

Computational Materials Simulation of Additively Manufactured Microstructures

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Powder Bed Fusion (PBF) Additive Manufacturing (AM)

❖ Powder spread, melt, & repeat...

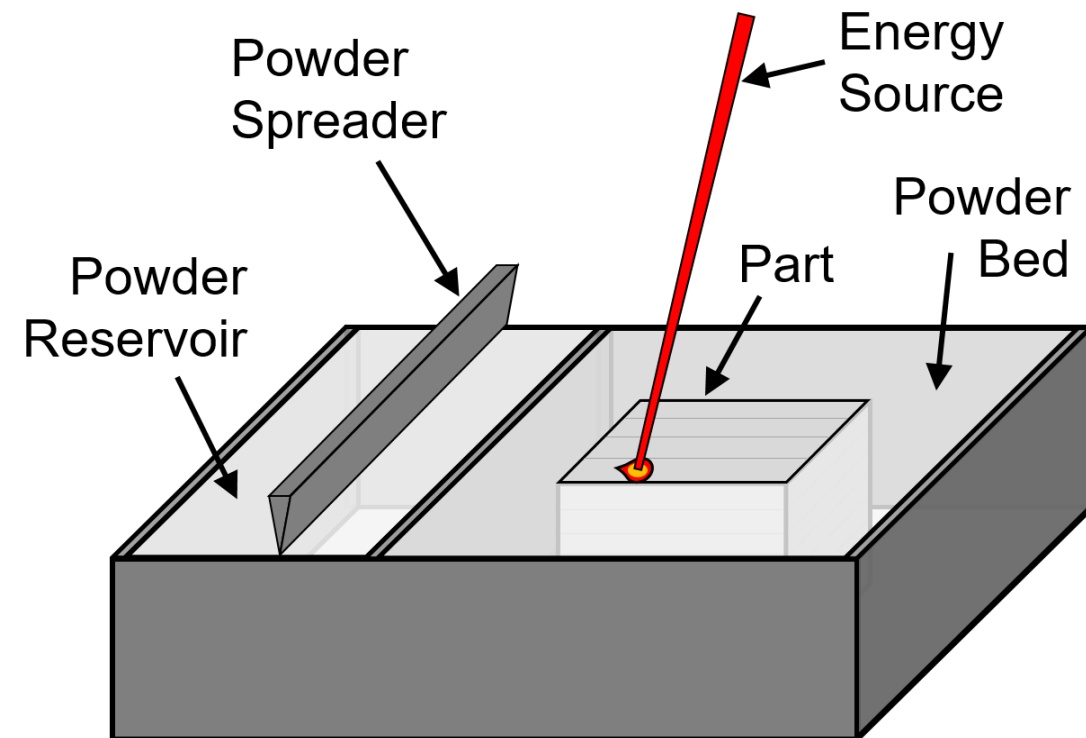
❖ Advantages:

- ❖ Design complexity
- ❖ Feature resolution
- ❖ Near-net-shape creation
- ❖ Reduction in tooling
- ❖ Low concept-to-production time

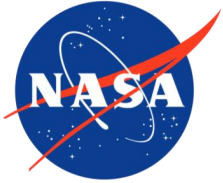
❖ Disadvantages:

- ❖ Build speed (low-to-medium runs)
- ❖ Part size
- ❖ Fatigue performance
- ❖ Performance uncertainty

Powder Bed Fusion AM Overview

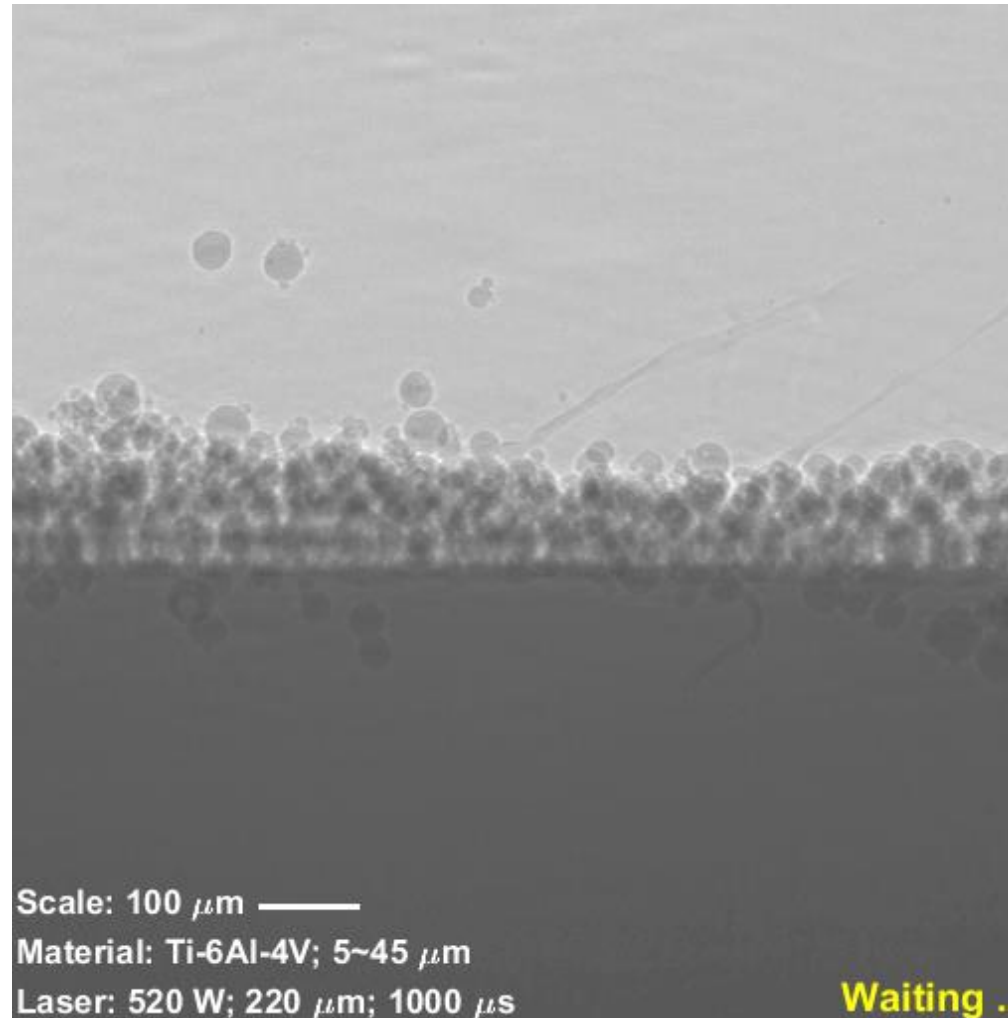


Complex Interaction of Multiple Phenomena in PBF



Simultaneous interactions between...

- ❖ Gas dynamics
- ❖ Plasma formation
- ❖ Fluid dynamics
- ❖ Granular/powder effects
- ❖ Phase transformations
- ❖ Heat transfer
- ❖ And more...



- ❖ Occurring constantly for hours or days
- ❖ Thousands or millions of melt events

Powder Layer

Bulk Material

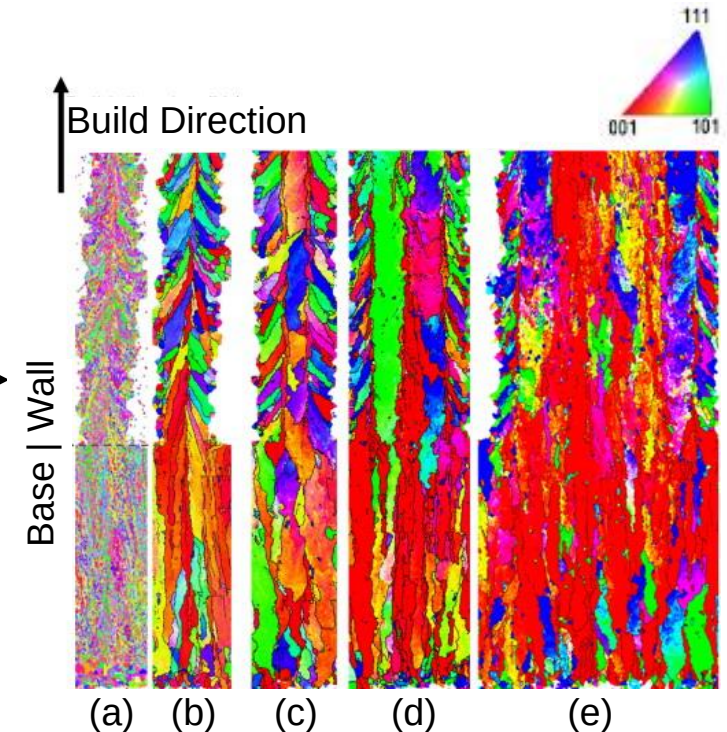
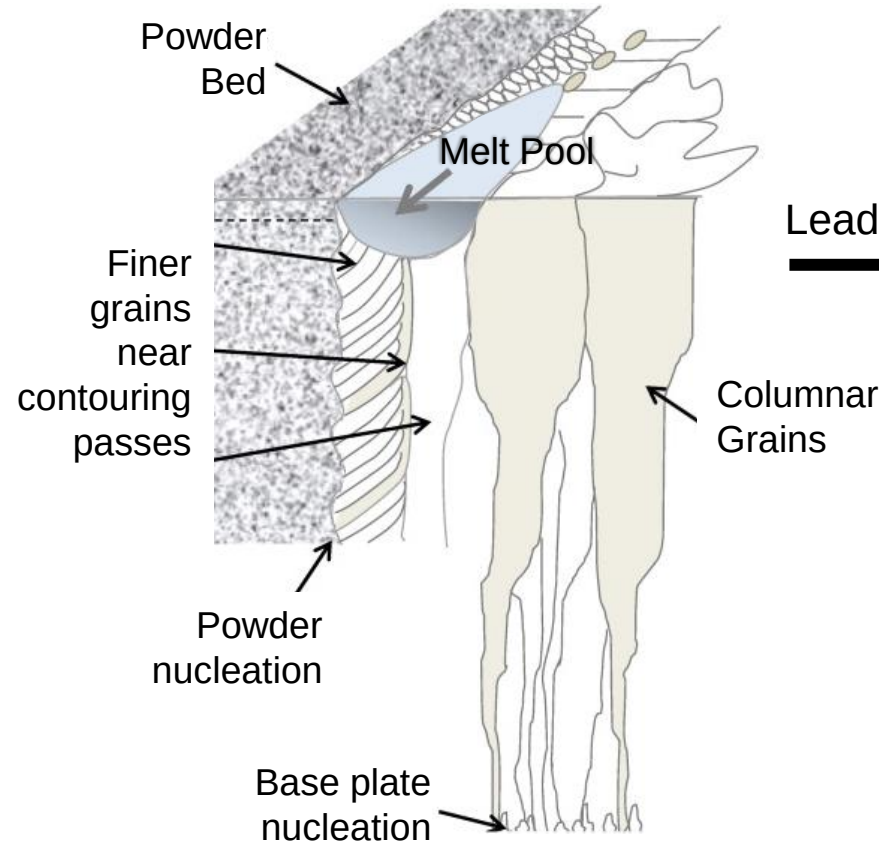
[1] C. Zhao, *et al.*, "Real-time monitoring of laser powder bed fusion process using high-speed X-ray imaging and diffraction." *Sci Rep* 7, 3602 (2017).
<https://doi.org/10.1038/s41598-017-03761-2>

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Bulk-Scale Effects of PBF on Microstructure

- ❖ Process involves repeated melting and solidification events
- ❖ Causes the formation of large, columnar grains orientated in the build direction



[2] Examples of reconstructed β -grain structures for (b) 1 mm, (c) 1.5 mm, (d) 2.0 mm, and (e) 5 mm wide walls in Ti64

[2] A.A. Antonysamy et al., "Effect of build geometry on the β -grain structure and texture in additive manufacture of Ti6Al4V by selective electron beam melting." *Materials characterization* 84 (2013): 153-168.

<https://doi.org/10.1016/j.matchar.2013.07.012>

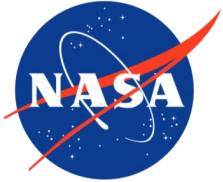
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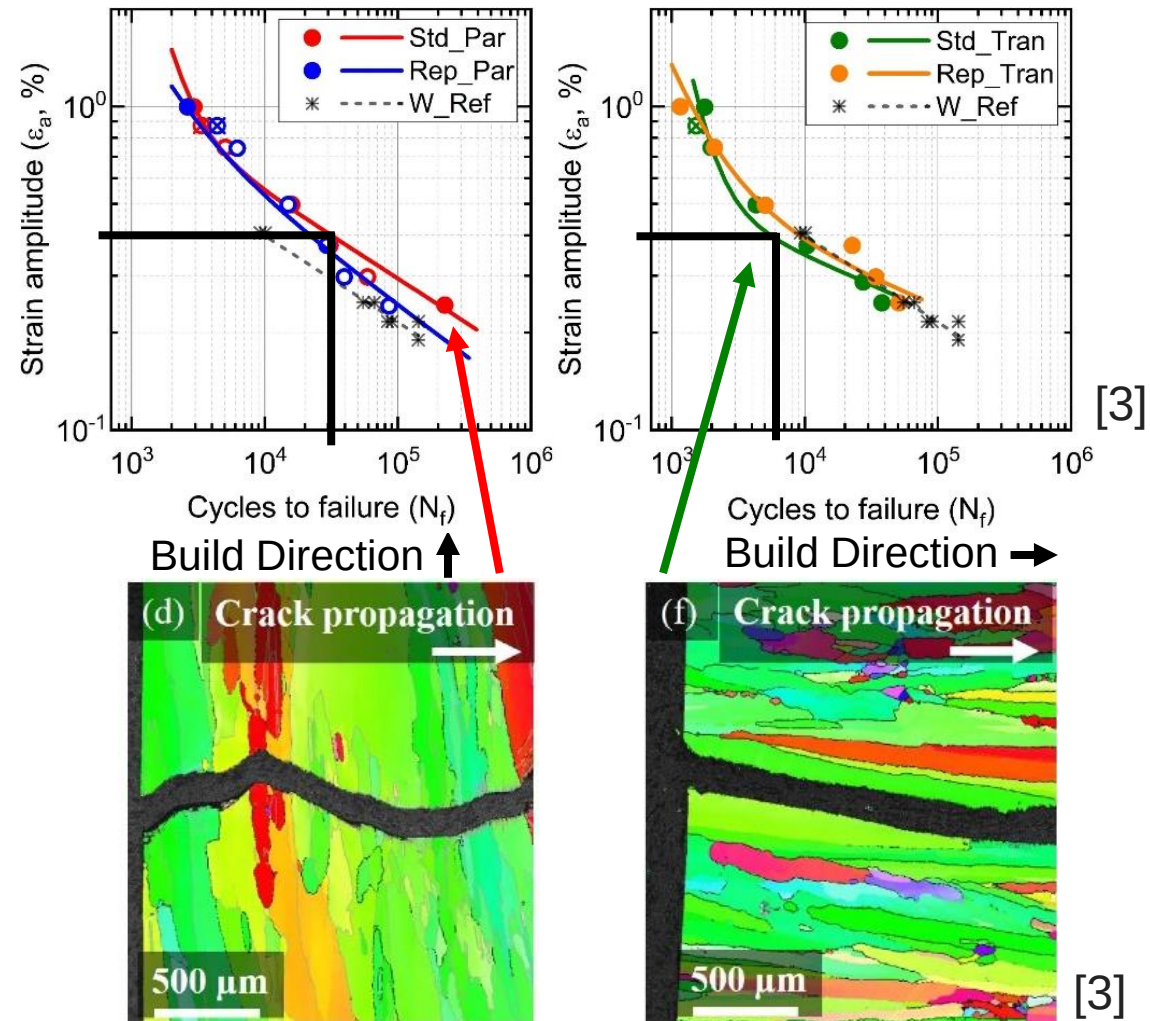
Figures cropped and relabeled vs. original

[2] Microstructure Development Mechanism

AM Microstructure – Why is it important?



- ❖ Columnar grains causes performance anisotropy and uncertainty based on orientation
- ❖ Makes qualification and certification (Q&C) of aerospace parts difficult
- ❖ Thousands of interacting melting events – how best to understand effect on final performance?



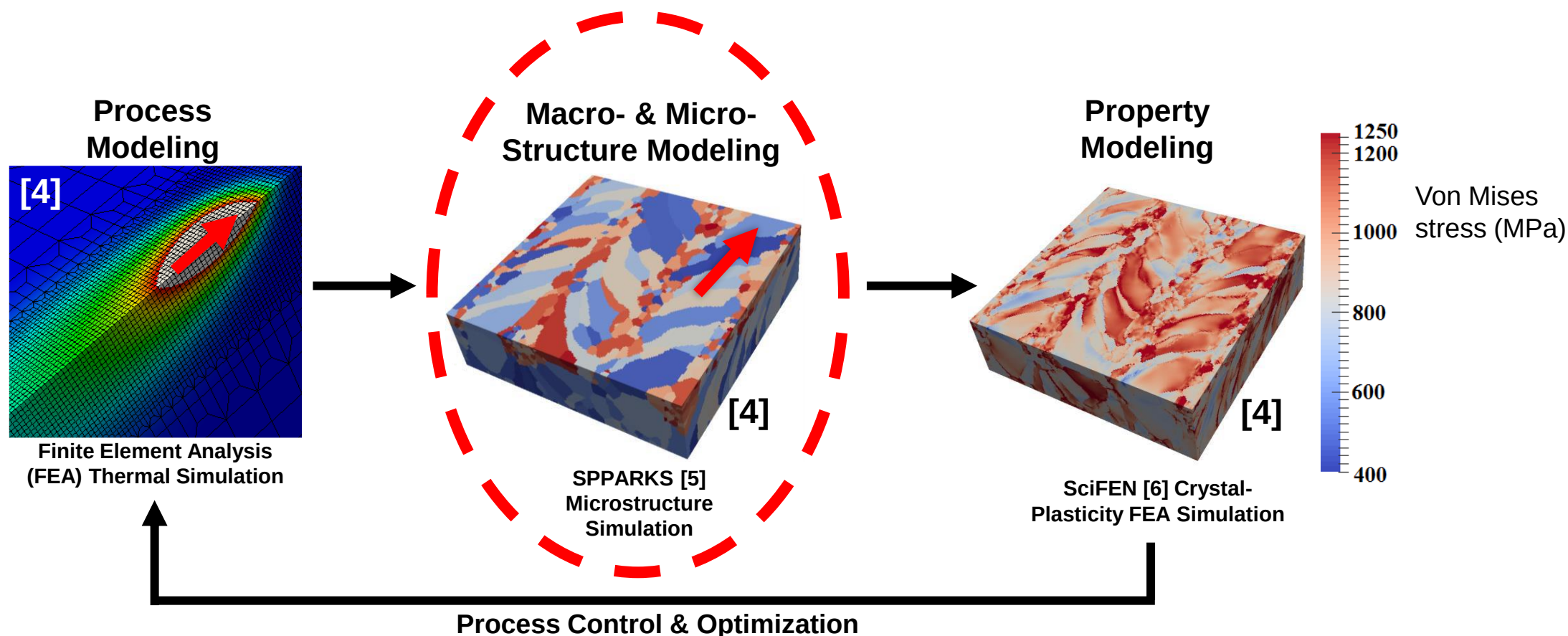
[3] A.R. Balachandramurthi, "Anisotropic fatigue properties of Alloy 718 manufactured by Electron Beam Powder Bed Fusion," Int. J. Fatigue 141 (2020)

Figures 10 & 13 used under CC BY 4.0 license <https://creativecommons.org/licenses/by/4.0/>
<https://doi.org/10.1016/j.ijfatigue.2020.105898>

Figures cropped, re-arranged, and lines added vs. original



Process-Structure-Property (PSP) Frameworks



[4] S.R. Yeratapally, Integrated Computational Materials Engineering to Establish Process-Structure-Property Relations in Polycrystalline Materials, *NIA Sandwich Series* (2020)
Available on the NASA Technical Reports Server (NTRS) (NTRS #20205001613)
Figures from Slide 12 modified from original

[5] Stochastic Parallel PARTicle Kinetic Simulator (SPPARKS), <https://spparks.github.io/>

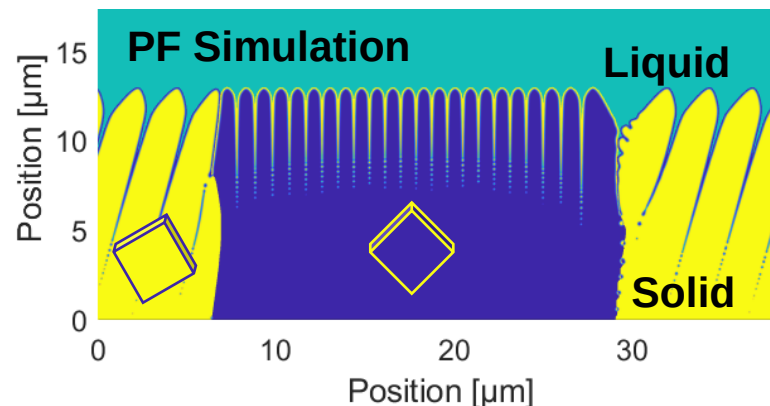
[6] SCalable Implementation of Finite Elements by NASA (SciFEN), <https://software.nasa.gov/software/LAR-18720-1>

Computational Microstructure Modeling for Additive Manufacturing (AM)

❖ Phase-Field (PF)

Simulates by solving governing partial differential equations

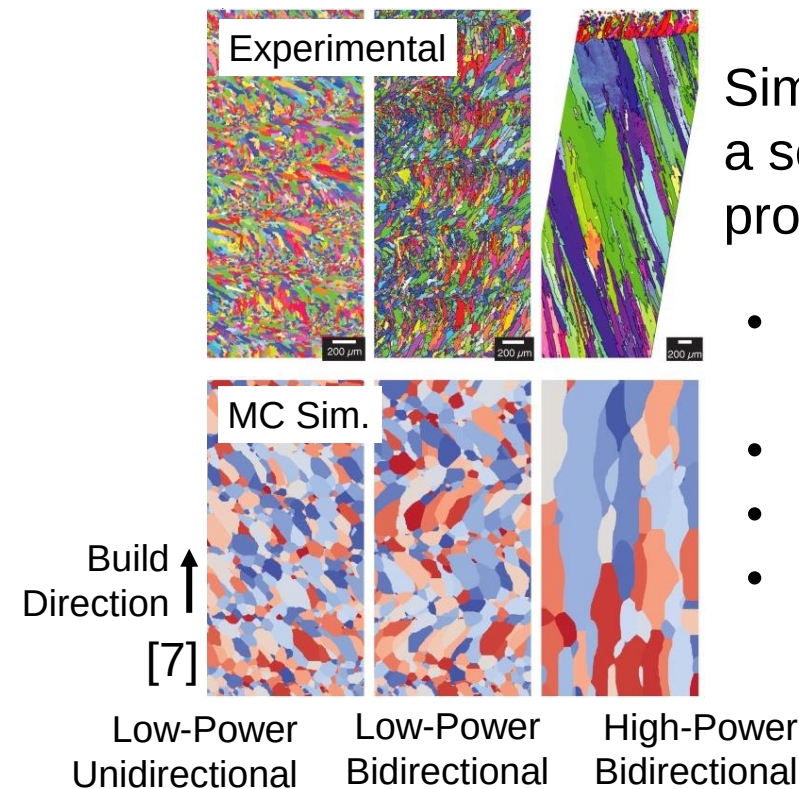
- Nanometer resolution
- High accuracy
- Expensive
- Fine details (texture)
- Strong physical basis



❖ Monte Carlo (MC)

Simulates through a series of probabilistic flips

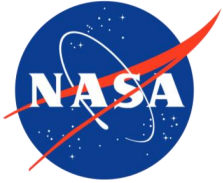
- Micrometer resolution
- Highly flexible
- Cheap
- Weak physical basis



[7] T.M. Rodgers et al., Simulation of metal additive manufacturing microstructures using kinetic Monte Carlo, *Comp. Mater. Sci.* (2017) <https://doi.org/10.1016/j.commatsci.2017.03.053>
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Figure cropped and relabeled vs. original

Leveraging Strengths of Complementary Models



- ❖ Current work is leveraging strengths of both techniques to produce advanced, composite model

Phase Field Modeling of AM Microstructures

Strong physical basis

Small domain size

Can predict fine resolution details

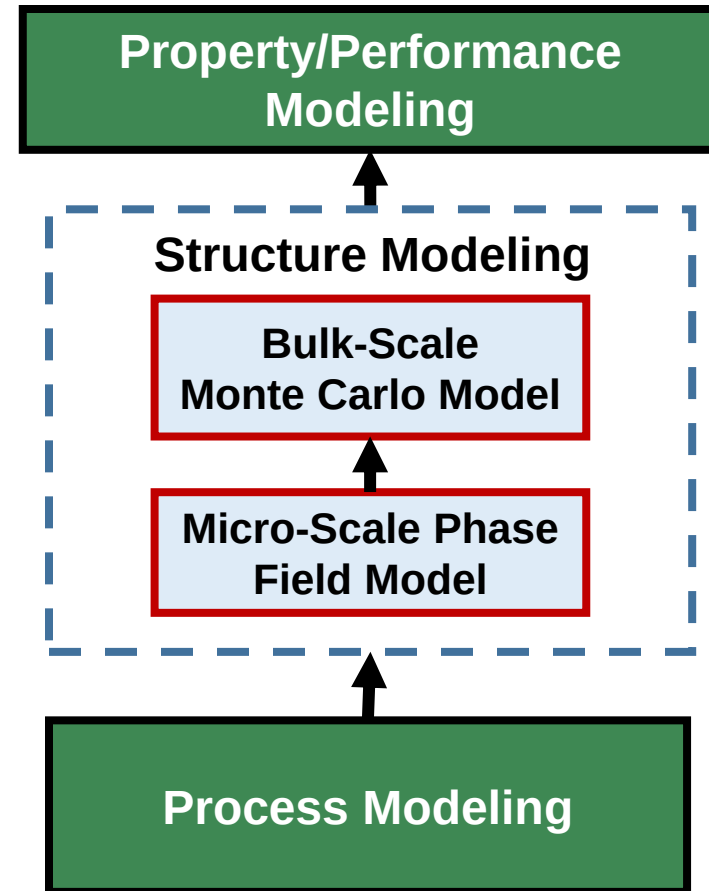
Monte Carlo Modeling of AM Microstructures

Weak physical basis

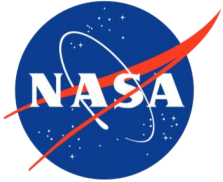
Large domain size

Easy to add/seed features (pores, segregation)

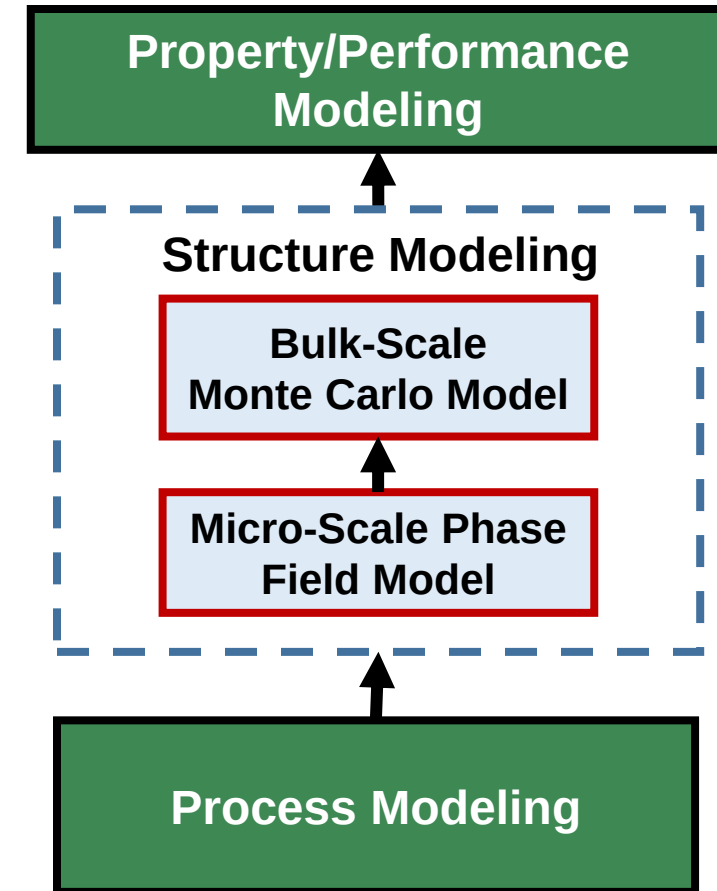
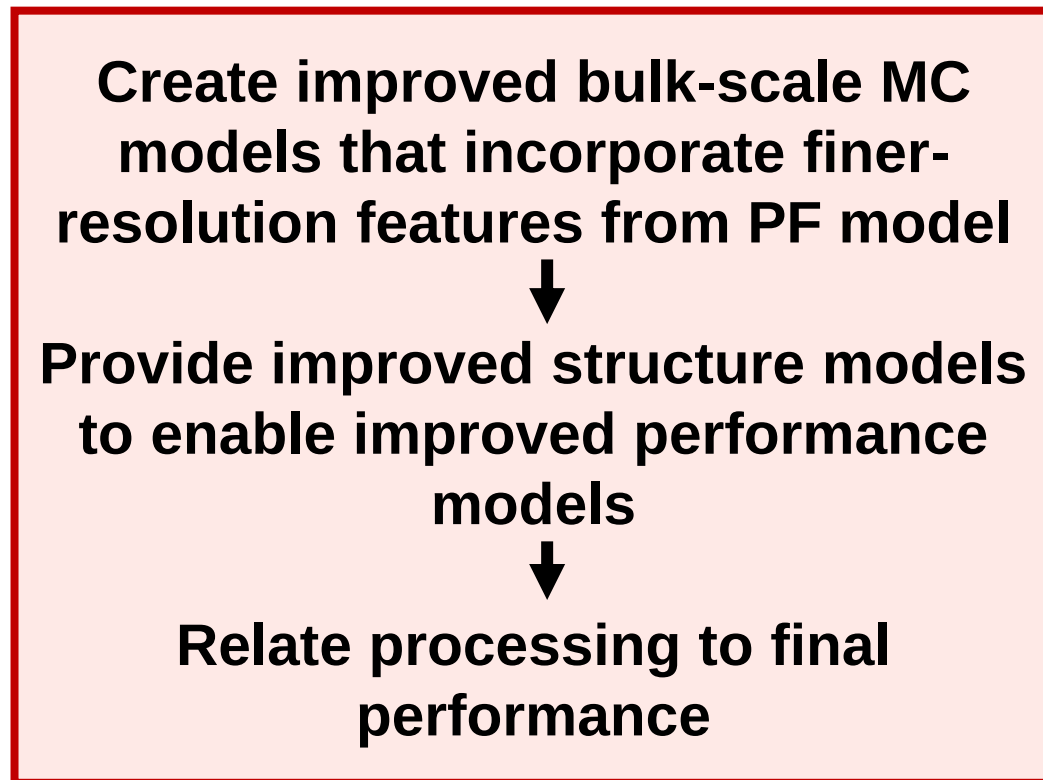
Utilize the MC models to attain higher domain size simulations with higher details from PF model



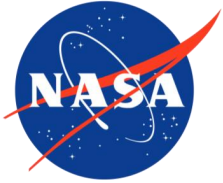
Leveraging Strengths of Complementary Models



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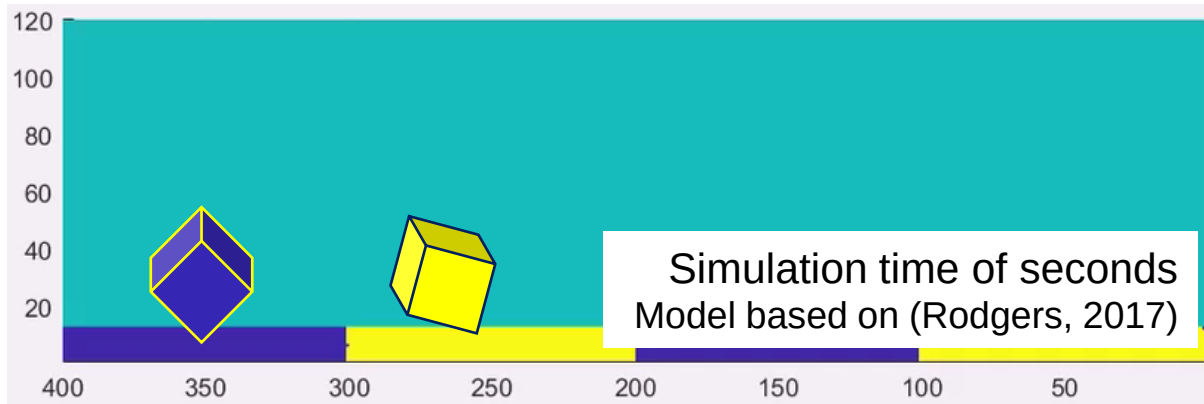


Crystal Orientation Evolution Modeling

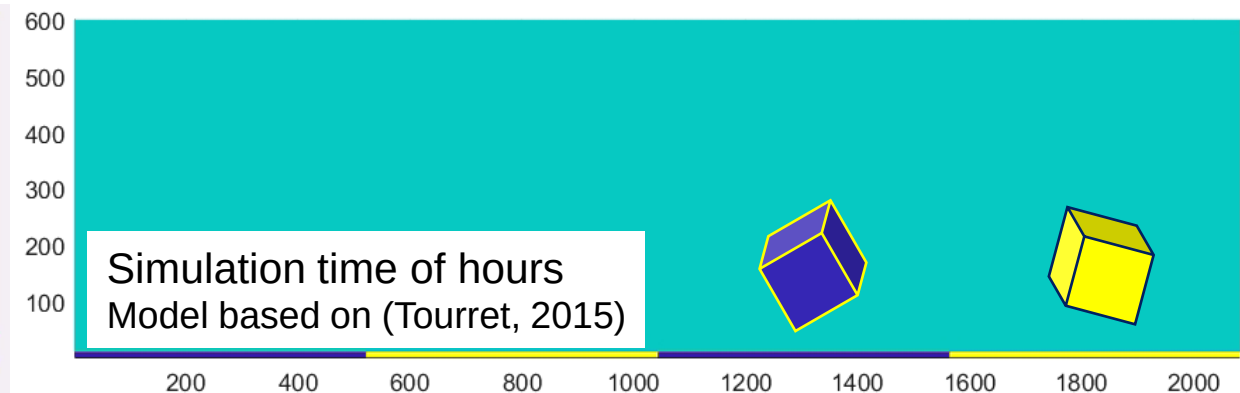


- ❖ Competitive grain growth contributes to the bulk-scale AM microstructure
- ❖ Drastic speed improvements achievable by implementing PF aspects in MC model

Monte Carlo Implementation of Competitive Grain Growth



Phase Field Implementation of Competitive Grain Growth



$$E = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^M (1 - \delta(q_i, q_j))$$

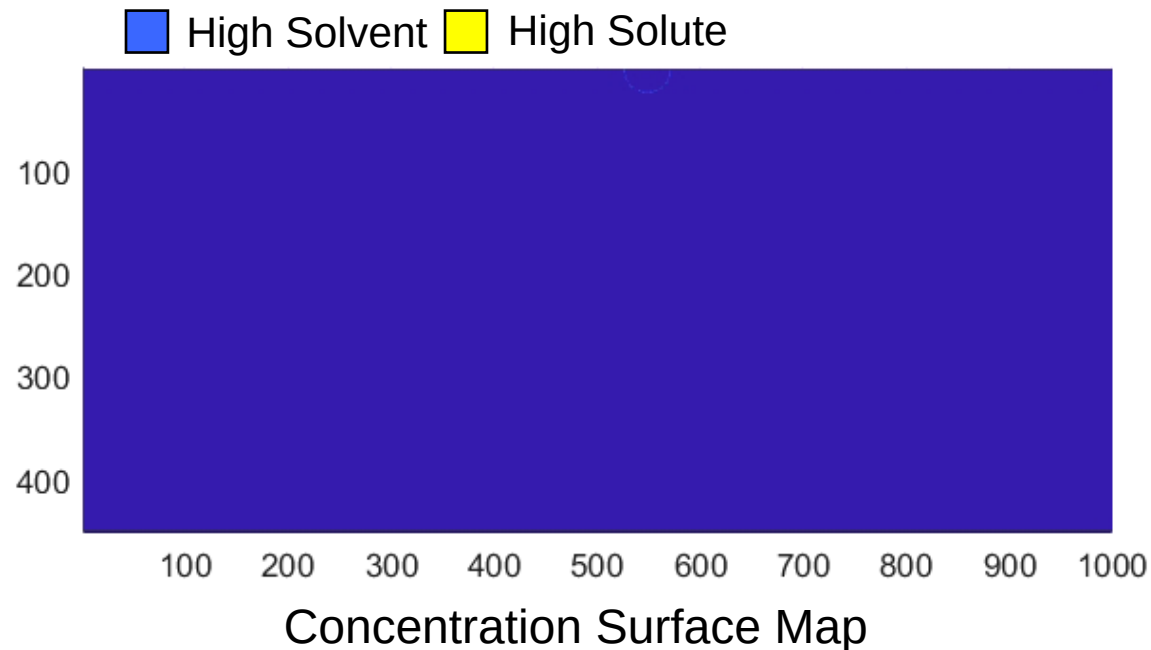
$$\left(\frac{1+k}{2} - \frac{1-k}{2} \phi \right) \frac{\partial U}{\partial t} = \nabla \cdot \left(\tilde{D} \frac{1-\phi}{2} \nabla U + \frac{1}{2\sqrt{2}} \tilde{U} \frac{\partial \phi}{\partial t} \frac{\nabla \phi}{|\nabla \phi|} \right) + \tilde{U} \frac{1}{2} \frac{\partial \phi}{\partial t}$$

$$[1 - (1-k)\tilde{T}] a_s(\mathbf{n})^2 \frac{\partial \phi}{\partial t} = \nabla \cdot [a_s(\mathbf{n})^2 \nabla \phi] + \sum_{m=x,y} \partial_m \left(|\nabla \phi|^2 a_s(\mathbf{n}) \frac{\partial a_s(\mathbf{n})}{\partial (\partial_m \phi)} \right) + \phi - \phi^3 - \lambda(1 - \phi^2)^2 (U + \tilde{T})$$

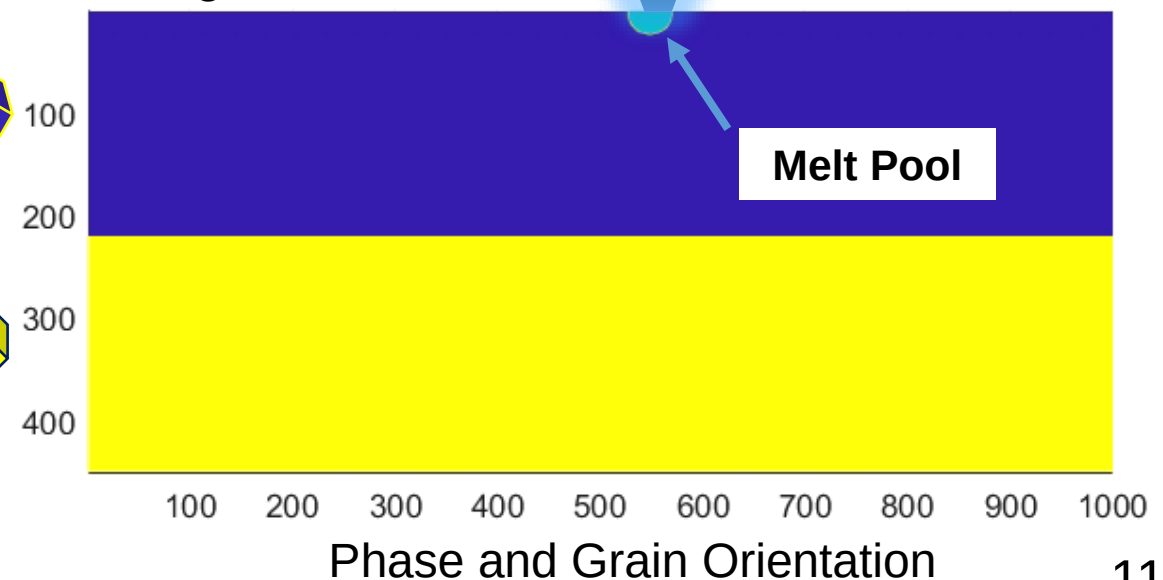


Moving Laser Melt Pool Modeling

- ❖ During PBF AM, a laser scans and melts the surface
- ❖ For alloys, solidification is solute field controlled
- ❖ Phase field modeling allows modeling dendritic growth during AM
 - ❖ Hours on high performance cluster GPUs for 2D domain of $100\text{ }\mu\text{m} \times 200\text{ }\mu\text{m}$



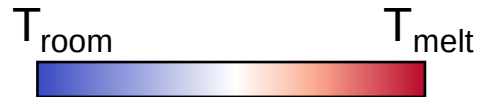
Moving laser heat source



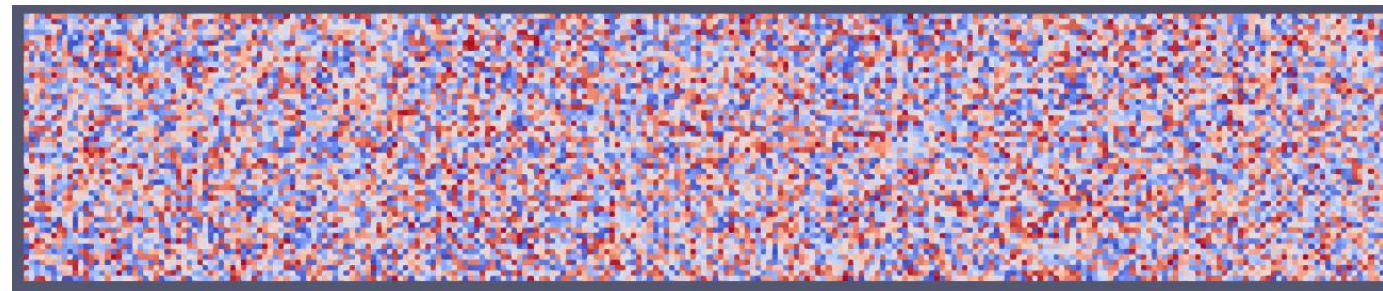
Moving Laser Melt Pool Modeling

- ❖ MC model loses the ability to model the solute field – but can calibrate MC to account for its effects
- ❖ Enables drastic speed and domain size improvements
 - ❖ Minutes on laptop for 3D domain of $1260\ \mu\text{m} \times 375\ \mu\text{m} \times 250\ \mu\text{m}$

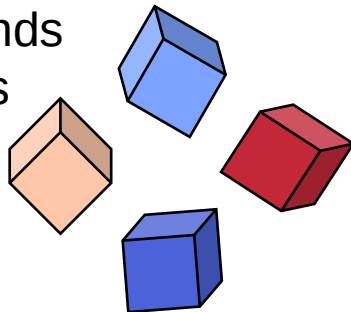
Temperature Field

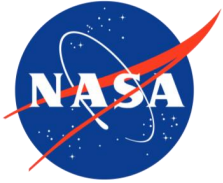


Grain Orientation Field



Thousands
of grains





Summary & Acknowledgement

- ❖ PBF AM - complex interactions and many melting events
- ❖ These melting events impacts the bulk-scale microstructure
- ❖ The anisotropic microstructure makes Q&C difficult

Thank you!

- ❖ Process-Structure-Property frameworks enable process understanding
- ❖ Composite structure models can leverage strengths of multiple models

Any Questions?

- ❖ This work was supported by NASA's Aeronautics Research Mission Directorate's Transformational Tools and Technologies (TTT) Project

