Need
Develop, implement and validate physics based modeling system for Additive Manufacturing that can predict microstructure evolution of a Ni-superalloy system e.g. IN718 in full 3D.
• Base model with binary assumption developed and validated at UTRC in 2D1.
• Requirement of running the problem in 3D to identify grain structure and mutually competing dendrites identified – too computationally expensive and requires supercomputers
• Extending the problem from a model binary alloy to multicomponent alloys requires linking to thermodynamic and kinetic databases
• National laboratories are well suited to solve the above industry need

Approach
Utilize a phase-field model to capture solidification microstructure and validate using experimental data from UTRC

Phase field model
• Eliminates need to explicitly track the interface
• Assumes a diffuse interface between solid and liquid phases represented by an order parameter
• Model details based on an extension of the approach developed by Kim, Kim and Suzuki2
• Minimization of free energy of the system drives its evolution
• Alloy thermodynamics integrated using the Calphad3 approach

Solution of equations in phase field model is performed using a finite difference scheme

Finite Difference Scheme
• Evolution equations are set up for temperature, solute concentration and order parameter fields
• Semi-implicit finite difference scheme is used to develop a system of equations for each field
• Solution of resulting system of equations is carried out using conjugate gradient method with diagonal pre-conditioning

High Performance Computing
• Solution over large computational domains requires use of supercomputing resources
• Computation domain is subdivided among large number of processes
• Finite difference calculations require information from first nearest neighbors, which can lie on another process
• Data exchange routines based on MPI facilitate efficient communication among processes
• Sparseness of coefficient matrix is exploited to limit storage and speed up matrix-vector multiplication required for solving system of equations

Results

Benefits
• The physics-based modeling will be instrumental in reducing the significant experimental effort required for process certification and optimization, thus leading to a high reduction in AM energy consumption and expenses by at least 30%.
• In addition the model will provide fundamental understanding of the process physics and more accurate representation of microstructure in full 3D with segregation profiles and dendrite size within ±10%, enhancing the capability for predicting mechanical properties.
• Model will allow customization of AM powder alloy and process parameters to achieve the desired product microstructure
• Processing-microstructure predictions can be coupled with micromechanical models to predict and optimize desired mechanical properties.