Comparison of cellular automata and continuum phase-field models for grain growth estimation

Harrison Williams[a,b], David Korba[a,b], Dr. Like Li[a,b], and Dr. Matthew W. Priddy[a,b]
[a]Department of Mechanical Engineering, Mississippi State University, Mississippi State, MS, 39762;
[b]Center for Advanced Vehicular Systems, Starkville, MS, 39759

MISSISSIPPI STATE UNIVERSITY

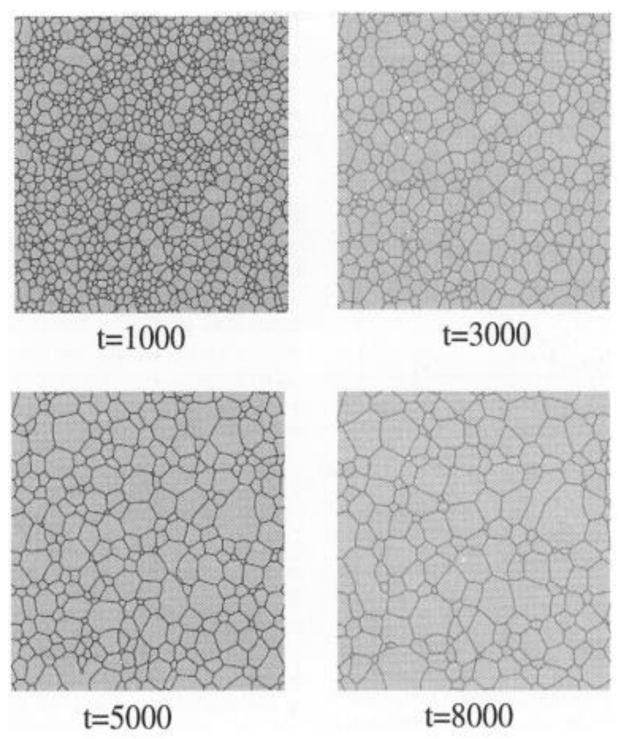
CMML Computational Mechanics and Materials Laboratory

Motivation

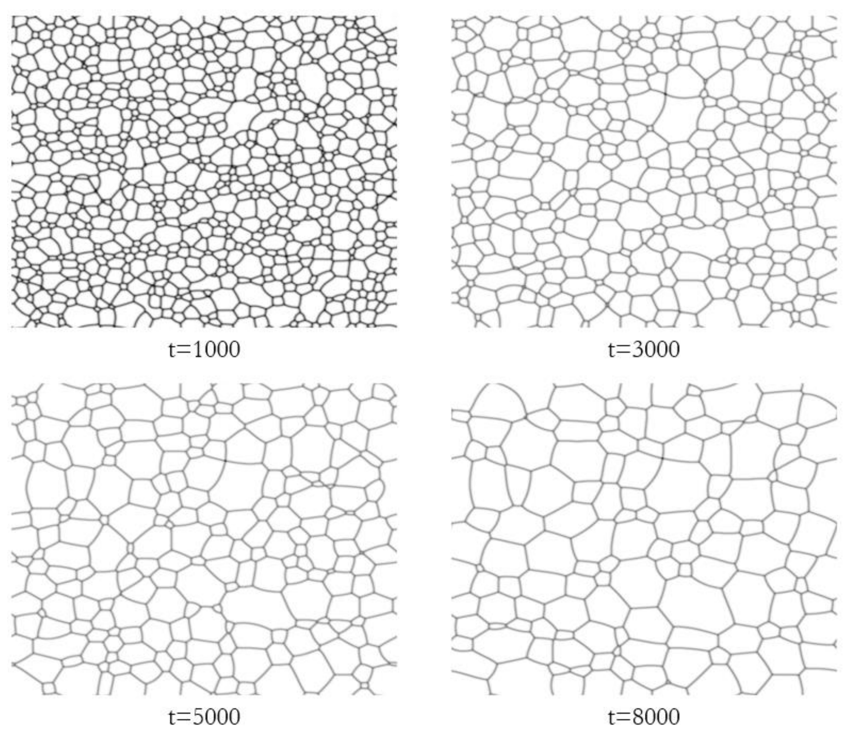
This work focuses on investigating the utility of cellular automata (CA) and phase-field (PF) modeling for estimating grain growth during additive manufacturing (AM) processes. Microstructure information, such as grain size and shape, was gathered via the two methods and will be used to inform higher length scale, thermomechanical models. The repeated thermal cycles in metal-based AM processes result in heterogeneous microstructures and can significantly affect the resultant mechanical properties. In addition, an informed thermomechanical model accurately predicts these changes in mechanical properties and ultimately allows for the study of residual stresses in AM parts.

Phase-field

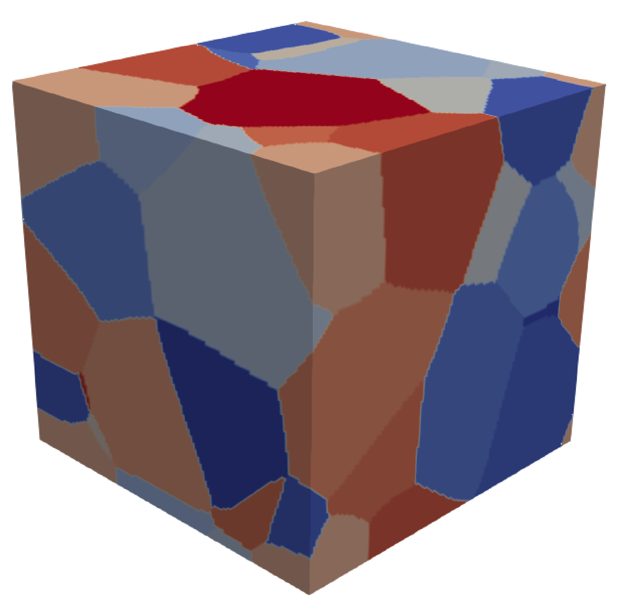
PF is a phenomenological model that is heavily used in studies of dendritic solidification, viscous fingering, hydrogen embrittlement, and vesicle dynamics. However, PF is also a suitable method for estimating grain growth. PF is well known for its ability to describe interface geometry, grain mobility/orientation, and morphological change in microstructure evolution based on the total free energy of the material.



1.a. Fan-Chen 2D, 1997 [1]



1.b. Fan-Chen 2D, 2022



1.c. Fan-Chen 3D

Figure 1. The 2D Fan-Chen code was modeled after the work of D. Fan and L.Q. Chen (1.a.). The 2D (1.b.) and 3D (1.c.) codes were scaled to 512x512 and 64x64x64 computational spaces.

Cellular Automata

CA is a discrete model commonly used in studies of anisotropic etching, particle flow, and microstructure evolution. CA inherently describes grain size, shape, and phase volume fraction while intrinsically scaling up to exascale simulations.

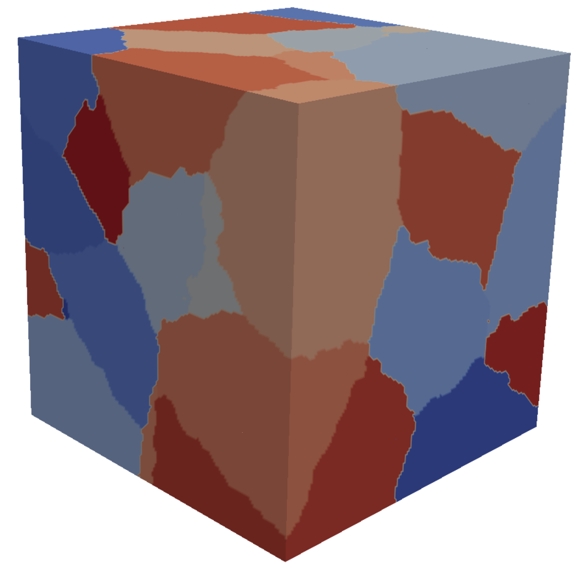
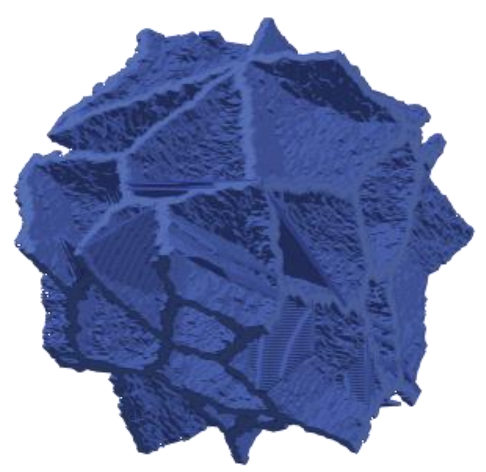
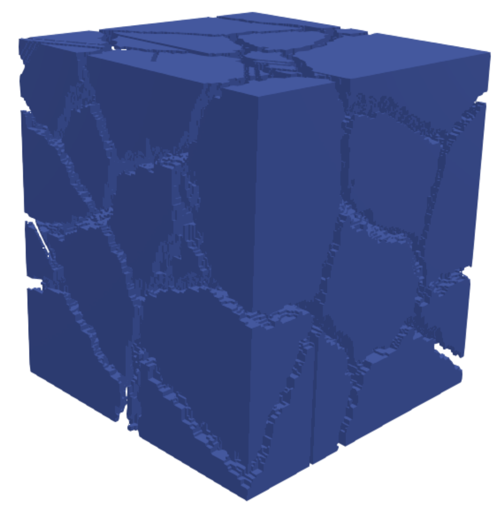


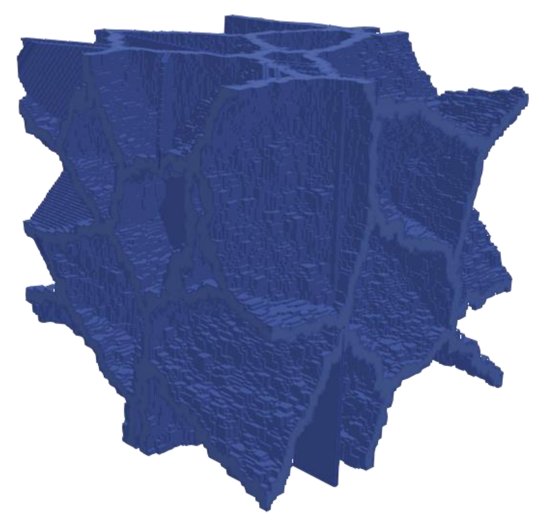
Figure 2. Cellular Automata 3D



3.a. Inverted Grain size/shape



3.b. Grain boundary and fatigue crack



3.c. Inverted GB and fatigue crack

Figure 3. Simulation of polycrystalline microstructure evolution and fatigue crack using CASUP [2].

Future Direction

Future work includes a formal report for the grain growth comparison and a transition of this work into thermomechanical modeling. Grain size, shape, density, and equivalent diameter will be pulled and examined from Figures 1.c. and 2. From this, we will determine which of the two methods can simulate more realistic structures.

Comparison

Grain Growth

Phase-field

- Computationally expensive, solves PDEs for continuous field variables
- Finite difference scheme for spatial components
- Grain orientation driven interface migration
- Thermodynamics driven; physically informed parameters
- Best describes interface geometry and grain mobility/orientation
- GB velocity is introduced through varying free energy parameters and grain boundary energy,

$$F(\eta_i) = \int_V \left(f_0 + \sum_{i=1}^{p} \frac{k_i}{2} |\nabla \eta_i|\right) dV$$

where $|\nabla \eta_i|$ is the grain boundary energy term.

Cellular Automata

- Computationally light, uses little memory
- Transition rules for spatial components
- Describes grain size/shape and phase volume fraction
- Scalable and easily coupled with lower and higher length scales
- Applicable in studies of texture evolution
- GB velocity is introduced through the local driving force and transition rules,

$$v = mF$$

where v is GB velocity, m is GB mobility, and F negative gradient in boundary energy across the interface.

Figure 4. Comparative chart of phase-field and cellular automata.

References

1. Fan, D., & Chen, L.-Q. (1997). Computer simulation of grain growth using a continuum field model. *Acta Materialia*, *45*(2), 611–622. https://doi.org/10.1016/s1359-6454(96)00200-5
2. *Cellular Automata Library for Supercomputers*. CASUP. (2018). Retrieved from https://cgpack.sourceforge.io/