Collaborative Efforts Between NASA Langley Research Center and the University Leadership Initiative at Carnegie Mellon University

Samuel Hocker[1], Brodan Richter[1], Joshua Pribe[2], Saikumar Yeratapally[3], George Weber[1], Andrew Kitahara[2], Ed Glaessgen[1]

[1] NASA Langley Research Center, Hampton, VA
[2] Analytical Mechanics Associates, Hampton, VA
[3] Science and Technology Corporation, Hampton, VA

University Leadership Initiative Closeout Meeting – September 8, 2023
Carnegie Mellon University
Pittsburgh, Pennsylvania

Images are credit NASA

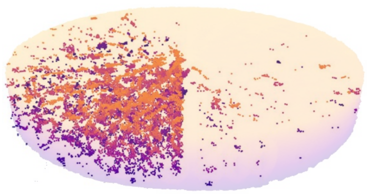
Area of Research

Computational Materials-Informed Qualification and Certification (Q&C) of Additively Manufactured (AM) Flight Hardware

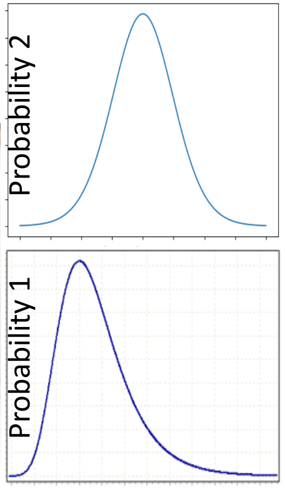
Photograph

5 [mm]

Porosity



AM Component



Process → Structure → Property/Performance

Small deviations in processing parameters may result in large differences in performance.
Current approaches for Q&C of metallic materials (including AM) are entirely based on test data.

Change the Paradigm for Q&C

Develop a computational materials-informed ecosystem for quantifying sources of variability in fatigue performance of additively manufactured metallic materials through integrated multi-scale, multi-physics simulation, characterization and monitoring.

Outline

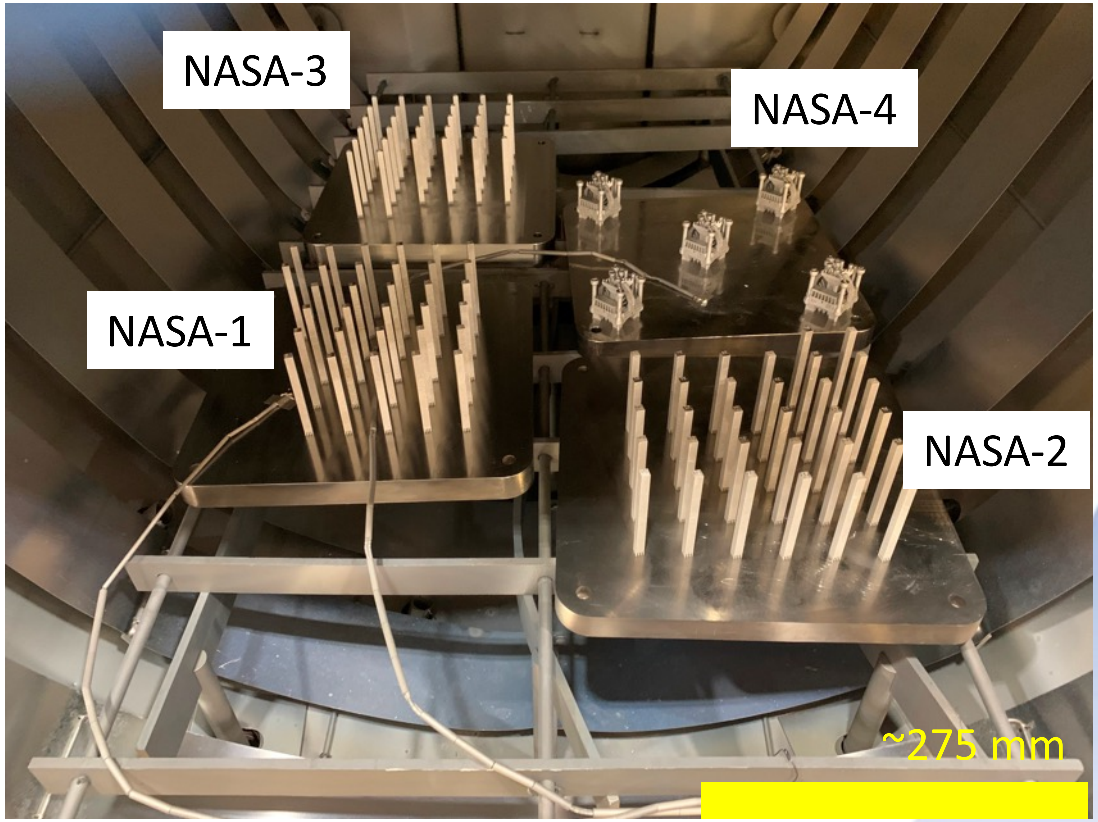
- "NASA-built specimens", process-structure metrics and monitoring of powder bed fusion laser beam metals (PBF-LB/M)
  - Samuel Hocker
- Microstructure evolution modeling of PBF-LB/M parts
  - Brodan Richter (NASA) in collaboration with Evan Adcock and Joseph Pauza (Carnegie Mellon University)
- Microstructure performance predictions of PBF-LB/M parts
  - Sai Yeratapally and George Weber
- Process-structure-property frameworks
  - Josh Pribe
- Database and data structures
  - Andrew Kitahara

Outline

- "NASA-built specimens", process-structure metrics and monitoring of powder bed fusion laser beam metals (PBF-LB/M)
  - Samuel Hocker
- Microstructure evolution modeling of PBF-LB/M parts
  - Brodan Richter (NASA) in collaboration with Evan Adcock and Joseph Pauza (Carnegie Mellon University)
- Microstructure performance predictions of PBF-LB/M parts
  - Sai Yeratapally and George Weber
- Process-structure-property frameworks
  - Josh Pribe
- Database and data structures
  - Andrew Kitahara

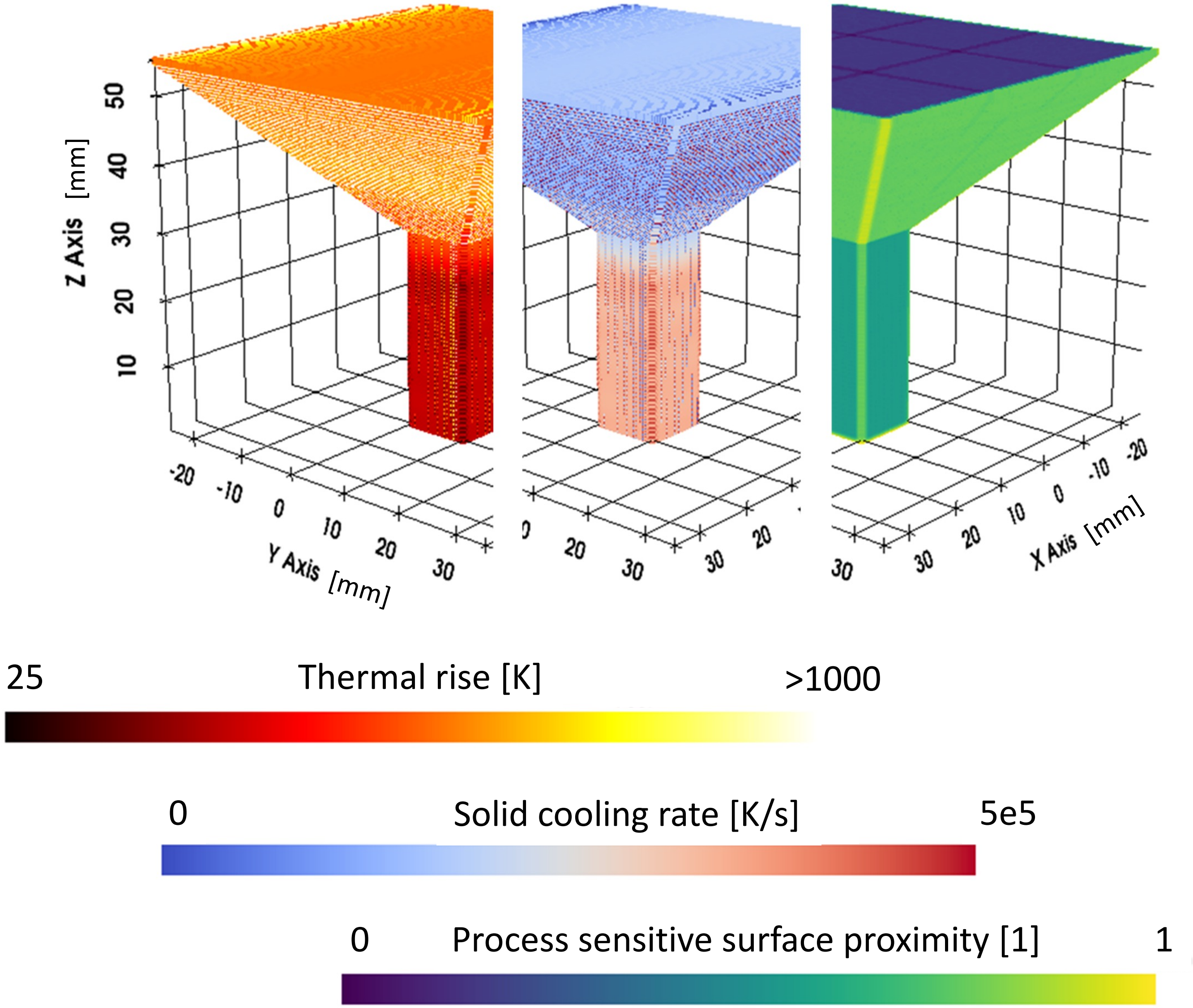
Builds Supporting University Leadership Initiative Round Robin

- 4 round robin builds
  - EP07: agreed round robin build with 8 different parameters
  - 32 x-ray computed tomography scans have been taken
  - NASA-1, EP07 (interrupted)
  - NASA-2, SLM nominal parameters
  - NASA-3, EP07
  - NASA-4, UTEP test artifacts



UTEP = University of Texas at El Paso; EP07 = UTEP build design #7; NASA = National Aeronautics and Space Administration; NASA-1 = first build conducted at NASA; NASA-2 = second build conducted at NASA; NASA-3 = third build conducted at NASA; NASA-4 = fourth build conducted at NASA

Inverted Pyramid at LaRC



- Process metrics calculated from modeled process point field
  - Thermal rise
  - Surface cooling rate
  - Process sensitive proximity to surface
  - …
- GPU accelerated
  - 38 million points
  - Calculation cost ~30 minutes
- Synchronized with in-situ monitoring data-streams

Additive Manufacturing Model-based Process Metrics (AM-PM)

Success: Develop a computational approach that can be used to model and quantify deviations in process conditions throughout the AM process.

Discovery and Development

Used reduced order AM models to calculate process metrics (AM-PM) throughout the build process and designed to be fully scalable.

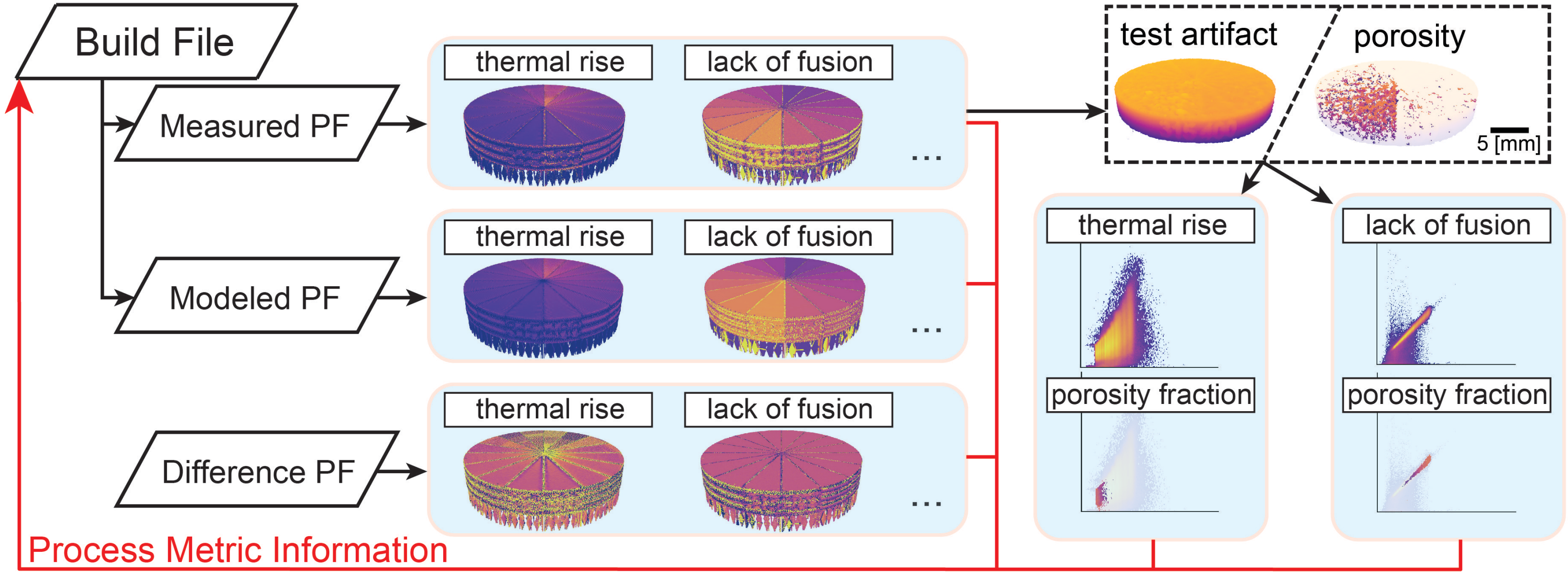
Performance
vs. current state-of-the-art process models

>650x Faster Compute

Fully Parallel and Analytical

***new* Modeled vs Measured Process Conditions**

Point Field (PF) Driven Additive Manufacturing Model-based Process Metrics



Benefits

- Directly model and compute process conditions from a build file or measured conditions alike and compare.
- Scalable across GPU clusters.
- Provides foundation and framework to evaluate process conditions against structure throughout an AM process.

Hocker, S.J.A., Richter, B., Spaeth, P.W., Kitahara, A.R., Zalameda, J.N., Glaessgen, E.H., 2023. A Point Field Driven Approach to Process Metrics Based on Laser Powder Bed Fusion Additive Manufacturing Models and In-Situ Process Monitoring. JMR. https://doi.org/10.1557/s43578-023-00953-7

Configurable Architecture Additive Testbed at LaRC

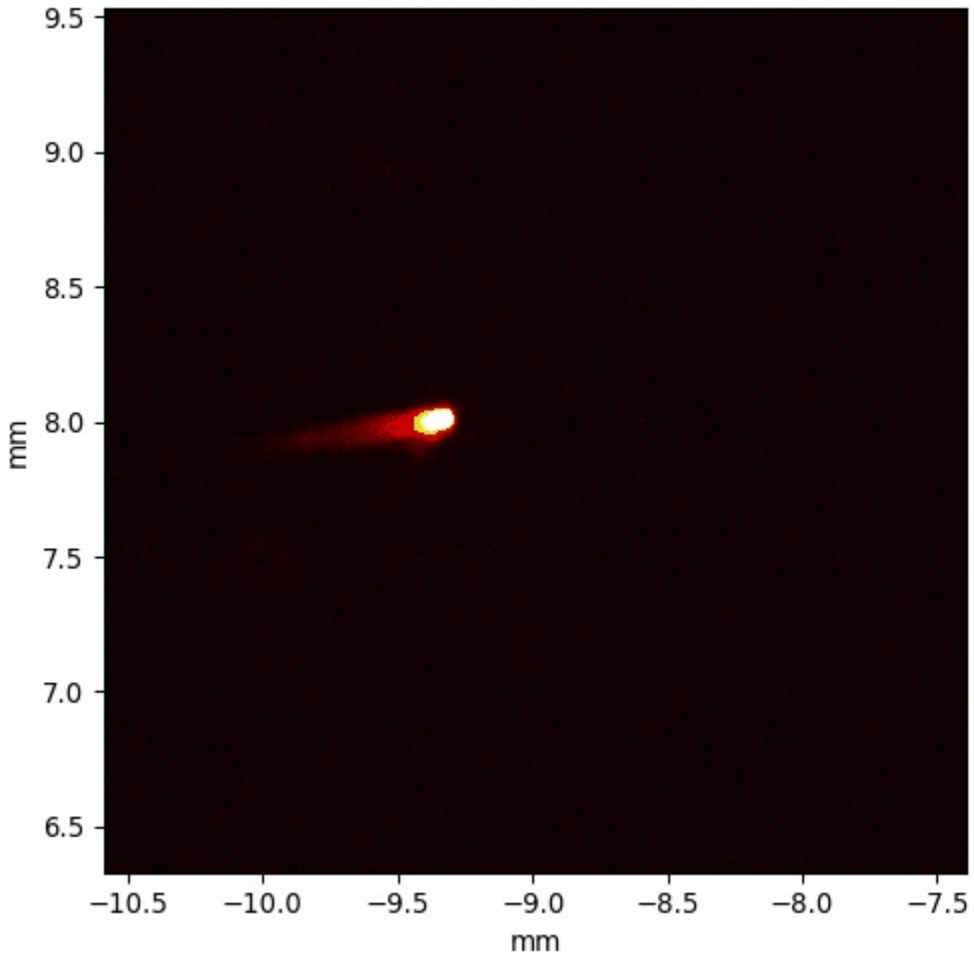
Synchronized Suite of In-situ Monitoring

- Laser real-time control feedback
  - Process point field (measured)
    - Position
    - Power
    - Focus
- Long-wave infrared camera
  - Layer-wise thermal imaging
- Dual near infrared high speed cameras
  - Melt-pool imaging
- Visible spectrum imaging (photography, Basler cameras)
  - Layer-wise images (spread consistency, as welded surface)
  - Dual moderate framerate spatter tracking

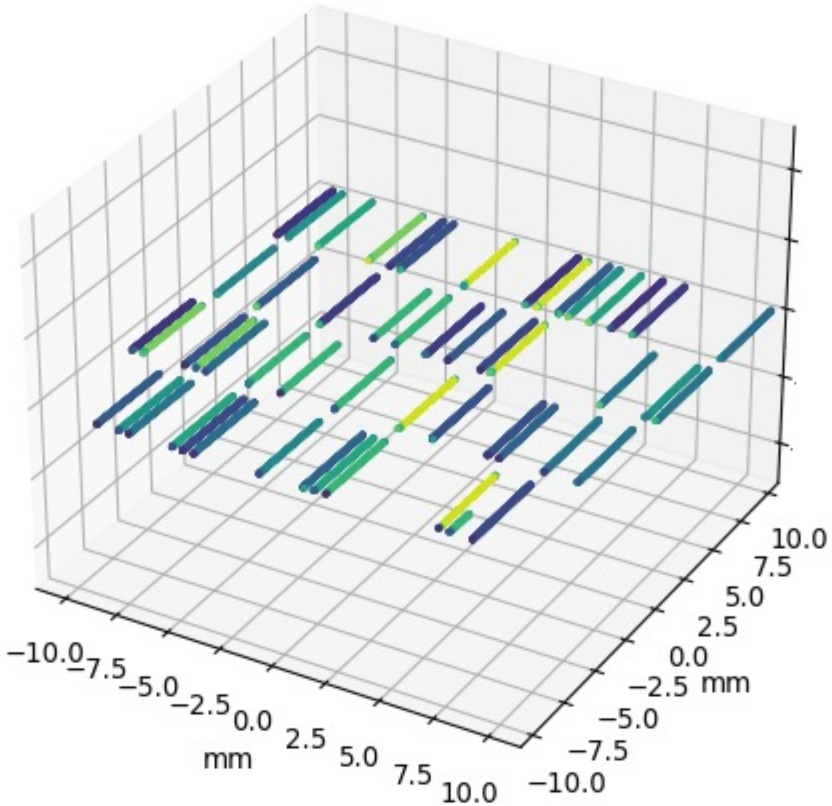
Configurable Architecture Additive Testbed at LaRC

Synchronized High Speed Melt-pool Imaging

Co-axial Melt-pool Images



AM-PM: speed [mm/s]



Outline

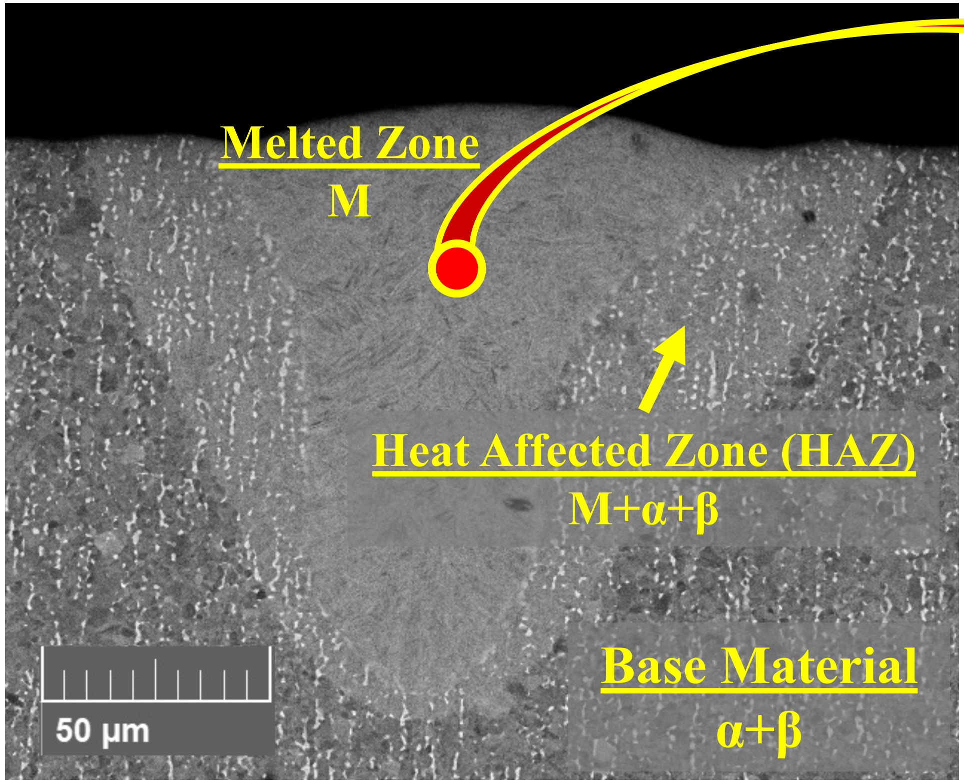
- "NASA-built specimens", process-structure metrics and monitoring of powder bed fusion laser beam metals (PBF-LB/M)
  - Samuel Hocker
- Microstructure evolution modeling of PBF-LB/M parts
  - Brodan Richter (NASA) in collaboration with Evan Adcock and Joseph Pauza (Carnegie Mellon University)
- Microstructure performance predictions of PBF-LB/M parts
  - Sai Yeratapally and George Weber
- Process-structure-property frameworks
  - Josh Pribe
- Database and data structures
  - Andrew Kitahara

Phase Prediction for Ti-6Al-4V During Powder Bed Fusion

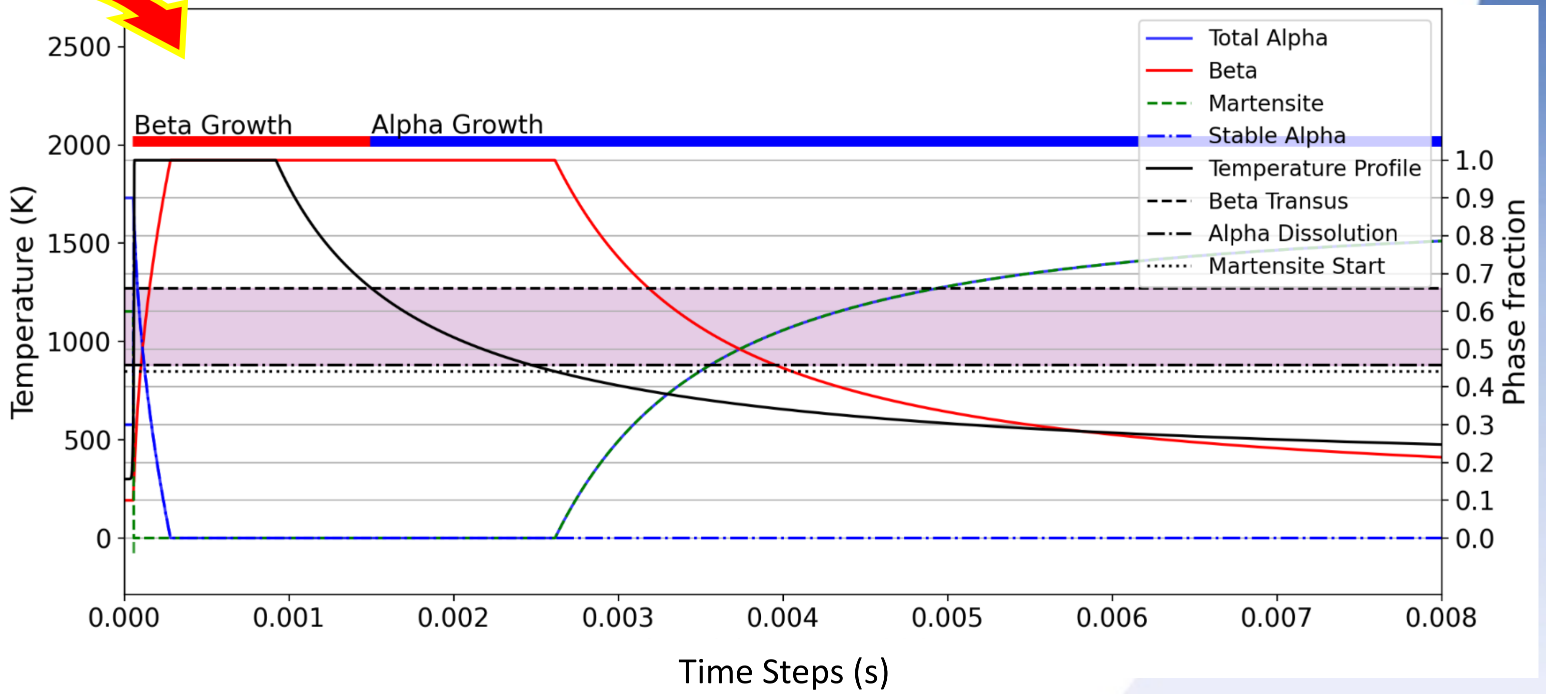
Brodan Richter (NASA) and Evan Adcock (NASA Intern and Carnegie Mellon University)

- Modeling change in alpha (α), beta (β), and martensite (M) phases during processing

Scanning electron micrograph of laser melted Ti-6Al-4V



Phase Change alongside Scanning Laser Heat Profile over a Single Point within the melt zone



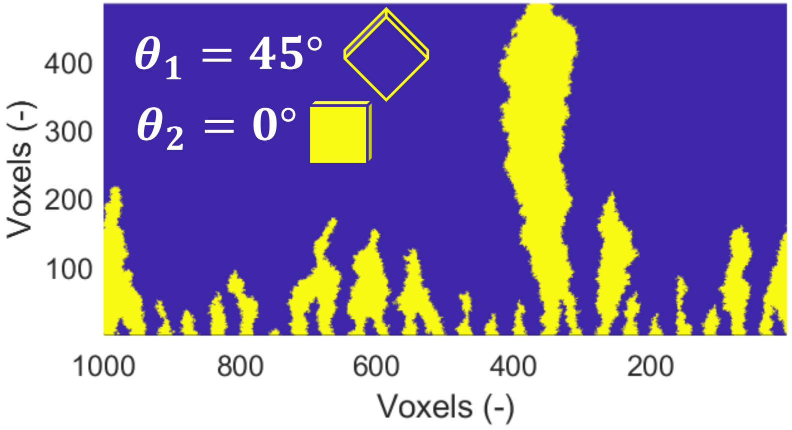
E. Adcock & B. Richter, “Non-Equilibrium Phase Evolution Prediction in Laser Power-Bed Fusion of Ti-6Al-4V,” Advanced Materials and Processing Student Research Symposium, August 2022.

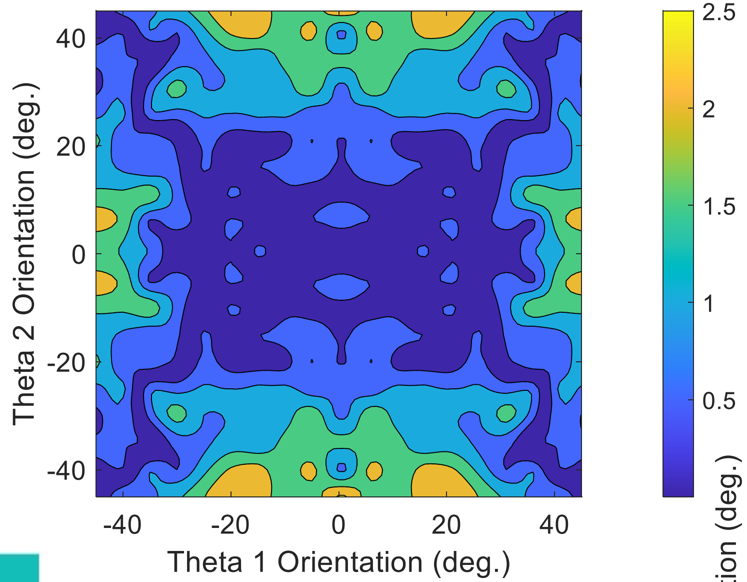
Phase Field vs. Monte Carlo Comparisons of Grain Overgrowth Rate

Brodan Richter (NASA) and Joe Pauza (Carnegie Mellon University)

- Modeling grain competition during solidification through phase field and Monte Carlo methods

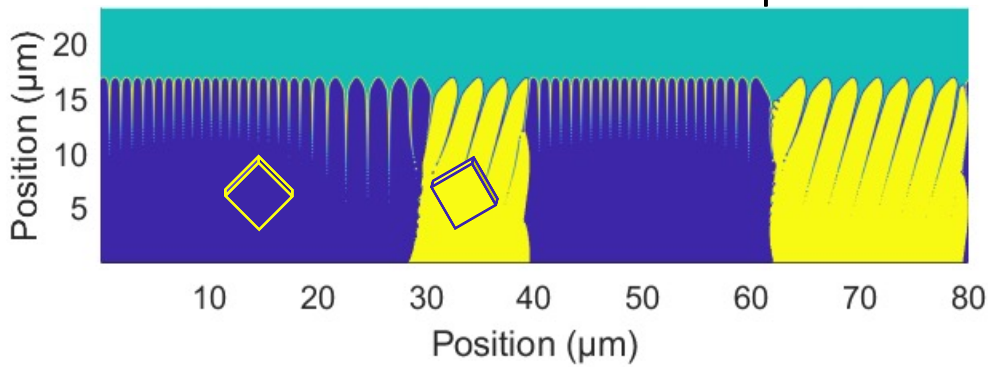
Monte Carlo Simulation Example



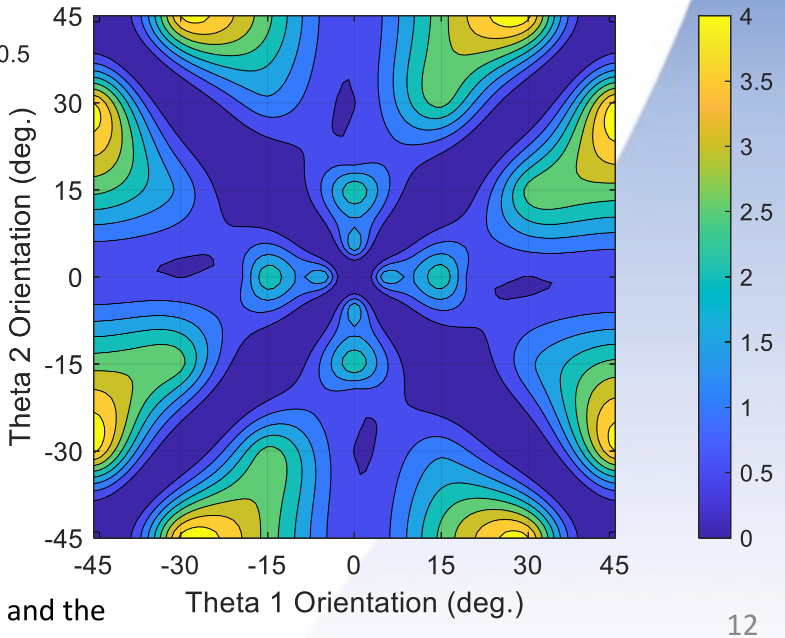


Monte Carlo Grain Overgrowth Rate

Phase Field Simulation Example



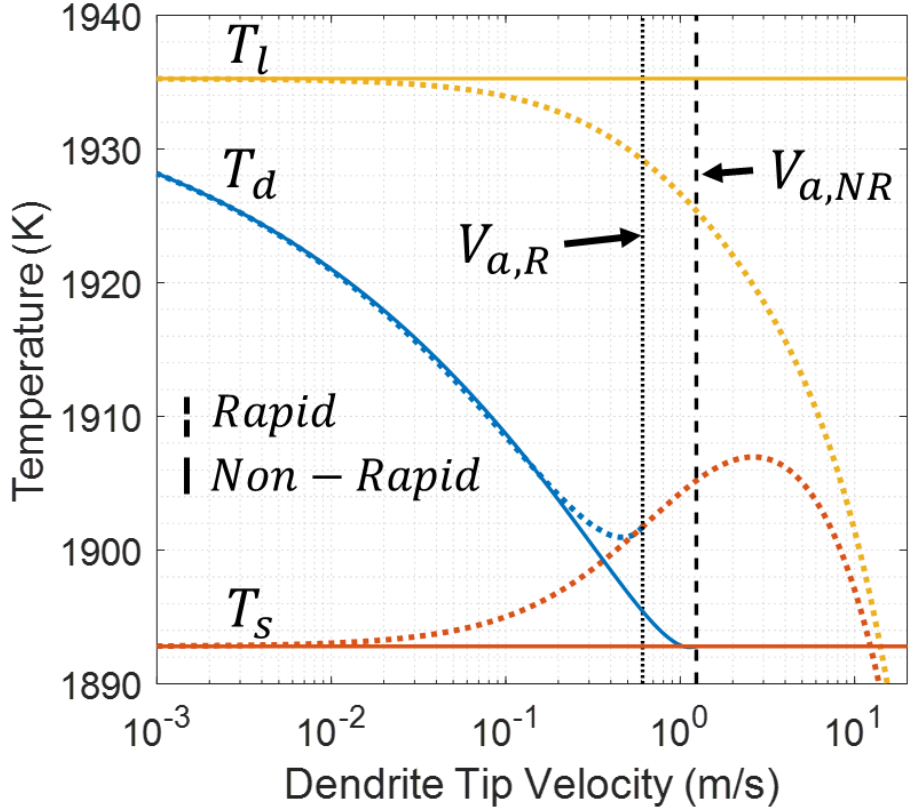
Phase Field Grain Overgrowth Rate



B. Richter, et al., "Phase Field Informed Monte Carlo Texture Evolution Models for Additive Manufacturing: Microstructure Simulation and the Need for Experimental Grain Competition Data," Materials Science & Technology Conference 2021, October 2021.

Impact of Dendrite Tip Velocity on Simulated Microstructures

- Modeling dendrite tip velocity vs. undercooling and how it affects simulated microstructures



Where:

T_d: Dendrite Tip Temperature

T_l: Liquidus Temperature

T_s: Solidus Temperature

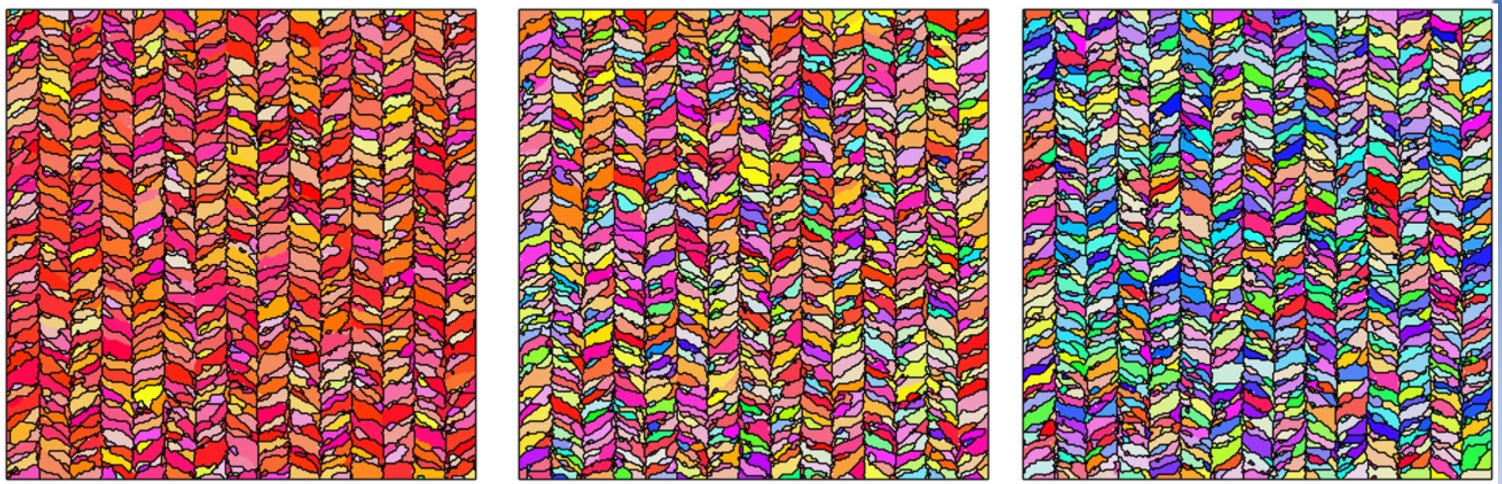
T_m: Pure Melting Temperature

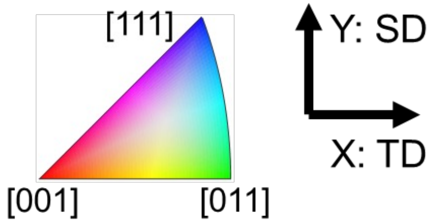
ΔT: Undercooling Temperature

V_c: Constitutional Undercooling Criterion

V_a: Absolute Stability Limit

Velocity Formulation 1	Velocity Formulation 2	Velocity Formulation 3





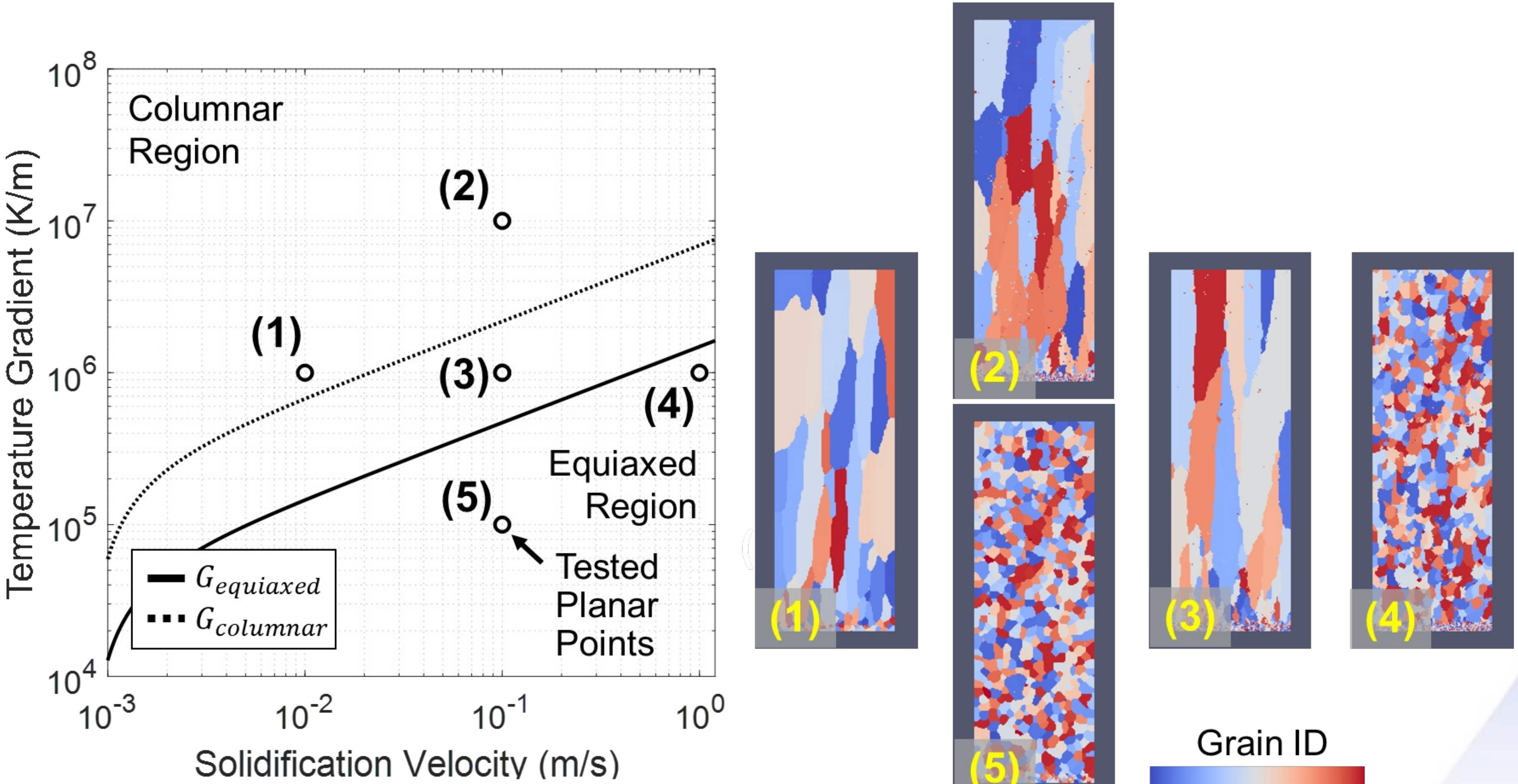
SD Reference Direction

SD: Scanning Direction
TD: Transverse Direction

B. Richter, et al., "Impact of Dendrite Tip Velocity Formulation on The Simulated Microstructures of Powder Bed Fusion Ti-6Al-4V ," ICME 2023, May 2023.

Simulating the Ti-6Al-4V Columnar-to-Equiaxed Transition

- Modeling how well microstructure simulations captures the columnar-to-equiaxed transition for directional and PBF simulations



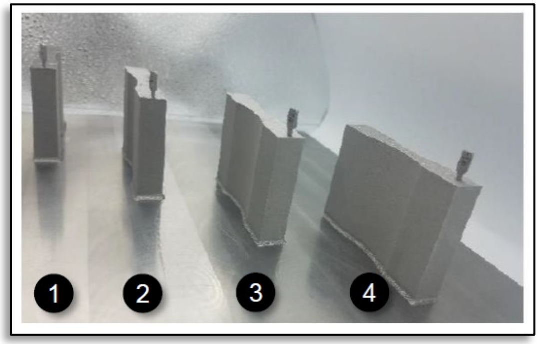
G: Temperature Gradient

B. Richter, et al., "Planar and Full-Process Modeling of the Powder-Bed Fusion Ti-6Al-4V Columnar-to-Equiaxed Transition Behavior," MS&T22, October 2022.

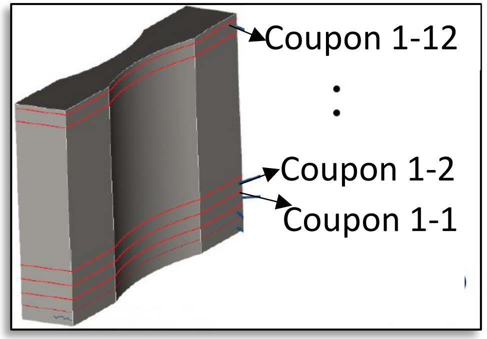
Outline

- "NASA-built specimens", process-structure metrics and monitoring of powder bed fusion laser beam metals (PBF-LB/M)
  - Samuel Hocker
- Microstructure evolution modeling of PBF-LB/M parts
  - Brodan Richter (NASA) in collaboration with Evan Adcock and Joseph Pauza (Carnegie Mellon University)
- Microstructure performance predictions of PBF-LB/M parts
  - Sai Yeratapally and George Weber
- Process-structure-property frameworks
  - Josh Pribe
- Database and data structures
  - Andrew Kitahara

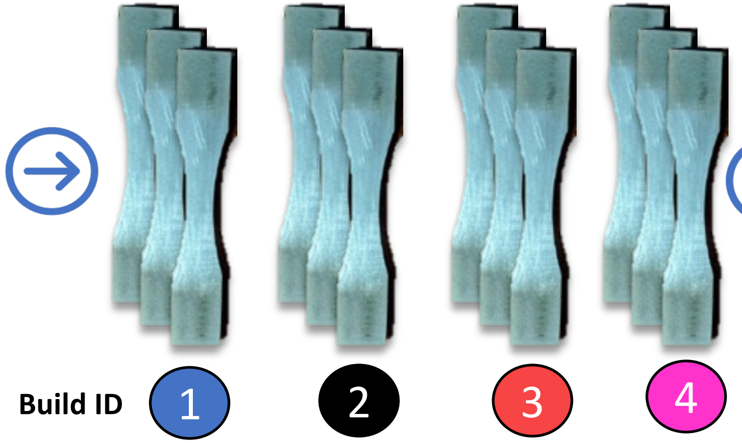
Characterization, Testing, and Modeling to Quantify the Effect-of-defects in as-built Ti-6Al-4V

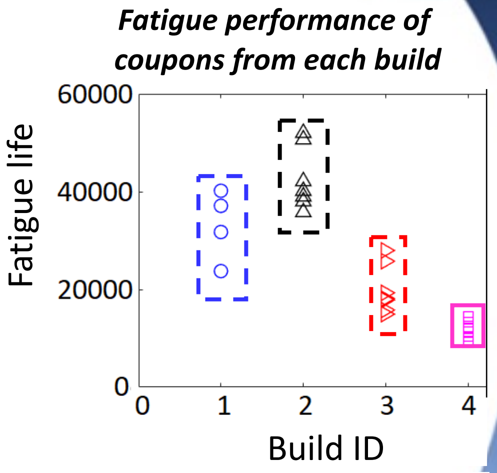


Build plate with four builds



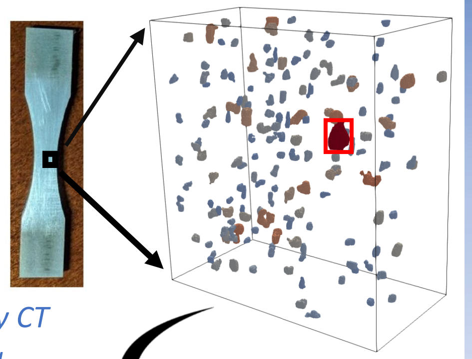
Coupon extraction for Build 1



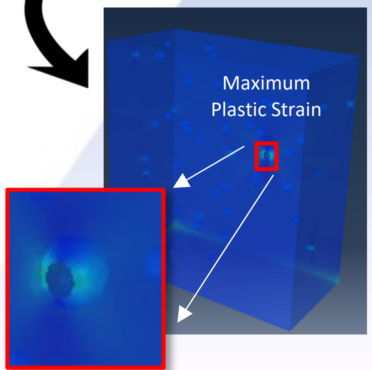


Micromechanical Modeling

- Established **correlations between defect distributions**, through X-ray computed tomography (CT), **and fatigue life** results from testing.
- Developed an Integrated Computational Materials Engineering (**ICME**) framework that generates idealized **defect-embedded micromechanical models** based on defect distributions from X-ray CT scans and **evaluates crack driving forces.**



Segmented X-Ray CT data showing heterogeneous porosity



Finite element simulation of pore instantiations from X-Ray CT data

Observations

- Specimens with large numbers of large defects showed up to a **70% reduction in fatigue life**.

Benefits of Modeling Approach

- Micromechanical simulations show a large plastic strain accumulation near large surface pores, adding insights into the detrimental nature of pores close to free surfaces.
- A validated ICME framework accelerates model-assisted qualification and certification efforts.

1-4 References in the slide notes

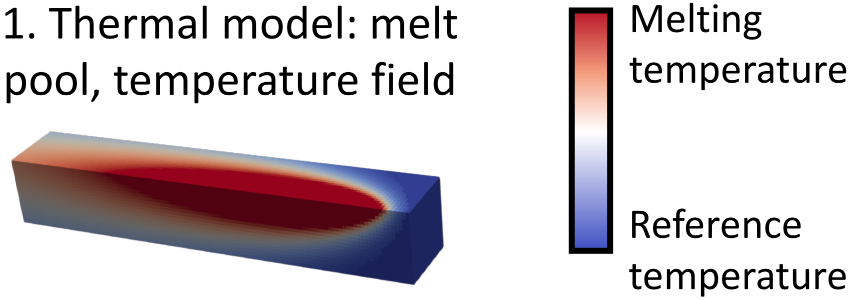
Outline

- "NASA-built specimens", process-structure metrics and monitoring of powder bed fusion laser beam metals (PBF-LB/M)
  - Samuel Hocker
- Microstructure evolution modeling of PBF-LB/M parts
  - Brodan Richter (NASA) in collaboration with Evan Adcock and Joseph Pauza (Carnegie Mellon University)
- Microstructure performance predictions of PBF-LB/M parts
  - Sai Yeratapally and George Weber
- Process-structure-property frameworks
  - Josh Pribe
- Database and data structures
  - Andrew Kitahara

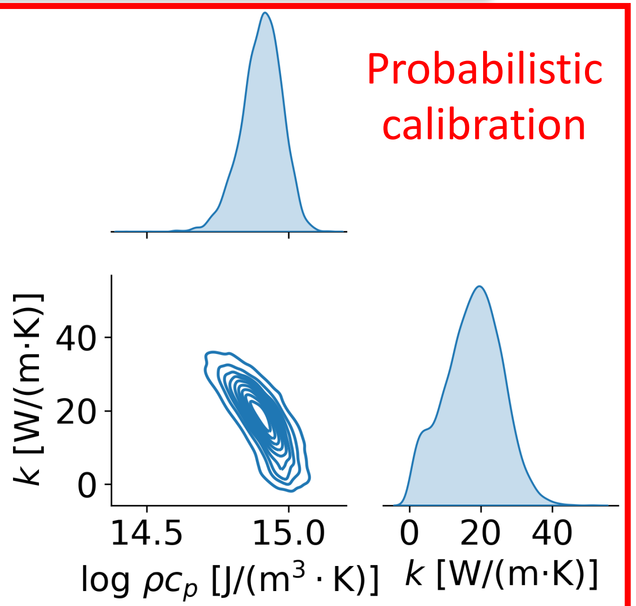
Process-Structure-Property Simulations with Quantified Uncertainty

Pribe, J.D., et al., 2023. A process-structure-property simulation framework for quantifying uncertainty in additive manufacturing: Application to fatigue in Ti-6Al-4V. Accepted for publication in Integrating Materials and Manufacturing Innovation.

1. Thermal model: melt pool, temperature field



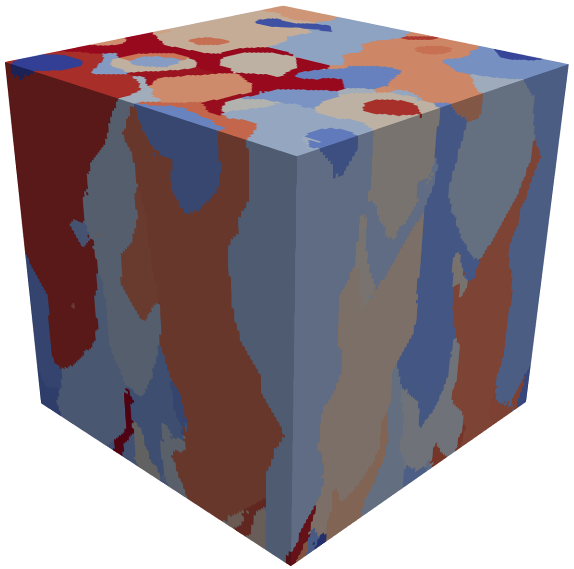
Probabilistic calibration



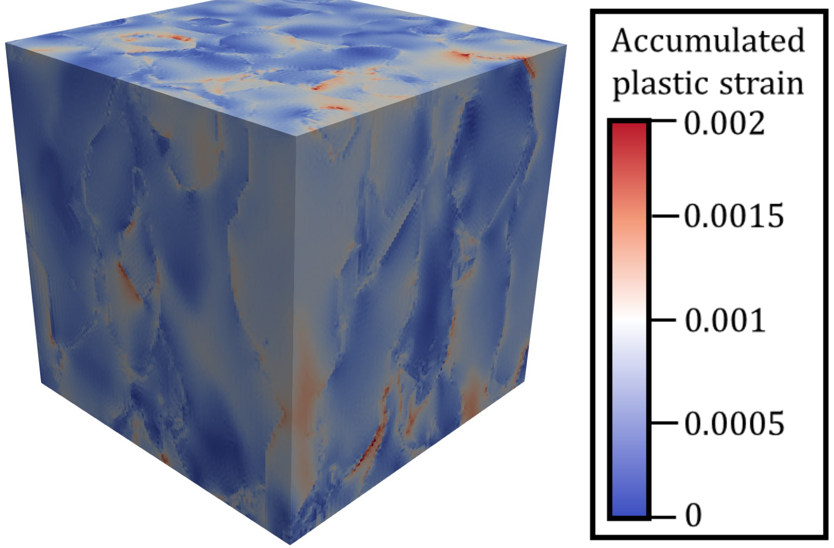
k: thermal conductivity
ρc_p : volumetric heat capacity

Repeat simulations

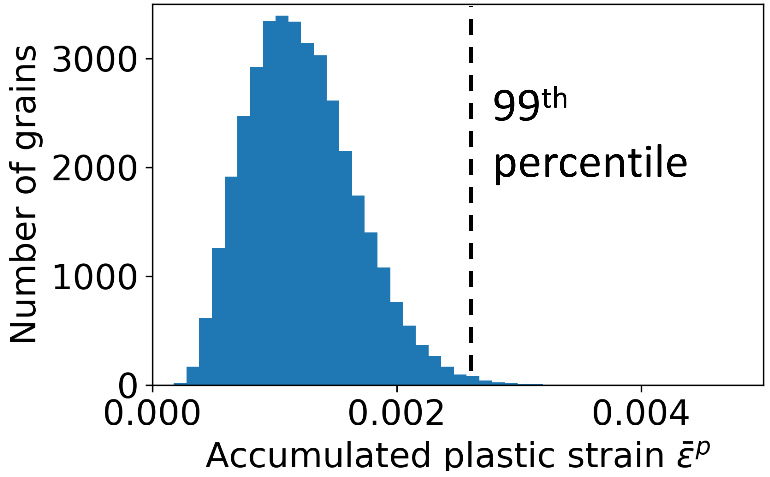
2. Process-structure model: solidification, texture, defects



3. Structure-property model: stress and strain fields, fatigue indicator parameters



Fatigue indicator parameter statistics

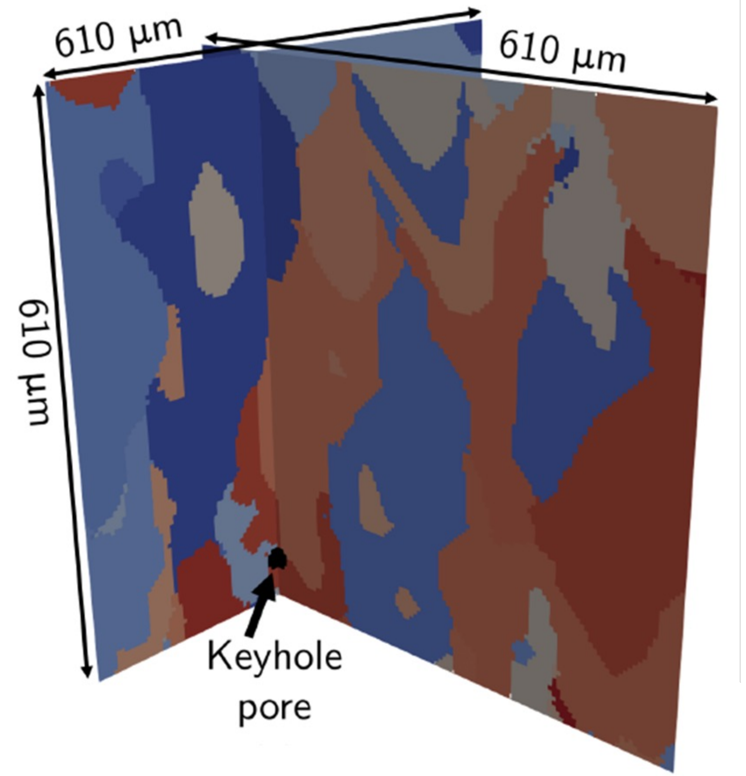


Connections with ULI Work

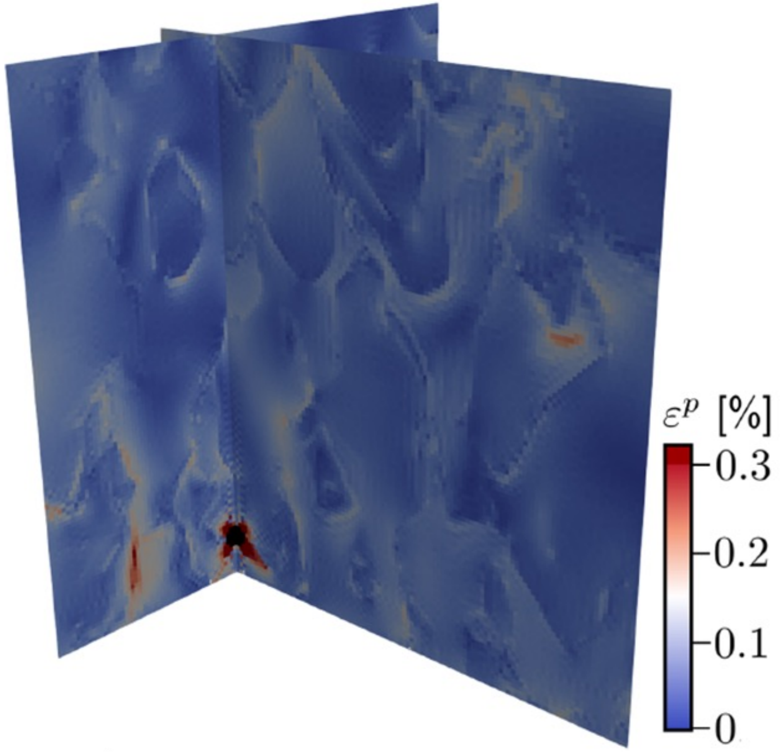
Defect development and interactions

- Pore-microstructure interaction and its influence on fatigue behavior
- Detrimental impact of interacting spherical/keyhole pores relative to isolated lack-of-fusion pores

Simulated microstructure with keyhole pore



Plastic strain (ε^p) concentration near keyhole pore



Outline

- "NASA-built specimens", process-structure metrics and monitoring of powder bed fusion laser beam metals (PBF-LB/M)
  - Samuel Hocker
- Microstructure evolution modeling of PBF-LB/M parts
  - Brodan Richter (NASA) in collaboration with Evan Adcock and Joseph Pauza (Carnegie Mellon University)
- Microstructure performance predictions of PBF-LB/M parts
  - Sai Yeratapally and George Weber
- Process-structure-property frameworks
  - Josh Pribe
- Database and data structures
  - Andrew Kitahara

Data Framework Development

Andrew Kitahara (NASA/AMA), Alex Gonzalez (Colorado School of Mines), Kirk Rogers (The Barnes Global Advisors)

Approaches Pursued	Outcomes / Observations
Organize data into tree structure	Tree structure works well for depths of attributes
Original records primarily in Excel format	Manual data entry is a bottleneck
Transfer Excel to Granta MI	Workable, but Excel macros present learning curve
Extract data from Granta MI with Python Software Toolkit	Determined unsuitable by team

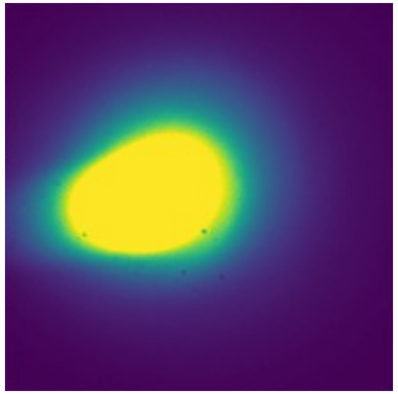
Research Organizations

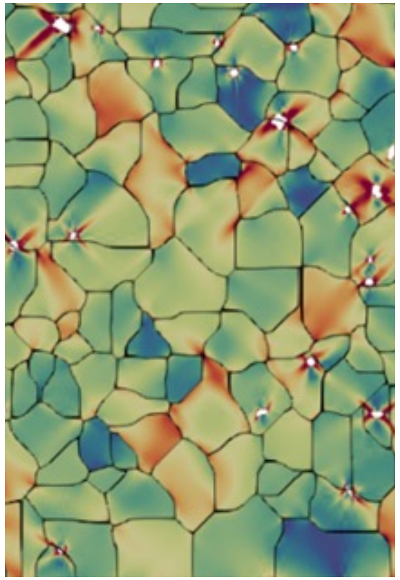
Universities:
Carnegie Mellon University
Case Western Reserve University
Colorado School of Mines
University of Pittsburgh
University of Texas - El Paso

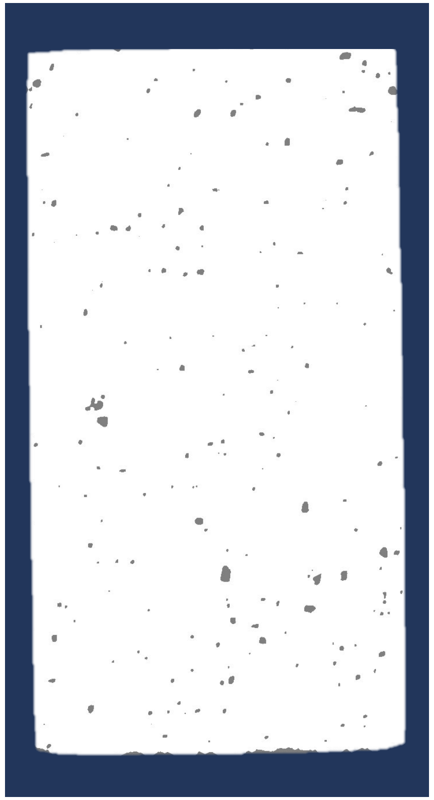
Public Sector:
NASA Langley Research Center

Private Sector:
Materials Resources, LLC
The Barnes Global Advisors

Direct Impact







Specimen Design
- Design of experiment
- Engineered research coupons

Process Modeling
- Melt pool
- Microstructure

NDE and CNDE
- Pre-testing
- Post-testing

Serial Sectioning
- Microscopy
- EBSD

Performance Modeling
- Crystal plasticity
- Effect of defects

In-Situ Testing and Imaging
- Fatigue / Tensile
- Video image correlation

NDE: Non-destructive evaluation
CNDE: Computational non-destructive evaluation
EBSD: Electron backscatter diffraction

Related Efforts

ASTM AM Center of Excellence

- Data acquisition and management
- Data use and practices
- Data security
- Established a common data dictionary

NIST

- Research Data Framework
- Additive Manufacturing Materials Database
- Materials Data Curation System

ASTM: ASTM International, formerly known as American Society for Testing and Materials

NIST: National Institute of Standards and Technology