Computational and Analytical Methods in AM: Linking Process to Microstructure

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Modeling and Simulation Can Link Process to Performance

- **Process Parameters**
  - Laser power
  - Scan speed
  - Scan direction
  - Material
  - Powder size
  - Layer thickness
  - Etc...

- **Microstructure**
  - Porosity
  - Grain structure
  - Surface roughness
  - Precipitates
  - Voids
  - Defects
  - Residual stress

- **Properties/Performance**
  - Strength
  - Fatigue life
  - Ductility
  - Hardness
  - Toughness

The focus of this talk
Problem Overview

- Focus on LENS / SLM / EBM for metals

Powder Delivery
(Feed or Bed Formation)

Heat Source
(Laser or Electron)

Part Scale
Heat Transfer
Phase Change
Thermo-Mechanics

Powder & Sub-Powder Scale
Melting and Solidification
Deformation and Flow
Microstructure Formation

Mesoscale
Homogenization
Computational Method Needs

• Q8: What are those drivers and what fundamental advancements are needed for computational methods and optimization techniques?

• These problems are difficult because of:
  • Multiple length and time scales
  • Complicated or unknown physics models
  • Complex moving interfaces
Computational Method Needs

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**Vision for Concurrent Multiscale Modeling**

- AM phenomena occur on multiple time/length scales, imposing serious tradeoff between solution resolution and computational efficiency of simulations

*New method for concurrent multiscale modeling*

- Send in conservative fluxes
- Upscale to macroscale solution
- Evolve microstructure with higher resolution

Global Analysis: Part Size
- ~ minutes thermal-Solid

Melt-pool: ~Laser Size
- ~ milliseconds thermal-fluid-solid

Solidification: ~Particle Size
- ~ Nano-milliseconds thermal-fluid-Solid

*Require a multiscale method to optimize the tradeoff*

Macroscale FEM Coupled with Microscale Thermo-Calc Simulations

- Thermo-Calc can give properties (such as H vs. T curve) based on composition
  - Equilibrium phases (e.g. FCC vs. BCC) predicted
  - Future goal is to couple concurrently to get effects of cooling rate

J. Smith et al., Northwestern University
Effect of Properties on Thermal Simulation

“Handbook” Properties

Thermo-Calc Properties
Multiscale Subcycling: Microstructure Formation

- AM process is inherently multiphysics and multiscale
- Large thermal gradients lead to complex microstructure evolution during manufacturing

We want to understand phase evolution from process parameters (energy density, layer thickness etc.)

Want to capture evolution at critical points with phase field models (or other fine scale representations)

\[ \alpha' \text{ acicular phase} \]

Concurrent Multiscale Method: Preliminary Results with Isotropic Solidification

Typical Temperature Profile During Solidification:

a) Cooling of material in liquid phase
b) Energy absorption due to solidification, negligible temperature change
c) Full solidification of material

Supercooled from left edge

Material in fully liquid state

Solidification behavior at specified point

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Concurrent Multiscale Method: Possible future goals

- For AM applications, we want to be able to simulate anisotropic microstructure/dendrite formation.
- Modeling these phenomena will give a greater insight into process control.

Anisotropic surface energies lead to dendrite growth.

Solidification behavior at specified point.
Need: Reduced-Order Modeling Techniques

- Full fine-scale modeling of a part is unrealistic
- Opportunity in application of High Performance Computing (Q2, Q7): Reduced Order Models

ROM: Pre-computed large scale simulation to compute mode shapes for fast approximate solves

Can we use nonlinear dimensionality reduction or similar methods to classify and query databases of fine-scale solutions?

Carlberg et al., 2012, J. Comp. Phys

Tenenbaum et al., 2000, Science

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Example: Modeling E-Beam Heating

- Correct form of thermal source term due to beam heating is unknown
- Monte Carlo simulations of electron-atom interaction may elucidate this

Physics Model Needs

- Q5: What tools are needed?
- Non-isothermal, multicomponent phase field models for solidification of complex materials

![Phase field simulation of martensitic transformation under plastic strain](image1)


- Meso-scale models for powder beds with different levels of particle consolidation

![Meso-scale models](image2)

How do we Deal with Model Uncertainty?

Q4: How can AM benefit from fundamental advances in verification, validation, and UQ methodologies?

“There’s not a person on the planet right now who can tell me exactly how high the temperature gets during additive manufacturing.”

-- Anonymous Thermal Modeler, Personal Communication

- We in the modeling community can do more to help determine what quantities that can be measured will best inform model selection.
- Verification of macro-scale thermal models takes some thought as meshes are refined to the particle scale.
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Powder Scale Models

Important physics:

- Melting
- Solidification
- Flow
- Vaporization
- Pore formation
- Surface tension

- Conduction
- Convection
- Radiation
- Thermo-capillary motion
- Dendrite formation

Powder Scale Models

- Progress is being made on modeling powder melt/solidification

Arbitrary Lagrangian-Eulerian Method

Layer 1, speed 2 m/s, 200 W: Severe balling effects

Layer 1, speed 1.6 m/s, 166 W: Discontinuous track

Layer 2, speed 1.6 m/s, 166 W: Continuous track with dross

King et al., 2015, Matl. Sci. Tech.

Lattice-Boltzmann Method


Northwestern U. group approach
**Need:** Development of New and Existing Methods for Capturing Complex Interfaces

**Conserved Level Set Method**

Turbulent spray breakup  

**Phase Field Models**

Jet pinch-off  

Al-Si solidification  
A. Yamanaka  
*Tokyo U. of Agriculture and Tech.*
Need: Development of New and Existing Methods for Capturing Complex Interfaces

**Finite Cell Method**

Complex part simulation with non-conforming mesh

**XFEM**

Non-conforming mesh simulations of randomized microstructures
Jifeng Zhao, Northwestern University

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Summary

• Interdependence between scales in AM calls for new computational methods
  • Concurrent macro/micro-scale simulations should be possible at localized regions of interest
  • Reduced order models informed by HPC simulations may bring real-time micro-scale simulations in reach

• Complicated physics can be understood through both simulation and experiment
  • There is a need for a coordinated validation plan between modeling and experiments

• Methods for modeling complex moving interfaces can impact AM simulations