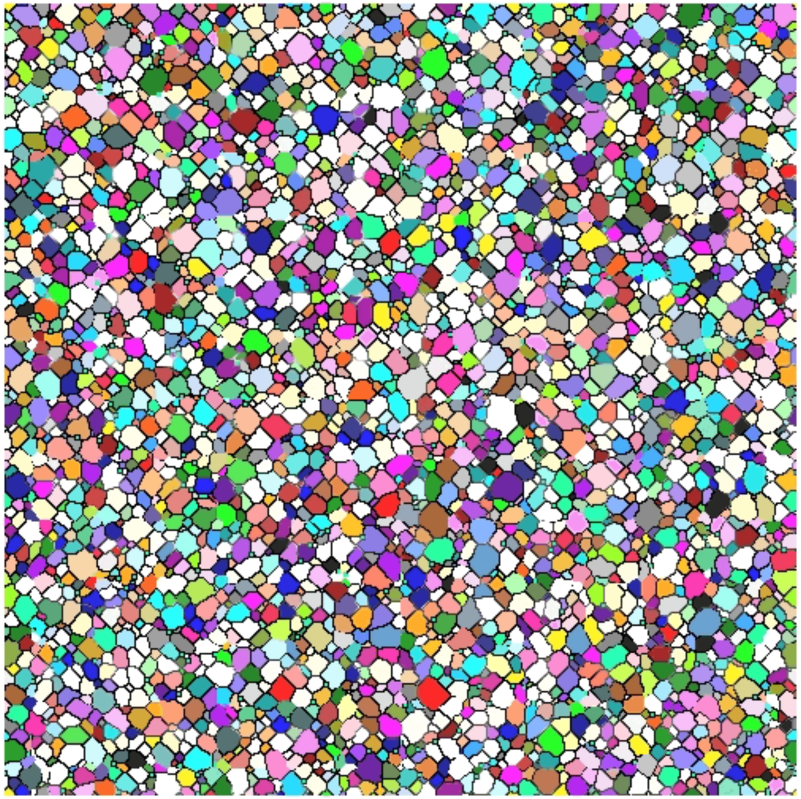
Frederick Hohman, David Montes de Oca Zapiain,
Evdokia Popova

Outline

- Background and Motivation
- Model Development (Data Driven)
- Results
- Conclusions

Background

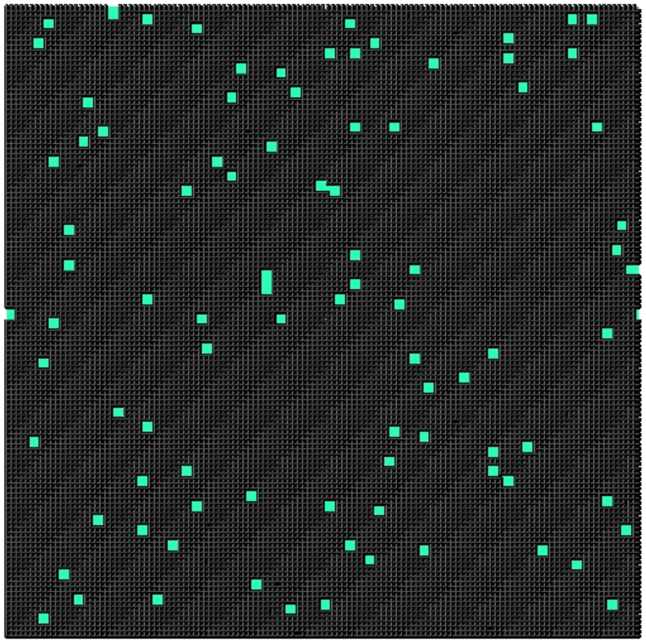
- The driving force for grain growth is the grain boundary interfacial free energy.
- Common practice in manufacturing to add "**pins**" to control the final grain size.



SPPARKS Grain Growth Simulations

- SPPARKS: a widely used open source tool to model pinned grain growth.
- SPPARKS uses Kinetic Monte Carlo equations to simulate the grain growth.

Sandia National Laboratories



Objective

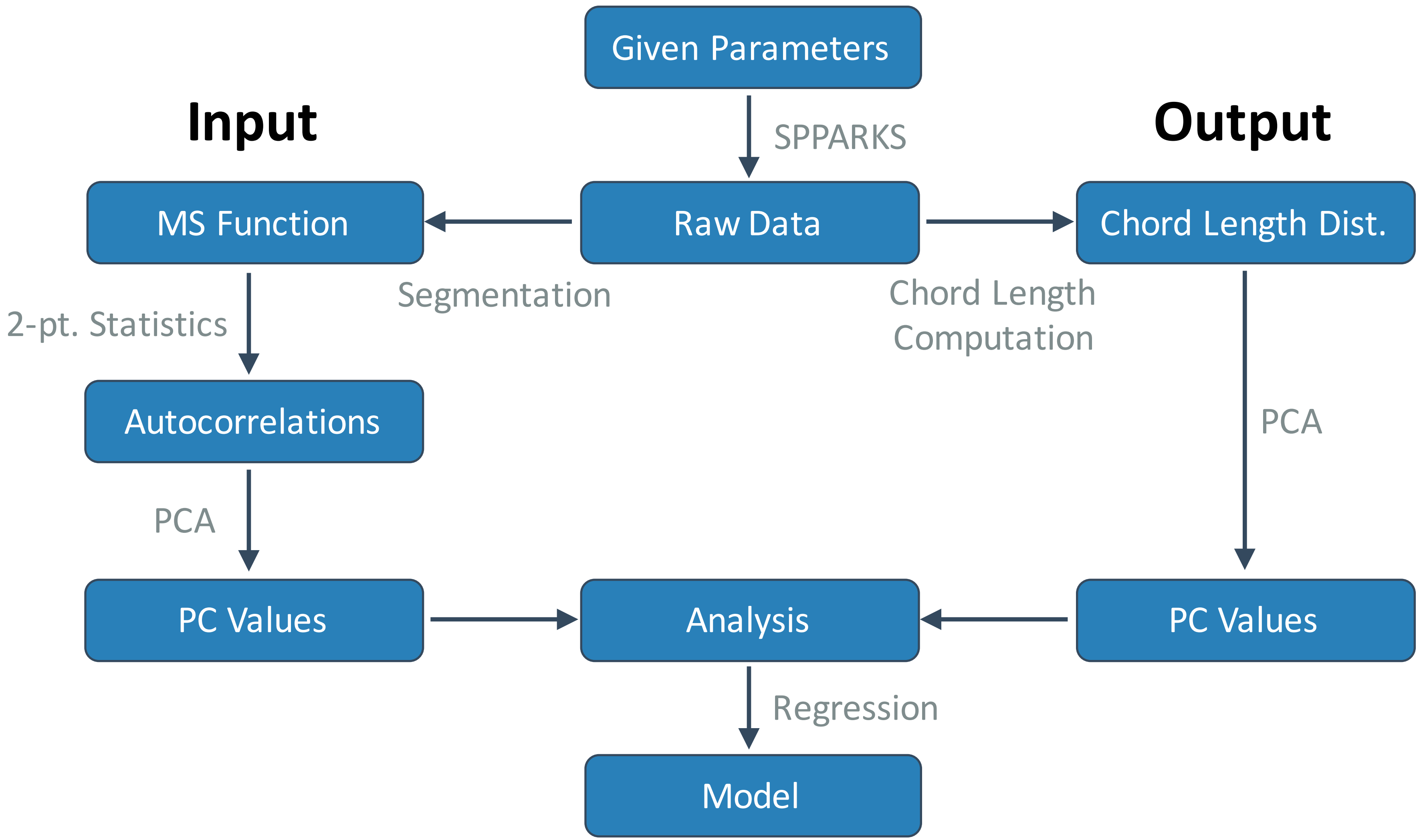
- Use **Data Science Approach** to extract **Process-Structure Linkages** for grain boundary pinning simulations during grain growth.
- Identify the correlations that exist between an initial **distribution of precipitates** and the **grain size** of a final microstructure.
- Build a **surrogate model** for SPPARKS grain growth simulations.

Data Science Approach

Four major steps for a material informatics problem.

I. Defining local states: 3-phase material (grains, boundaries, and pins)
II. 2-point statistics: autocorrelation of pins
III. PCA I/O, visualize with 3 components
IV. Model development: linear regression

Workflow / Data Pipeline



Data Generation

Simulation Parameters

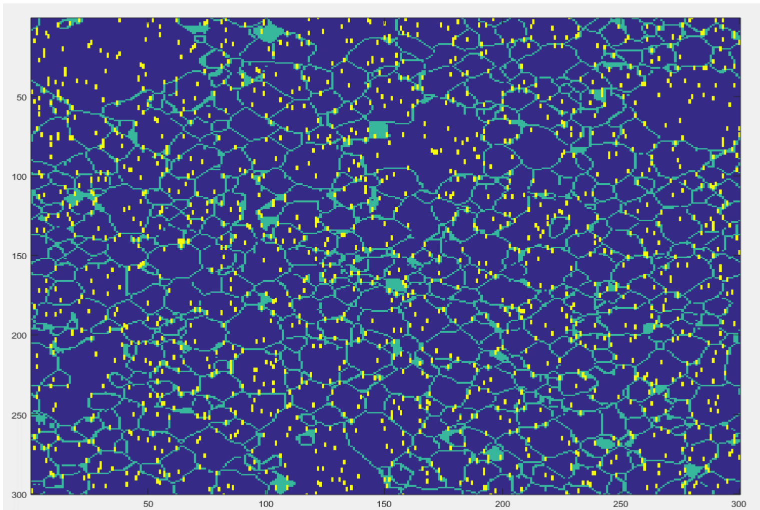
- 300x300x300 voxel microstructure
- Periodic boundary condition
- Randomized initial microstructure
- 20K Monte-Carlo time steps
- Constant temperature

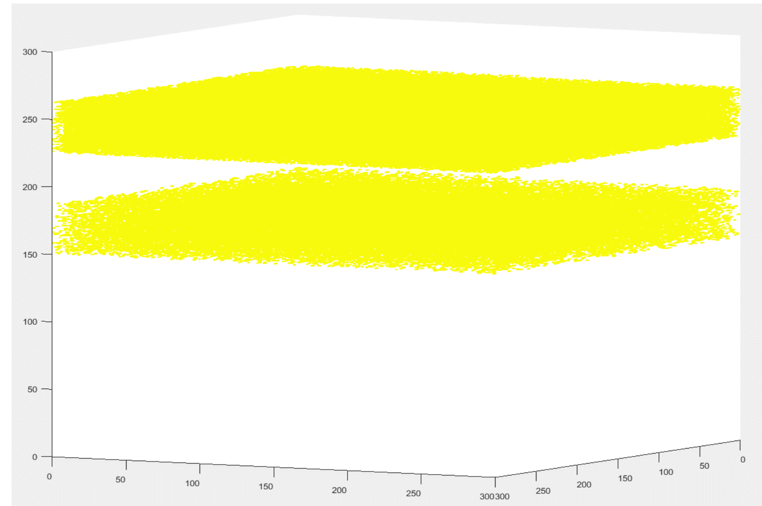
Data generated

- 5 different classes of precipitate distribution
- Total: **220** different grain growth simulations

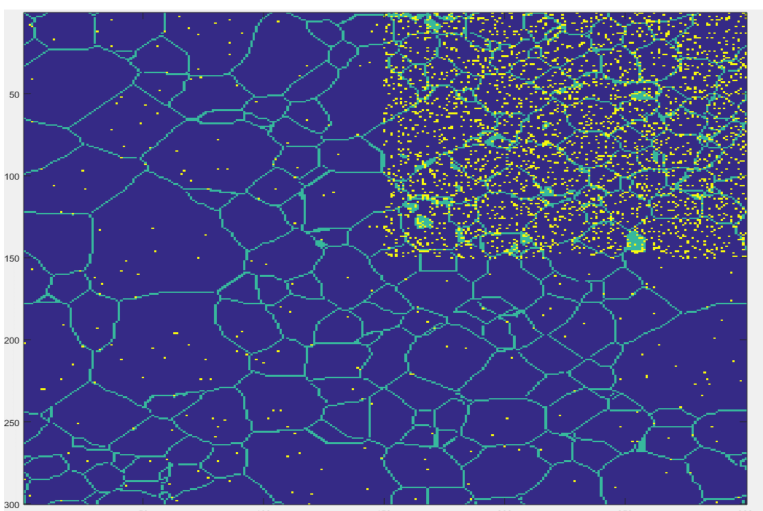
Precipitate Distribution Classes

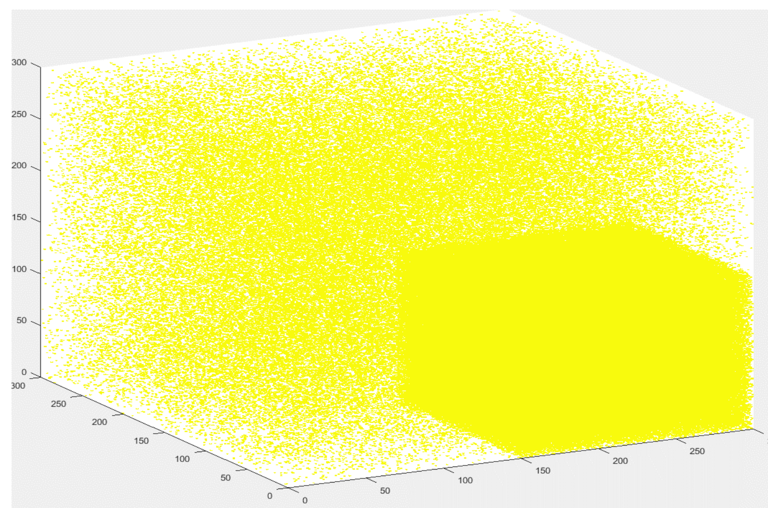
Band Cluster





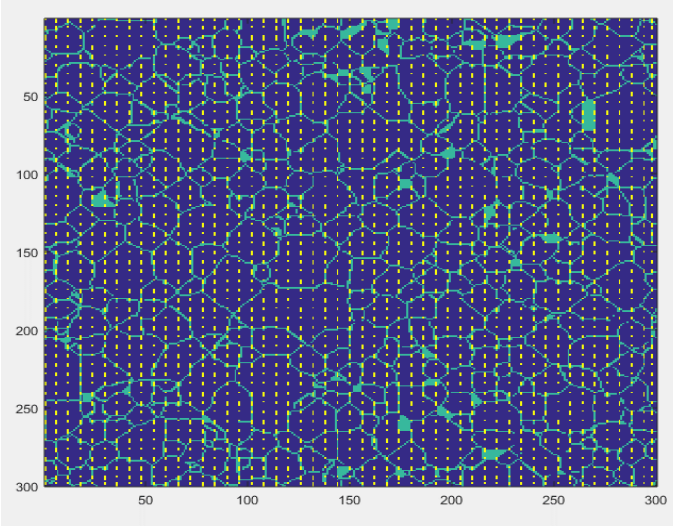
Quadrant Cluster

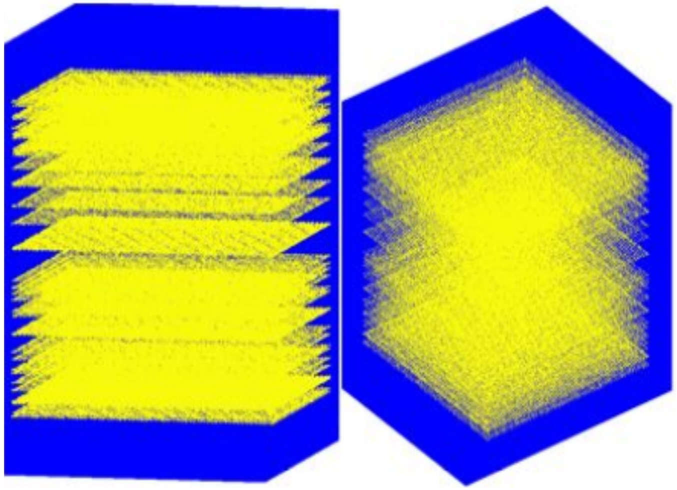




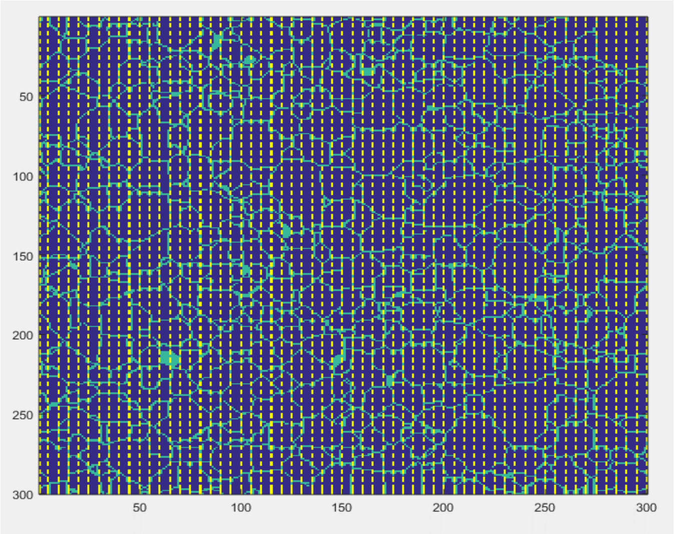
Precipitate Distribution Classes

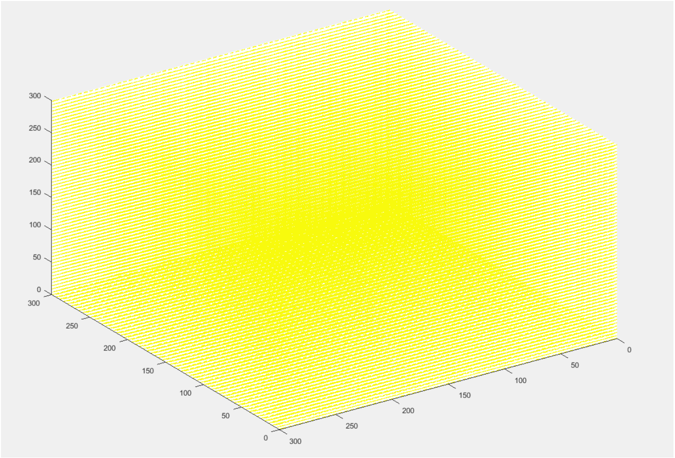
Rolling





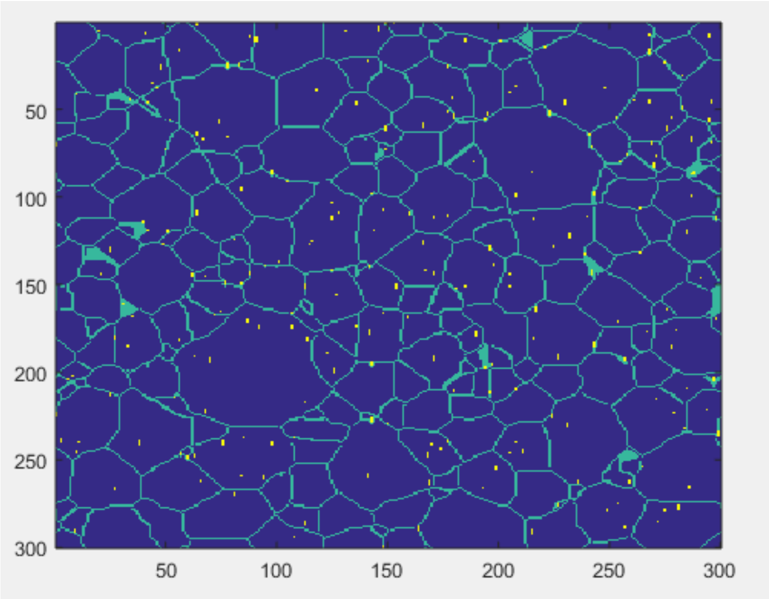
Uniform

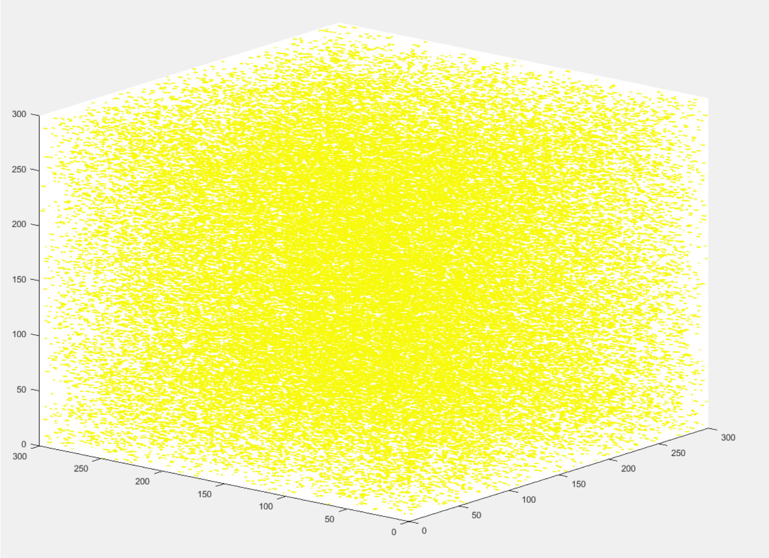




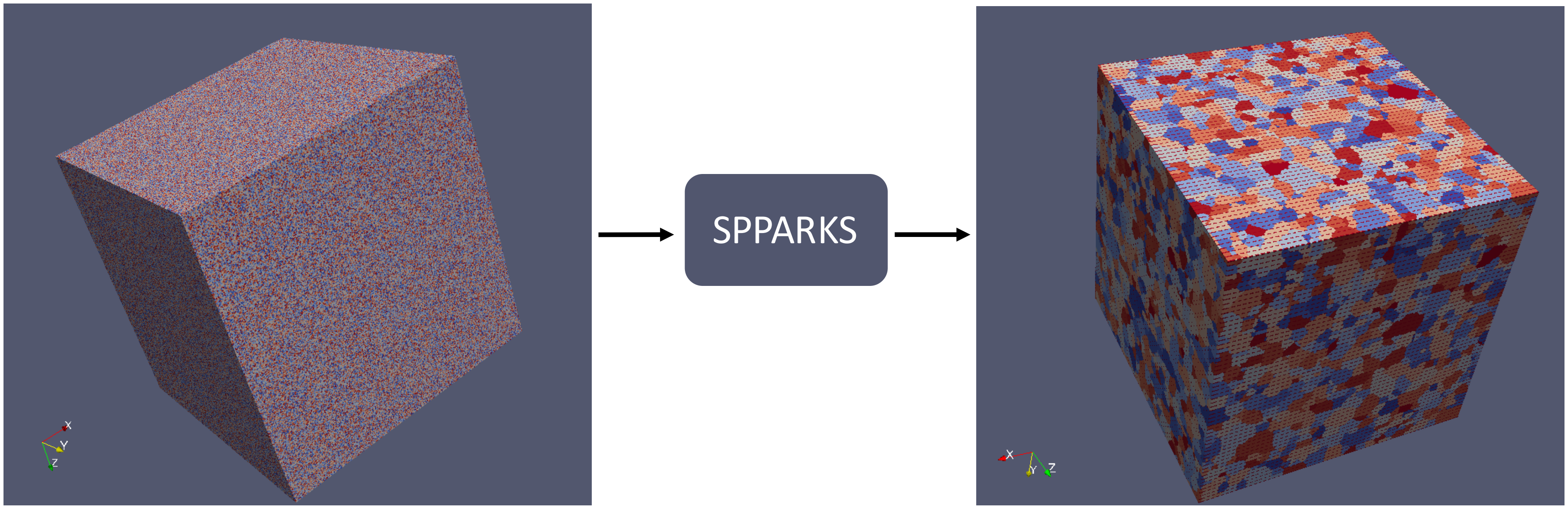
Precipitate Distribution Classes

Random





Input and Output of a Simulation



Input

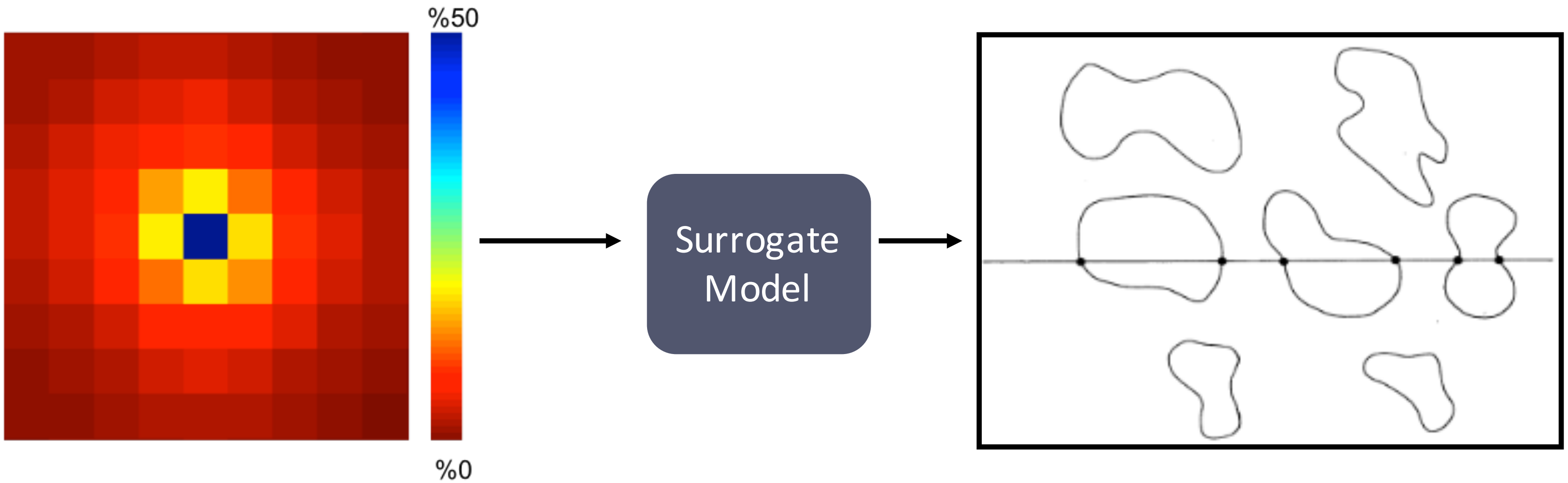
- Shape of precipitate (1, 2, and 3 voxel long precipitates)
- [.5%-3%] Volume Fraction of Precipitates
- Distribution of the precipitates

Output

- From which grain size distribution will be extracted

Define a correlation between process parameters and grain size distribution of a final microstructure to build a surrogate model.

Input and Output of the Surrogate Model

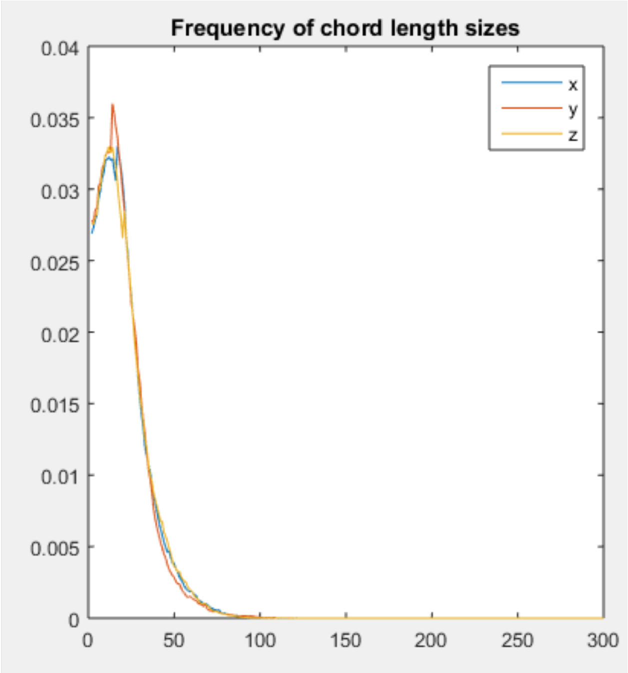


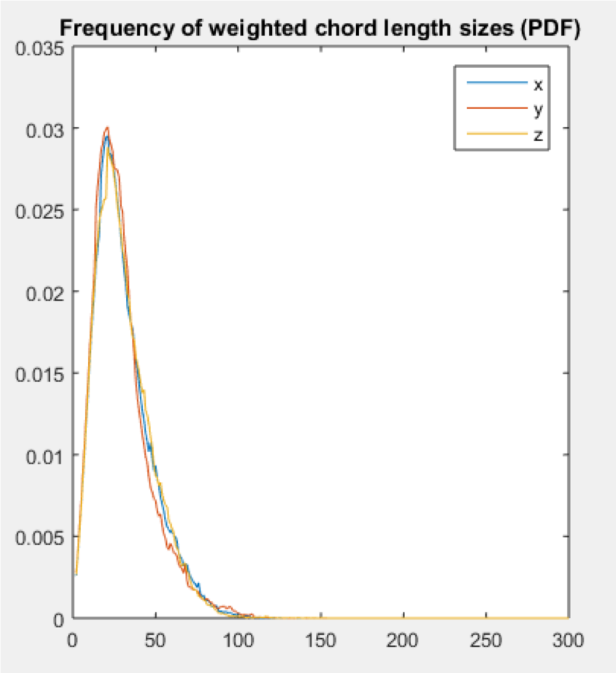
Input
2pt statistics
(autocorrelation of pins)

Output
Chord length distribution in the 3 orthogonal directions

Details on Chord Length Distribution

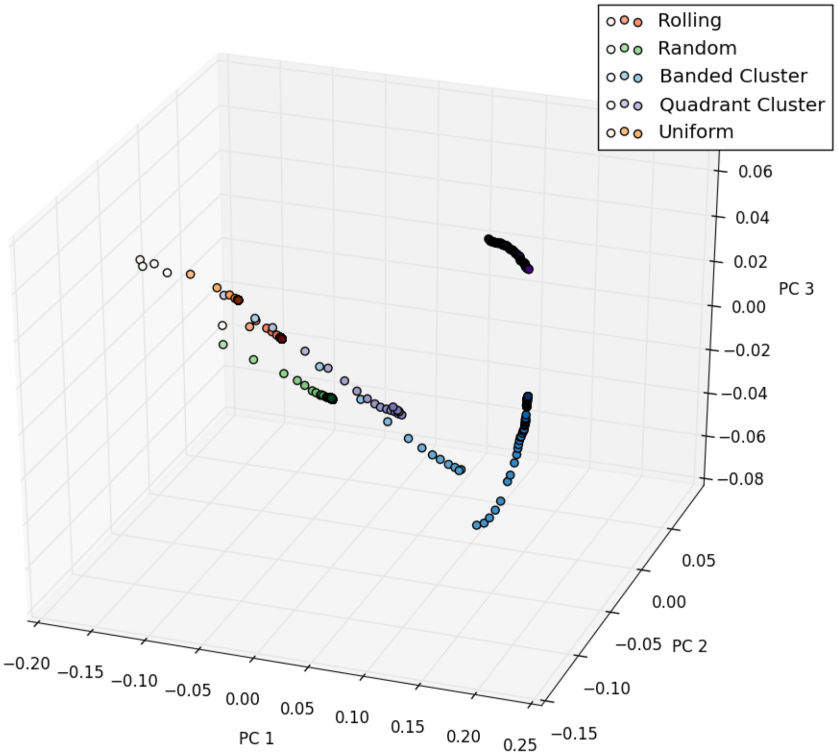
- Obtain a histogram of the different chord lengths in the three orthogonal directions.
- Assign a heavier "weight" to the bigger chords by multiplying frequency by its size and dividing by the cumulative sum.

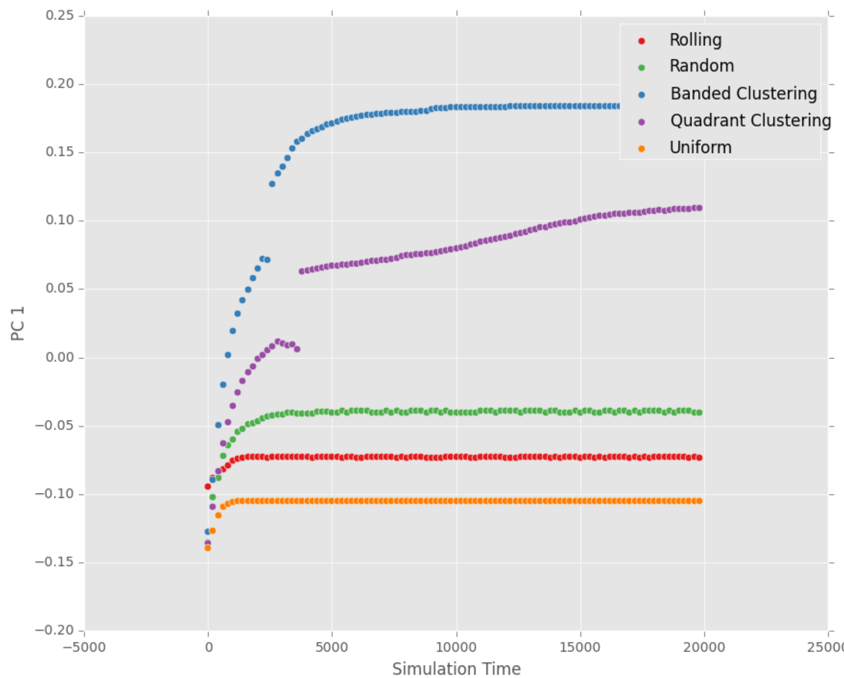




Confirming "Steady State"

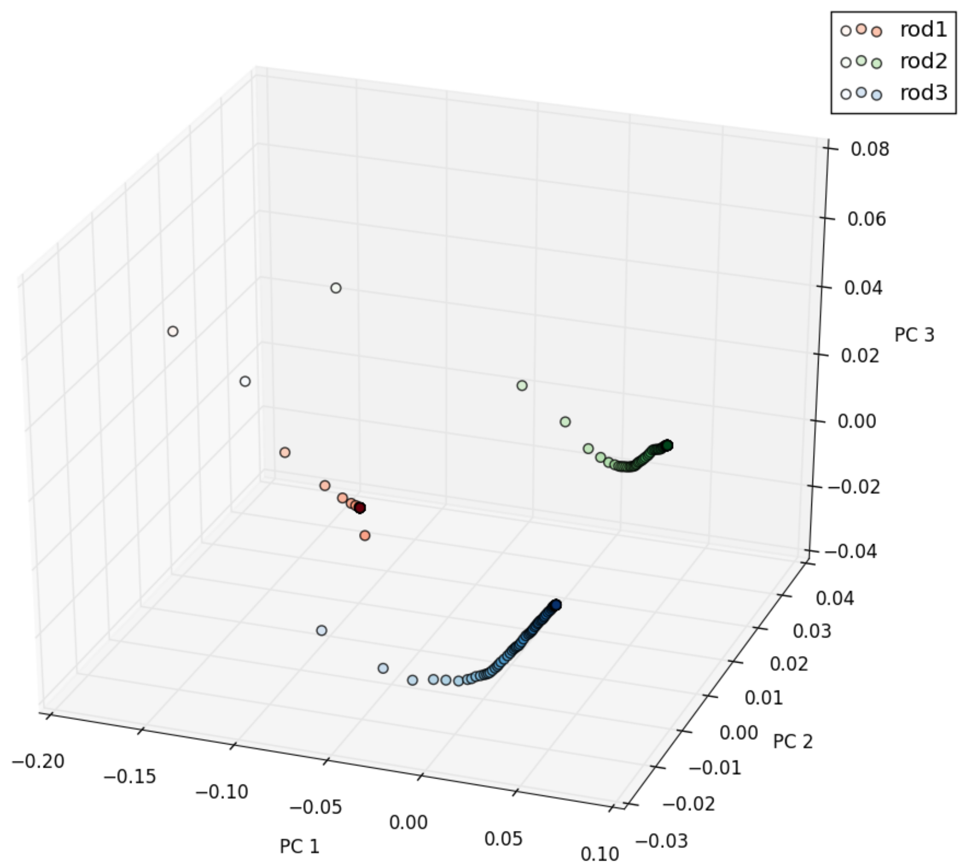
Verify SPPARKS simulation ran long enough to reach steady state.





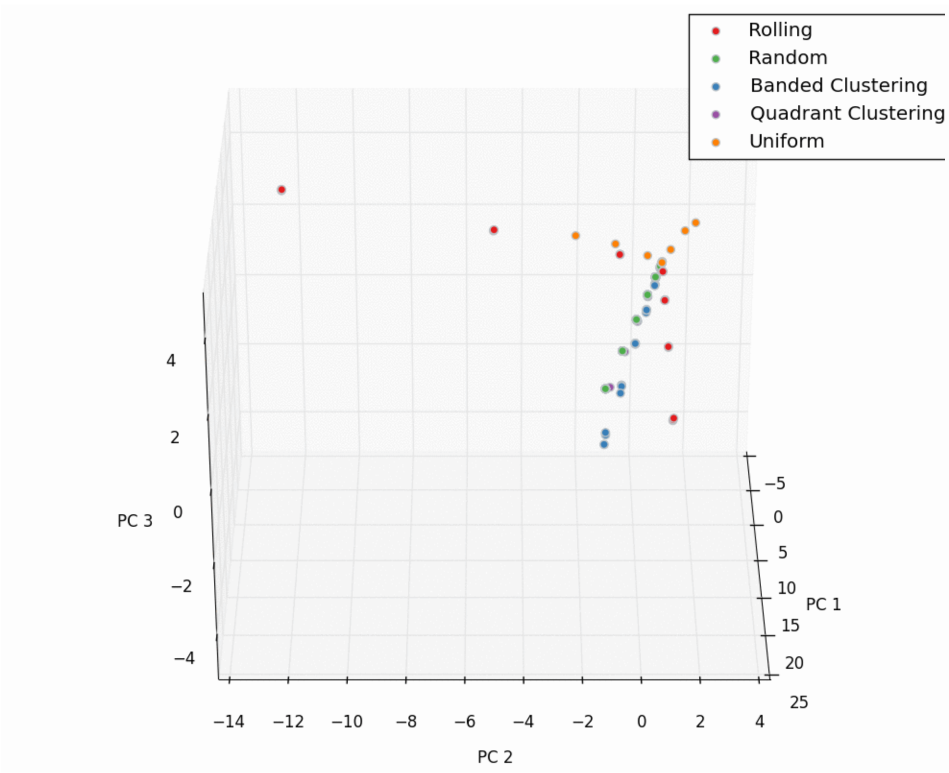
Confirming Output Effects

Verify pin shape affects chord length distribution.

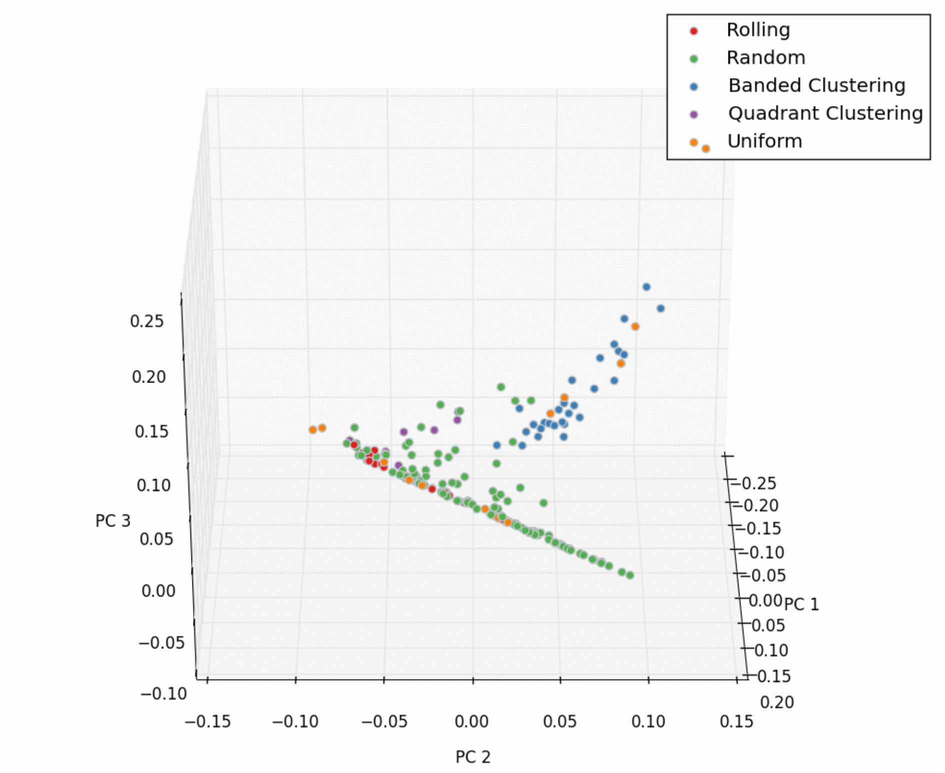


PCA: I/O

Input

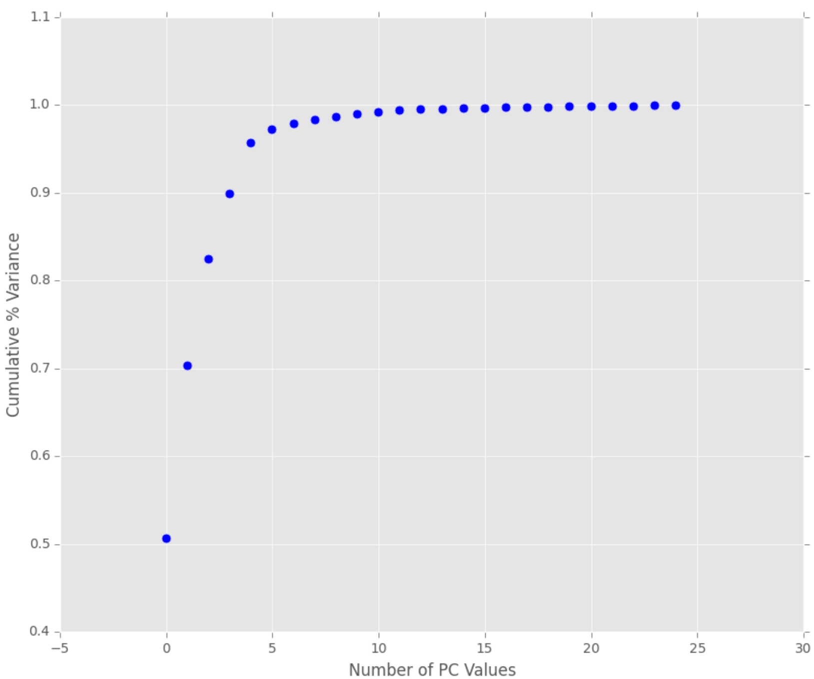


Output



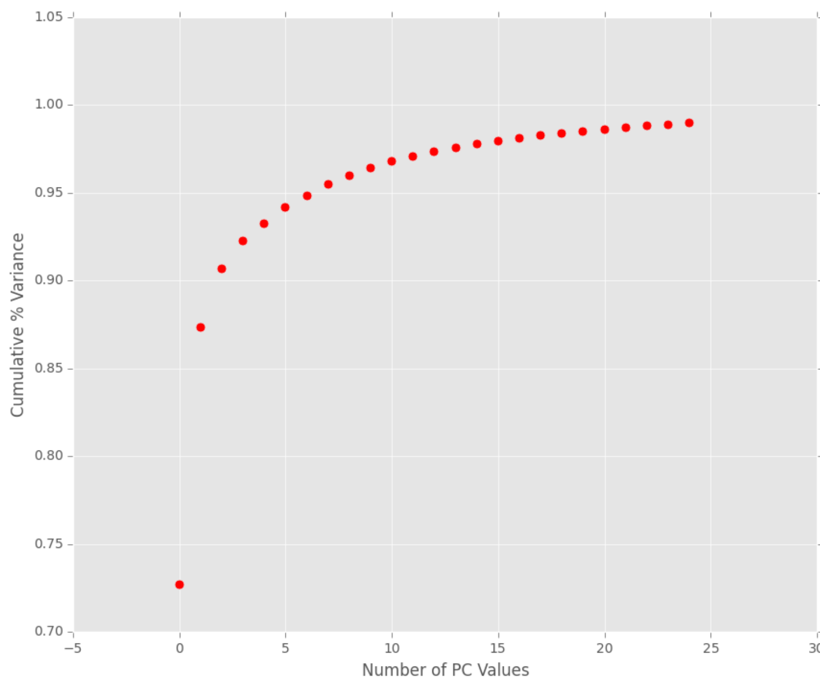
PCA: Scree Plot

Input



> 95% variance in first 5 PC components.

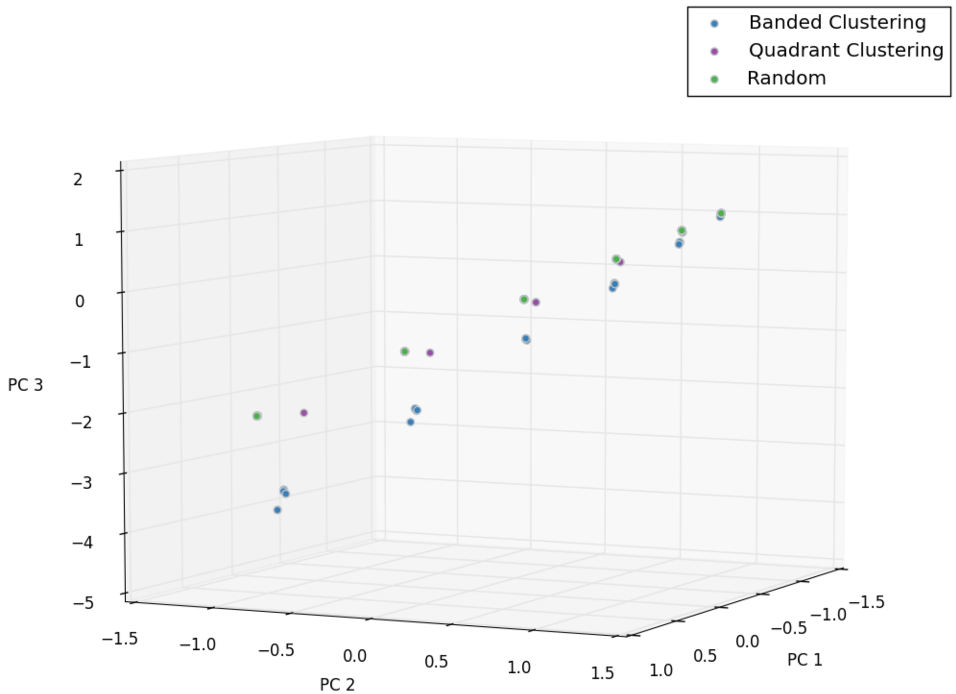
Output



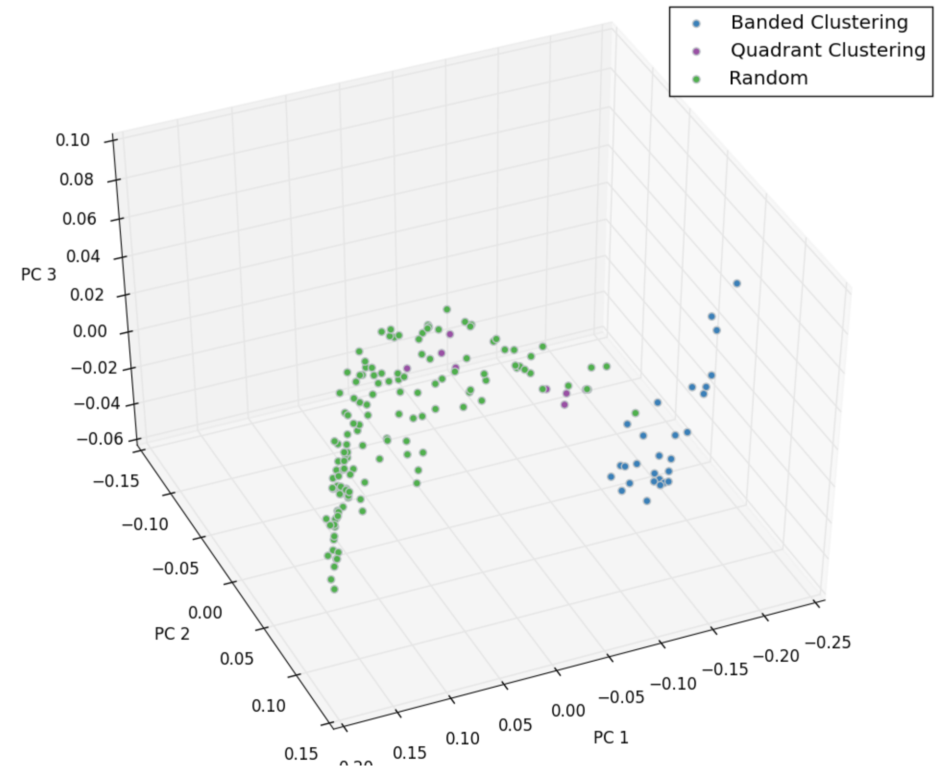
> 95% variance in first 8 PC components.

PCA: Trend Analysis I

Input

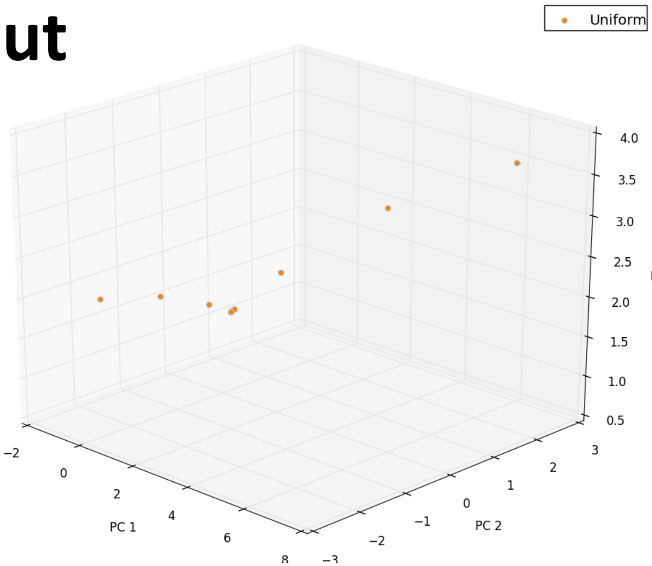


Output

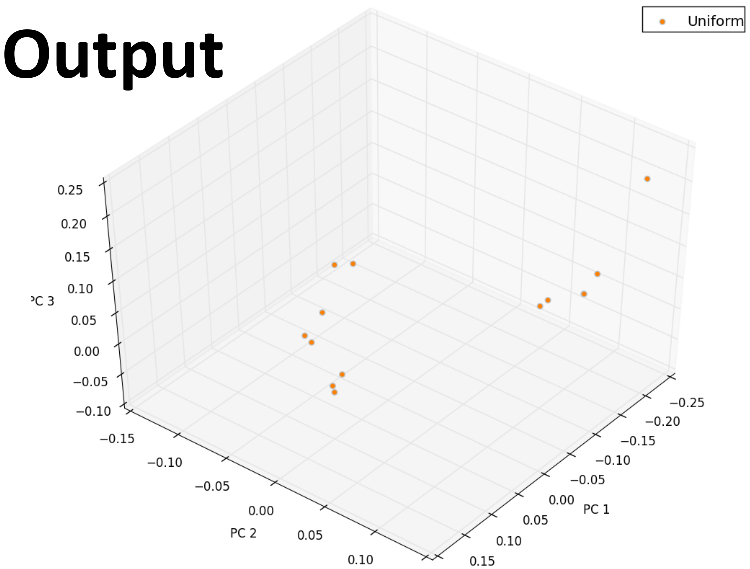


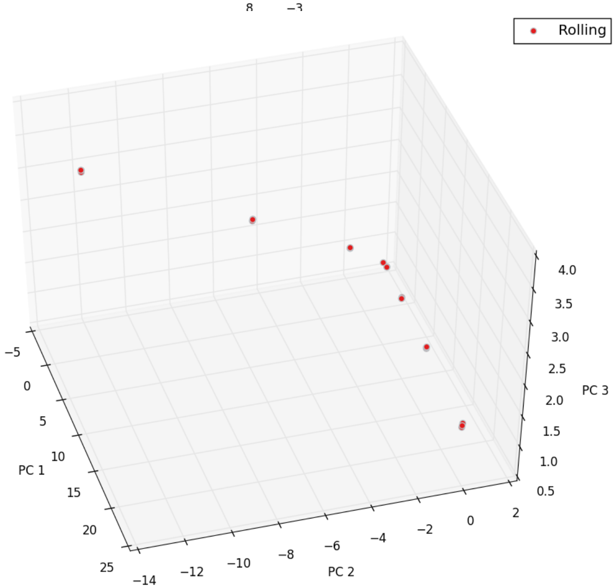
PCA: Trend Analysis II

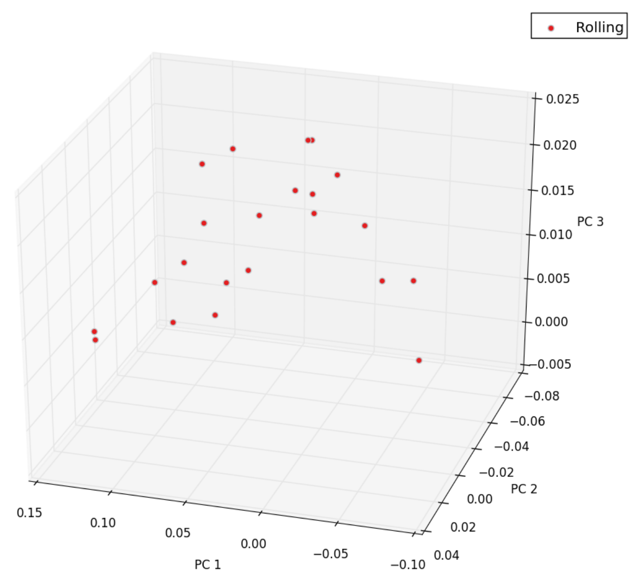
Input



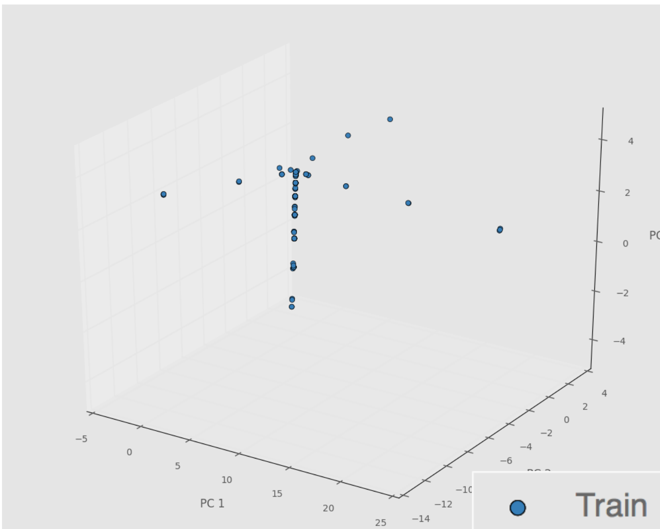
Output

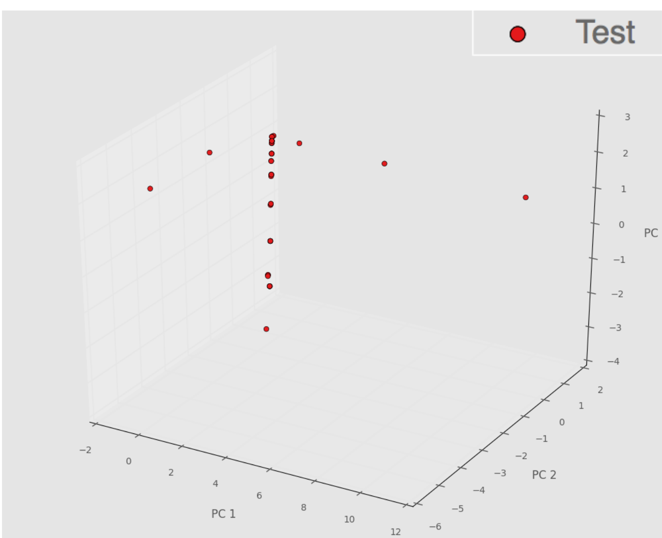




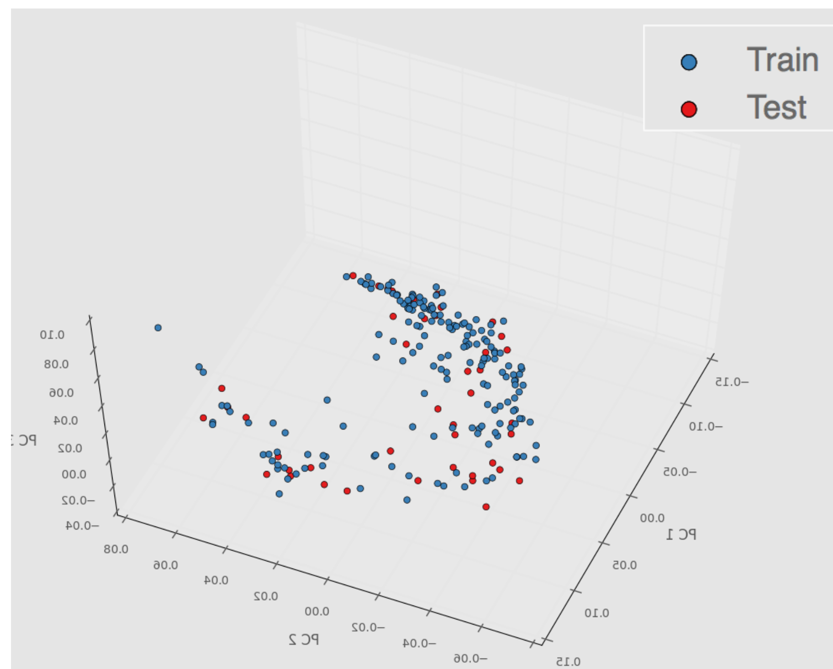


Regression



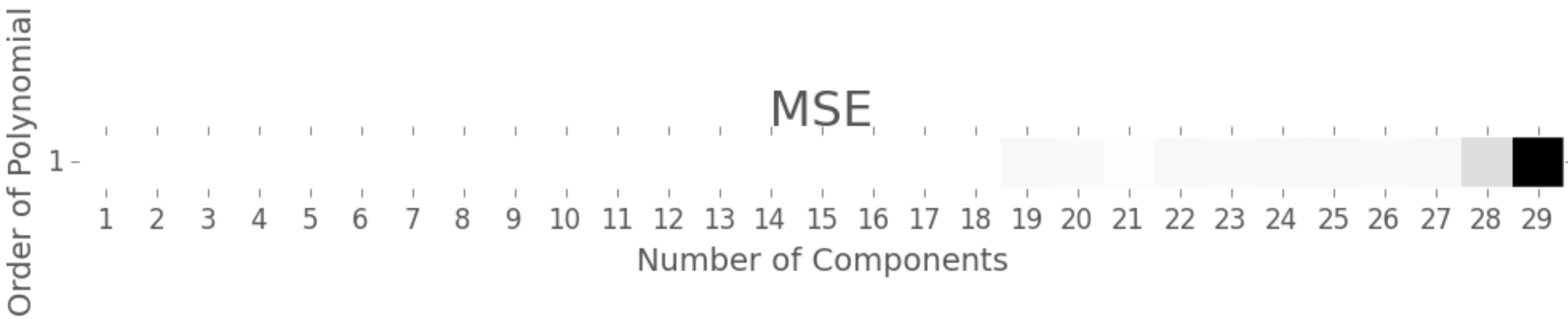


- Scikit-learn based linear regression
- Use 20% of our data to test



Regression Results

- Construct model for every combination of
  - Polynomial degree: [1-5]
  - Number of PC values: [1-30]
- Leave-one-out cross-validation to optimize MSE



Best Model

Linear Regression (Order 1 polynomial)

Number of Components: 10

MSE Value: 2.70392576062e-05

Conclusions

- Using novel data science tools a surrogate model is developed for grain boundary pinning problem during grain growth simulations.
- The work done establishes a **generalized**, **automated**, and **scalable** framework that can be extended to other models.

Future Work

- Evaluate current classes relevance.
  - Expand simulation pool to include more representative data.
- Expand model capabilities and predictions for newly generated data.
- Further model validation.

Acknowledgements

- Dr. Surya Kalidindi (GT)
- David Brough (GT, CSE)
- Ahmet Cecen (GT, CSE)
- Dr. John Mitchell (Sandia National Labs)

http://materials-informatics-class-fall2015.github.io/MIC-grain-growth/

References

- Gladman, T. (1966). On the theory of the Effect of Precipitate Particles on Grain Growth in Metals. Proceedings of the Royal Society of London.Series A, Mathematical and Physical Sciences (294), 298-309.
- Hillert, M. (1965). On the theory of normal and abnormal grain growth. Acta Metallurgica , 13, 227-238.
- Kalidindi, S. (2015). Hierarchical Materials Informatics. Oxford: Elsevier.
- Plimpton, S., Battaile, C., Chandross, M., Holm, L., Zhou, X., & al., e. (2009). Crossing the Mesoscale No-Man's Land via Parallel Kinetic Monte Carlo. Sandia report.
- SANDIA National Lab. (2009). SPPARKS Kinetic Monte Carlo Simulator. http://spparks.sandia.gov/index.html
- Wheeler, Daniel; Brough, David; Fast, Tony; Kalidindi, Surya; Reid, Andrew (2014): PyMKS: Materials Knowledge System in Python. figshare. http://dx.doi.org/10.6084/m9.figshare.1015761

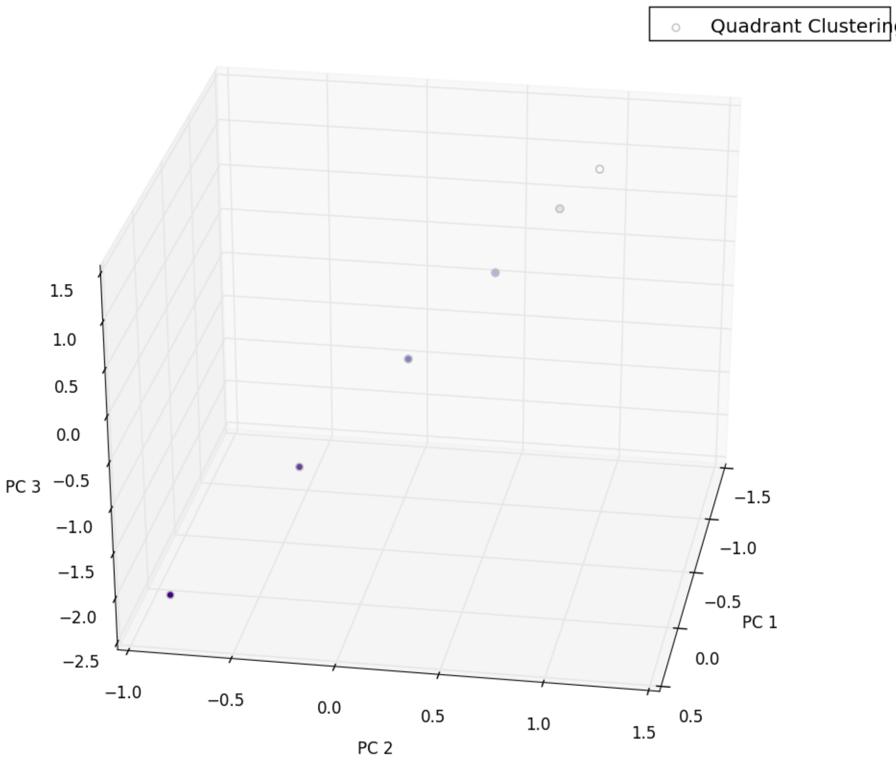
http://materials-informatics-class-fall2015.github.io/MIC-grain-growth/

Thank you for your attention!

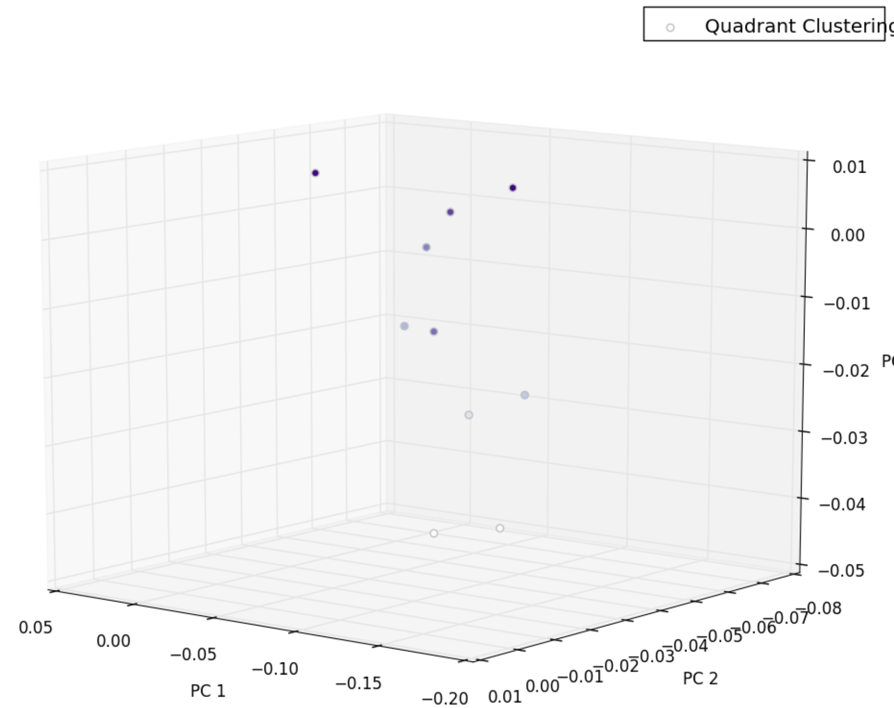
Questions?

PCA: Trend Analysis III

Input



Output



Varying percentage within one class show directionality.