

Translational AI Center (TrAC) Seminar Spring 2024

George Biros

April 10th at 1:00 PM (US Central Time)

Zoom link and more information: <https://trac-ai.iastate.edu/event/trac-seminar-series-george-biros/>

A Graph Neural Network Surrogate for Epitaxial Crystal Growth

Abstract

Predicting grain (crystal) formation and growth during alloy solidification is of great importance in additive manufacturing (AM) as it is one of the key factors in determining the final microstructure and the mechanical properties of the printed part. Numerical simulations of grain formation involve moving interfaces and require fine spatial and temporal discretizations that can be computationally expensive. In this talk, I will discuss GrainGNN, an efficient and accurate surrogate for epitaxial grain growth in additive manufacturing conditions. GrainGNN is a sequence-to-sequence long-short-term-memory (LSTM) graph neural network that evolves the dynamics of manually crafted features. We present results in which GrainGNN can be orders of magnitude faster than phase field simulations, while delivering 5%–15% pointwise error. This speedup includes the cost of the phase field simulations for generating training data. GrainGNN enables predictive simulations and uncertainty quantification of grain microstructure for situations not previously possible.

This is joint work with Yigong Qin (UT Austin), Steve DeWitt (ORNL), and Balasubramanian Radhakrishnan (ORNL)

References:

<https://arxiv.org/abs/2401.03661> (GrainGNN, 3D)

<https://www.sciencedirect.com/science/article/abs/pii/S0927025622006383> (GrainNN, 2D)

<https://www.sciencedirect.com/science/article/abs/pii/S0927025622000660> (Phase field DNS)

Short Bio

George Biros is the W. A. “Tex” Moncrief Chair in Simulation-Based Engineering Sciences in the Oden Institute for Computational Engineering and Sciences and has Full Professor appointments with the departments of Mechanical Engineering and Computer Science (by courtesy) at The University of Texas at Austin. From 2008 to 2011, he was an Associate Professor in the School of Computational Science and Engineering at Georgia Tech and The Wallace H. Coulter Department of Biomedical Engineering at Georgia Tech and Emory University. From 2003 to 2008, he was an Assistant professor in Mechanical Engineering and Applied Mechanics at the University of Pennsylvania. He received his BS in Mechanical Engineering from Aristotle University in Greece (1995), his MS in Biomedical Engineering from Carnegie Mellon (1996), and his PhD in Computational Science and Engineering also from Carnegie Mellon (2000). He was a postdoctoral associate at the Courant Institute of Mathematical Sciences from 2000 to 2003. With collaborators, he received the ACM Gordon Bell Prize in 2003 and in 2010. He is a 2023 SIAM Fellow.