Direct Numerical Simulation of Microstructure Evolution in Metal Additive Manufacturing Processes

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ABSTRACT

The Exascale Computing Project (ECP, https://exascaleproject.org/) is a U.S. Dept. of Energy effort developing hardware, software infrastructure, and applications for computational platforms capable of performing $10^{18}$ floating point operations per second (one “exaop”). The Exascale Additive Manufacturing Project (ExaAM) is one of the applications selected for development of models that would not be possible on even the largest of today’s computational systems. In addition to ORNL, partners include Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), the National Institute for Standards and Technology (NIST), as well as key universities such as Purdue Univ., UCLA, and Penn. State Univ.

We describe the physics components that comprise our simulation environment and report on progress to date using highly-resolved melt pool simulations to inform part-scale finite element thermomechanics simulations, drive microstructure evolution, and determine constitutive mechanical property relationships based on those microstructures using polycrystal plasticity. The coupling of melt pool dynamics and thermal behavior, microstructure evolution, and microscale mechanical properties provides a unique, high-fidelity model of the process-structure-property relationship for additively manufactured parts. We report on the numerics, implementation, and performance of the nonlinearly consistent coupling strategy, including convergence behavior, sensitivity to fluid flow fidelity, and challenges in timestepping.

We also provide initial comparisons of our highly-resolved simulations to reduced-order models with respect to both computational cost and accuracy.