Optimal Control under Uncertainty and Multiscale Heterogeneous Materials Modeling in Additive Manufacturing

Yuanxun Bao[1] George Biros[1] John A. Turner[2]

[1]Institute for Computational Engineering & Sciences, The University of Texas at Austin

[2]Computational Sciences and Engineering Division, Oak Ridge National Laboratory

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Advances in Experimental Design, Optimization and Learning for Uncertain Complex Systems

Abstract

Additive manufacturing (AM) has revolutionized manufacturing, allowing construction of complex parts not readily fabricated by traditional techniques. Yet, there are many open questions in how AM process variables impact the resulting material microstructure (the forward problem), and the ability to control the AM process to manufacture parts with desired properties (the optimization problem). In addition, the physical effects occurring during AM are tremendously complex, spanning multiple orders of length scales and timescales. This necessitates the development of multiscale models and simulations to gain further insights and to enable predictions by process parameter modifications suitable for further optimization of material properties. As a first step, we present a two-scale model that couples heat conduction (continuum model) and microstructure evolution (phase-field model) during solidification of materials, and propose a model optimization problem for process parameter control. This two-scale model will account for random coefficients and microstructure evolution via grain growth, solid-state phase transformations, multicomponent alloys and fluid flows at the microscale, and combined with thermo-mechanical continuum models at the macroscale. The optimization problem will be solved using adjoint-based algorithms.

Motivation: multiscale modeling in AM

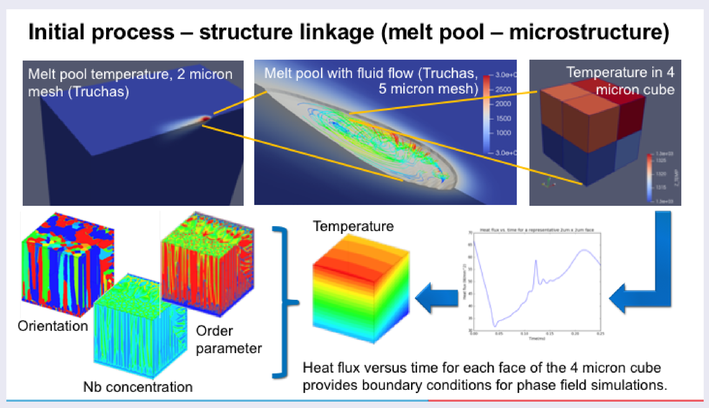

Figure 1:Example of multiscale simulation for additive manufacturing using laser powder bed fusion. In the coarse scale, a simple evaporation heat transfer with radiation boundary conditions is used. In the second scale, fluid flow is included; In the coarse scale, phase-field simulations for the solidification morphology [1]. Here the material is a Ni-Fe-Nb ternary alloy.

Full resolution AM models encompass spatial and temporal scales spanning orders of magnitude. Process control variables and material parameters determine microstructure (grain size, orientation, etc.), which in turn determines mechanical properties. Our formulation is a two-way coupled macroscopic scale (cm) and microstructure evolution (μm).

- Macroscale: thermo-mechanical models (FEM).
- Mesoscale: fluid dynamics and heat transfer in the melt pool (FEM/FVM)
- Microscale: microstructure evolution (phase-field models)

Our goal is to setup an optimization problem around this two scale forward problem.

Approach: a two-scale forward problem

We employ an computational homogenization framework (see figure from [2]) to bridge the macroscopic and microscopic scales. The main idea in computational homogenization is to obtain the constitutive closure relations for the macroscopic problem in a numerical form through the consistent construction and solution of a microstructural problem. In our simple model, we consider heat conduction at the macroscale, where heat conductivity and driving force are determined by the evolution of phase-field at the microscale.

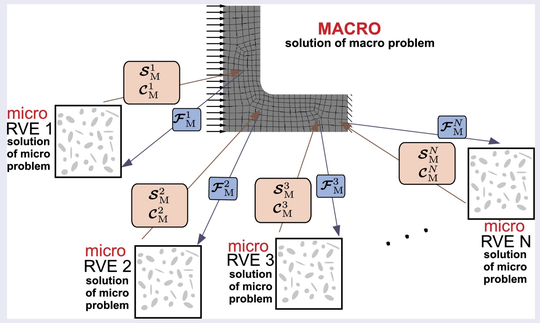

Figure 2:A schematic illustration of multiscale computational homogenization framework [2].

- **Macroscale model:** We consider the heat equation with conductivity $\bar{K}(\phi)$ a function of solid-liquid / solid-solid interface homogenized from the microscale. Averaged quantities from the microscopic model (like phase-field ϕ) are coupled back to the macroscale:

$$\frac{\partial T}{\partial t}(\boldsymbol{x},t) = \nabla_{\boldsymbol{x}} \cdot (\bar{K}(\phi)\boldsymbol{\nabla}_{\boldsymbol{x}} T) + \frac{L}{c_p}\frac{\partial \bar{\phi}}{\partial t} + f, \quad \boldsymbol{x} \in \Omega \tag{1}$$

  where L is half the latent heat, c_p the heat capacity, and f external source term.
- **Microscale model:** we employ a simple phase-field model for dendritic growth [3],

$$\begin{aligned}\tau A^2(\theta)\frac{\partial \phi}{\partial t}(\boldsymbol{x},\boldsymbol{y},t) = W_\phi^2 \nabla_{\boldsymbol{y}} \cdot (A^2(\theta)\boldsymbol{\nabla}_{\boldsymbol{y}}\phi) - g'(\phi) - \frac{L(T(\boldsymbol{x},\boldsymbol{t})-T_m)}{HT_m}p'(\phi) \\ - W_\phi^2 \partial_{y_1}[A(\theta)A'(\theta)\partial_{y_2}\phi] + W_\phi^2 \partial_{y_2}[A(\theta)A'(\theta)\partial_{y_1}\phi],\end{aligned} \tag{2}$$

  where W_ϕ is the diffusive interface parameter, the function $A(\theta) = 1 + \epsilon\cos(4\theta)$ modulates the anisotropy of the interface kinetics, T_m is the melting temperature.
- **Microscale averaging:**

$$\bar{\phi}(x,t) = \frac{1}{|\omega|}\int_\omega \phi(x,y,t)\,dy \quad ; \quad \bar{K}(\phi) = \frac{1}{|\omega|}\int_\omega \kappa_0\phi + \kappa_1(1-\phi)\,dy \tag{3}$$

  Note the complexity of this simple multiscale model: at every spatial point in the macroscale thermodynamics model (1), we must solve the microscale phase field model (2) on an RVE/unit cell to evaluate the heat conductivity $\bar{K}(\phi)$. Notice that here we have not included random coefficients. Such coefficients can be related to the initial condition of ϕ (the order parameter), the heat forcing f and other material properties. Such randomness has significant effects in the microstructure.
- **Optimization:** our goal is decide on the right initial conditions and model parameters in order to control some quantity of interest, for example the average diffusivity. Some of the challenges in solving this optimization problem include:
  1. The coupled set of partial differential equations;
  2. The computational cost of phase-field solvers and long time history that makes adjoint calculations difficult;
  3. Differentiability issues;
  4. The presence of random coefficients and noise;
  5. The need to characterize the uncertainty and variability of the predicted microstructure.

Preliminary results

We have initial implementations for single-scale and multiscale forward problems for our model problem.

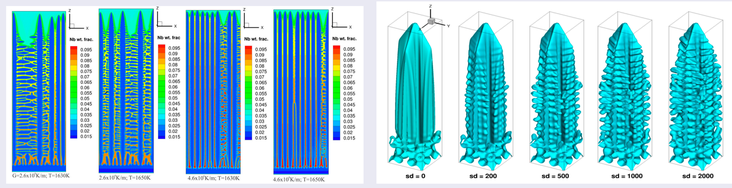

Figure 3:Results from phase field simulation of solidification [1]. Effects of changing the diffusivity (left) and noise on order parameter (right).

Synergy

- The proposed solvers find applications in many multiscale problems in which the microscale problem has an evolving microstructure. For example, problems include materials science (crystal plasticity), block-copolymers (also part of our project), but also transport phenomena for complex fluids.
- Solving the outer loop optimization problem with a 3D multiscale forward problem as an inner loop is a formidable task. Ideas from reduced-order modeling and machine learning communities can greatly reduce the computational cost and applicability of the method for industrial applications.

Ongoing work

- Develop fast solver for the macroscale and microscale problems;
- Incorporate hydrodynamics due to fluid flow, and phase-field models for alloys [4], mixture, and extends to multiple phase-field models;
- Develop a reduced order model for the microscale model;
- Develop a reduced order model for the input-output map that couples the micro to the microscale;
- Incorporate uncertainty into multiscale modeling and optimization, e.g. stochastic forces at the level of phase-field models.

References

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