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Computational and Analytical Methods in AM: Linking Process to Microstructure

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Northwestern University

Workshop on Predictive Theoretical and Computational Approaches for AM
Washington D.C.
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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

→

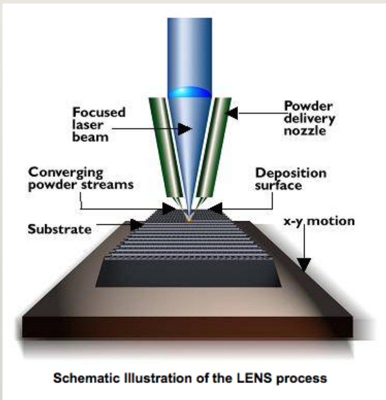
Properties/ Performance

- Strength
- Fatigue life
- Ductility
- Hardness
- Toughness

The focus of this talk

Problem Overview

- Focus on LENS / SLM / EBM for metals

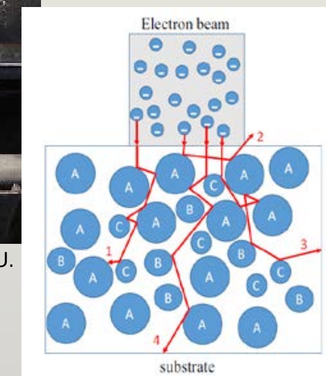


Sabreen Group, Inc.

Powder Delivery
(Feed or Bed Formation)

Heat Source
(Laser or Electron)

Prof. F. Lin, Tsinghua U.

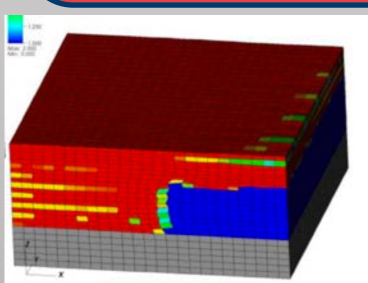


W. Yan, Tsinghua U. & NU

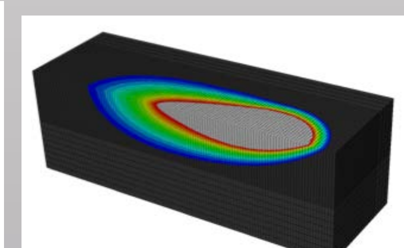
Part Scale
Heat Transfer
Phase Change
Thermo-Mechanics

Mesoscale
Homogenization

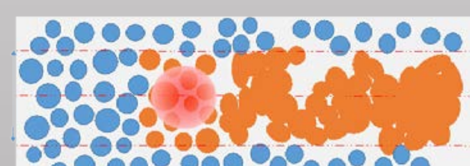
Powder & Sub-Powder Scale
Melting and Solidification
Deformation and Flow
Microstructure Formation

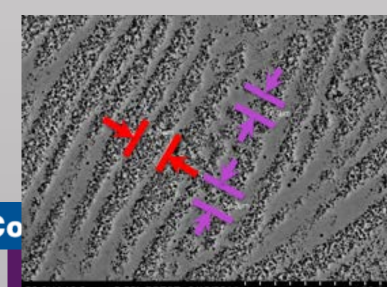


King et al., 2015, *Mat. Sci. Tech.*



W. Yan et al. 2015, *Comp Mech*





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

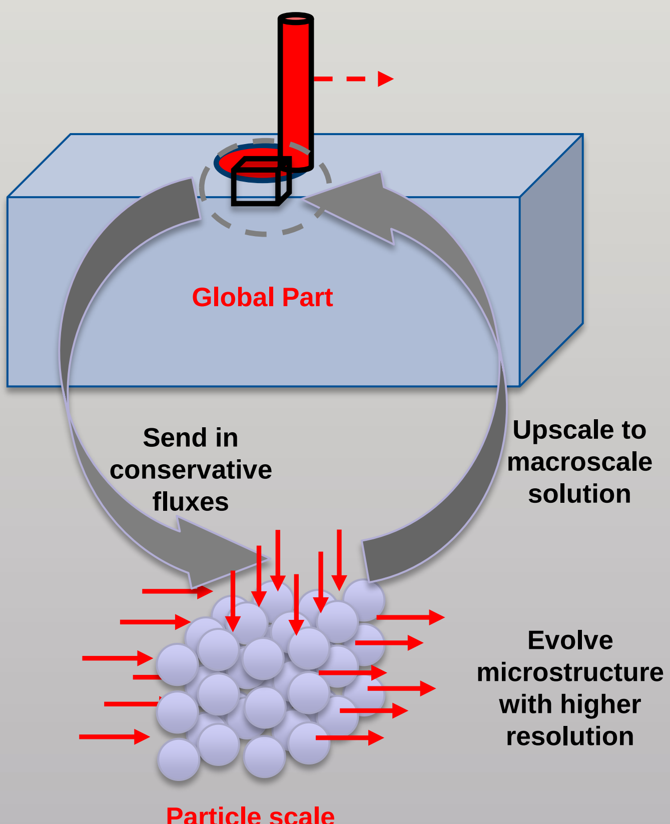
Computational Method Needs

- 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

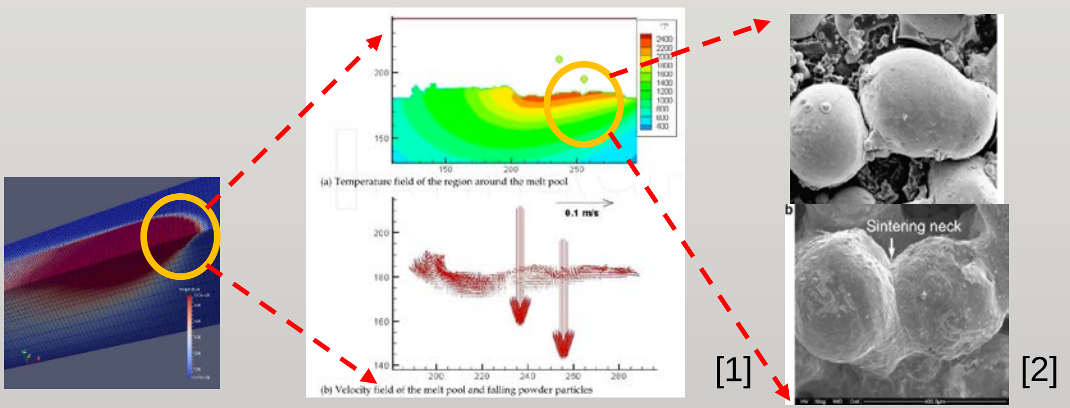
Vision for Concurrent Multiscale Modeling

- 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



* Require a multiscale method to optimize the tradeoff



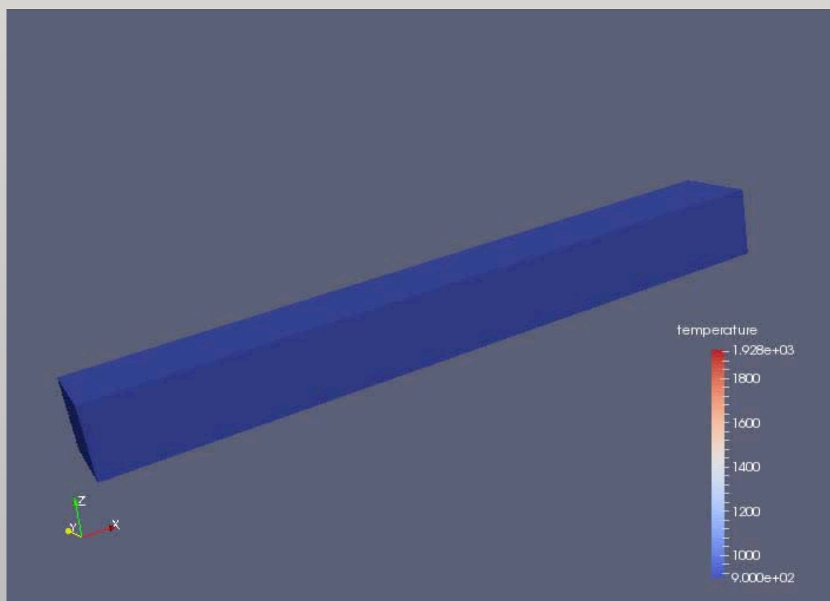
Global Analysis: Part Size	Melt-pool: ~Laser Size	Solidification: ~Particle Size
~ minutes thermal-Solid	~ milliseconds thermal-fluid-solid	~ Nano-milliseconds thermal-fluid-Solid

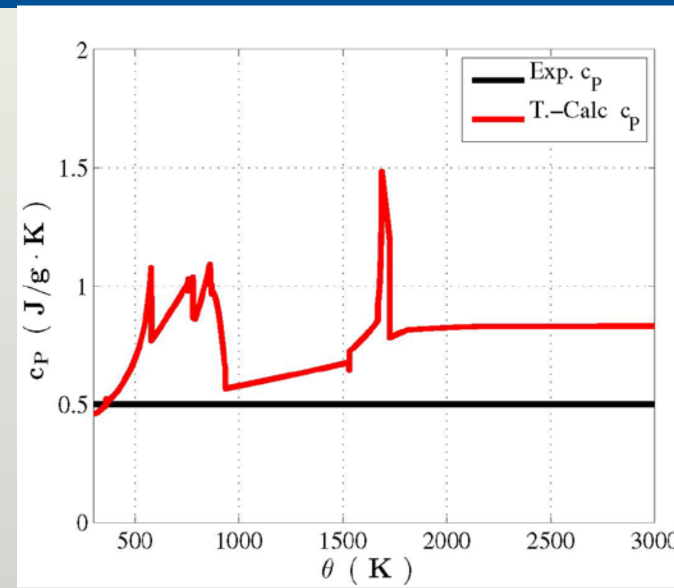
[1] Numerical modeling of the additive manufacturing (AM) processes of titanium alloy. Fan and Liou, 2012.

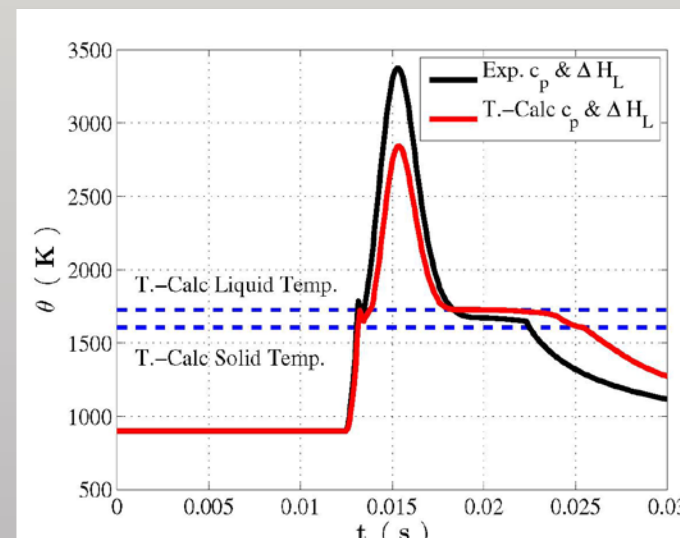
[2] Balling phenomena in direct laser sintering of stainless steel powder: Metallurgical mechanisms and control methods, Gu, 2009

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**



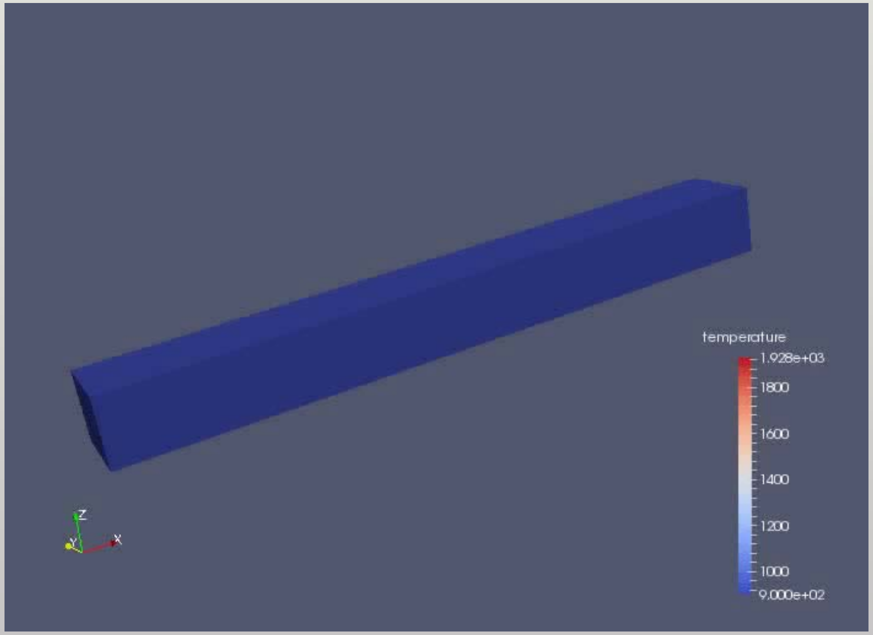




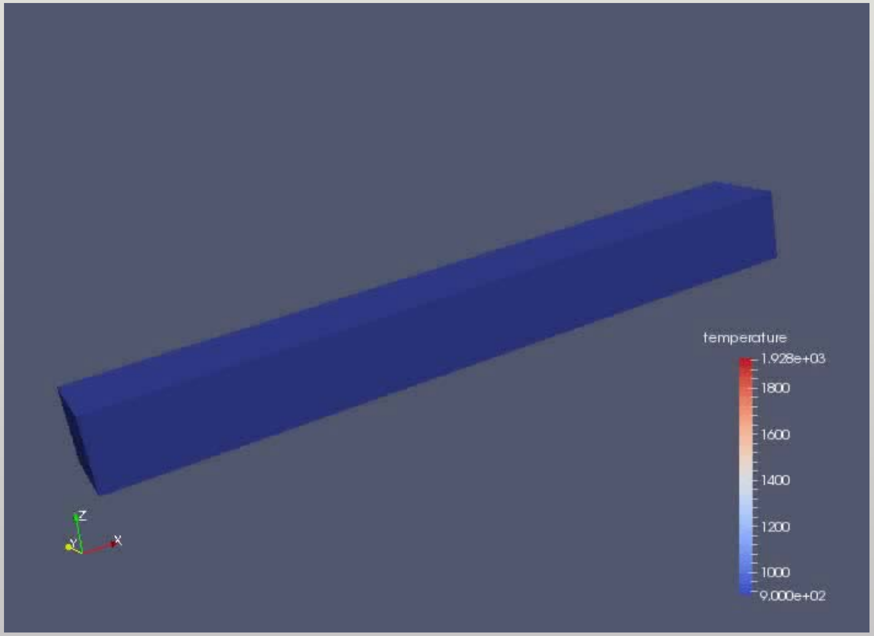
J. Smith et al., Northwestern University

Effect of Properties on Thermal Simulation

“Handbook” Properties



Thermo-Calc Properties



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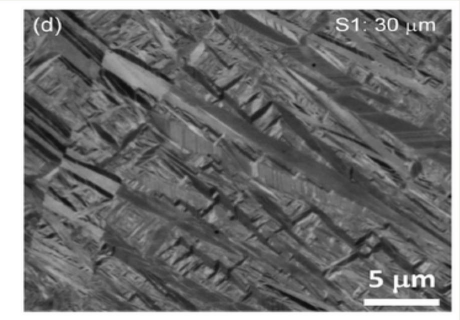
Multiscale Subcycling: Microstructure Formation

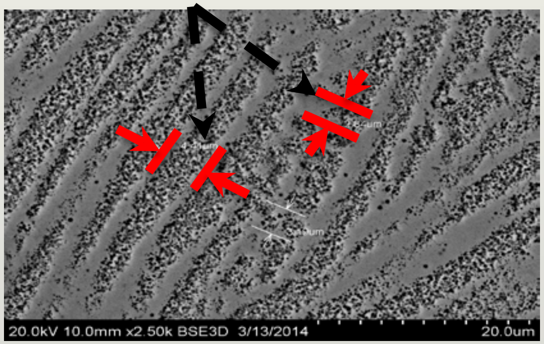
- AM process is inherently multiphysics and multiscale
- Large thermal gradients lead to complex microstructure evolution during manufacturing

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

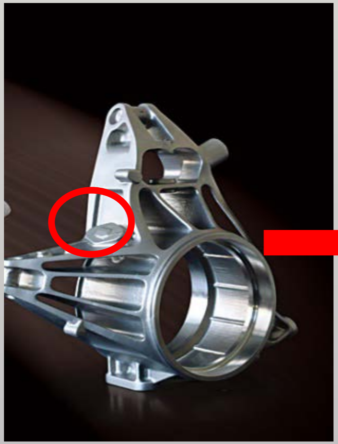


α' acicular phase

Dendrite Formation

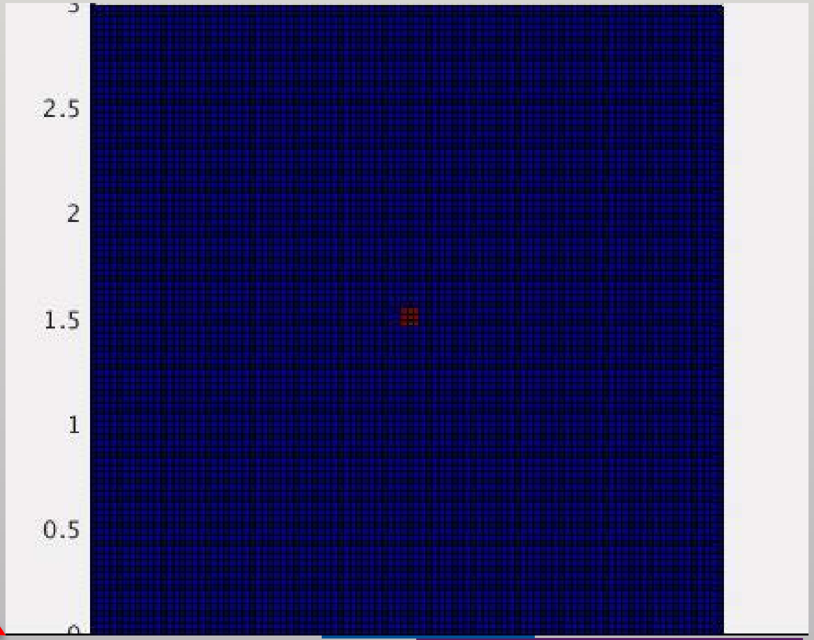


W. XU, S. SUN, J. ELAMBASSERIL, Q. LIU, M. BRANDT, and M. QIAN, Ti-6Al-4V Additively Manufactured by Selective Laser Melting with Superior Mechanical Properties 2015 The Minerals, Metals & Materials Society



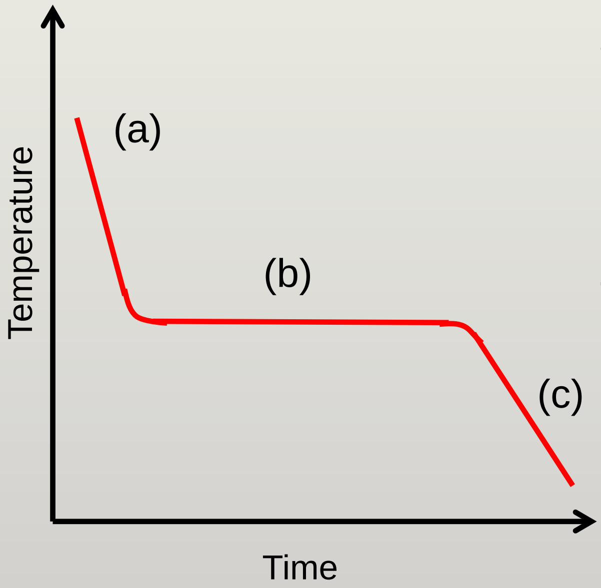
Part to be manufactured

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

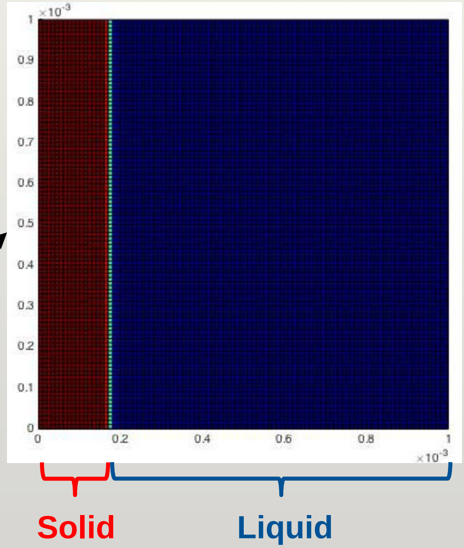


Concurrent Multiscale Method: Preliminary Results with Isotropic Solidification

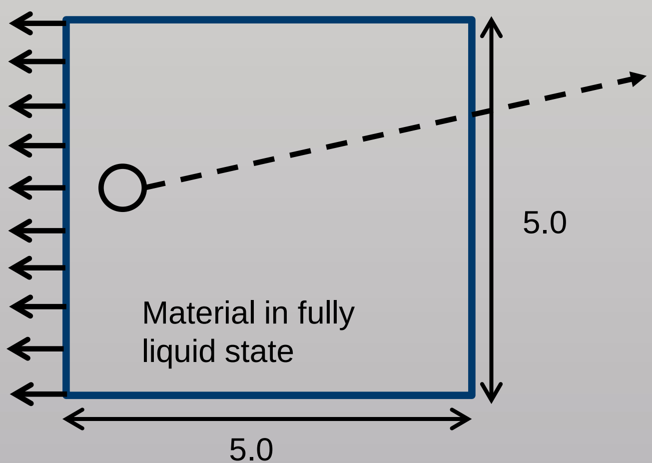
Typical Temperature Profile During Solidification:

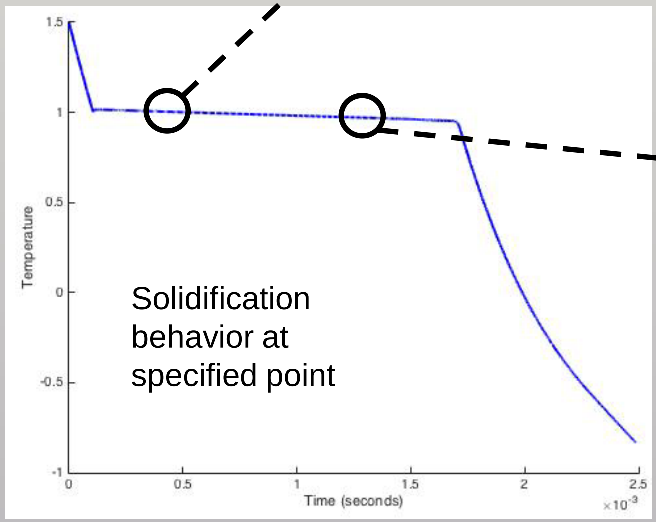


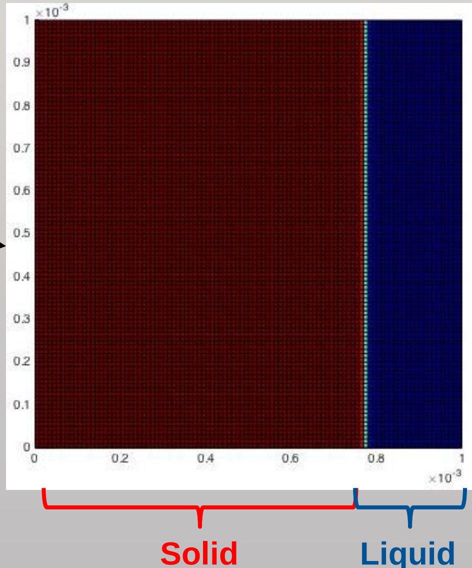
a) Cooling of material in liquid phase
b) Energy absorption due to solidification, negligible temperature change
c) Full solidification of material



Supercooled from left edge







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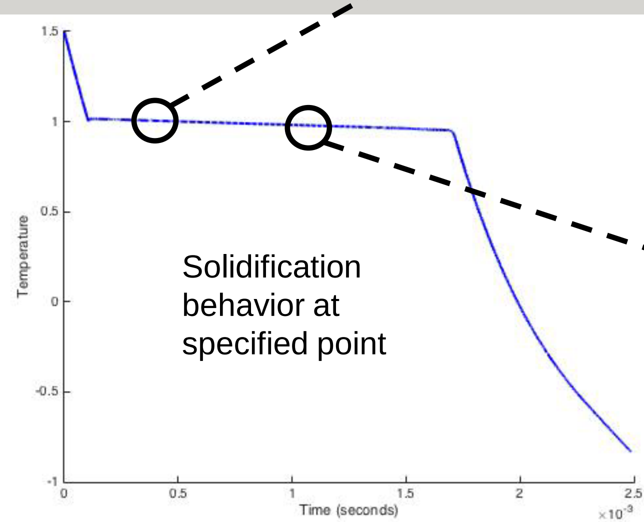
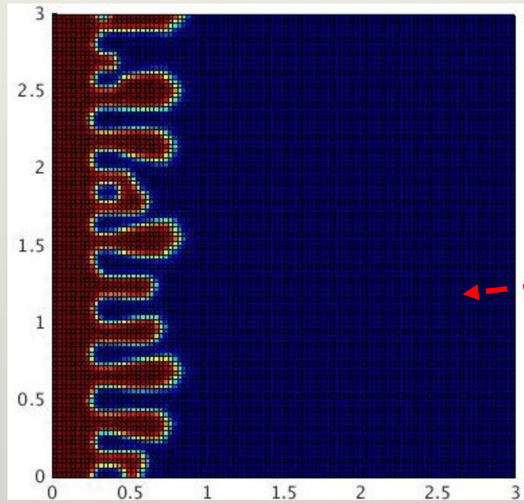
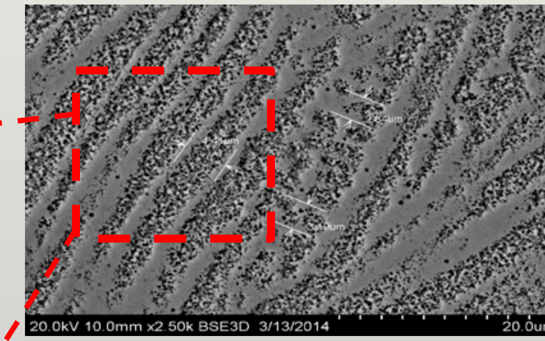
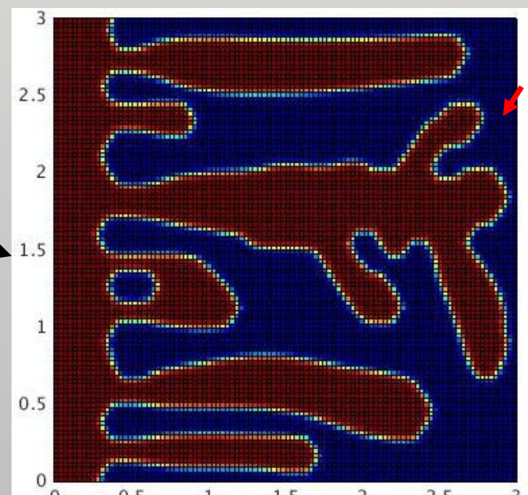
Concurrent Multiscale Method: Possible future goals

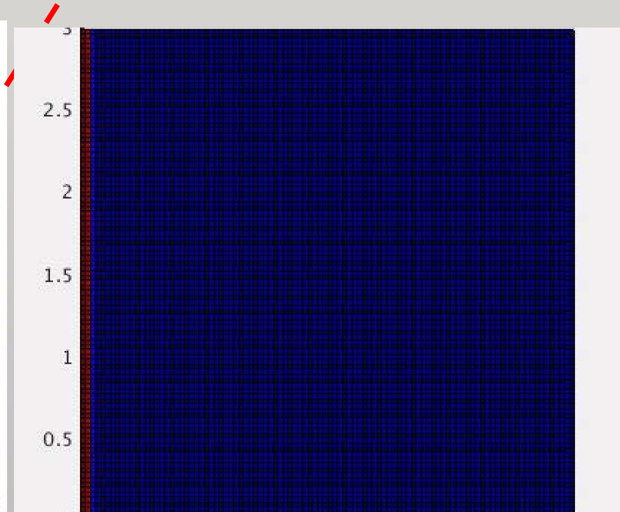
- For AM applications, we want to be able to simulate anisotropic microstructure/dendrite formation
- Modeling these phenomena will give a greater insight into process control











Anisotropic surface energies lead to dendrite growth

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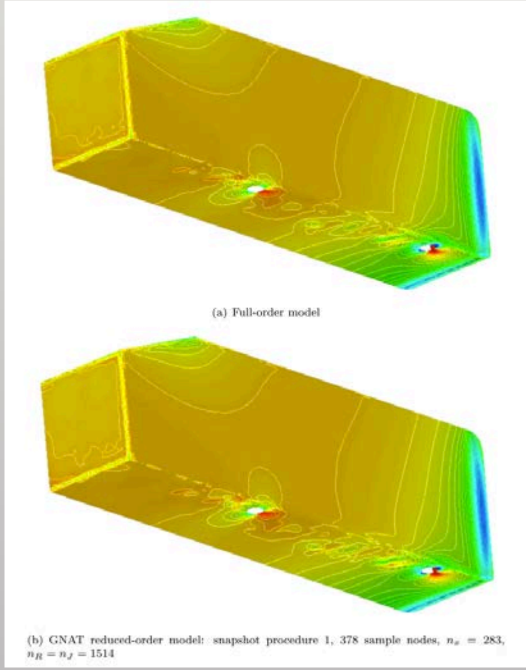
Need: Reduced-Order Modeling Techniques

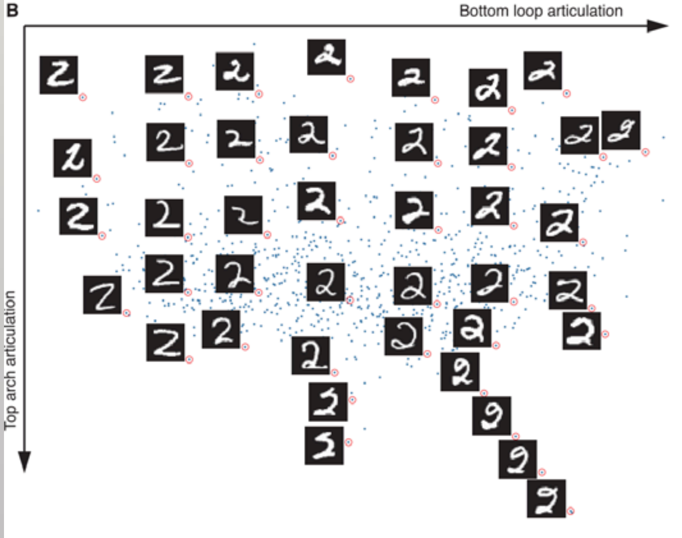
- Full fine-scale modeling of a part is unrealistic
- Opportunity in application of High Performance Computing (Q2, Q7): Reduced Order Models

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



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

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



Tenenbaum et al., 2000, *Science*

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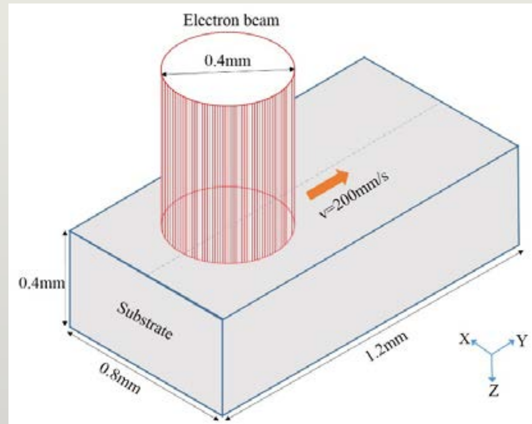
Computational Method Needs

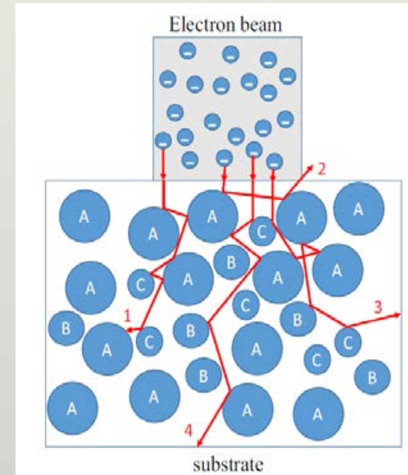
- Q8: What are those drivers and what fundamental advancements are needed for computational methods and optimization techniques?
- These problems are difficult because of:
  - Multiple length and time scales
  - **Complicated or unknown physics models**
  - Complex moving interfaces

Example: Modeling E-Beam Heating

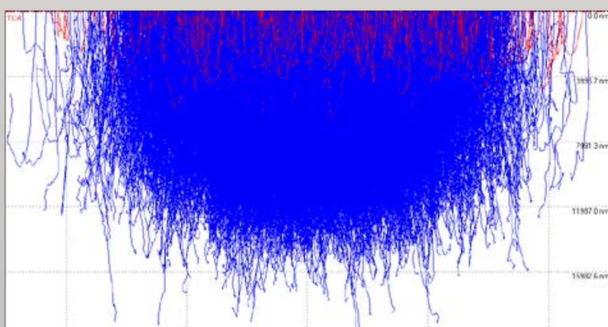
- Correct form of thermal source term due to beam heating is unknown
- Monte Carlo simulations of electron-atom interaction may elucidate this



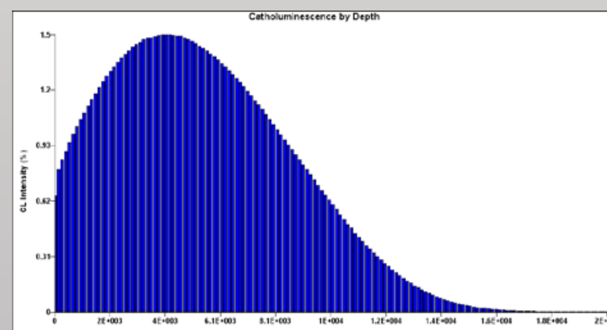
W. Yan et al. (2015) "Multiscale modeling of electron beam and substrate interaction: A new heat source model"



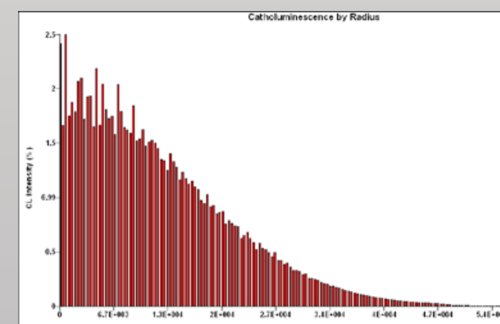
Electron-atom interaction



Trajectories



Distribution in Z



Distribution in R

Fit:

$$q(x,y,z) = Q * \left[\frac{1}{\delta \cdot \int_{-\frac{z_0}{\delta}}^{+\infty} \exp(-t^2)dt} \exp\left(-\frac{(z-z_0)^2}{\delta^2}\right) \right] * \left[\frac{N}{\pi R_b^2} \exp\left(-N \cdot \frac{(x-x_s)^2 + (y-y_s)^2}{R_b^2}\right) \right]$$

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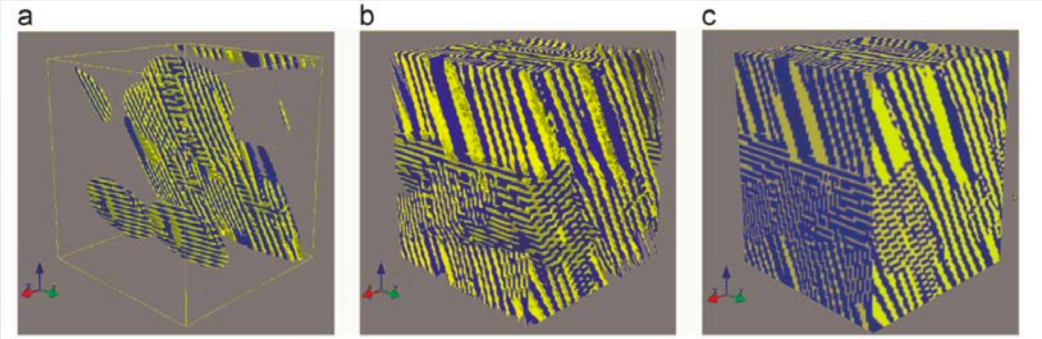
Physics Model Needs

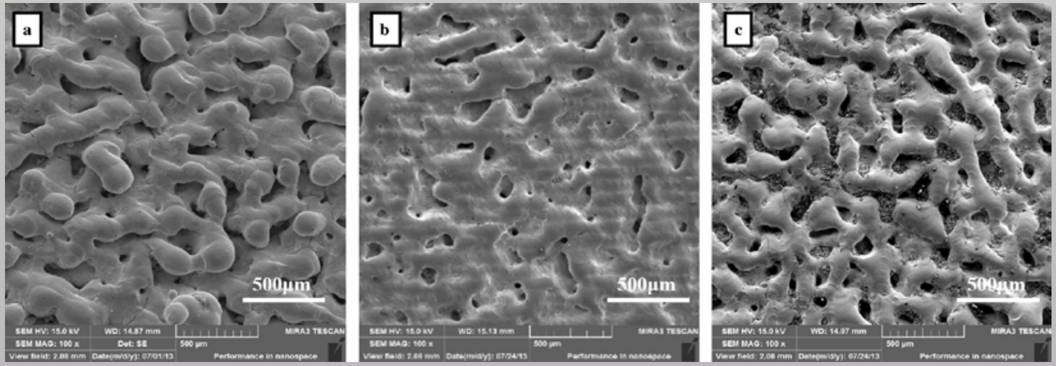
- Q5: What tools are needed?
- Non-isothermal, multicomponent phase field models for solidification of complex materials

Phase field simulation of martensitic transformation under plastic strain



Kundin et al. (2015), *J. Mech. Phys. Sol.*

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



Zhou, X., et al. (2015) *U. Mat. Proc. Tech.*

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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

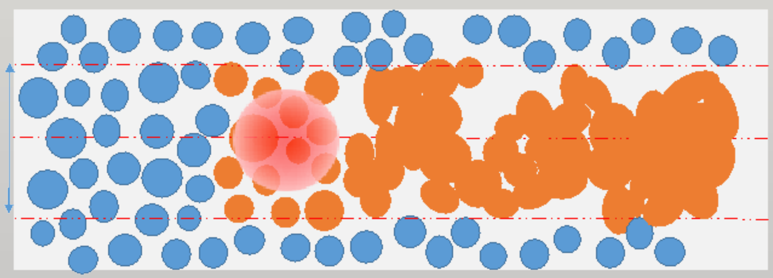
Computational Method Needs

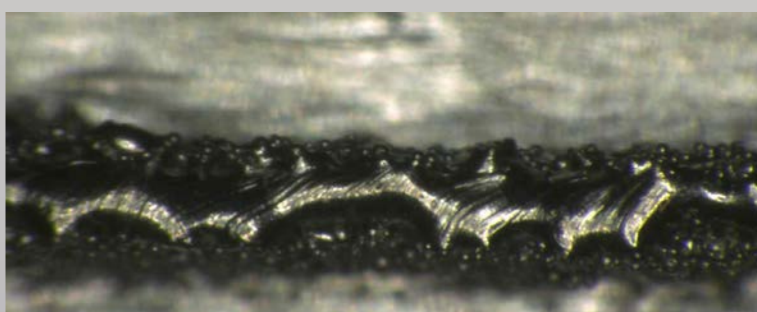
- Q8: What are those drivers and what fundamental advancements are needed for computational methods and optimization techniques?
- These problems are difficult because of:
  - Multiple length and time scales
  - Complicated or unknown physics models
  - **Complex moving interfaces**

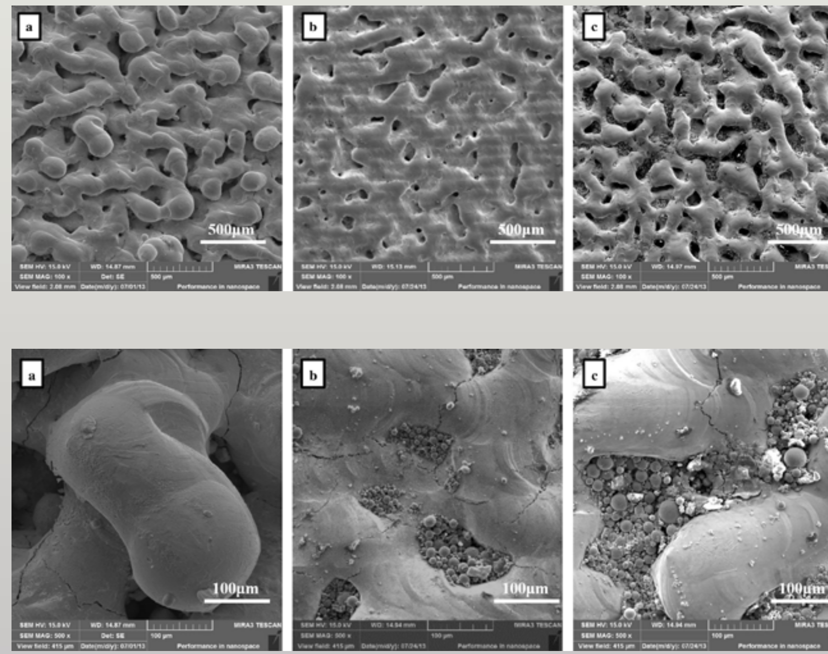
Powder Scale Models

Important physics:

- Melting
- Solidification
- Flow
- Vaporization
- Pore formation
- Surface tension
- Conduction
- Convection
- Radiation
- Thermo-capillary motion
- Dendrite formation







Zhou, X., et al. (2015). "Balling phenomena in selective laser melted tungsten." Journal of Materials Processing Technology **222**(0): 33-42.

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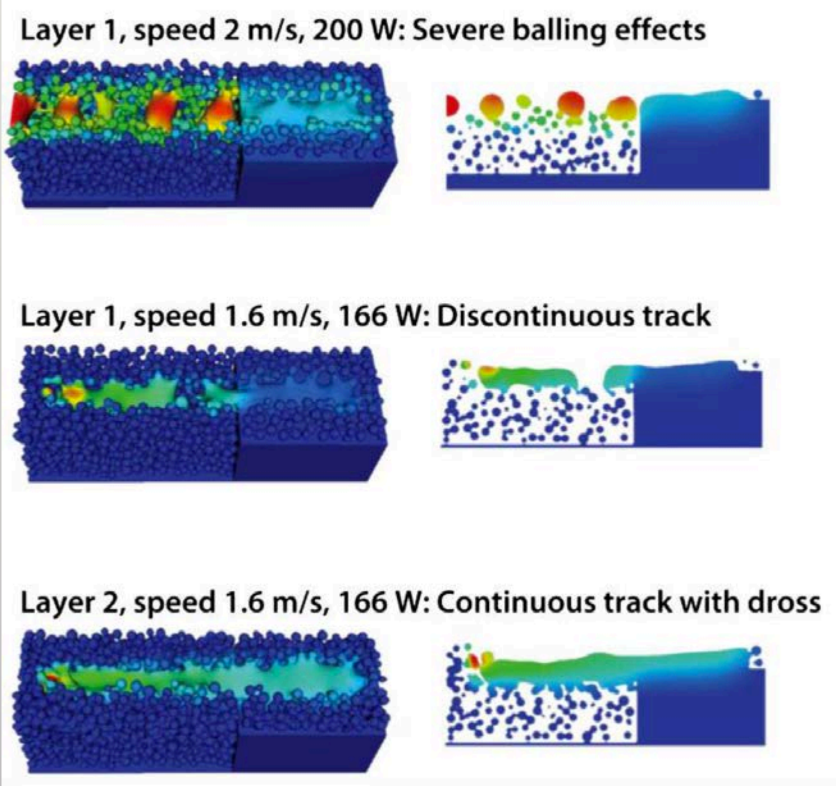
Powder Scale Models

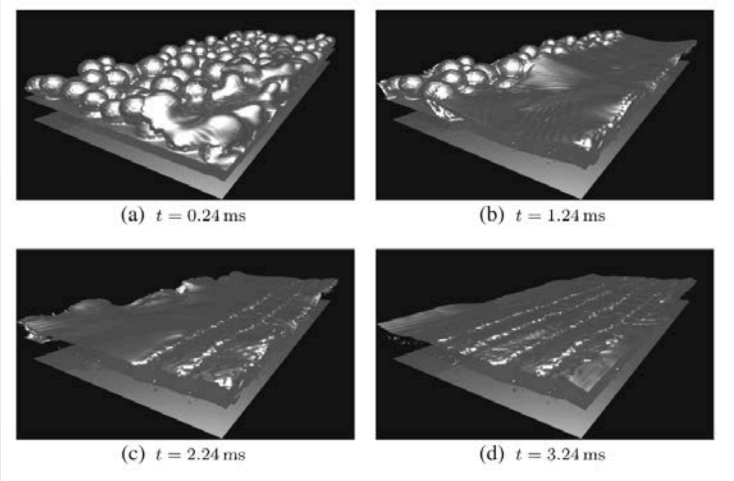
- Progress is being made on modeling powder melt/solidification

Arbitrary Lagrangian-Eulerian Method

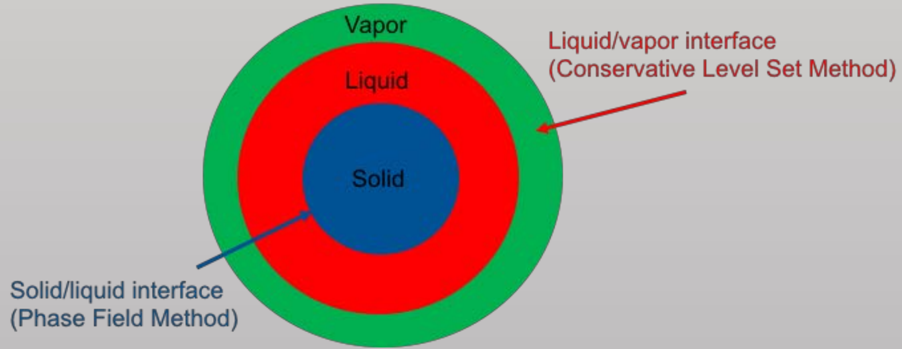


King et al., 2015, *Matl. Sci. Tech.*

Lattice-Boltzmann Method



Markl et al., 2014, *Int. J. Adv. Manuf. Tech.*



Northwestern U. group approach

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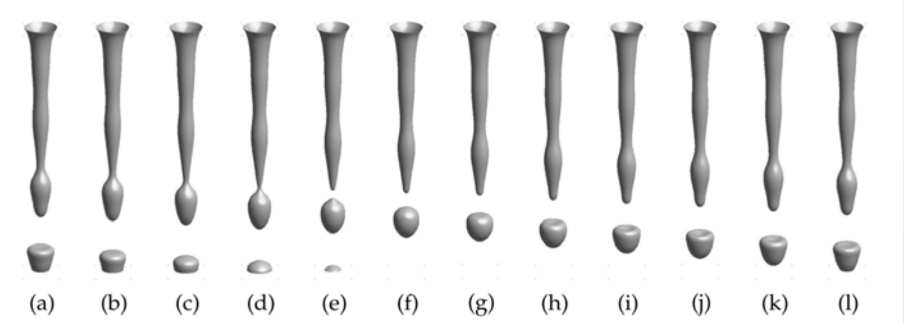
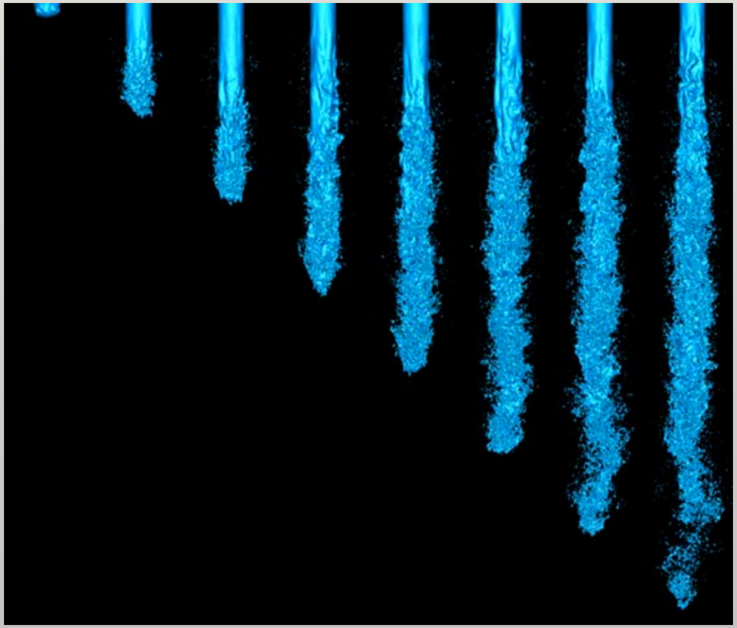
Need: Development of New and Existing Methods for Capturing Complex Interfaces

Phase Field Models

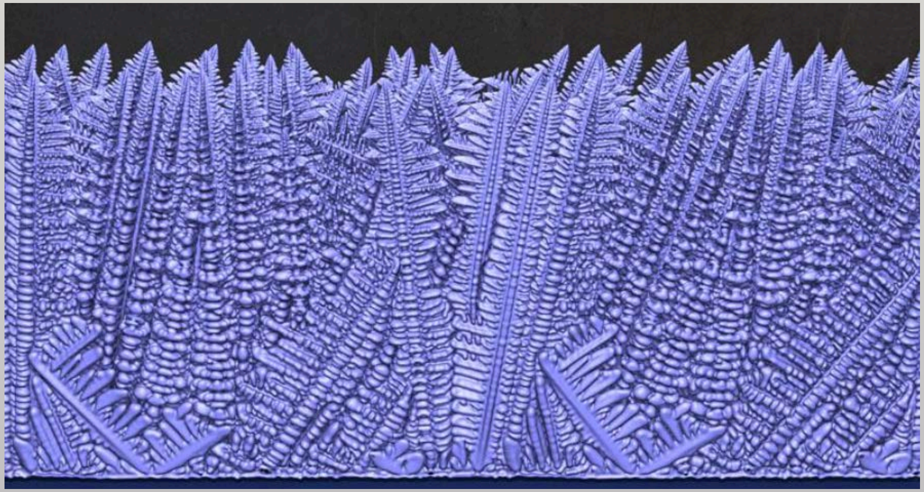


Jet pinch-off
Kim, 2012, *Commun. Comput. Phys.*

Conserved Level Set Method



Turbulent spray breakup
Desjardins et al., 2008, *J Comp Phys.*



Al-Si solidification
A. Yamanaka
Tokyo U. of Agriculture and Tech.

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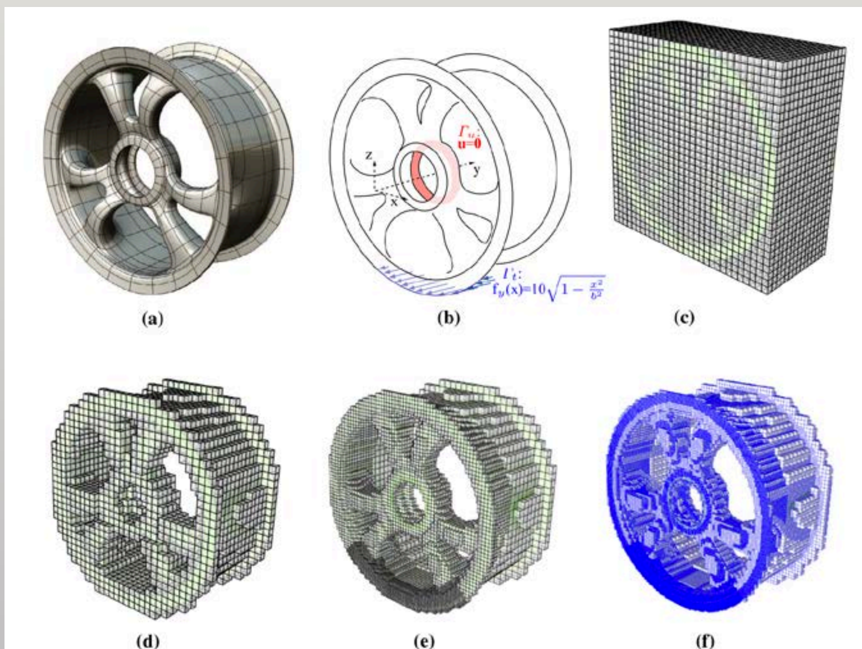
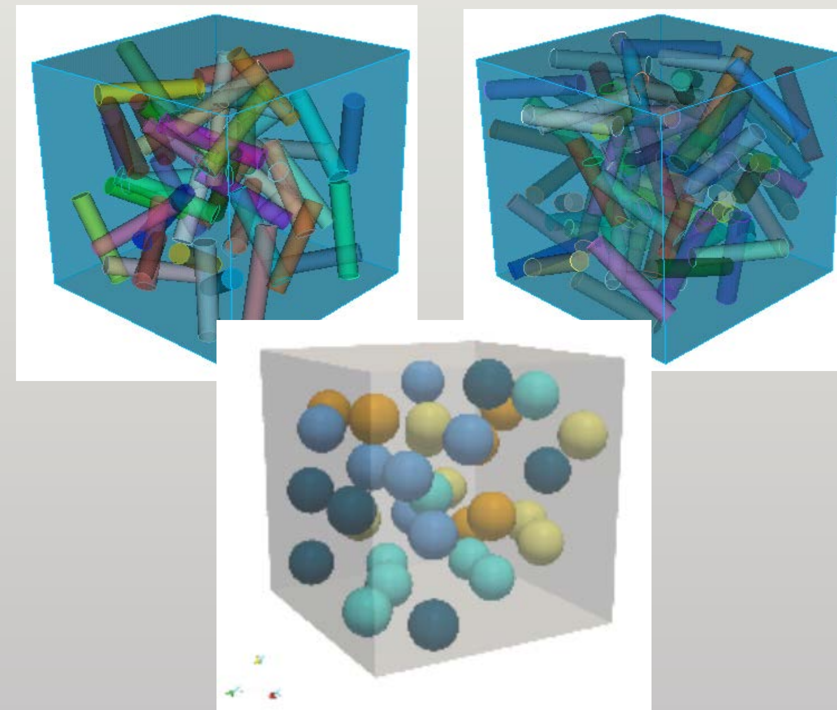
Need: Development of New and Existing Methods for Capturing Complex Interfaces

XFEM

Finite Cell Method



Complex part simulation with non-conforming mesh
Schillinger & Ruess, 2014, *Arch. Comp. Meth. Eng.*



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