# Developments and Challenges Related to Thermal Process Modeling of Metallic Laser Powder Bed Fusion to Advance Certification of Flight Hardware

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# Introduction

## NASA’s Transformational Tools and Technologies (TTT) Project:

- Funded by Aeronautics Research Mission Directorate
- Project objective: advance computer-based tools and models for understanding and prediction of flight performance
- https://www.nasa.gov/aeroresearch/programs/tacp/ttt

## Sub-Group Working Under TTT:

- Develop computational and experimental tools to promote metallic additively manufactured (AM) parts for flight
- Ti-6Al-4V alloy (commercial aviation applications)
- Primary hurdle to adopting AM parts for flight is certification

## Objective of Current Work:

- Reduced order (fast) micro-scale (fine) thermal process model toward improved part-scale property predictions
- Better part-scale property predictions may lead to improved as-built part quality, which bolsters the business case for metallic AM parts for flight applications

# Laser Powder Bed Fusion (L-PBF)

## Primary Advantages of AM:

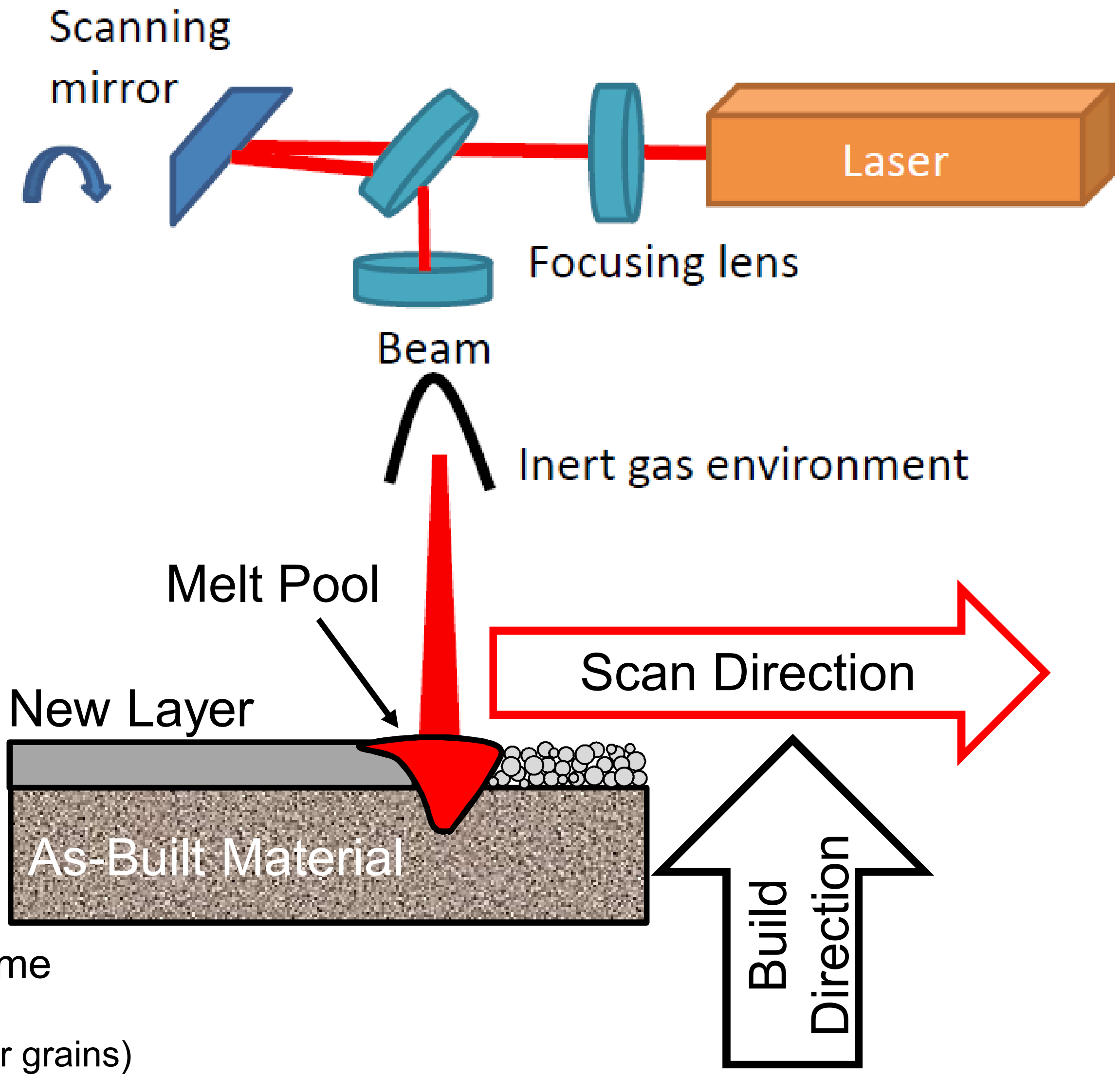
- Reduced part count assemblies
- Rapid manufacture of complex parts (few design constraints)

## L-PBF:

- Powder spread over part in thin layers (~40 µm)
- Small diameter laser rapidly traces part cross section (~70 µm)
- Well established AM process; relatively high feature resolution
- Part size constrained by build chamber volume (< 1 $m^3$)

## Some Hurdles to Adoption in Aerospace:

- Cost of powder vs. wrought
- High variability in properties from part to part
- Post processing reduces many of these issues but adds cost/time
    - Surface roughness (30 – 40 µm)
    - As-built property anisotropy (build – direction oriented columnar grains)
    - Residual stress distortions/cracking
    - Porosity




Wallace, T., Lang, C., Timucin, D., et. al., 2016, 'NASA's Materials Genome Initiative for Additive Manufacturing,' JANNAF Additive Manufacturing TIM.

# Qualification of AM Parts in Aerospace

## General:

- As-built AM part properties are notoriously inconsistent
- No widely accepted comprehensive “industry standard” for AM part production requirements

## Example of Current Requirements for Load Critical AM Parts (NASA):

- NASA self certifies flight vehicles; need to ensure reliable part properties throughout supply chain
- Comprehensive requirements for AM process control and part production (manned and high dollar spacecraft only)
    - MSFC-STD-3716 and MSFC-SPEC-3717: specific to L-PBF for IN718
    - Upcoming: NASA STD-6030/6033: adaptation of 3716 and 3717 not material or process specific
- Requirements in these standards to address variable part performance narrow AM business case:
    - Strict powder feedstock specifications
    - Large battery of mechanical tests (establish expected statistical distribution of material properties)
        - Witness samples (evaluated against this reference)
    - Equipment and software locked down after qualified process established
    - Each individual machine must be process qualified for critical flight parts
    - 100% part inspection, 100% heat treatment post processing

## TTT Objective to Improve As-Built Part Quality to Promote Adoption of AM for Flight Parts

# Opportunities for AM Process Models

## Opportunities for Process Modeling to Help:

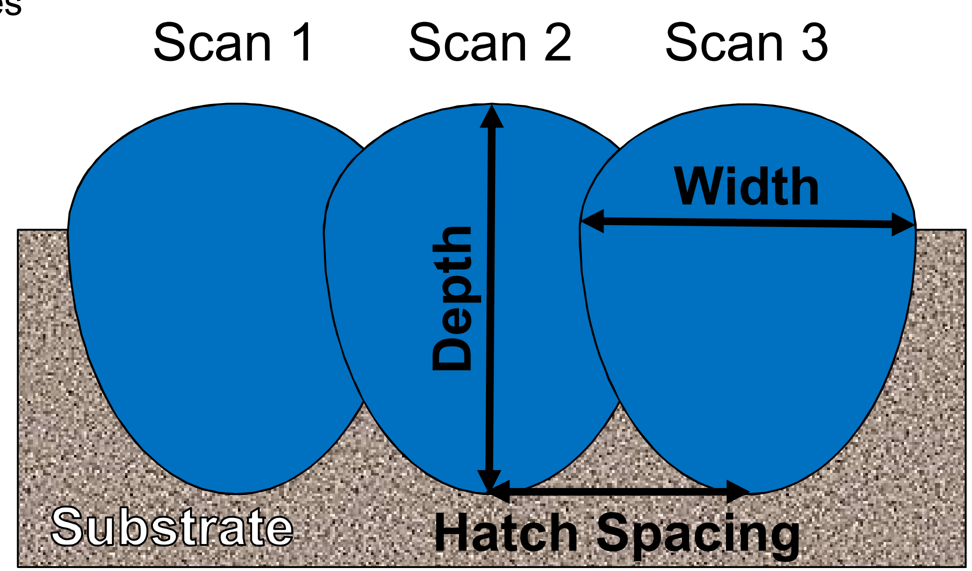
- Point heat source means a lot of opportunities for defects
- AM is a relatively immature process, mechanisms not well understood
- Measurement data tells us what not why or how to improve

## How Process Modeling Can Help:

- Understand physical mechanisms
  - Cause and effect relationships between process parameters and properties
  - Variable sensitivity and effects on property variation
- In-situ process monitoring (includes opportunities for machine learning)
- Mitigate need for post processing steps by improving as-built part quality

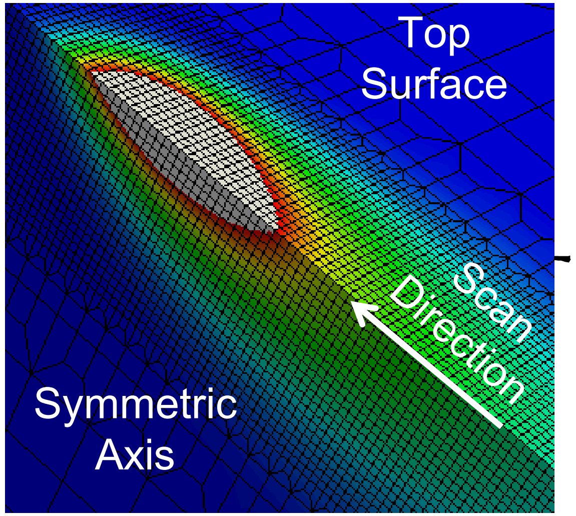
## Examples of Process Effects of Interest:

- Melt pool dimensions (MPDs)
  - Effect on porosity (Lack of Fusion (LoF))
  - Stability (powder particle interactions, mode of heating, etc)
- Temperature history
  - Microstructure growth and part properties (micro-scale)
  - Residual stress distribution and deformation (part-scale)



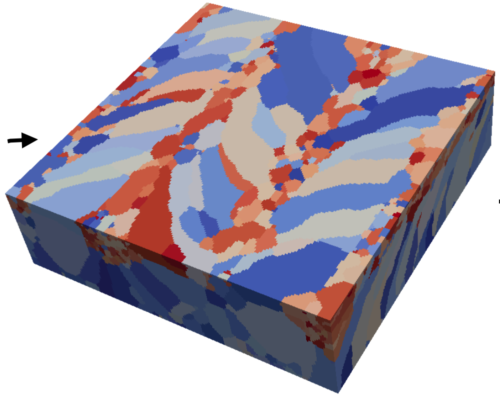

Melt Pool Dimensions
Cross section of single layer
(Laser traveling in/out of page)

# Overview of Process Modeling Relationships (TTT)

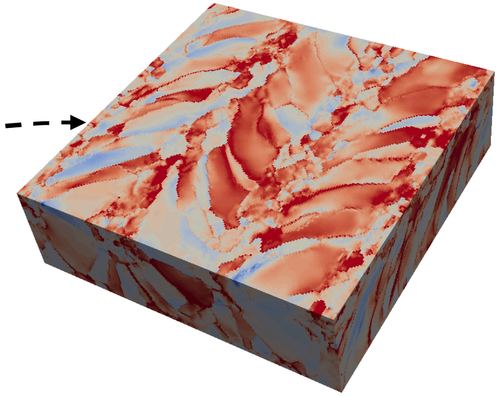



Single Scan Track Finite Element (FEA) Thermal Model

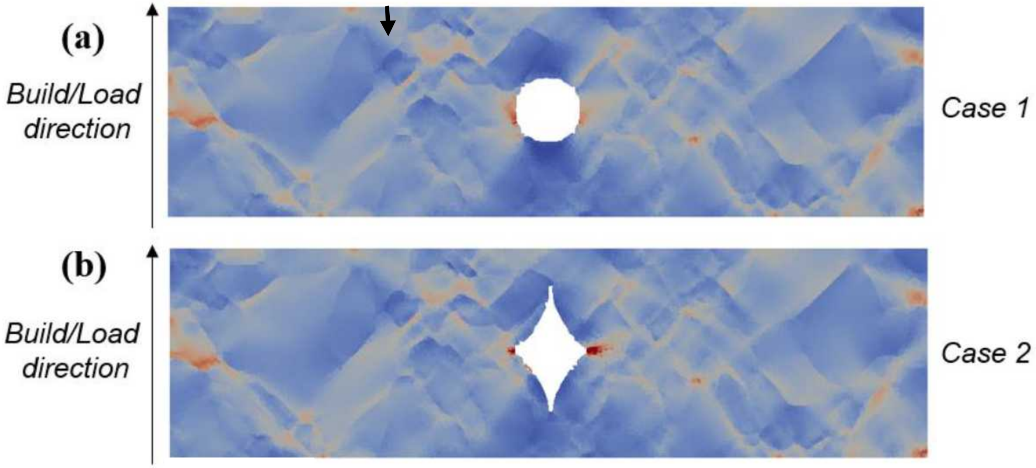
Focus for this talk



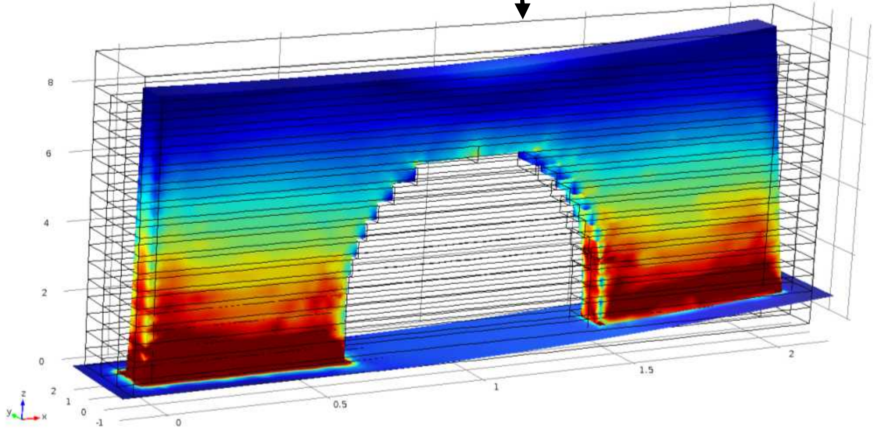
Microstructure Prediction (SPPARKS) **



Heterogenous Stress/Strain Fields (ScIFEN) **




Effect of Defects **



Residual Stress and Distortion *

* Wallace, T., Lang, C., Timucin, D., et. al., 2016, ‘NASA’s Materials Genome Initiative for Additive Manufacturing,’ JANNAF Additive Manufacturing TIM.

** Yeratapally, S.R., Lang, C.G., Glaessgen, E.H., A computational study to investigate the effect of defect geometries on the fatigue crack driving forces in powder-bed AM materials, AIAA SciTECH 2020

# FEA Thermal Process Model Challenges

## Computer Resource Intensive:

- Fine mesh and small timesteps
  - Steep thermal gradients (e.g., boiling to solidus ~50 μm)
    - Resolve melt pool and solid-liquid phase change front
  - Melt pool transits a given point (e.g., ~0.5 ms)
- Complex/coupled physics

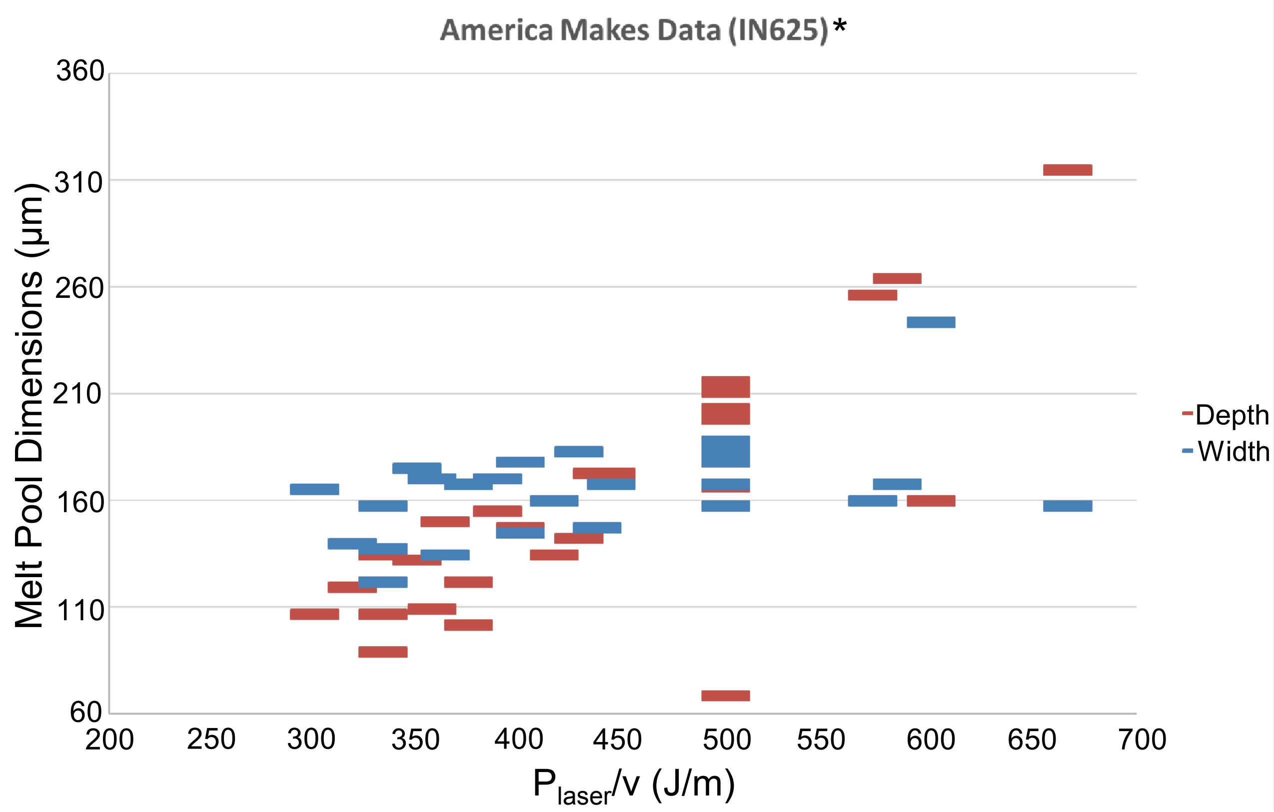
## Uncertainty in Modeling:

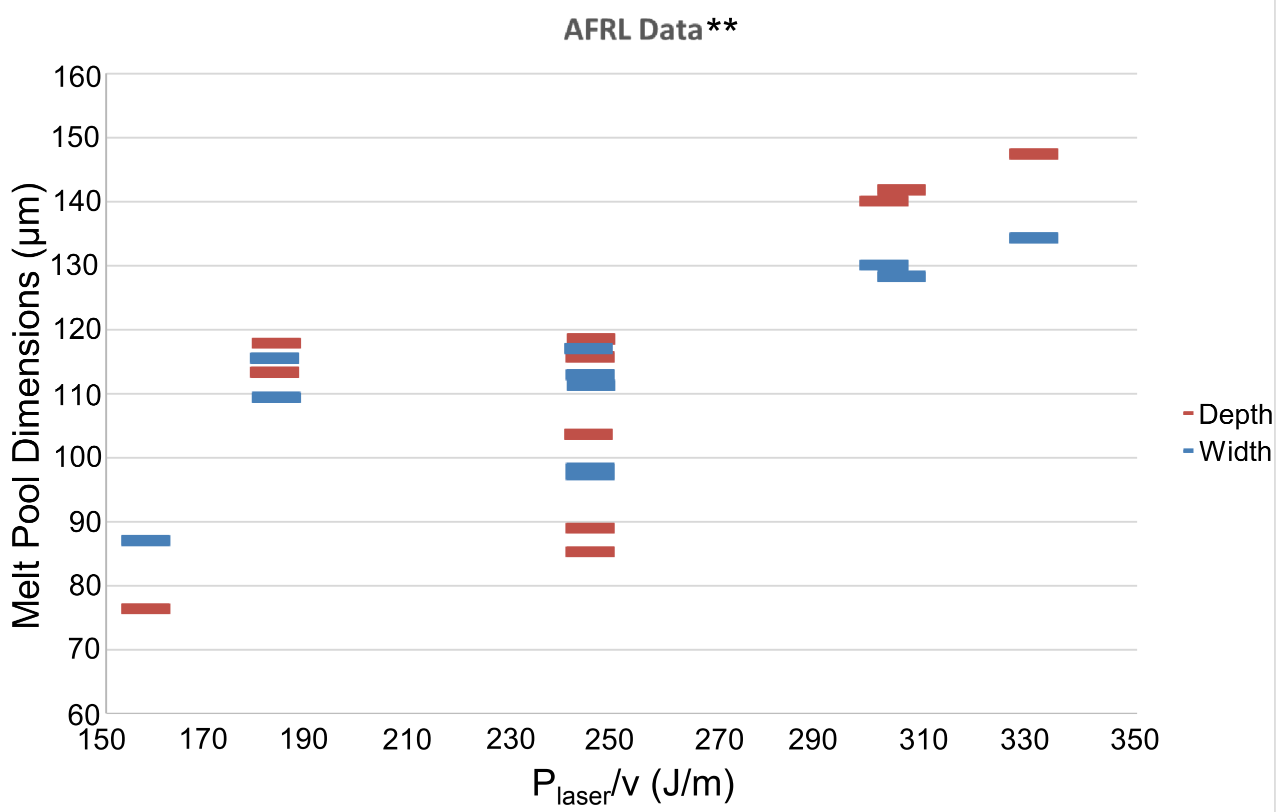
- Material properties difficult to measure (especially near and above melting)
  - Absorptivity varies with process parameters
- Physics models (evaporation, heat source, etc.)

## Validation Data:

- Data sources expensive or limited (micro-graphs, x-ray diffraction, etc.)
- Measurement uncertainty can be high or accurate measurements are infeasible
  - Temperature distribution: thermocouples, IR camera data, etc.
  - MPDs: micrographs, Dynamic X-Ray Radiography (DXR), etc.

# FEA Thermal Process Model Challenges: Data Variability




$$Plaser = laser\ power; \mathrm{v} = \mathrm{laser\ scan\ speed}$$

Challenges with High Variability Data:

- Model validation
- Target for auto-parameter tuning (more on this soon)

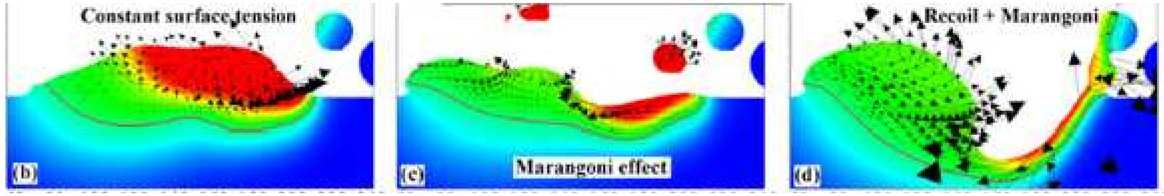
* Groeber, M., Schwalbach, E., Donegan, S., et. al., 2018, 'The Air Force Research Laboratory, Additive Manufacturing (AM) Modeling Challenge Series: Challenge Problem 2: Microscale Process-to-Structure,' Supplemental Data. Extracted from America Makes Project 4026 final report

** Groeber, M., Schwalbach, E., Donegan, S., et. al., 2018, 'The Air Force Research Laboratory, Additive Manufacturing (AM) Modeling Challenge Series: Challenge Problem 2: Microscale Process-to-Structure,' Challenge Problem Statement.

# Thermal Process Model Fidelity

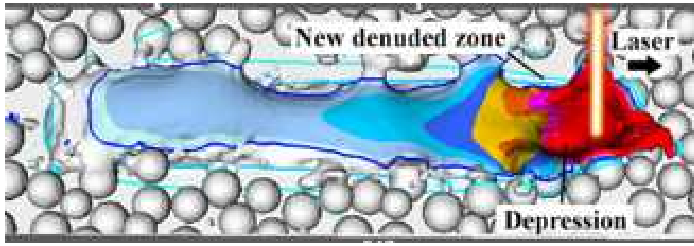
## Model Scale (Micro, Macro, and Part Scale):

- Ideally, part-scale would be most directly useful for all analysis
- Larger scale models require more computer resources
- Part scale models are low fidelity (order)




## High Fidelity Micro-Scale Model Example:

- Understand physical mechanisms cause and effects
    - Powder particle interactions, keyhole formation mechanism, melt pool convection, etc.
- Example Lawrence Livermore National Lab's Model*:
    - Excellent micro-scale mechanism simulation; does not scale well
    - 100,000 CPU hours; requires high performance computing (~3 years with 4 core desktop)
        - Parametric study infeasible: variability in part properties, effect of variables, etc.
        - Changing process parameters and alloys requires unique study ($a_{laser}$ manually adjusted)




* Khairallah, S., Anderson, A., Rubenchik, A., et. al., 2016, "Laser powder-bed fusion additive manufacturing: Physics of complex melt flow and formation mechanisms of pores, spatter, and denudation zones," Acta Materialia, Vol. 108, p. 36-45.

## Part-Scale Models:

- Commonly start with thermal agglomeration (lumping) assumption
- Macro-effects considered: edge effects, scan patterns, build orientation, etc.
- Topology optimization, residual stress and part distortion, geometric parameter optimization, etc.

## One Current Approach (TTT):

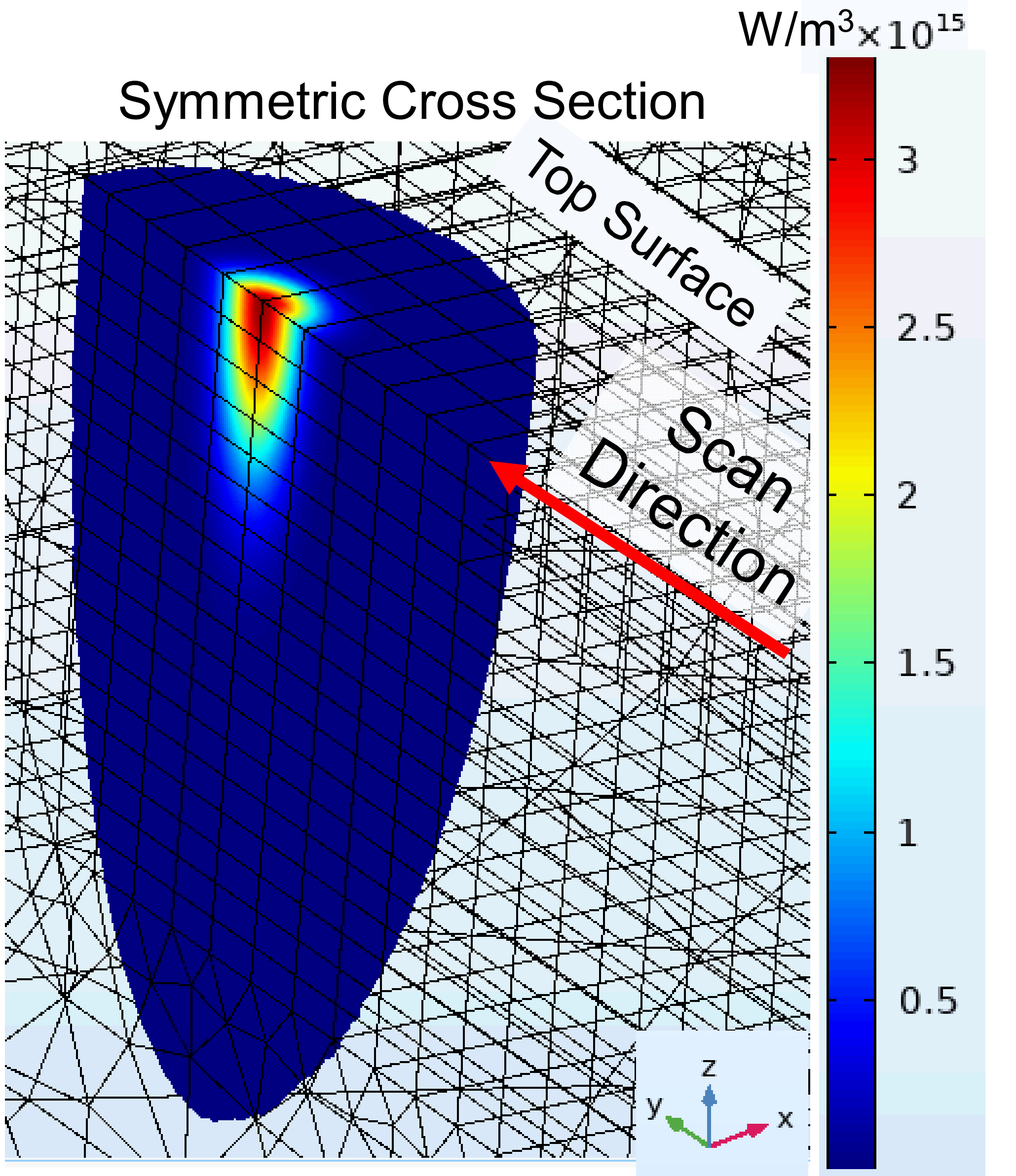
- Unique contribution: reduced order (fast) micro-scale (fine) thermal model to improve input for part-scale analyses

# Current Approach: Volumetric Heat Source

$$Q_{laser} = a_{laser}\frac{6\sqrt{3}P_{laser}}{abc\pi\sqrt{\pi}}e^{-3(x-x_0)^2/a^2}e^{-3(y-y_0)^2/b^2}e^{-3(z-z_0)^2/c^2}\,*$$

$$a_{laser} = laser\ absorptivity$$
$$a = b = \sigma_{laser} * spot\ size\ parameter$$
$$c = \sigma_{laser} * depth\ parameter$$
$$\sigma_{laser} = laser\ diameter/4$$
$$x_0, y_0, z_0 = laser\ location$$

* Goldak, J., Chakravarti, A., Bibby, M., 1984, "A New Finite Element Model for Welding Heat Sources," Metallurgical Transactions B, Vol. 15B, p. 299-305.

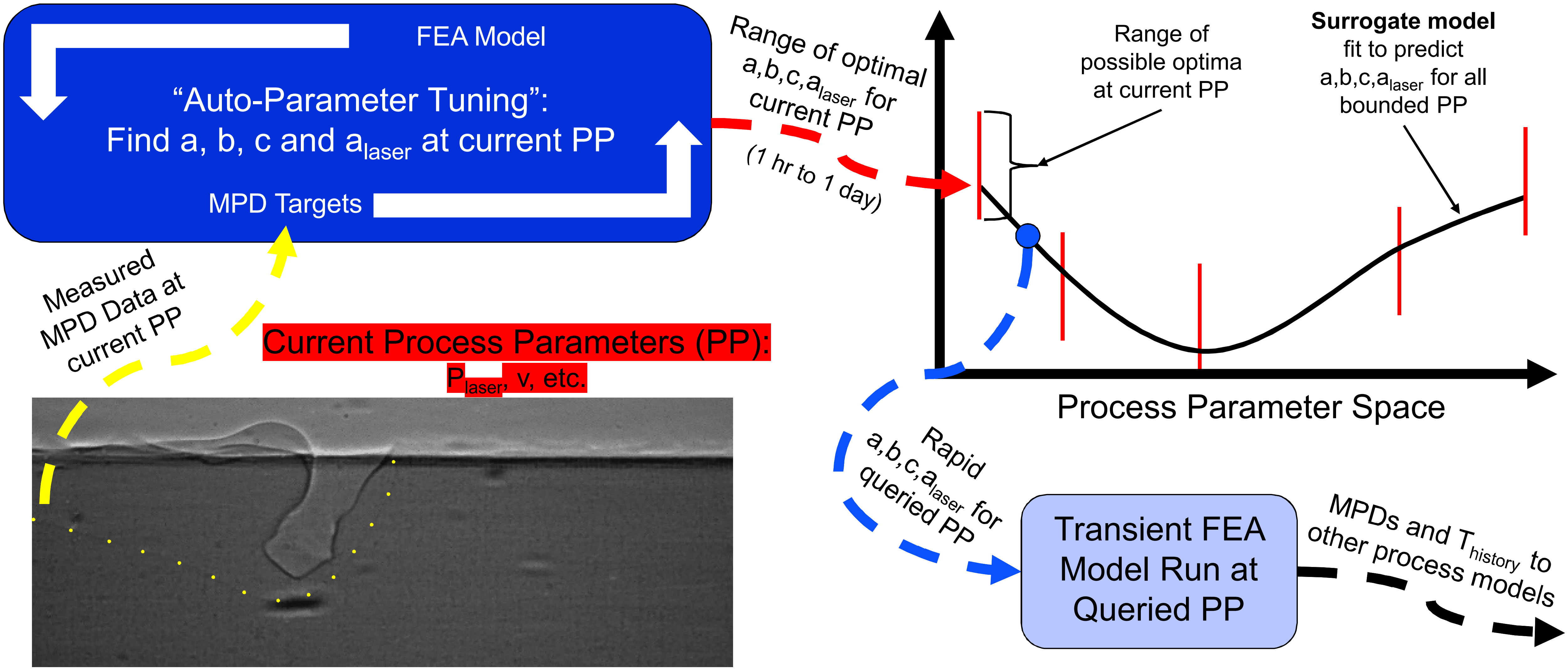



Predict MPDs → temperature history outside of melt pool
- Required inputs for other process models
- Region with highest certainty in physics and material properties

"Working Predictive Measure" is the goal:
- Significant increase in solution speed (reduced model fidelity)
  - Substitute volumetric source for complex melt pool physics
  - Study of effects of variables and variation
- Relative increase in fidelity of inputs for higher scale models
  - LoF porosity predictions
  - High resolution microstructure – properties

Selecting "optimal" parameters (a, b, c, $a_{laser}$):
- Predicted MPDs that match measured values

# Current Approach: Working Predictive Model Overview




Melt Pool Imaged Via Dynamic X-Ray Radiography (DXR)*
MPDs Acquired Via Machine Vision

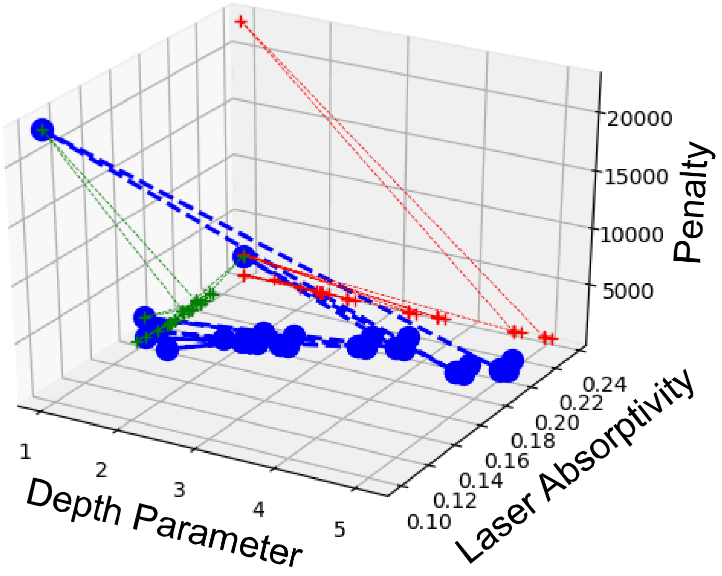
*Image Courtesy Dr. Anthony Rollett, Carnegie Mellon University

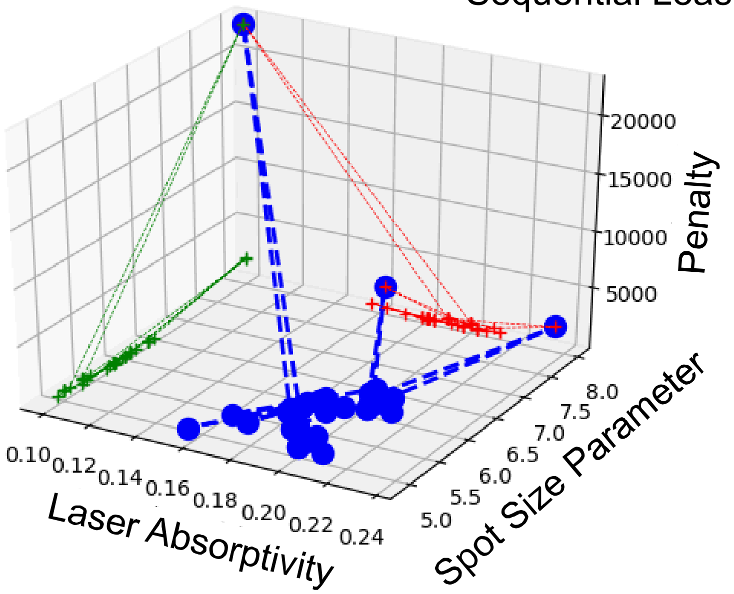
# Current Approach: Auto-Parameter Tuning Approaches

Example Methods Investigated to Automatically Find Parameters:

- Direct optimization:
  - Optimization algorithm iteratively runs thermal model
  - Minimization of penalty function
    - $penalty = (W_{measured} - W_{predicted})^2 + (D_{measured} - D_{predicted})^2$
  - "Optimum" a,b,c and $a_{laser}$

Showing convergence on optimum (this example):
Sequential Least SQuares Programming (SLSQP)

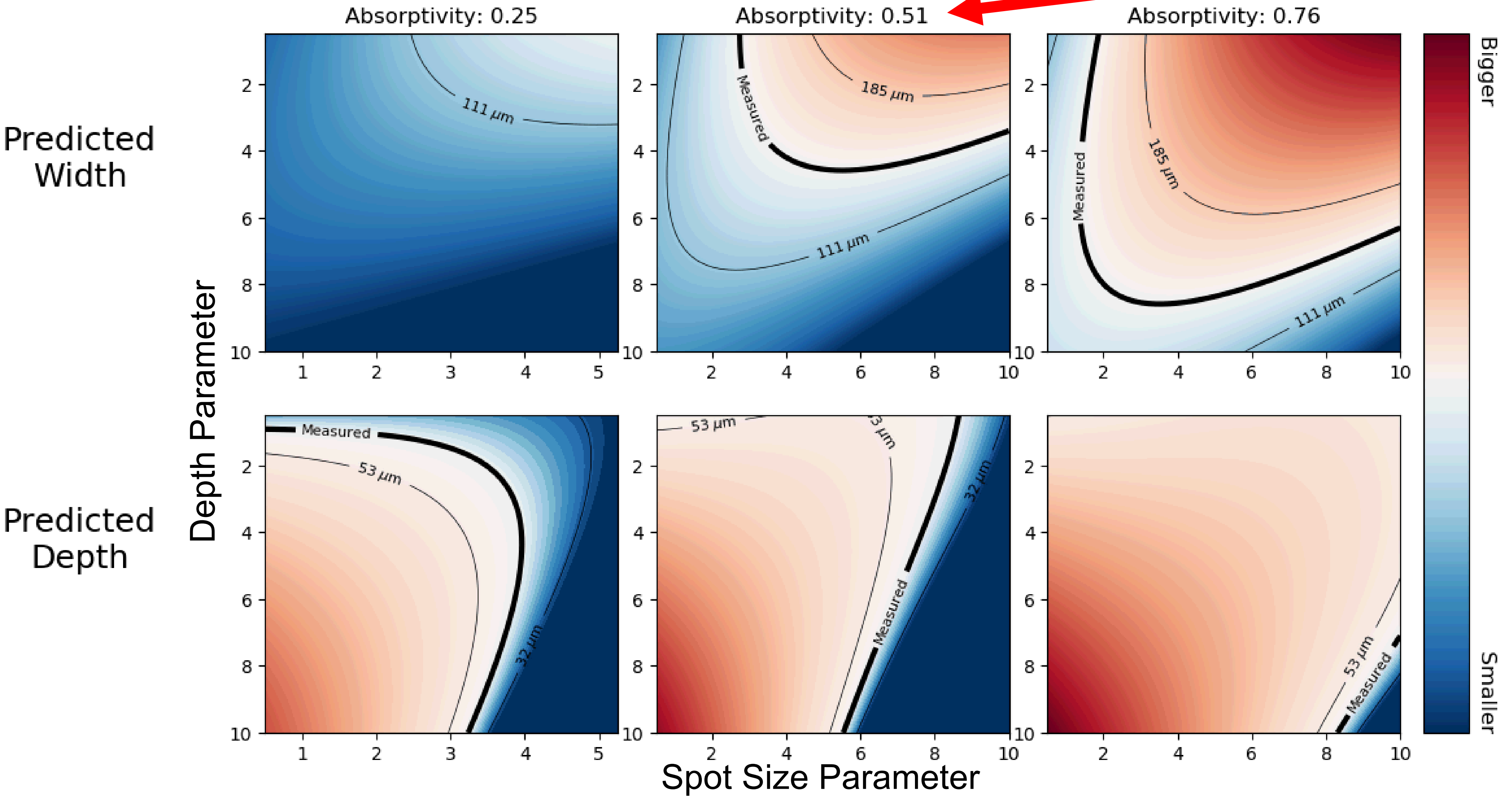


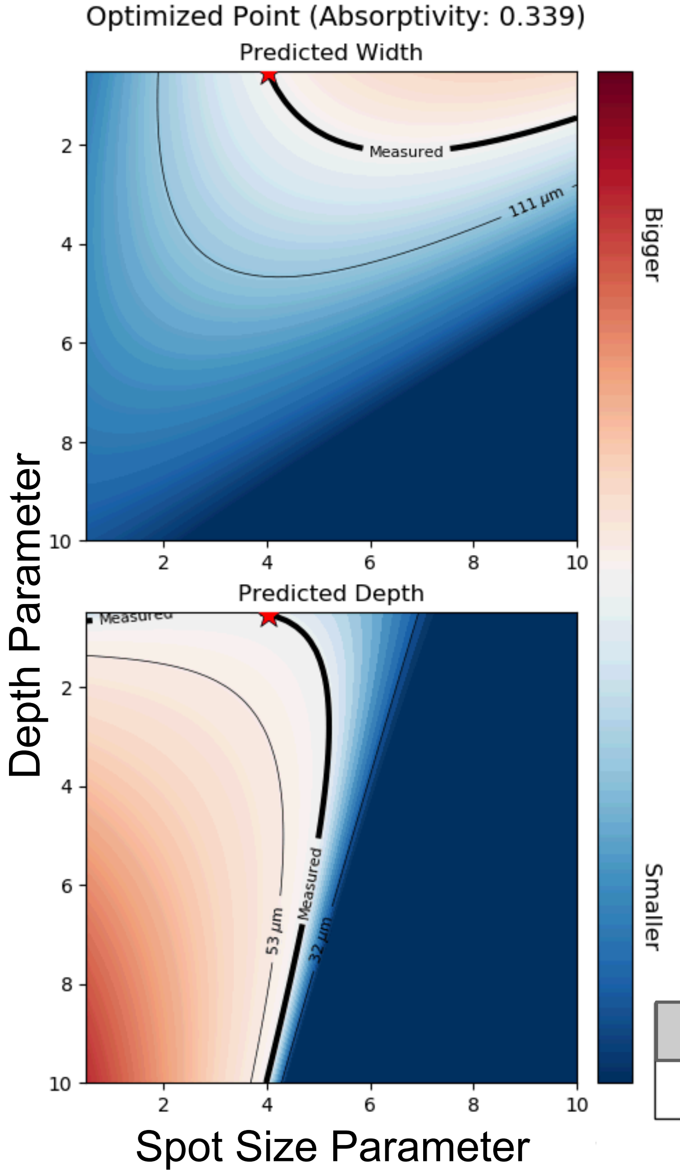

- Optimization and Machine Learning (next slides):
  - Run thermal model parametrically over a range of model space
  - Fit a cross validated surrogate model
  - Optimization algorithm locates "optimum" a,b,c and $a_{laser}$ in surrogate model

# Current Approach: Surrogate of FEA Thermal Model

Must be additional optima around 0.51



# Current Approach: Optimization of Surrogate Model



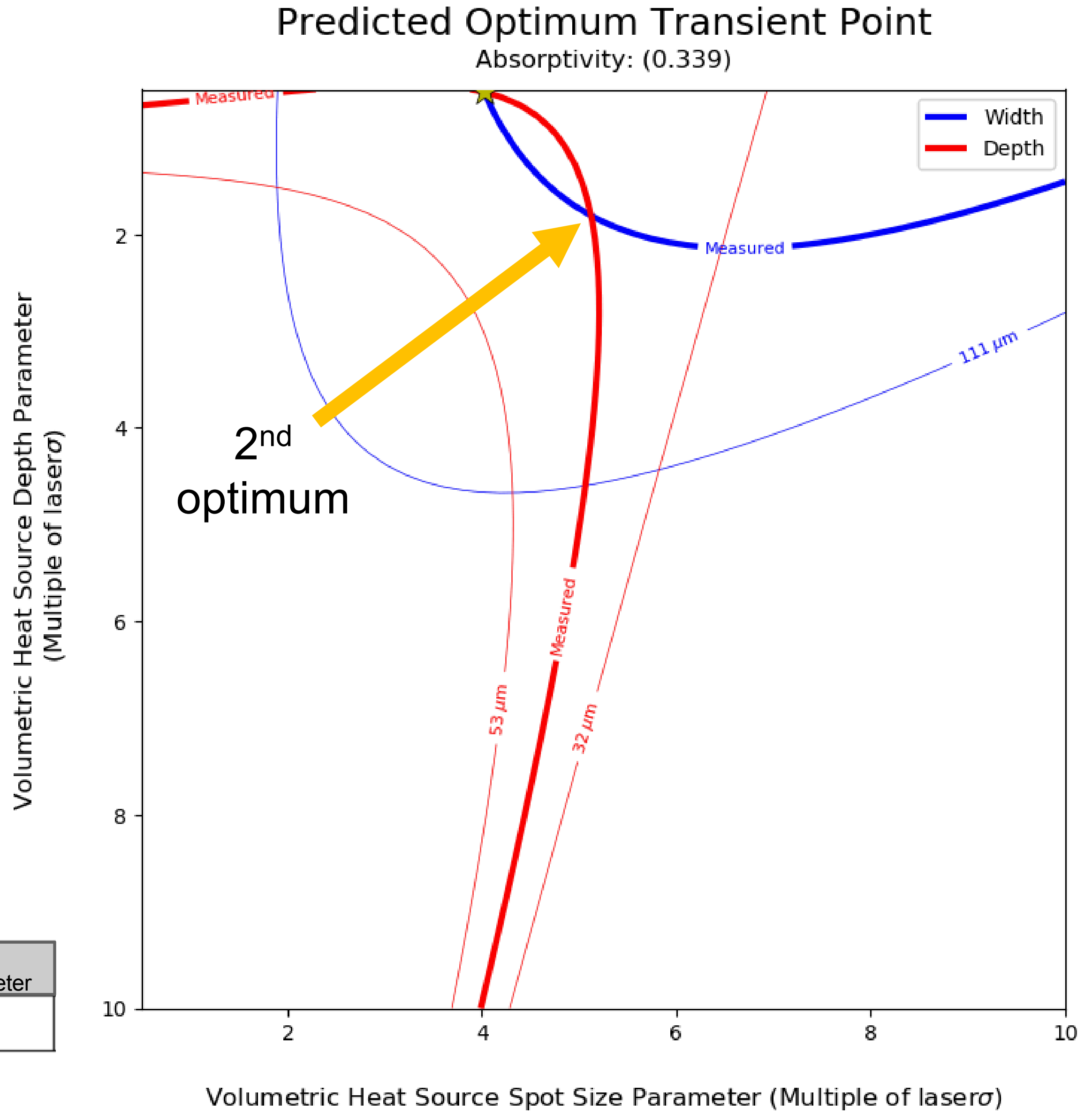

Target is NIST AM Bench "Case A" *
(IN625 no powder)

* National Institute of Standards and Technology (NIST) Additive Manufacturing Benchmark Test Series (AM-BENCH) AMB2018-02 (2018).

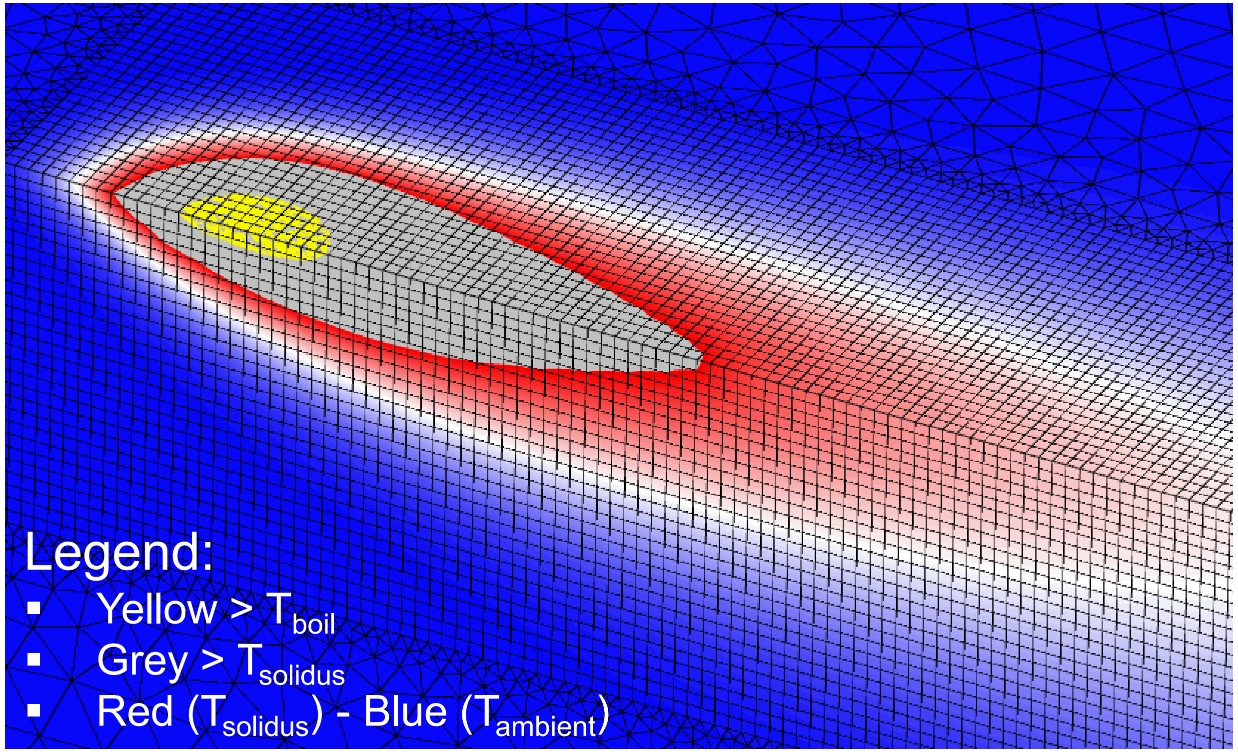
| *Predicted Transient Depth (μm)* | *Measured Depth (μm)* |
|---|---|
| 42.5 | 42.5 |

| *Predicted Transient Width (μm)* | *Measured Width (μm)* |
|---|---|
| 147.9 | 147.9 |

| Optimized Depth Parameter | Optimized Absorptivity | Optimized Spot Size Parameter |
|---|---|---|
| 0.52856 | 0.33884 | 4.02151 |

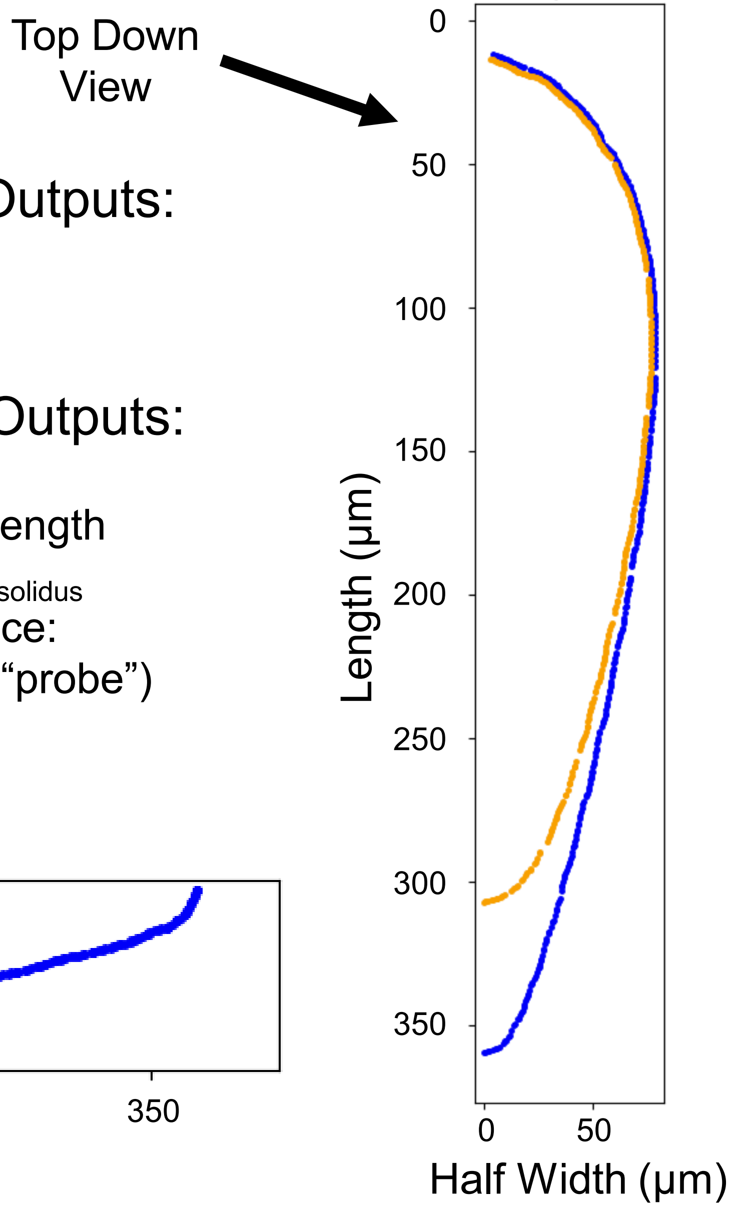


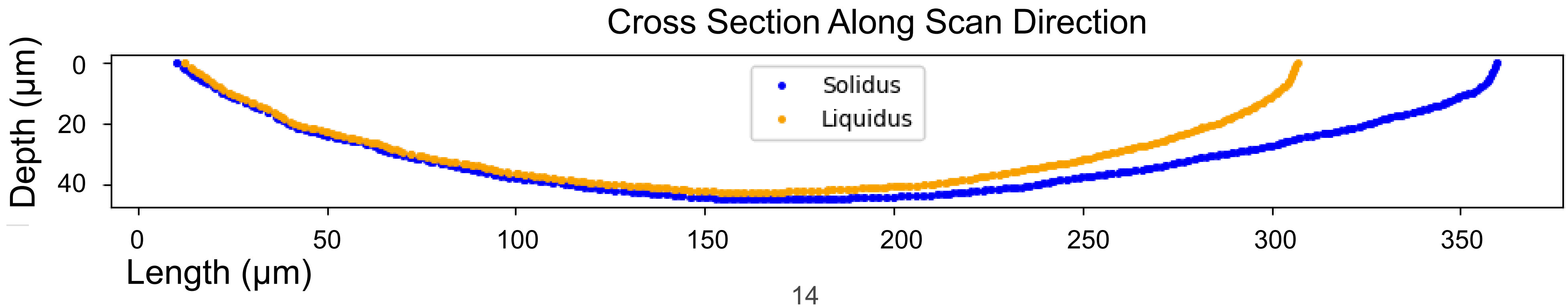
# Current Approach: Transient Model Predictions




Parameter Tuning Outputs:
- Maximum Width
- Maximum Depth

Full Transient Run Outputs:
- MPDs:
  - Width, Depth, Length
  - Point cloud at $T_{solidus}$
- Temperature transience:
  - At a fixed point ("probe")
  - Point cloud



# Concluding Remarks

Developing Computational Capabilities to Better Understand Mechanisms and Cause and Effects

Model Fidelity and Scale

- If computational resources were unlimited large scale – high fidelity models obvious choice
- High fidelity models for understanding process mechanisms; large scale models for design and production guidance
- Niche exists where micro-scale resolution inputs drive part-scale predictions at a useful speed

This Work: Low Fidelity (Fast) Micro-Scale (Fine) Thermal Model to Improve Part-Scale Process Model Predictions

- Auto-parameter tuning of volumetric heat source to reduce model fidelity
- Opportunities for parametric studies on property variation and process variable sensitivity
- Successfully predicts MPDs based on width and depth; future work toward melt pool shape prediction

Promote Adoption of AM for Flight Parts:

- As-built AM part properties highly variable; current requirements to guarantee quality narrow business case
- More accurate and articulate part-scale model thermal input assumptions mean better as-built property predictions

# Symbols

$a_{laser}$: surface laser absorptivity
$C_p$: Specific heat at constant pressure
D: Melt pool maximum depth
f: phase fraction indicator
h: convective heat flux coefficient
$L_v$: latent heat of vaporization
M: molar mass
$m_v$: evaporative mass flux
n: surface normal
$P_{laser}$: laser power
$p_o$: ambient pressure
$p_v$: vapor pressure
$Q_{laser}$: laser volumetric heat

$q_{cond}$: conductive heat flux
$q_{conv}$: convective heat rflux
$q_{evap}$: evaporative surface heat flux
$q_{rad}$: radiative heat flux
R: ideal gas constant
T: Temperature
$T_{ambient}$: Ambient build chamber temperature
$T_{boil}$: Boiling temperature
$T_{solidus}$: Solidus temperature
t: time
v: laser scan speed
W: Melt pool maximum width
ε: surface emissivity
ρ: density
$\sigma_{laser}$: Standard deviation of Gaussian distribution of laser heating

# Backup Slides

# Current Approach: Single Track Transient FEA Model

**Volume (heat source next slide):**

$$\rho Cp\frac{\partial T}{\partial t} + \nabla \cdot q_{cond} = 0$$ **(Heat diffusion)**

$$C_p = \frac{1}{\rho}\left(\theta_1\rho_1 C_{p_1} + \theta_2\rho_2 C_{p_2}\right) + L_{1-2}\frac{\partial f}{\partial T}$$ **(Melting phase change)**

$$f = \frac{1}{2}\left(\frac{\theta_2\rho_2 - \theta_1\rho_1}{\theta_1\rho_1 + \theta_2\rho_2}\right)$$ θ = phase indicator

**Top surface:**

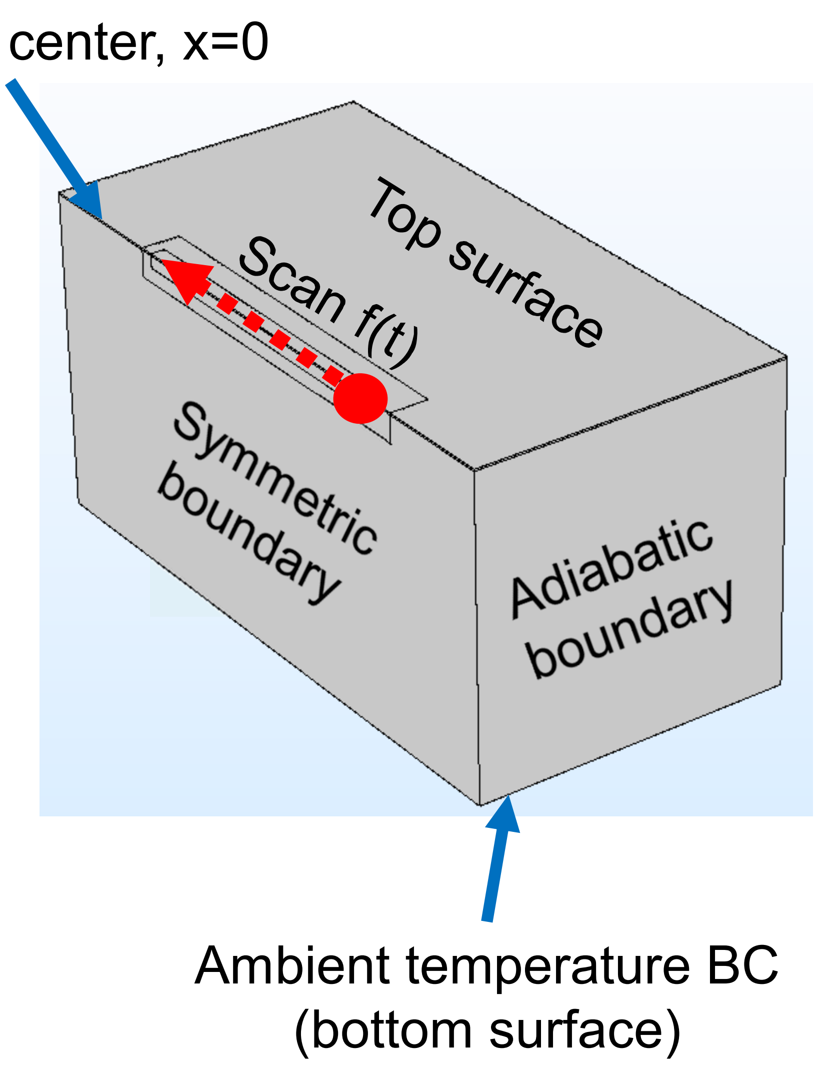
$$-n \cdot q_{rad} = \varepsilon\sigma\left({T_{ambient}}^4 - T^4\right)$$ **(Heat lost to radiation)**

$$-n \cdot q_{conv} = h(T_{ambient} - T)$$ **(Convection)**

$$-n \cdot q_{evap} = -\frac{\partial f}{\partial T}L_v m_v\,;\, m_v = (p_v - p_o)\sqrt{\frac{M}{2\pi RT}}$$ **(Evaporation)**

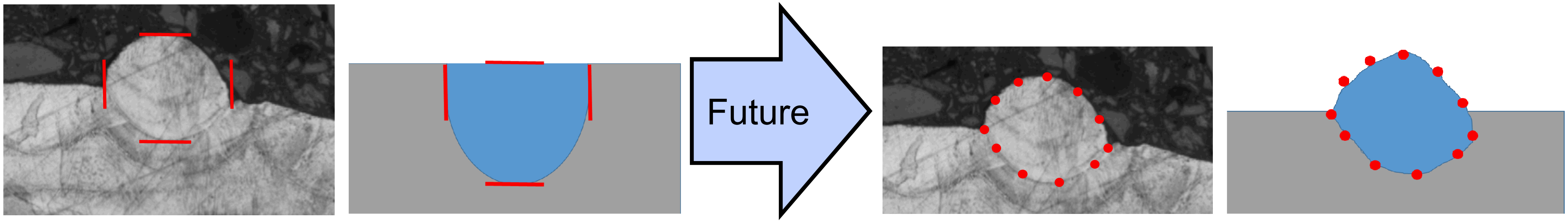
**Notable Simplifications:**

- Homogenous powder layer (powder bed and substrate continuum)
- Eliminates some melt pool physics:
  - Liquid fluid dynamics (CFD)
  - Recoil pressure/vapor depression
  - Marangoni induced flow/surface tension effects



# Current Approach (TTT): Future Work

Improve Fidelity of MPD targets:




Measured MPDs | Predicted/Target MPDs | Measured MPDs | Predicted/Target MPDs

## Variability in Part Properties Assessment

- Identify sensitive process variables (unique advantage of current approach)
- Effect of powder (machine learning approaches)

## Scale Up Thermal Model

- “Unit Cell” for stable MPDs aggregate layers and adjacent scans
- Vary scan patterns

## Generate Validation Data to Build Surrogate Model

- Unique in-house capability: Configurable Architecture Additive Testbed for in-situ observations (CAAT)
- Look at in-situ monitoring opportunities