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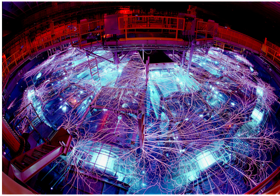

Employing a Bézier curve model for simulating microstructure generation during the AM process

WCCM-ECCOMAS Congress 2022

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U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

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Outline

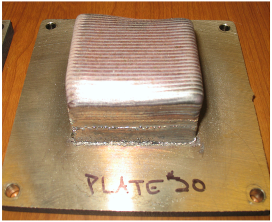
1. Background and motivation
2. Goals
3. The model
4. Comparisons with experiments
5. Future work
6. Conclusions and acknowledgments

Background and Motivation

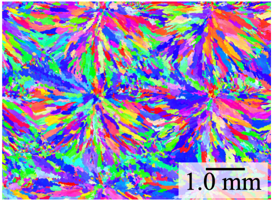
In additive manufacturing (AM), material is incrementally and layerwise added to a part by fusing it together with existing material using a moving heat source.

Challenges:

1. Length scale.
2. Complex multiphase material physics, 3D heat transfer, and fluid flow.
3. Complex AM process of layerwise material deposition, fusion, and solidification.



(a) AM block of SS 304L [1]



(b) EBSD image of SS 304L [1]

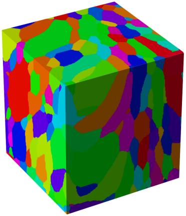
[1] Adams, David, et al. "Mechanical response of additively manufactured stainless steel 304L across a wide range of loading conditions." Sandia National Laboratories. SAND2019-7001, 2019.

Goals

- Develop a reduced-order model which can predict the evolution of microstructure in the AM process.
- Model is applicable to multiple AM processes, e.g., powder bed fusion and Laser Engineered Net Shaping.
- Enable microstructure aware simulations of AM component parts.

Grain Evolution Model

1. Domain is discretized into lattice sites.
2. Spins are assigned to sites and groups of contiguous sites with the same spin correspond to grains.
3. Grain evolution is simulated with a modified Potts Metropolis Monte Carlo model.
4. The growth of grains is driven by the normal curvature-driven grain growth model; however, there is a temperature-dependent grain boundary mobility.



Grains in an AM block.

[2] Rodgers, Theron, et al. "Predicting mesoscale microstructural evolution in electron beam welding." Jom 68 (5). 2016. 1419-1426.

[3] Rodgers, Theron, et al. "A Monte Carlo model for 3D grain evolution during welding." Modelling and Simulation in Materials Science and Engineering 25 (6). 2017.

Grain Evolution Model

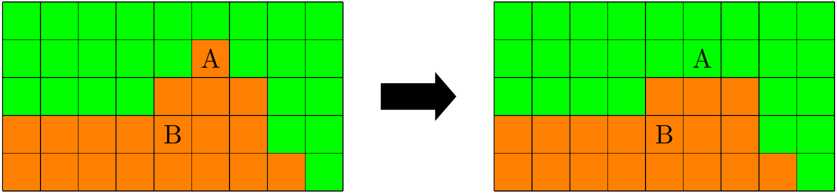
The grain boundary energy for a site i is given by

$$E_i = \frac{J}{2} \sum_{j}^{n} (1 - \delta_{ij}) \,. \qquad (1)$$

The probability P_i of site i changing its spin to that of the selected dissimilar neighboring site is estimated as

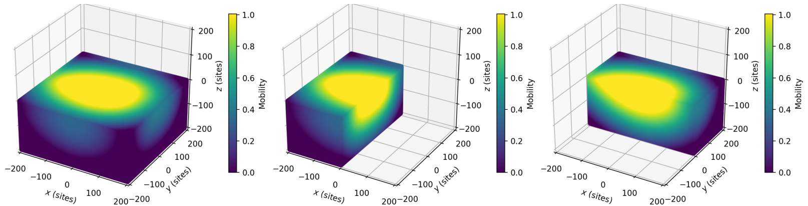
$$P_i = \begin{cases} M & \Delta E_i \leq 0 \\ M e^{-\frac{\Delta E_i}{kT}} & \Delta E_i > 0 \end{cases} , \qquad (2)$$

where T: temperature, k: Boltzmann constant, and M: mobility.



Surrogate Temperature Profile

- We employ a geometric representation of the melt pool.
- The temperature profile is simulated by propagating the melt pool through the material domain.
- The mobility is made a function of the distance from the melt pool, $M(\mathbf{x}) = 1 - \frac{d(\mathbf{x})}{mz}$ for $d(x) < mz$.



Bézier Curves

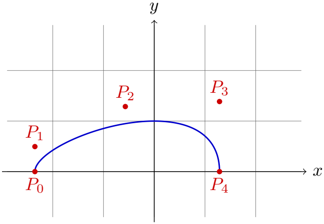
The **Bernstein polynomials** of degree n are defined by

$$B_{i,n}(u) := \frac{n!}{i!(n-i)!} u^i (1-u)^{n-i}, \quad i \in [0, 1, \ldots, n], \quad u \in [0, 1]. \quad (3)$$

A **Bézier curve** in dimension d of degree n is defined by

$$\mathbf{C}(u) := \sum_{i=0}^{n} \mathbf{P}_i B_{i,n}(u), \quad u \in [0, 1], \quad (4)$$

where $\{\mathbf{P}_i\} \in \mathbb{R}^d$ are referred to as control points and govern the shape of the curve.

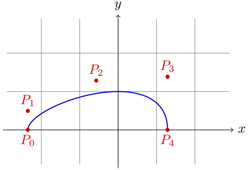


Fourth-order Bézier curve.

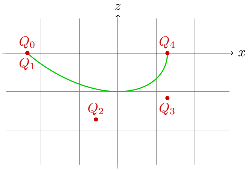
Melt-Pool Geometry

- Two fourth-order Bézier curves $C^{\text{surf}}(u)$ and $C^{\text{spine}}(u)$ are employed to define the surface and spine of the melt pool.
- The melt pool boundary is formulated as a degree three Bézier curve $\mathbf{S}^{\beta}(u, v)$ with control points $R_i[u]$ defined by the functions $\mathbf{C}^{\text{surf}}(u)$ and $\mathbf{C}^{\text{spine}}(u)$:

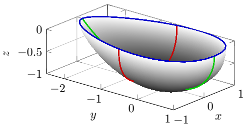
$$\mathbf{S}(u, v) := \sum_{i=0}^{3} \mathbf{R}_i[u] B_{i,3}(v), \quad u \in [0, 1], \quad v \in [0, 1]. \qquad (5)$$



(a) Surface boundary with control points.



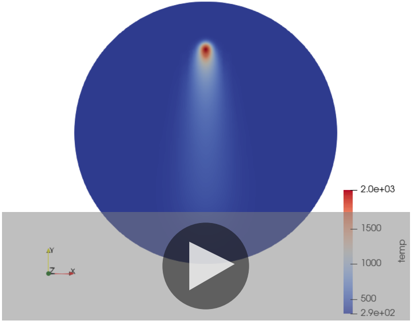
(b) Spine boundary with control points.



(c) Melt pool boundary with surface and spine curves.

Simulated Melt Pool

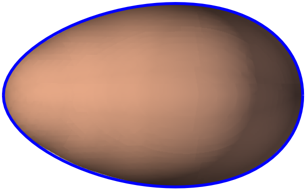
- There are several challenges to determining the melt pool shape experimentally.
- We simulated a heat source moving through the medium and captured a contour of the melt boundary.



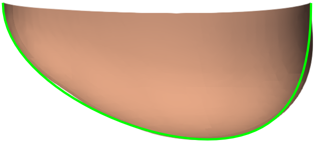
Fitting a Bézier Melt Pool to the Simulated Pool

Steel	x	y	z
P_0	-2.2597	0.00000	0.00000
P_1	-2.2597	0.85711	0.00000
P_2	1.29865	1.50644	0.00000
P_3	2.23368	0.88308	0.00000
P_4	2.23368	0.00000	0.00000

Steel	x	y	z
Q_0	-2.2597	0.00000	0.00000
Q_1	-2.2597	0.00000	-0.78114
Q_2	1.29865	0.00000	-1.62087
Q_3	2.23368	0.00000	-1.78114
Q_4	2.23368	0.00000	0.00000



(a) Surface curve with simulated MP.



(b) Spine curve with simulated MP.

SPPARKS (Stochastic Parallel PARticle Kinetic Simulator)

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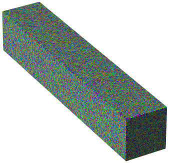
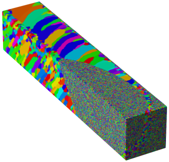
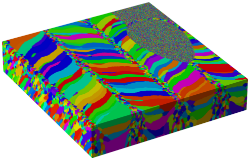
- SPPARKS is a parallel Monte Carlo code for lattice models [4].
- The model is implemented as an application “am_ bezier”.



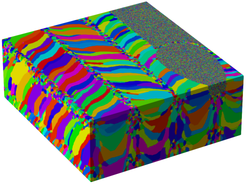
(a) Sites are randomly initialized.



(b) First pass.



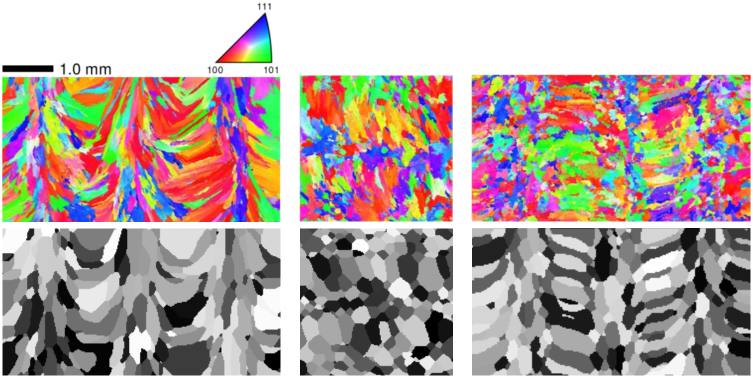
(c) First layer.



(d) Second layer.

[4] S. Plimpton, et al. Crossing the mesoscale no-man’s land via parallel kinetic Monte Carlo. Tech. Rep. SAND2009-6226. Sandia National Laboratories. 2009.

Comparison with experiments



X-Cut Y-Cut Z-Cut

EBSD microstructures (top) [1] compared with SPPARKS am_bezier generated microstructures (bottom). EBSD coloring corresponds to crystallographic orientation while the grayscale for the simulated microstructure distinguishes grains.

Future work

- Simulate multiphase materials.
- Consider other AM processes, e.g., powder bed fusion.
- Include the temperature profile into the simulation instead of distance.
- Develop microstructure aware models.

Conclusions and Acknowledgements

- Developed a model describing microstructure evolution during the AM process.
- Implemented the model into the parallel Monte Carlo code SPPARKS.
- Compared simulated microstructure with EBSD data for stainless steel 304L.

Acknowledgments

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