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Simulating Additive Manufacturing with Potts Kinetic Monte Carlo and SPPARKS

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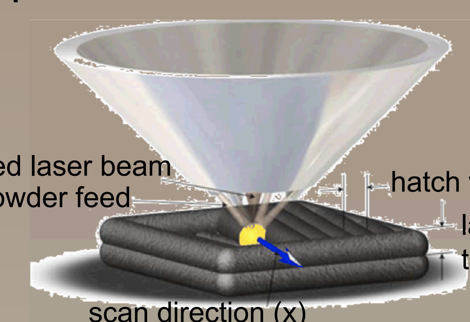
Introduction

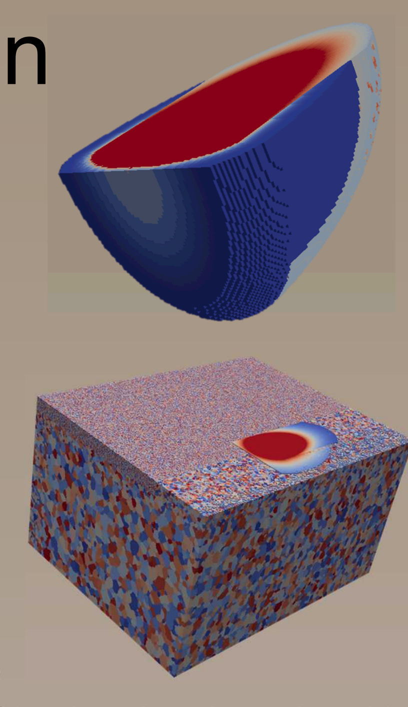
Additive manufacturing processes offer the ability to create metallic components with complex shapes without the expense and time commitment required with traditional approaches. However, the complex, non-uniform temperature histories of these processes result in materials with complex, anisotropic microstructures. Here, a Potts Kinetic Monte Carlo method is introduced to model microstructure evolution during additive manufacturing and autogenous welding processes, along with approaches to quantify and validate the results.



Schematic of LENS additive manufacturing process with adjustable process parameters

Model description

A user defined melt pool is scanned through the simulation domain on a specified trajectory. The material is represented as a cubic lattice of sites with “spins” that represent specific grains. When the melt pool travels through a lattice site, the spins are randomized and any existing grain assignment is lost. Rapid grain growth occurs in the high temperature region surrounding the melt pool, and results in the formation of elongated grains oriented along the temperature gradient.

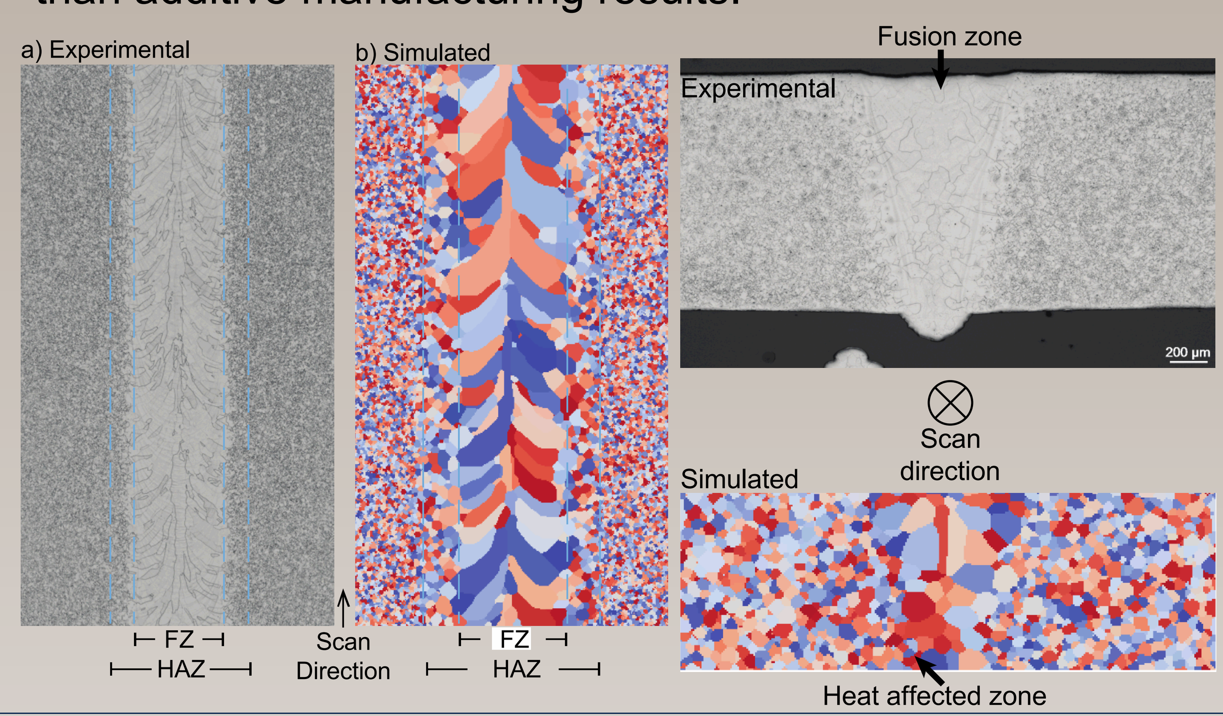


Simulated melt pool and in-process simulation domain

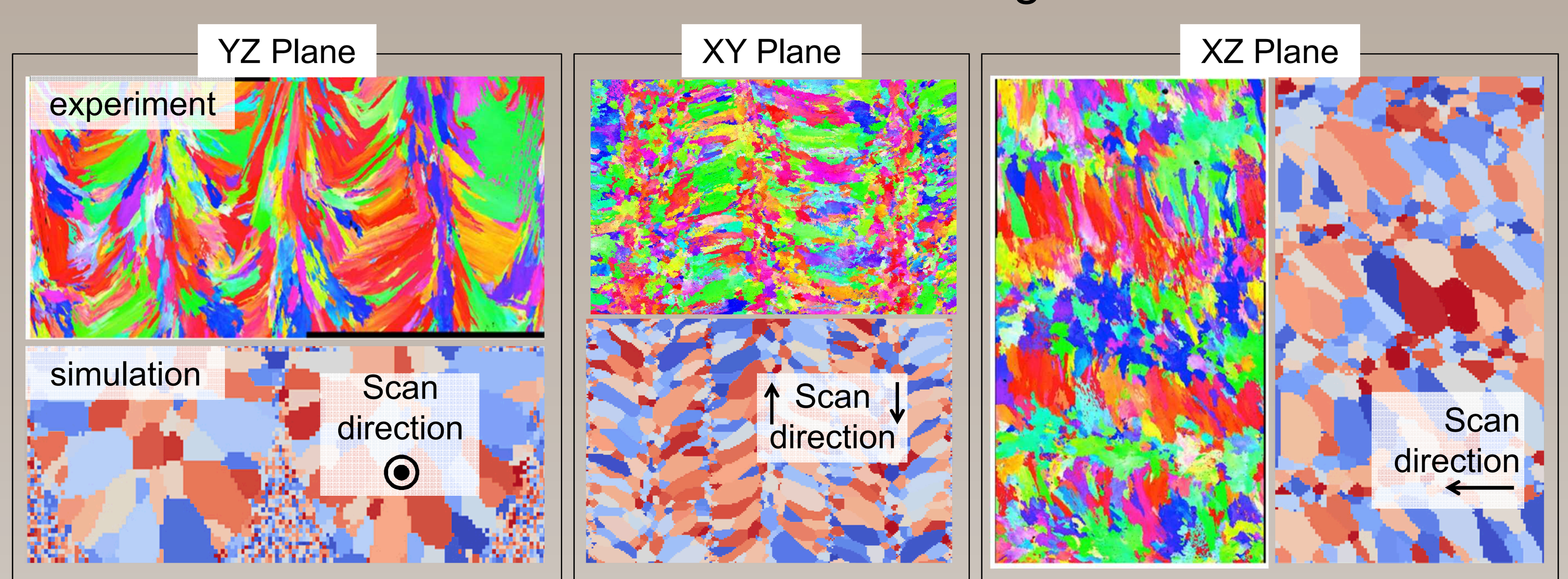
Qualitative Comparison with experiment

Autogenous welding

Autogenous welding experiments involve a single-pass of a heat source (typically an electron or laser beam) through a domain. The resulting microstructure contain oriented, elongated grains with a simpler overall structure than additive manufacturing results.



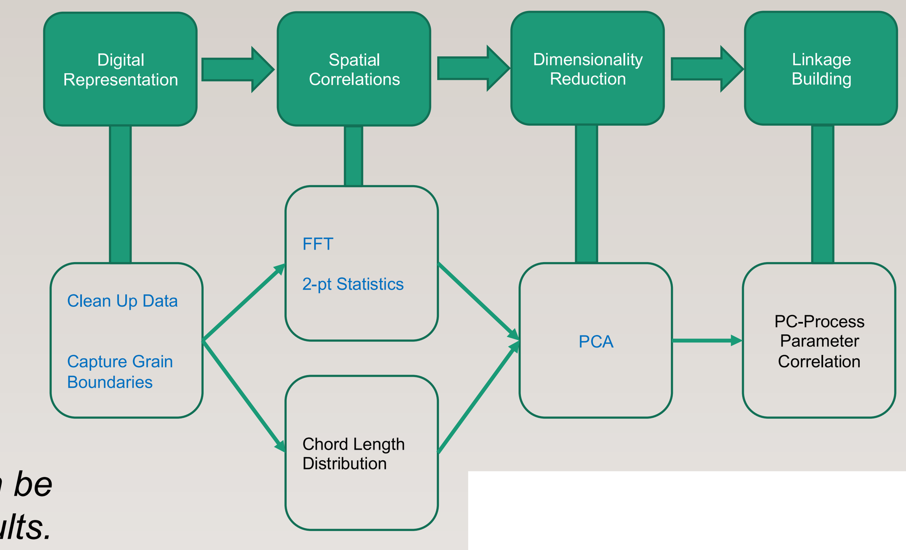
Laser Engineered Net Shaping (LENS) Additive manufacturing



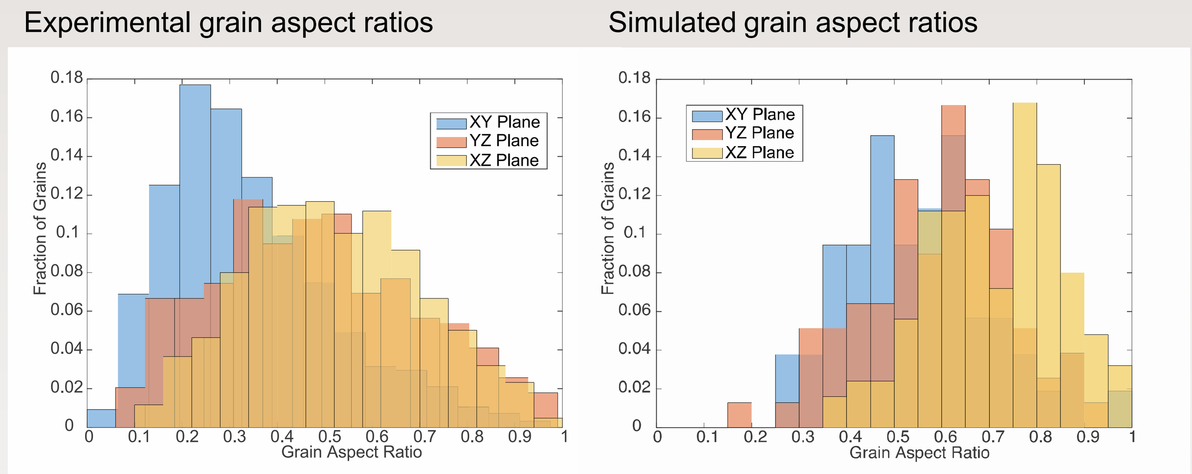
An important feature of additive microstructures is the anisotropic nature of the as-processed grain structures. This is demonstrated by comparison of experimental EBSD images with simulated grain structures. The simulations provide a reasonable reproduction of essential microstructure characteristics as shown above.

Quantitative Analysis Methods

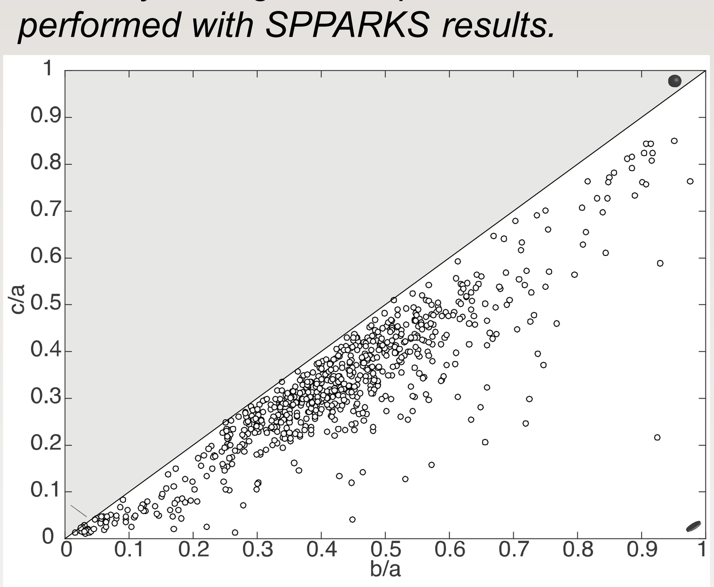
SPPARK simulation results allow for the application of several quantitative approaches, including 2D slice analysis, full 3D grain shape studies, and emerging data science approaches using n-point statistics and principle component analysis. Direct, quantitative comparisons between simulation and experimental microstructures, such as grain size, shape, and orientation distributions, are also possible.

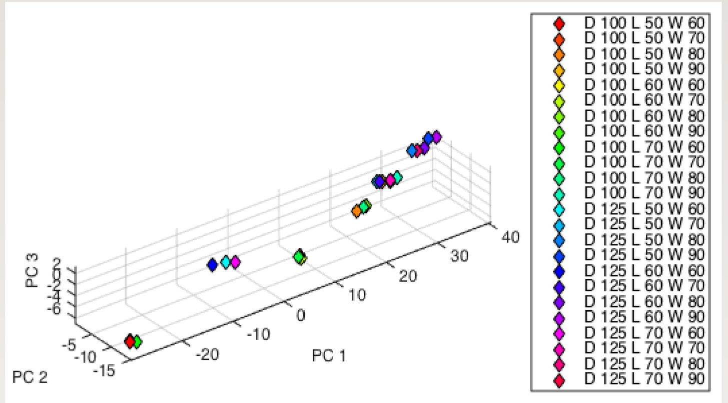


2D slices of experimental and simulated microstructures can be compared directly.



3D analysis of grain shape can be performed with SPPARKS results.

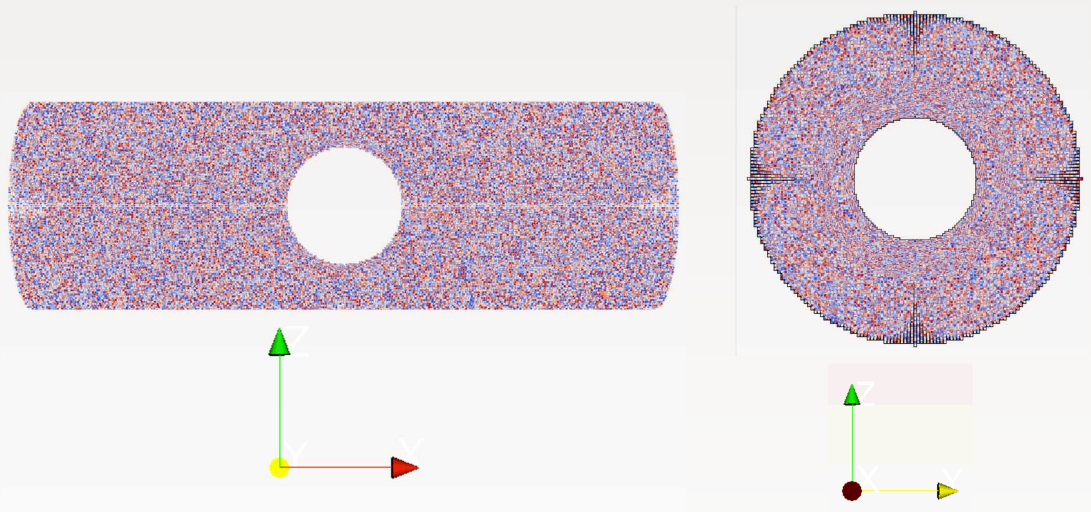




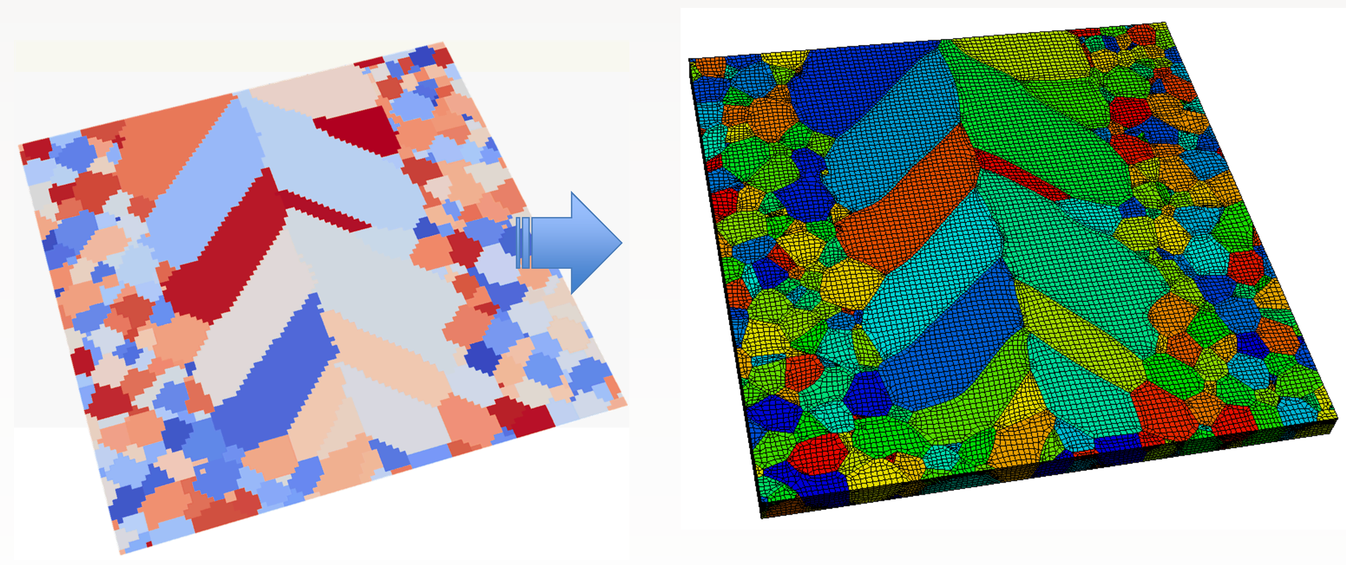
Data science-based approaches are in development to determine process-property linkages from complex grain structures (in conjunction with Surya Kalidindi, Andriy Dotsenko, Xinyi Gong, and Evdokia Popova at Georgia Tech)

Ongoing work

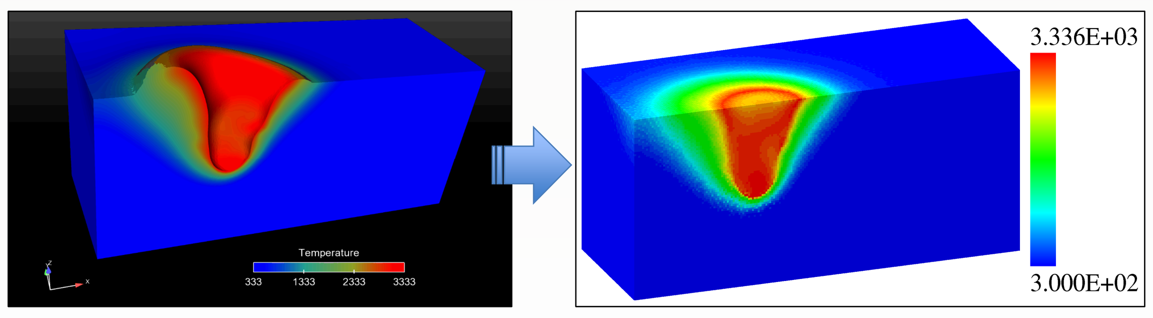
Current work is focused on improving the simulation’s integration within the process-structure-property linkage through the implementation of more realistic melt pool physics and the implementation of component-shaped domains for mechanical behavior simulations.



Extension to component-shaped domains (Joe Bishop, Org. 1554)



Meshing output microstructures for material mechanics simulations (Hojun Lim, Org. 1814 and Ben Reedlunn, Org. 1554



Incorporating more rigorous physics models for melt pool behavior (Mario Martinez, Org. 1516)

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