Variational quantitative phase-field modeling and simulation of powder bed fusion additive manufacturing: Challenges of non-isothermal Allen-Cahn-Navier-Stokes system

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Powder bed fusion (PBF) additive manufacturing is a versatile process that offers significant advantages in optimizing material microstructure and properties across a wide range of materials. However, the PBF process involves complex multiphysical phenomena that can produce varying effects on the resulting components. This complexity necessitates a thorough investigation of the PBF process through both experimental methods and computational modeling and simulation. The phase-field model has emerged as a powerful tool for describing the intricate pore structure evolution and multiphysical interactions within the PBF process. However, as a diffuse-interface approach, the phase-field model employs a finite interface width to represent the transient microstructure, which requires asymptotic projection onto corresponding sharp-interface equations to ensure quantitative validity. While this issue has been solved for several processes, there is no related work specifically addressing interface phenomena in PBF.

A comprehensive non-isothermal phase-field model for the PBF process must account for a range of phenomena, including mass transfer, heat transfer, structural relaxation, solidification, and melt dynamics. During the first funding period, we developed a variational quantitative phase-field model to address the challenges of quantitative validity in non-isothermal sintering, focusing on mass transfer, heat transfer, and structural relaxation. This model eliminates artificial interface effects arising from the diffuse-interface representation of the grain-pore interface and was derived in a variational manner consistent with non-equilibrium thermodynamics. In the second funding period, we are extending this work by developing a variational quantitative phase-field model for non-isothermal solidification, incorporating melt flow dynamics. This model is developed as an extension of the non-isothermal Allen-Cahn-Navier-Stokes (NACNS) system, and various numerical benchmarks were performed to compare the simulated melt velocity profiles with sharp-interface solutions.

Additionally, we developed an energy- and entropy-stable numerical discretization of the non-isothermal ACNS system by reformulating the heat transfer equation in terms of entropy rather than internal energy. The resulting non-isothermal ACNS model will be applied to simulate melt dynamics in the PBF process for model material systems such as stainless steel 316L and yttria-stabilized zirconia.