

# Critical Issues and Gaps in Testing and Characterization Data for Computational Materials in Qualification and Certification of Additively Manufactured Metallic Materials

## *Part 2*

***Presented at:***

MS&T 2021 Conference

*October 17-21, 2021*

Columbus, OH

**Presented by:**

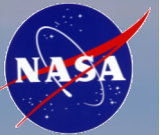
***Dr. E.H. Glaessgen***

*NASA Senior Technologist for Computational Materials*

*NASA Langley Research Center*

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Tracking Number: 20210020916



# Outline

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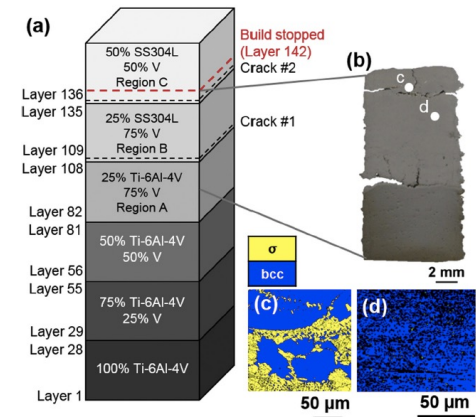


- Additive Manufacturing (AM) Opportunity Space
- Engagement with the Community
- NASA's Capability Development
- Concluding Remarks

# Increasing Complexity of AM Parts



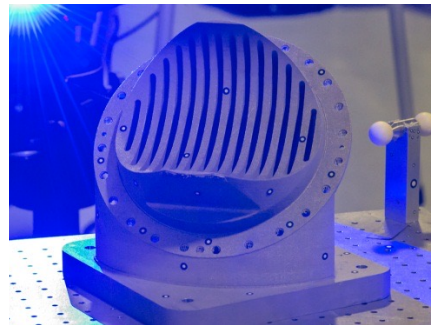
Image: DARPA Transformative Design (TRADES) Program



Graded Materials  
Image: Jet Propulsion Lab\*



Topology Optimized Bracket  
Image: AutoDesk



Pogo Z-Baffle  
Image: NASA



Fuel Injector  
Image: General Electric

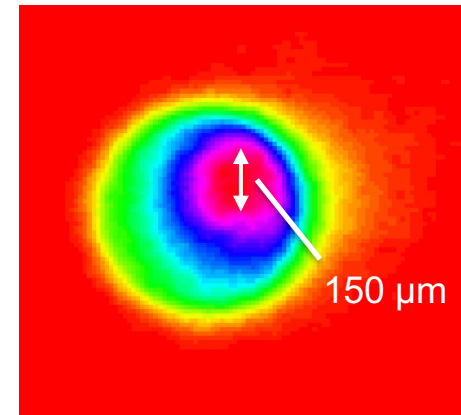
Increasing Complexity

\*Bobbio et al. (2018) *J. Alloys and Compounds*, **742** 1031

# Laser - Powder Bed Fusion (L-PBF) Process



Dynamic X-Ray Radiography of L-PBF



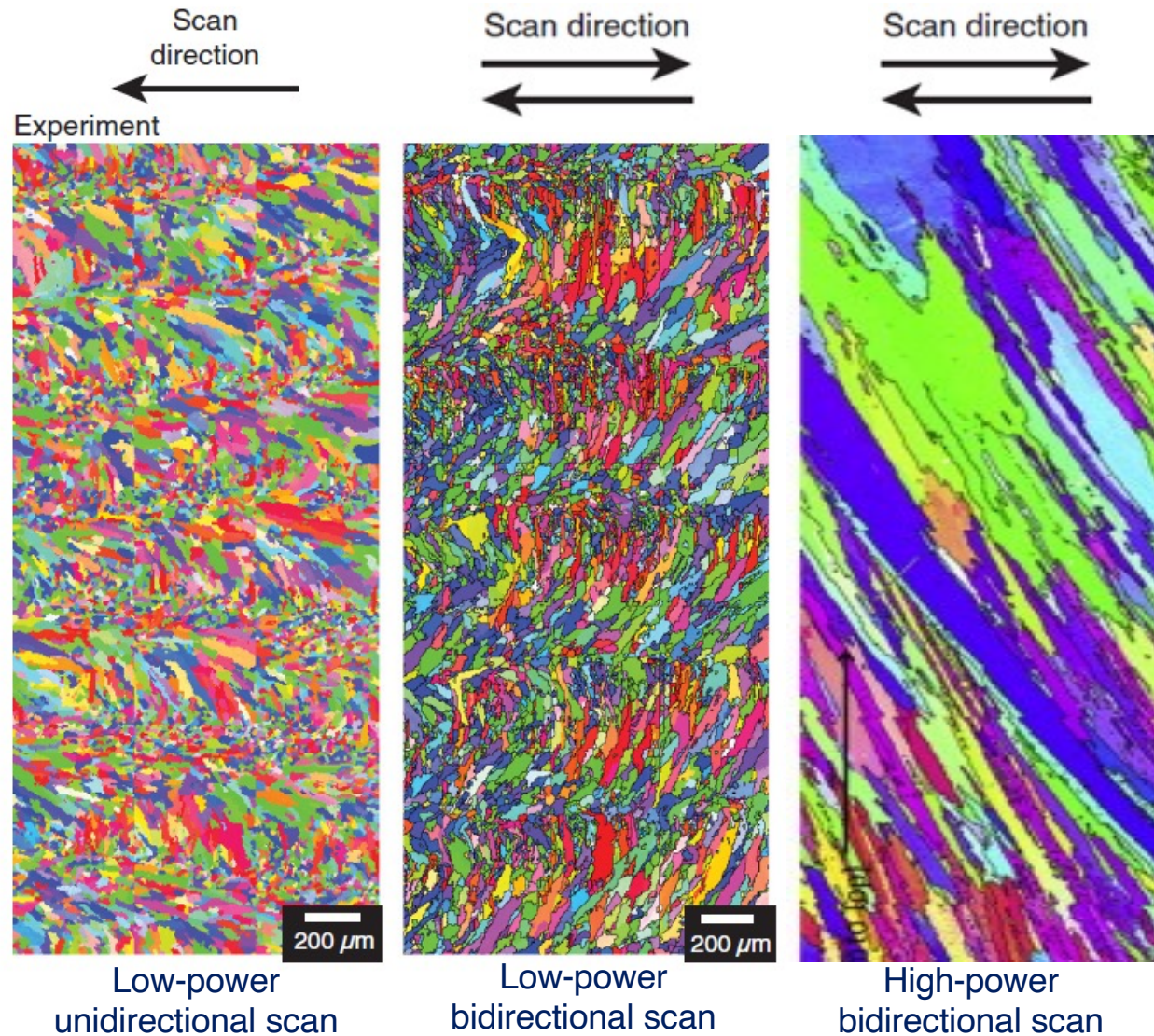
In-situ Thermal Image  
of Melt-Pool



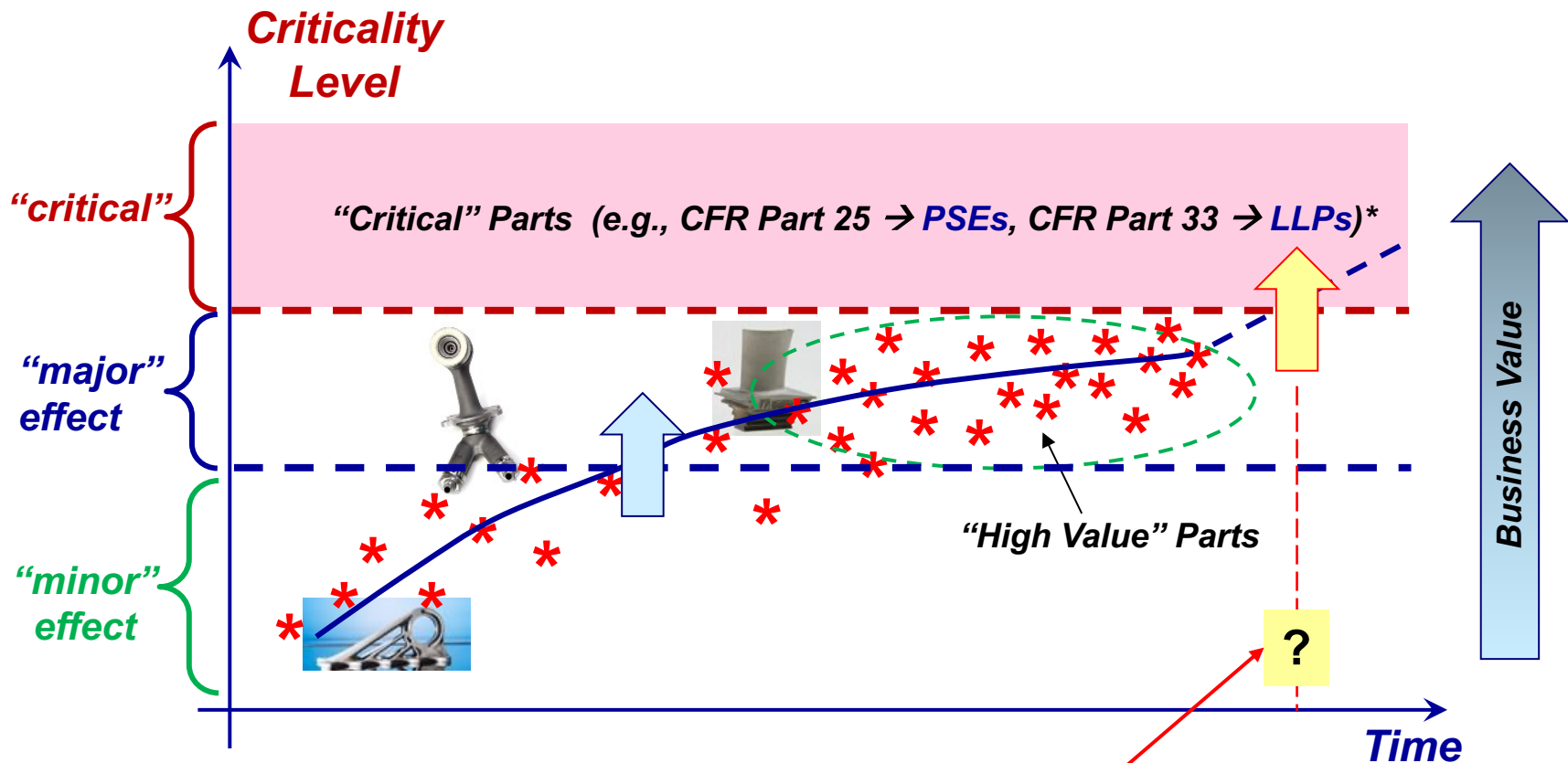
Advanced Photon Source (APS) at  
Argonne National Laboratory

Image: \*Argonne National Lab, \*\*Tao Sun (APS) & Tony Rollett (CMU)

# Complex/Variable AM Microstructure\*



# Evolution of Criticality of AM Parts\*



**Transition to “safety-critical” applications in aviation will occur sooner than initially expected**

\*CFR - Code of Federal Regulations  
**PSE** – Principal Structural Element  
**LLP** – Life Limited Part

\* Adapted from Michael Gorelik, FAA 6

# Examples of “Model-Friendly” Domains\*



## Reference to Title 14 CFR Parts 25 (Airframe) and 33 (Engines)

- Damage Tolerance → Part 25 (AC 25.571-1D)
  - In general, “**analysis supported by test evidence**” is accepted
- Damage Tolerance → Part 33 (AC 33.70-1)
  - Analysis is accepted (e.g., stress, heat transfer, crack growth, ... )
    - However, “**...the analysis approach should be validated against relevant test data**”



# Input from the Aerospace Community



NASA/CR—2018-219771



## Vision 2040: A Roadmap for Integrated, Multiscale Modeling and Simulation of Materials and Systems

*Xuan Liu and David Furrer  
Pratt & Whitney, East Hartford, Connecticut*

*Jared Kusters and Jack Holmes  
Nexight Group, Silver Spring, Maryland*

NASA/CR-2018-219771

March 2018

NASA/TM—2019-220428



## ARMD Workshop on Materials and Methods for Rapid Manufacturing for Commercial and Urban Aviation

*Jonathan B. Ransom, Edward H. Glaessgen, and Brian J. Jensen  
Langley Research Center, Hampton, Virginia*

NASA/TM-2019-220428

November 2019

NASA/TM—20210015175

DOT/FAA/TC-20/38



## NASA / NIST / FAA Technical Interchange Meeting on Computational Materials Approaches for Qualification by Analysis for Aerospace Applications

*Edward H. Glaessgen  
Langley Research Center, Hampton, Virginia*

*Lyle E. Levine, Paul W. Witherell, and M. Alkan Donmez  
National Institute of Standards and Technology, Gaithersburg, Maryland*

*Michael Gorelik  
Federal Aviation Administration, Scottsdale, Arizona*

*Nathan A. Ashmore  
Boeing Research and Technology, St. Louis, Missouri*

*Richard R. Barto  
Lockheed Martin Advanced Technology Laboratories, Cherry Hill, New Jersey*

*Corbett C. Battaile  
Sandia National Laboratory, Albuquerque, New Mexico*

*Harry R. Millwater  
University of Texas at San Antonio, San Antonio, Texas*

*Gerard J. Nanni  
Bell, Fort Worth, Texas*

*Anthony D. Rollett  
Carnegie Mellon University, Pittsburgh, Pennsylvania*

*Edwin J. Schwalbach  
Air Force Research Laboratory, Dayton, Ohio*

*Vasisht Venkatesh  
Pratt and Whitney, East Hartford, Connecticut*

May 2021

NASA/TM-2021-15175

## **NASA / NIST / FAA Technical Interchange Meeting on Computational Materials Approaches for Qualification by Analysis for Aerospace Applications**

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- Held at NASA Langley Research Center on January 15-16, 2020.
- Motivated by three related factors:
  - The aerospace industry's increasing interest in expanding the use of computational materials for Q&C of process-intensive metallic materials.
  - The rapid maturation of computational materials capabilities across a range of applications.
  - A general lack of coordination of development and investment in these capabilities by funding organizations.
- Included 60 subject matter experts (SMEs) representing 8 aerospace manufacturers, 7 government organizations and 2 universities.
- Participation was evenly divided into Processing-Microstructure and Microstructure-Performance tracks.
- Key objectives were to:
  - Understand existing gaps in model-based, e.g., computational materials, capabilities for processing and performance prediction for aerospace materials and components.
  - Forecast how capabilities can be matured to support material, process and part-level Q&C.

# Questions to Participants



## Group 1 questions - **Qualification Gaps, State of the Art (SOA) and Challenges**

Q1: What gaps cannot be addressed using traditional qualification methods or processes?

Q2: What is the current SOA for computational materials, including examples of success stories?

Q3: What are the main qualification challenges that may be addressed by computational materials-enabled capabilities?

## Group 2 questions - **Leveraging of Related Capabilities and Organizations**

Q4: How can the current or near-term use of computational materials in non-qualification frameworks be leveraged to mature the capabilities for qualification, developing a pathway for leveraging?

Q5: Are there any competition insensitive ways to share information? Is there a pathway to leverage internal company capabilities for use by the larger community?

Q6: Is there a role that industry working groups/standards organizations could play in this process? Where do the standards opportunities lie?

## Group 3 questions - **Capability Development**

Q7: What is the role of Verification and Validation (V&V) and Data Science in the maturation of computational materials capabilities?

Q8: What is the appropriate balance between modeling and testing for a fully mature computational materials framework (end state vision) to achieve the desired state for next-generation (computational materials-enabled) qualification?

Q9: What capabilities should NASA & NIST champion to enable next-generation qualification of process intensive metallic materials (e.g., AM). What is the timeline and phased approach at 5, 10, 20 years?

# Some Comments Related to Material Properties and Microstructure

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- Data that is missing or of questionable fidelity:
  - Critical thermo-physical data for materials models as a function of temperature (e.g., viscosity and surface tension) of molten material.
  - Melt pool solidification boundaries.
  - Microstructure and properties as a function of location within a complex geometry.
  - Critical initial flaw size.
- Variability and sensitivity:
  - Increase focus on understanding and accounting for machine-to-machine variability and its effect on microstructure and properties.
  - Determine sensitivity of the build process to each input parameter and how accurately these parameters must be maintained to provide a reliable and interoperative build system.
  - Develop sensitivity analyses and design of experiment approaches to determine parameters that have most important effect on the manufacturing processes.

# Some Comments Related to Data Storage and Data Exchange

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- Data storage:
  - Increase support for standardized raw data formats and data storage protocols.
  - Establish rigorous standards and requirements for meta-data.
  - Establish common formats for acquisition and storage (e.g., fields of view, contrast).
  - Develop requirements for data quality and inter-applicability (e.g., between machines) of training data to support Machine Learning.
- Data exchange:
  - Establish mechanisms for sharing competitive data within the community that is non-attributable yet has an adequate pedigree.
  - Develop means for enabling trust with data/models generated by others (i.e., establishing industry-accepted data/model pedigree).
  - Develop standardized forms of data exchange among different but related communities (e.g., mechanics, materials science).
  - Develop protocols for sharing government-owned/produced data.

# Some Comments Related to Gaps in Existing Methodologies

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- Development of capabilities to support:
  - Rigorous validation framework for simulation that will help to establish credibility with certification authorities (i.e., show that models are as credible as test data/results.)
  - Clear understanding of precision and accuracy requirements in simulation.
  - Uncertainty quantification in three key areas: simulations, processing and measurement.
  - Experiments that are driven by model validation and calibration needs.
  - Calibration of non-linear material model parameters under uncertainty.
  - Determination of clear bounds on the conditions for which a code has been “validated.”

# Some Comments Related to Community Relationships

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- Develop closer relationships between simulation and experimental communities focusing on the intersection between measurement outputs and modeling requirements.
- Improved coordination and communication between measurement teams (NIST, NASA, AM-Bench, etc.) and industry simulation teams would allow measurement priorities to better reflect industrial needs.
- Lessons learned from other domains (e.g., aerosciences including computational fluid dynamics) may provide guidance regarding the extent to which simulation can replace testing.

# Computational Materials for Qualification and Certification (CM<sup>4</sup>QC) Steering Group

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The ***primary goals*** of this Steering Group are to

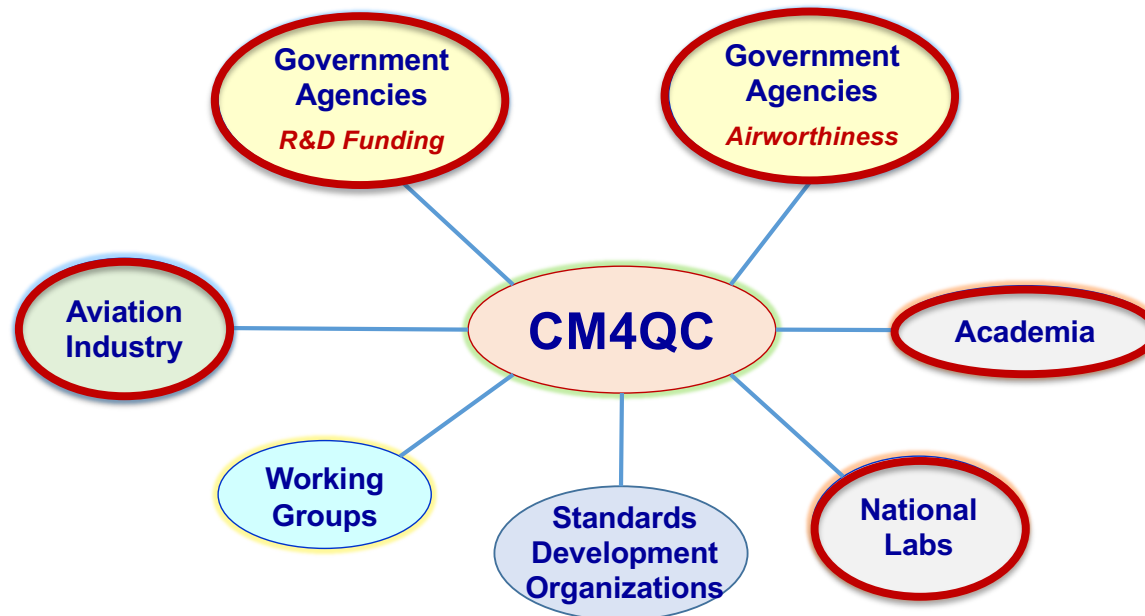
- Provide **coordination for and focus to investments** made by U.S. industry and the U.S. government toward development of computational materials-based (CM) approaches for qualification and certification (Q&C) of process intensive metallic materials (PIM).
- Identify key considerations and enablers required to **increase airworthiness / certifying authorities' acceptance of CM methods** used for Q&C of structural or flight-critical PIM parts.
- **Increase dialogue among the stakeholder organizations** and seek opportunities for **collaboration**.

Membership includes subject matter experts from the aerospace industry, various government laboratories and academia

# Operation of the CM4QC Steering Group



- Working Group 1: Understanding **industry priorities** / timeline and key regulatory implications (High TRL\*)
- Working Group 2: Strategies for **maturation and transition** of Research to Engineering (Mid TRL)
- Working Group 3: Development of required **computational materials and measurement capabilities** (Low TRL)



**Expected initial outcome –  
Multi-year implementation plan (late Spring 2022)**



# Complementary Investments

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**Carnegie  
Mellon  
University**

**NASA University Leadership Initiative at Carnegie Mellon University on *Development of an Ecosystem for Qualification of Additive Manufacturing Processes and Materials in Aviation* (6 universities, 2 small businesses)**

Focused on development of defect-based process maps that guide AM production machine settings to minimize or eliminate those manufacturing defects.

→ **Process Windows to Guide AM Machine Settings**



**Transformation Tools and Technologies Project's effort on *Qualification and Certification of Advanced Manufacturing-Based Materials and Structures***

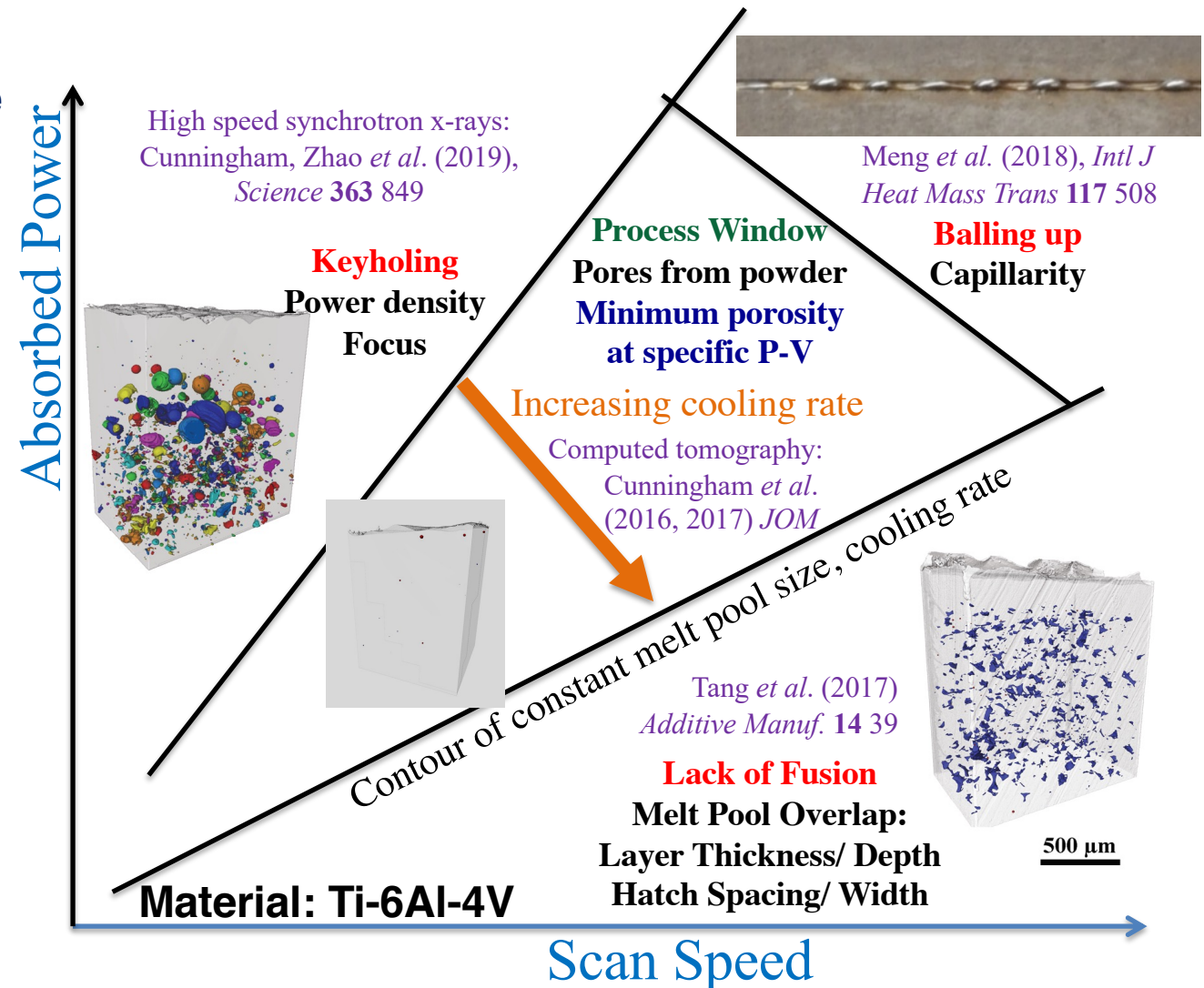
Focused on understanding the effect of processing on evolution of material microstructure and defects and the resulting effects of microstructure and defects on lifecycle performance

→ **Microstructurally-Informed Durability and Damage Tolerance**

# Process Window: Porosity\*



- Key-holing: excessive power density
- Lack-of-fusion: geometry of melt pool relative to layer depth & hatch spacing
- Capillarity causes “balling up”; complicated by fluid flow behind the heat source
- Note the sharp increase in porosity predicted in the lower right (lack of fusion) and upper left (key-holing).

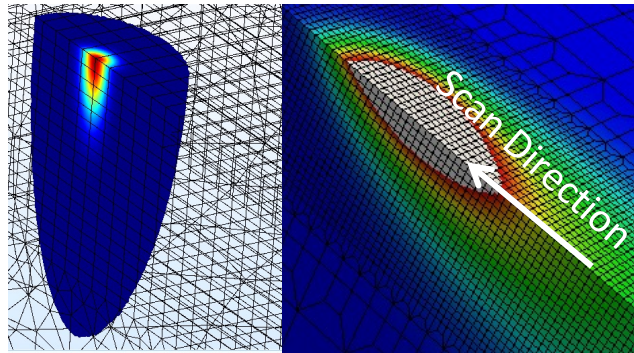


\*A.D. Rollett, NASA Aeronautics Research Mission Directorate's University Leadership Institute on Development of an Ecosystem for Qualification of Additive Manufacturing Processes and Materials in Aviation

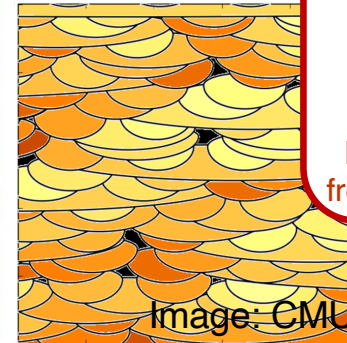
# Development of Microstructurally-Informed Durability and Damage Tolerance (D&DT) (1/4)



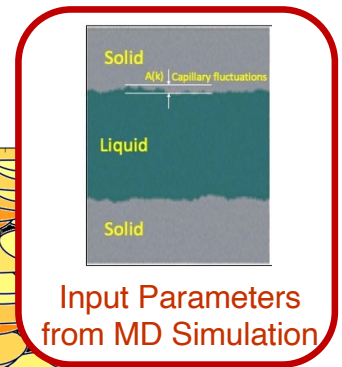
## Simulation of AM Processes



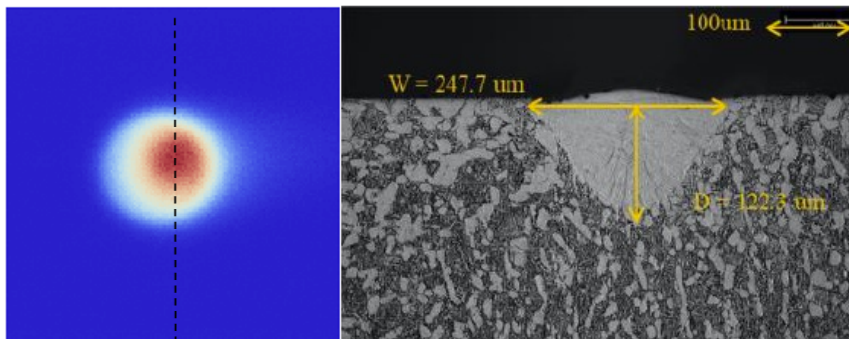
*Thermal Modeling*



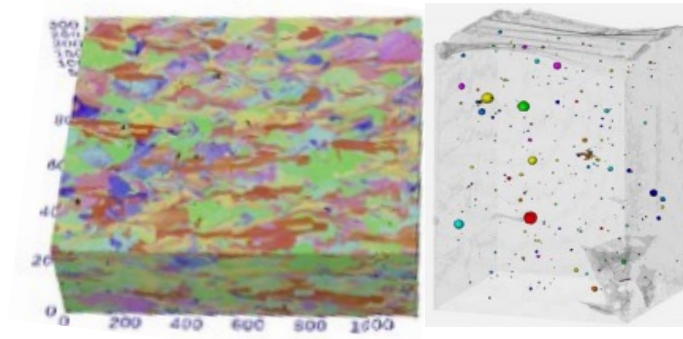
*Simulation of Microstructure & Defect Evolution*



## Measurement and Characterization



*Examination of the Melt Pool*



*Microstructure & Defects*

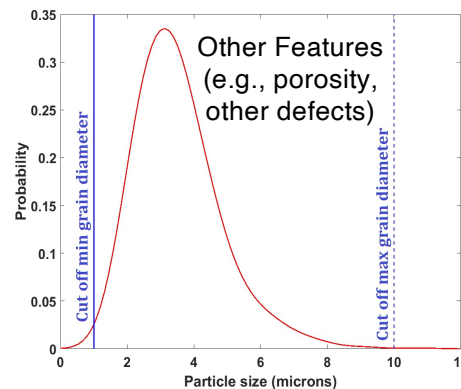
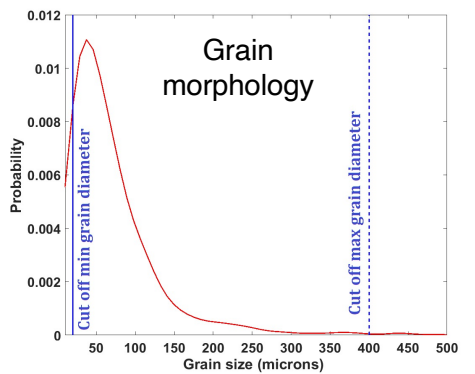
**Physics-based simulation and high-fidelity characterization of AM processing provide input to microstructure performance simulations**

# Development of Microstructurally-Informed D&DT (2/4)

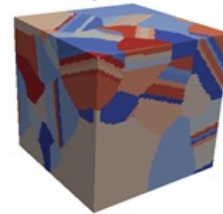
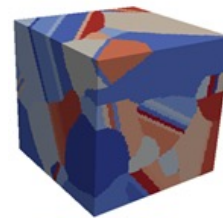


## FEA Simulations Consider Representative Microstructures Developed from Processing Simulation and Characterization Data – Capture Microstructural Details and Responses

Combined simulation and characterization to consider microstructure variability\*\*

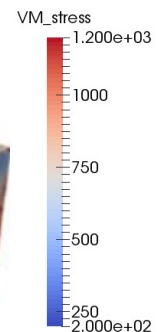


Microstructure instantiations for FEA\*



- 
- 100-1000 independent simulations
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FEA Simulations\*



**Finite element simulations account for variability in microstructure**

\*Yeratapally, et al., NIA

\*\*DREAM.3D (<http://dream3d.bluequartz.net/>)

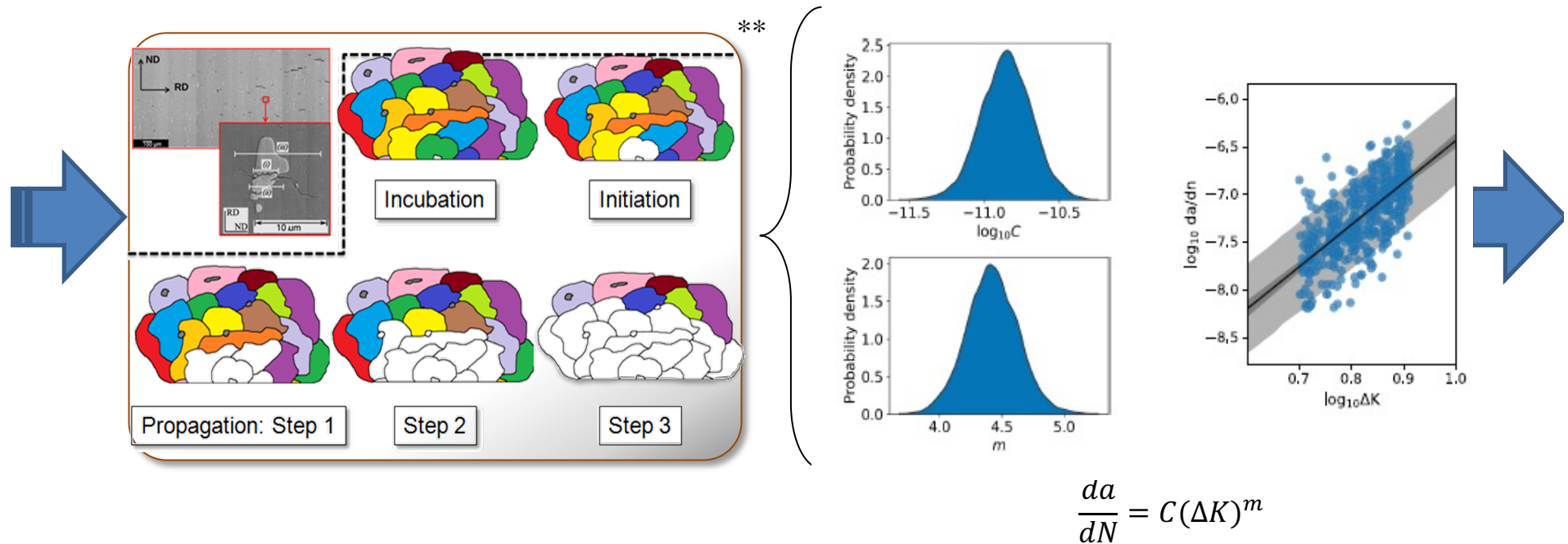
# Development of Microstructurally-Informed D&DT (3/4)



## Transition from Microstructurally Small Crack Growth Estimates to Engineering Codes

$$N_{failure} = N_{incu} + N_{init} + N_{MSC} + N_{MLC}^*$$

Fatigue Crack Growth Material  
Parameter Distributions\*\*\*



## Nondeterministic prediction of fatigue life considering effects of microstructure

\*Sum of the cycles to incubation, initiation, microstructurally small crack growth and microstructurally large crack growth

\*\*McDowell, et al, GaTech

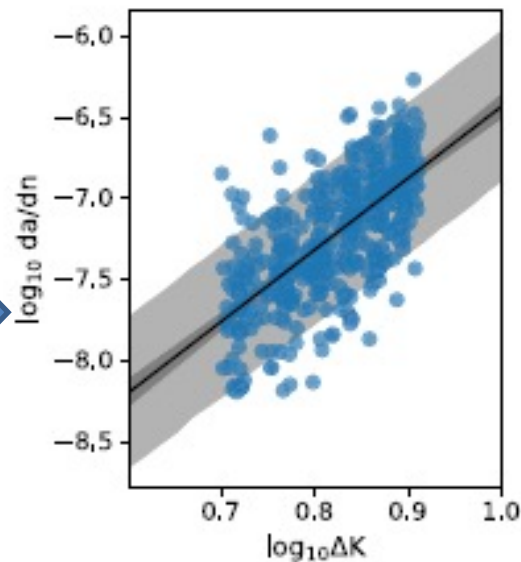
\*\*\*Hochhalter, Yeratapally, Leser, et al., LaRC 21

# Development of Microstructurally-Informed D&DT (4/4)



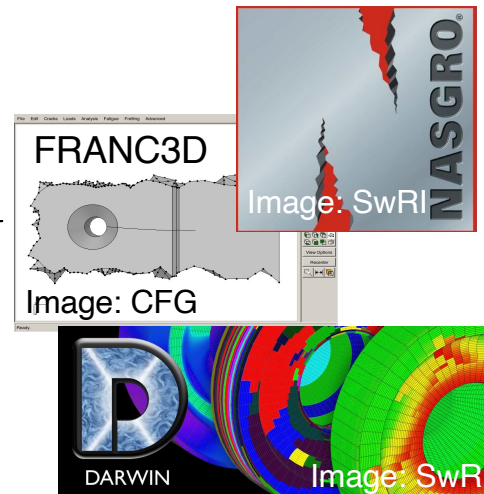
## Microstructurally-Informed D&DT of Fracture-Critical Components

Microstructure-Informed Variability in Crack Growth Rates

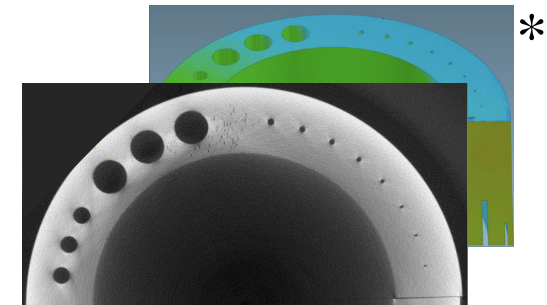


$$\frac{da}{dN} = C(\Delta K)^m$$

Embed these Relationships within Engineering Codes



Component Level Inputs



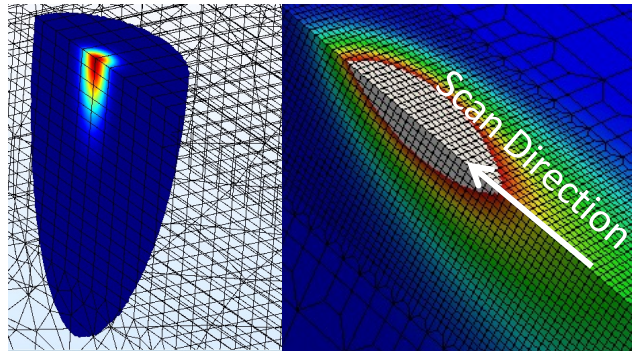
**Microstructurally-informed D&DT simulation applied to determine distribution in fatigue life of fracture-critical AM components with variable microstructures**  
**→ Maturing Computational Materials Science to Solve Engineering Problems**

\*Beshears, R., "Computed Tomography Inspection and Analysis for Additive Manufacturing Components," ASNT Annual Conference, November 2, 2017. **22**

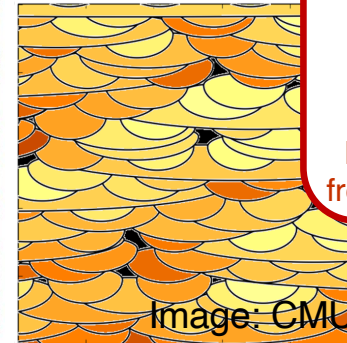
# Development of Microstructurally-Informed Durability and Damage Tolerance (D&DT)



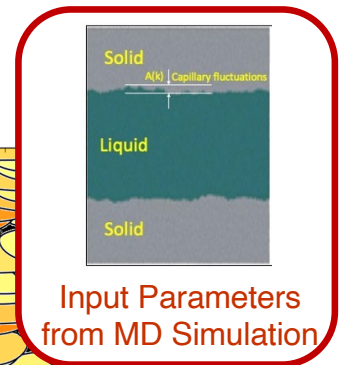
## Simulation of AM Processes



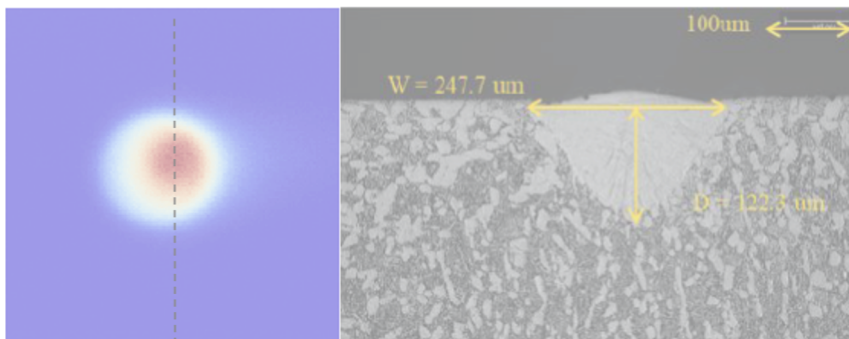
*Thermal Modeling*



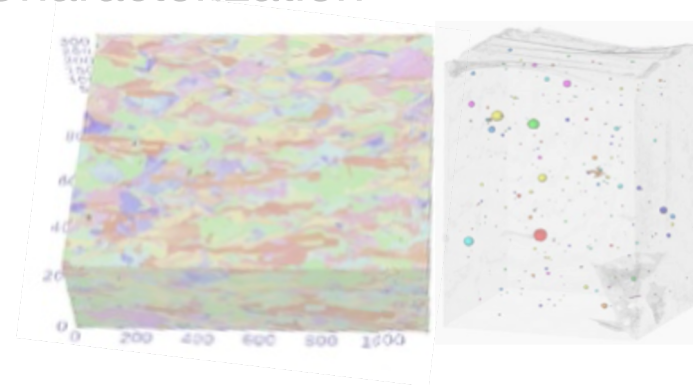
*Simulation of Microstructure  
& Defect Evolution*



## Measurement and Characterization



*Examination of the Melt Pool*



*Microstructure & Defects*

**Physics-based simulation and high-fidelity characterization of AM processing provide input to microstructure performance simulations**

# Predicting Melt Properties Using Atomistic Simulations



**Development of techniques based on molecular dynamics simulations to estimate melt properties of pure aluminum (Al) and pure titanium (Ti) for melt pool predictions and solidification processes in additive manufacturing.**

## APPROACH

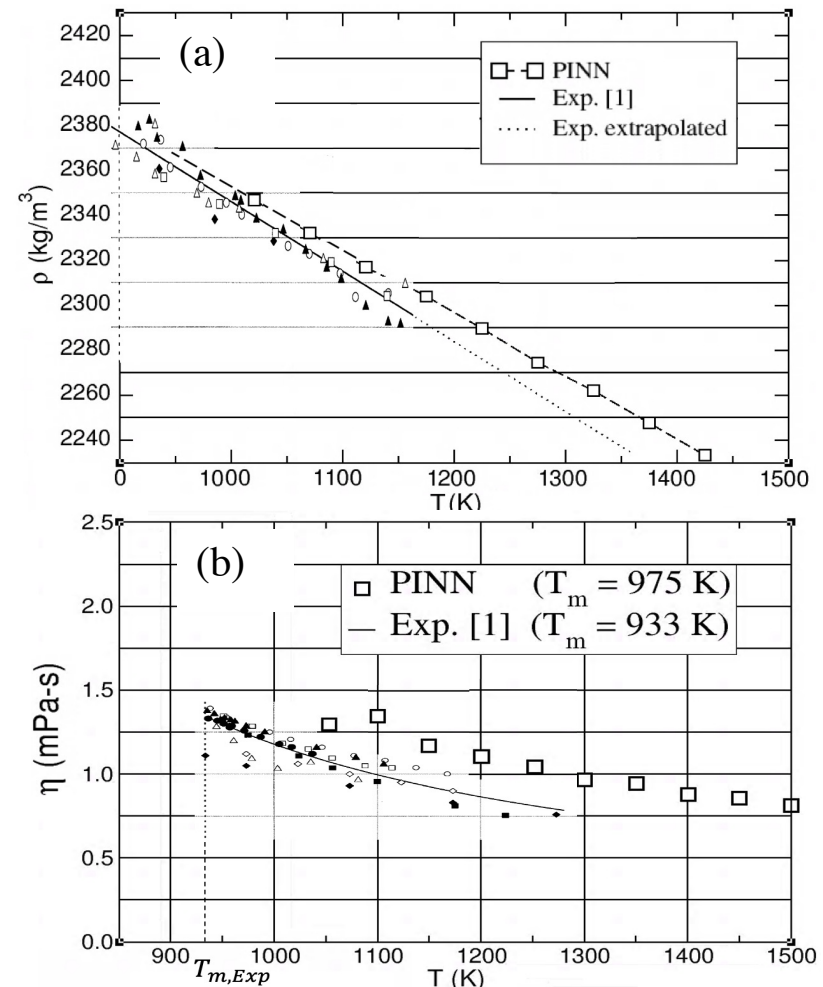
- Al system simulated using physically-informed neural network (PINN) potential. Ti system simulated using state-of-the-art embedded-atom method (EAM) empirical potential.
- PINN potential trained using density functional theory (DFT) and achieves high accuracy ( $\sim 1\text{meV/atom}$ ).
- Melt properties calculated using Green-Kubo statistical mechanics formula.
- Molecular dynamics used to simulate the evolution of Al and Ti melts to collect sufficient statistics on velocity, energy, and pressure fluctuations at temperature range from 1050 K to 1500 K (Al) and 1900 K to 2300 K (Ti).

## RECENT ACCOMPLISHMENTS and IMPACT

- Melt properties predicted within 20% of the experimentally reported values.
- The very high heating and cooling rates in AM ( $\sim 10^4\text{-}10^5$  K/sec), make accurate calculation of melt properties from first principles a key factor in predicting the correct microstructure and properties of the resulting material.

## NEXT STEPS

- Use the developed methodology to develop an accurate potential for Ti-6Al-4V system.



**Simulation vs. experiment comparison for pure aluminum for (a) density; (b) viscosity** 24

# Probabilistic Calibration and Validation of Simplified AM Thermal Process Model



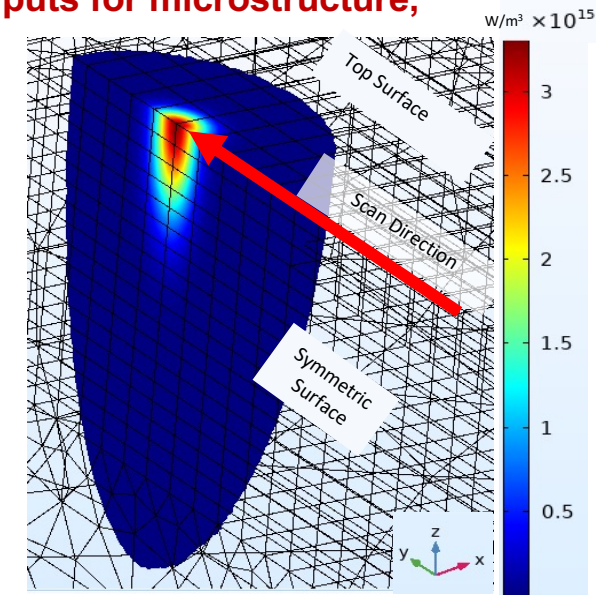
**Automated calibration and validation of a single scan track thermal process finite element model to build a data driven rapid predictor of local scale thermal inputs for microstructure, defect, and part scale models.**

## APPROACH

- Simplified thermal process model using a parameterized, volumetric heat source that simulates effect of transport mechanisms:

$$Q = \alpha_{laser} \frac{6\sqrt{3}P}{abc\pi\sqrt{\pi}} e^{-3(x-x_0)^2/a^2} e^{-3(y-y_0)^2/b^2} e^{-3(z-z_0)^2/c^2}$$

- $Q$  is the power density,  $P$  is the laser power,  $\alpha_{laser}$  is the laser absorptivity, and  $a, b$  and  $c$  are geometric parameters, and  $x_0, y_0$  and  $z_0$  are reference coordinates.
- Parameters ( $\alpha_{laser}, a, b, c$ ) calibrated to match observed melt pool data.
- Ex-situ melt pool measurements are limited and noisy; probabilistic approach addresses challenges due to natural variations in heating/part scale property variation.
- Gaussian Process Regression for probabilistic calibration using scant data.
- Iterative validate-calibrate adaptive learning algorithm employed to converge after minimal FEA model calls.



Volumetric Heat Source (Symmetric Cross Section)

## RECENT ACCOMPLISHMENTS and IMPACT

- Modeling framework has produced calibrated/validated predicted melt pool width and depth variability along a single beam on plate scan track.
- Melt pool morphology uncertainty can be directly propagated to predictions of microstructure and porosity.

## NEXT STEPS

- Machine vision algorithm to automate micrograph image analysis/measured data importation.
- Incorporate melt pool cross-sectional shape in place of simplified width and depth measurements.
- Test the method for a wider variety of processing conditions (e.g., those that induce keyhole porosity).

# Coupled Fluid-Thermal Process Simulation



**Provide high-fidelity process simulation for moving heat source with melt pool physics to predict temperature history, melt pool and vapor cavity, porosity formation, surface topology, and establish process parameter linkage.**

## APPROACH

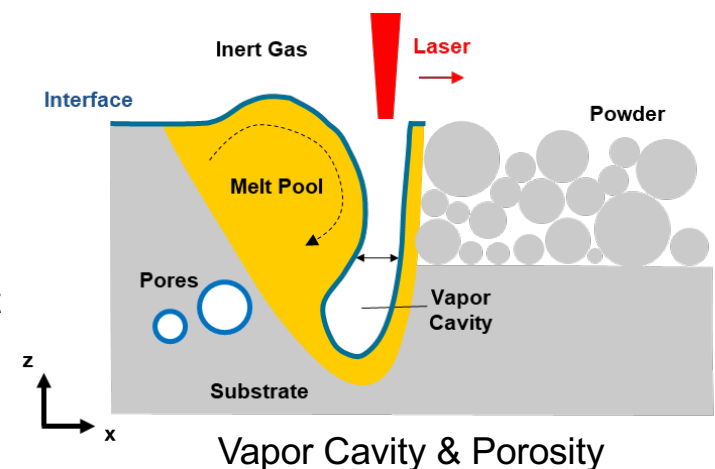
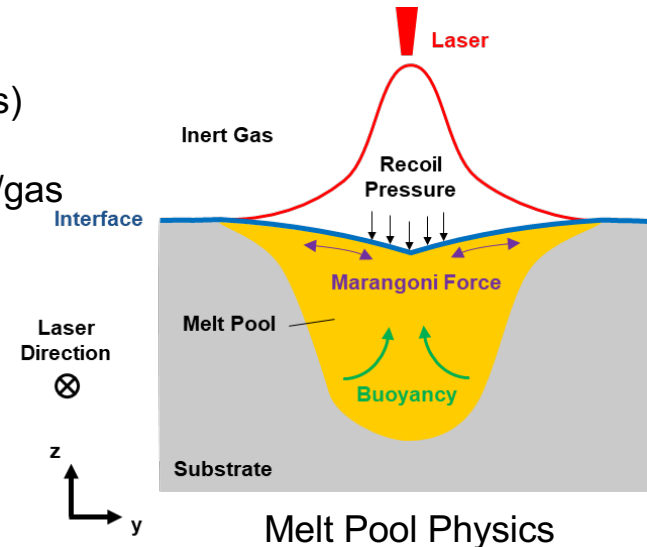
- Solve the coupled Energy, Mass, and Momentum (Navier-Stokes) conservations equations.
- Sharp interface: use the levelset method to evolve the substrate/gas interface according to the fluid velocity.
- Incorporate melt pool physics:
  - Fluid Flow
  - Buoyancy
  - Surface Tension
  - Recoil Pressure
  - Marangoni Shear Stress
- Develop adaptive mesh strategy for moving heat source.

## RECENT ACCOMPLISHMENTS and IMPACT

- Recent accomplishments
  - Diffuse interface implemented.
  - Spot weld analysis completed with comparison to a transient thermal analysis.
- Impact.
  - High-fidelity solution capability for process parameter linkage.
  - Predict porosity formation at root of vapor cavity for impact to property and performance.

## NEXT STEPS

- Implement conformal mesh for sharp interface.
- Develop adaptive mesh strategy to address computational expense.



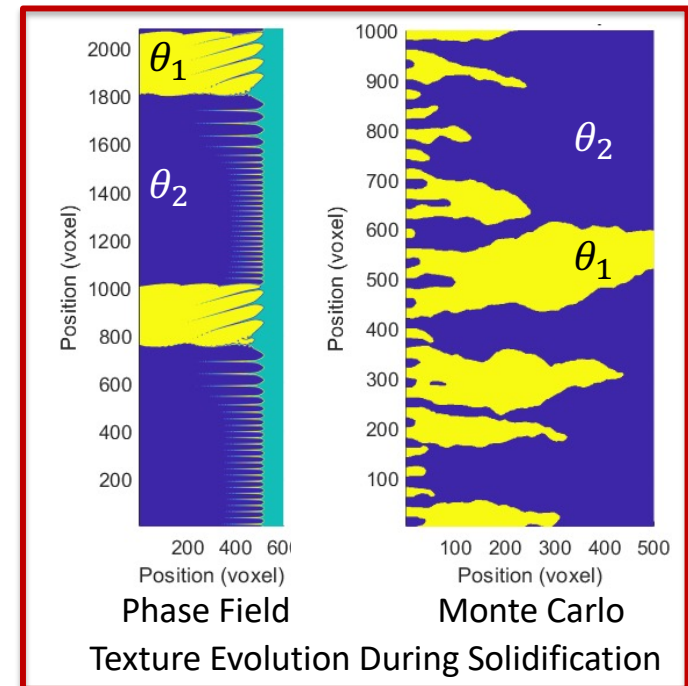
# Phase-Field Informed Monte Carlo Modeling of Microstructure Evolution



**Developing high-fidelity, physics-based Monte Carlo microstructure models with Phase-Field informed design for simulating additively manufactured microstructures.**

## APPROACH

- Phase-field method (high fidelity, specific, micro-scale method) used to provide inputs and calibrations for enabling improved Monte Carlo (low-fidelity, flexible, meso-scale) modeling of grain competition, seeding of micro-segregation regions, and calibrating grain coarsening behavior.
- Monte Carlo problem solved using rejection kinetic Monte Carlo algorithm by Rodgers (2017).
  - Randomly flip sites to neighboring orientations, accept flip if it lowers overall energy of system. Basis probability of acceptance based on temperature and grain orientation.
- Phase-Field model for binary alloy solidification by Karma (2001).
  - Coupled parabolic partial differential equations for chemical concentration and melt interface.
  - Solved numerically with explicit Euler time stepping and finite-difference method with 2<sup>nd</sup> order conserved and isotropic spatial derivative formulations.



## RECENT ACCOMPLISHMENTS and IMPACT

- Implemented quantitative binary-alloy phase-field model with support for multiple grains of various orientations.
- Performed large phase-field and Monte Carlo study on texture development comparing rate of grain overgrowth vs. input grain orientation.

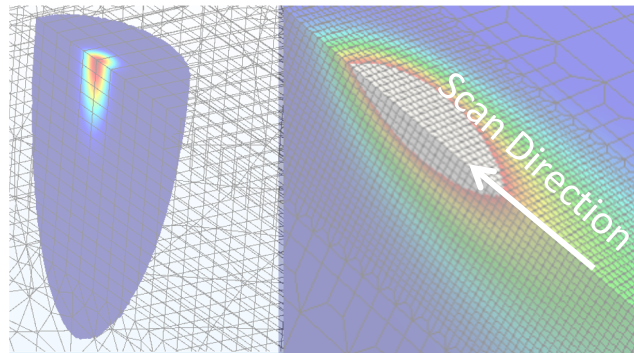
## NEXT STEPS

- Implement more advanced phase-field informed method for texture evolution in Monte Carlo models.
- Characterize role of curved melt pool and rapid solidification on texture evolution using phase-field models as input to Monte Carlo models.

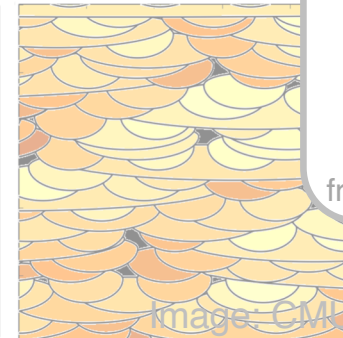
# Development of Microstructurally-Informed Durability and Damage Tolerance (D&DT)



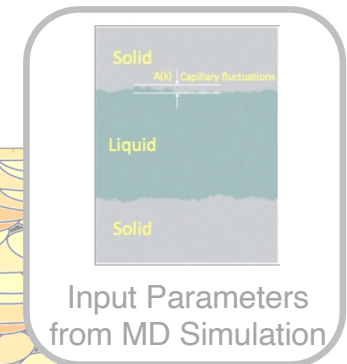
## Simulation of AM Processes



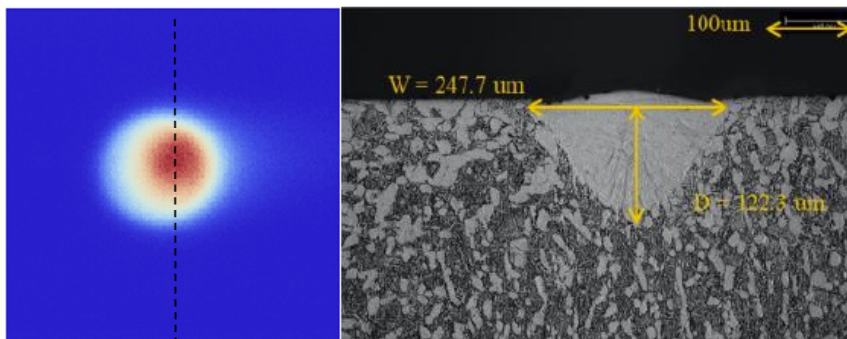
*Thermal Modeling*



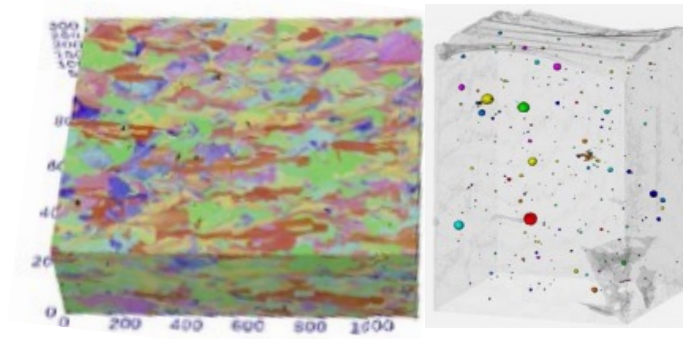
*Simulation of Microstructure  
& Defect Evolution*



## Measurement and Characterization



*Examination of the Melt Pool*



*Microstructure & Defects*

**Physics-based simulation and high-fidelity characterization of AM processing provide input to microstructure performance simulations**

# In-situ Process Monitoring for Powder-Bed Additive Manufacturing



**Reliable and traceable in-situ inspection techniques are needed to identify process anomalies and material defects.**

## APPROACH

- Implement imaging sensors in infrared and visual wavebands.
- Calibration of the sensors allows for conversion of measured intensity counts to radiance/temperature.

$$Radiance = \int_{\lambda_1}^{\lambda_2} \frac{c_1}{\lambda^5 (e^{\frac{c_2}{\lambda(T+273.15)}})} * sensor(\lambda) * filter(\lambda) * d\lambda$$

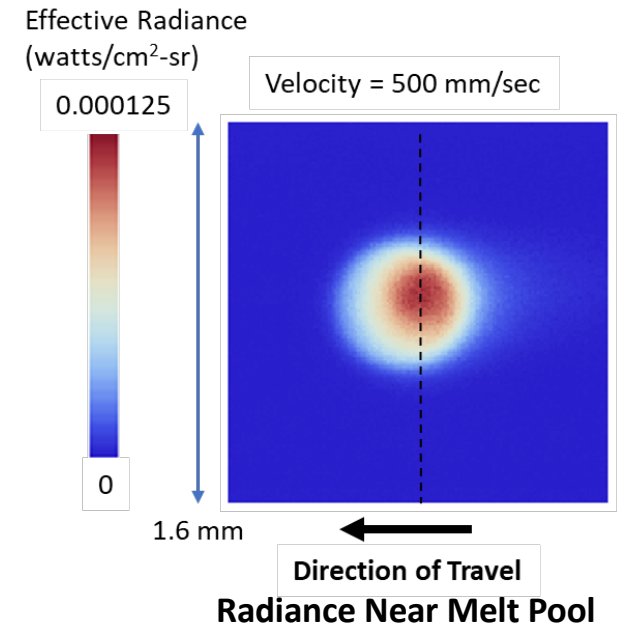
- $\lambda$  is the wavelength variable,  $T$  is temperature,  $c_1$  and  $c_2$  are functions of the speed of light, Planck's constant and Boltzmann's constant.
- Effective radiance is related to temperature considering the sensor's spectral response over the wavelength bounds, per optical path, and solved using numerical integration.
- Microscopy and materials laboratory measurements are used to inform and validate in-situ measurements.
- High performance computing and machine learning tools used to enable process anomaly detection via in-situ measurements over large data sets.

## RECENT ACCOMPLISHMENTS and IMPACT

- In-situ thermal measurements compared to finite element-based thermal model for melt pool width given various process parameters. In-situ measures enable process tomography for comparison to X-ray CT and serial-sectioned optical microscopy.

## NEXT STEPS

- Implement full build tomography with cross-correlation analyses of in-situ measurements with ex-situ measurements. Quantify measurement uncertainty and identify measurement requirements.



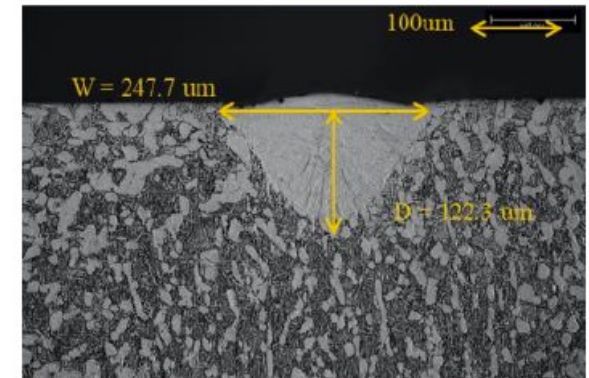
# Microstructure and Porosity Characterization in AM Parts



**Serial sectioning via RoboMet to characterize microstructure and porosity in AM parts.**

## APPROACH

- RoboMet provides means to serial section AM parts; automation enables greater consistency and repeatability.
- Combine with other microscopy techniques / equipment to generate data on melt pool dimensions, grain morphology, texture, porosity morphology and distribution.
- Reconstruct 2D slices into 3D datasets for visualization and quantification of internal part variability.
- Data is used to inform and validate in-situ sensor measurements during part fabrication and computational models.



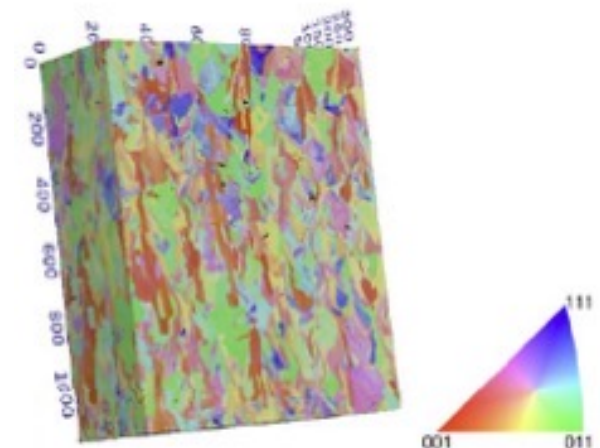
Single Track Melt Pool Measurement

## RECENT ACCOMPLISHMENTS and IMPACT

- Automated serial sectioning combined with quantitative imaging and analytical techniques enables 3D lab-based characterization.
- Data is critical for instantiation and validation of structure-property models; comparison / validation of NDE porosity measurements; quantifying melt pool dimensions to validate / calibrate thermal model.

## NEXT STEPS

- Use RoboMet to interrogate melt pool dimensions for varying build parameter combinations to validate in-situ AM sensor data.
- Expand analysis to more complex information (e.g., electron backscatter diffraction, EBSD), porosity quantification and crack initiation studies.



3D Reconstruction from RoboMet

Rowenhorst, et al. *Current Opinion in Solid State and Materials Science* 24.3 (2020): 100819.

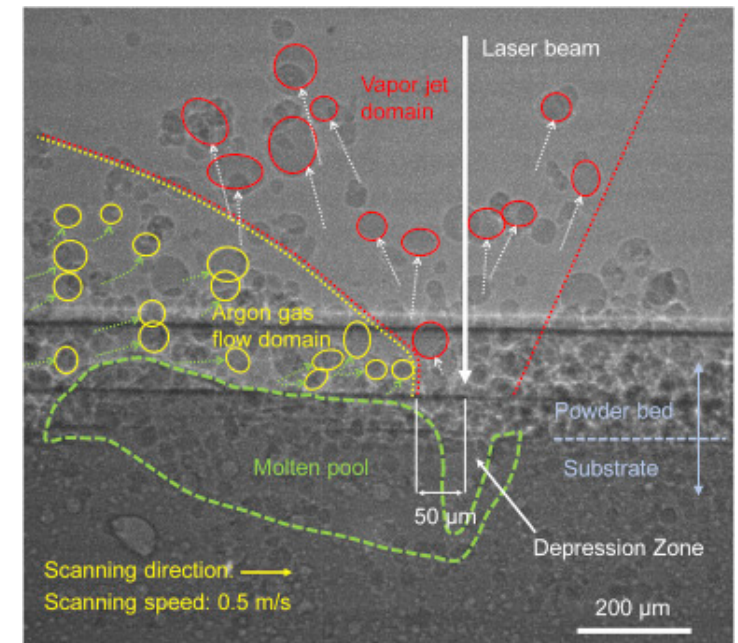
# Microstructure and Porosity Characterization in AM Parts via Synchrotron Experiments



High energy synchrotron sources for microstructure and porosity characterization in AM parts.

## APPROACH

- Leverage the multiple emerging synchrotron-based methods being developed for characterization of materials.
- *Dynamic X-ray Radiography (DXR)*
  - Enables real-time visualization of the laser interaction within the material.
  - Quantifies critical features of the AM process (vapor cavity size, melt pool depth and length, powder ejection, solidification rate, and porosity formation).
- *High Energy Diffraction Microscopy (HEDM)*
  - Near-field HEDM provides 3D non-destructive microstructure characterization (grain orientation and morphology).
  - Far-field HEDM enables in-situ grain-level stress-strain measurement to interrogate the influence of microstructure and porosity on local stress fields and damage accumulation.



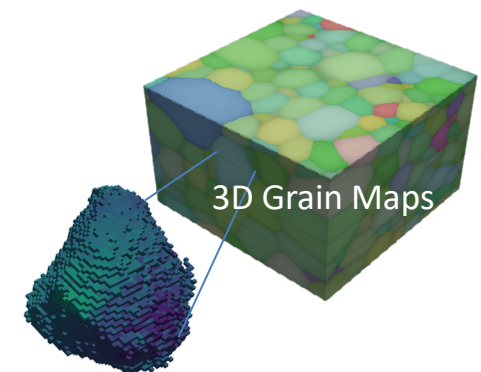
Dynamic X-ray Radiography

## RECENT ACCOMPLISHMENTS and IMPACT

- Developing relationships with university partners and other government labs to leverage access to experiments and data generated at synchrotron sources.
- DXR data shared by grantee used to validate thermal model for AM process.
- DXR and HEDM studies offer unprecedented in-situ data - highly valuable for characterization and model calibration / validation.

## NEXT STEPS

- Expand relationships with synchrotron users and develop funding to support experiments of interest.



Near and Far Field HEDM

# Artificial Intelligence for In-Situ AM Melt Pool Characterization



**Data driven modeling to develop relationships between processing parameters and resulting deformation, residual stresses and microstructure, including defect formation.**

## APPROACH

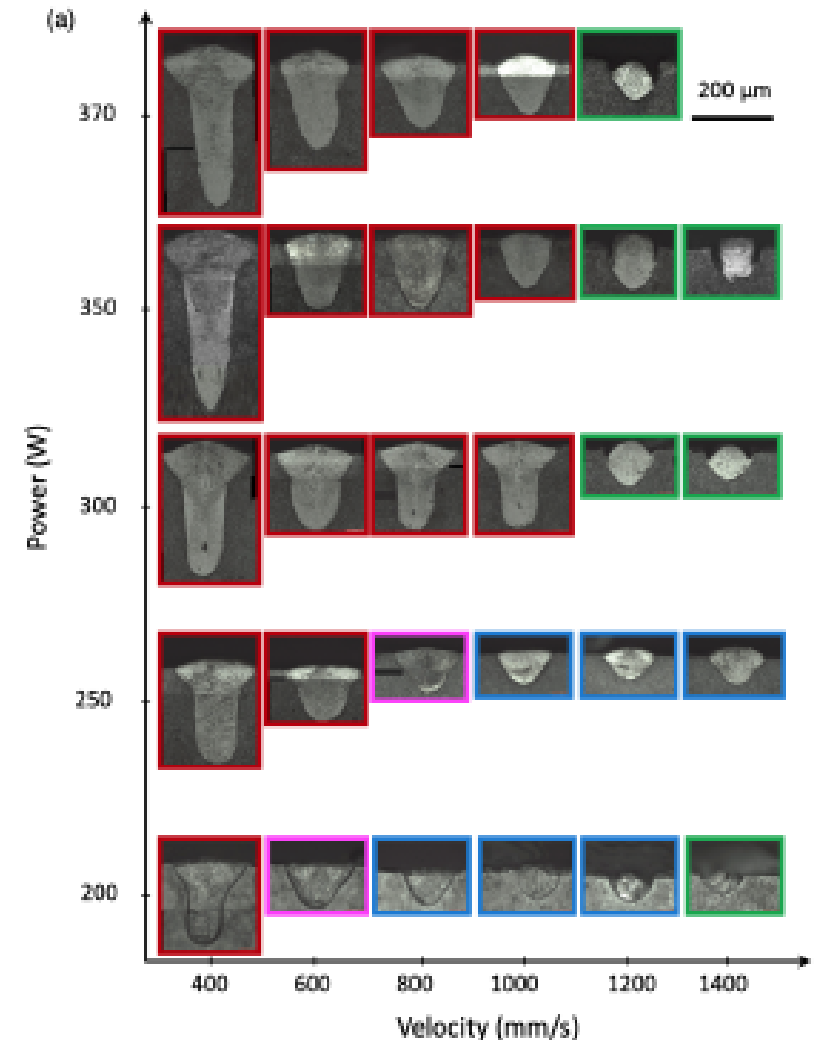
- Calibrated process models are needed to predict temperature history and enable simulation of melt pool dimensions, deformation, residual stresses and microstructure.
- Development of deep learning and recommender system methodologies, to include generative models, to predict and generate microstructure geometries.
- Can leverage smaller datasets, unlabeled data to identify latent features by mapping input data to a lower dimensional feature space.
- Predictions of power/velocity combinations for melt pool and keyhole dimensions.

## RECENT ACCOMPLISHMENTS and IMPACT

- Refined predictive accuracies for models generating keyholing depth, width, area, and convex hull area measurements.
- Established modeling approach to predict geometries based on laser absorption.

## NEXT STEPS

- Application of a conditional generative adversarial network (C-GAN) to incorporate thermophysics variables as input features.

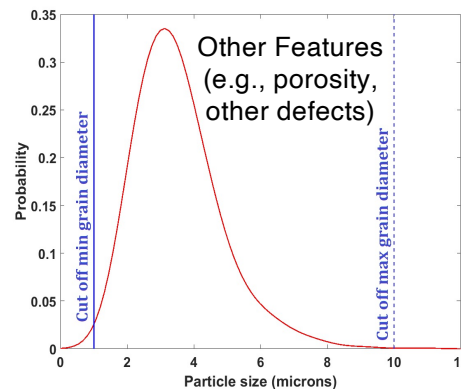
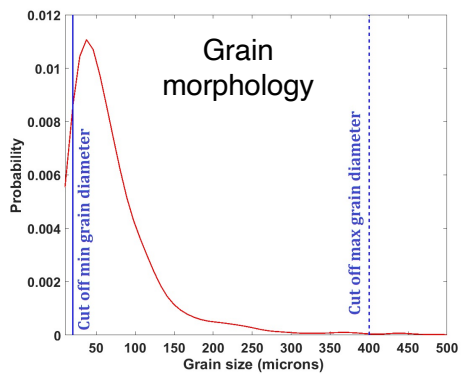


# Development of Microstructurally-Informed D&DT

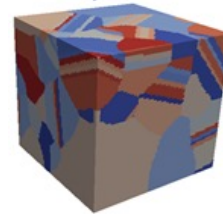
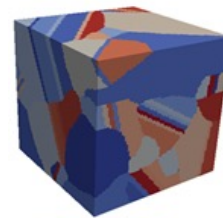


***FEA Simulations Consider Representative Microstructures Developed from Processing Simulation and Characterization Data – Capture Microstructural Details and Responses***

*Combined simulation and characterization to consider microstructure variability\*\**

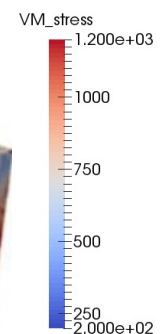


*Microstructure instantiations for FEA\**



•  
• 100-1000 independent simulations  
•

*FEA Simulations\**



**Finite element simulations account for variability in microstructure**

\*Yeratapally, et al., NIA

\*\*DREAM.3D (<http://dream3d.bluequartz.net/>)

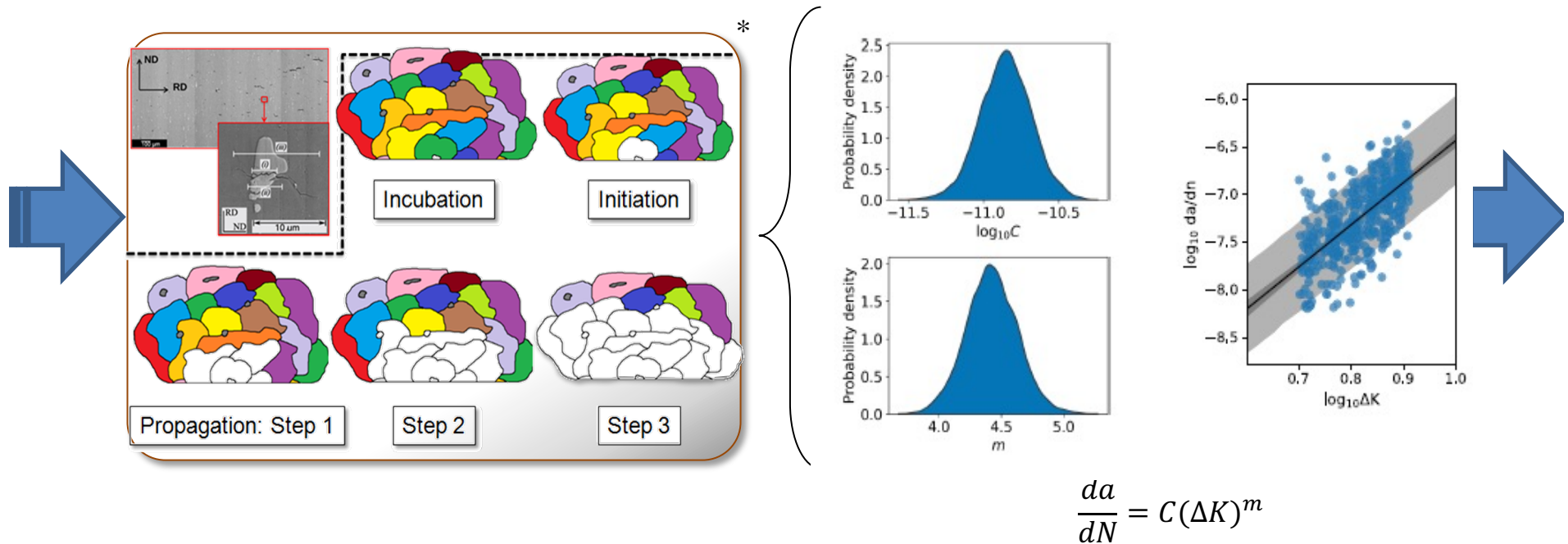
# Development of Microstructurally-Informed D&DT



## Transition from Microstructurally Small Crack Growth Estimates to Engineering Codes

$$N_{failure} = N_{incu} + N_{init} + N_{MSC} + N_{MLC}$$

Fatigue Crack Growth Material  
Parameter Distributions\*\*



**Nondeterministic prediction of fatigue life considering effects of microstructure**

\*McDowell, et al, GaTech

\*\*Hochhalter, Yeratapally, Leser, et al., LaRC

# Investigation of Effect of Defect Distributions on the Localization of Plastic Strain



**Use microstructure-based high-fidelity computational models to understand the effect of process-specific defects on the accumulation of damage and debit in mechanical performance.**

## APPROACH

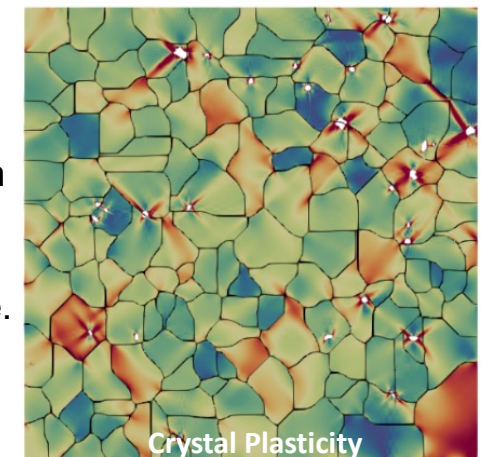
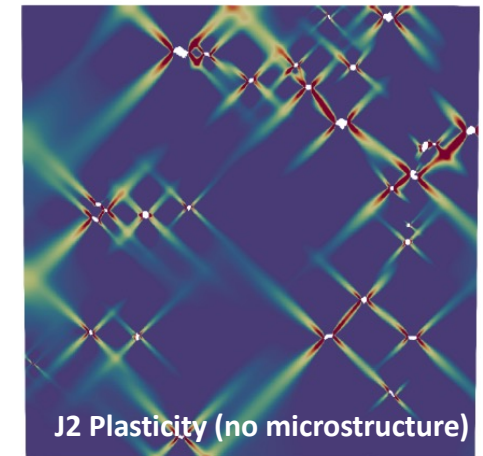
- Fuse the defect and microstructure data to feed the process-specific defect embedded microstructure model into a crystal plasticity (CP) simulation.
- CP simulation gives quantitative information on the heterogeneous distribution of stress and strain, governed by microstructure and defect character.
- Elasto-viscoplastic fast Fourier transform of Lebensohn (2001) was used.
- Crack initiation metrics:
  - Accumulated plastic slip ( $\Gamma$ ):  $\sum_{s=1}^N |\gamma^s|$ ;  $\gamma^s$  is slip on slip system,  $s$ .
  - Fatigue indicator parameter on slip plane  $p$ ,  $FIP^p = \int_0^t \Gamma \left( 1 + \frac{\sigma_p^n}{\sigma_Y} \right) dt$   
 $\sigma_p^n$  is normal stress on slip plane  $p$  and  $\sigma_Y$  is the yield stress
- Presence of defects raises the accumulation of plastic strain in its vicinity. Defects close to free-surface accumulate high plastic strain.

## RECENT ACCOMPLISHMENTS and IMPACT

- Integrated complementary characterization data (from X-ray CT and EBSD) with high-fidelity CP simulation to gain fundamental understanding on strain localization near defects.
- New methodology provides information that cannot be obtained by testing alone.

## NEXT STEPS

- Use serial sectioned data from RoboMet as input into models.
- Obtain HEDM data to perform in-situ microstructure characterization and strain measurements at the grain scale.
- Develop capabilities to simulate microstructurally-small fatigue crack growth.



**Equivalent Plastic Strain**

# Mechanical Testing of AM Ti-6Al-4V



**Mechanical testing to characterize the effect of processing defects on mechanical performance.**

## APPROACH

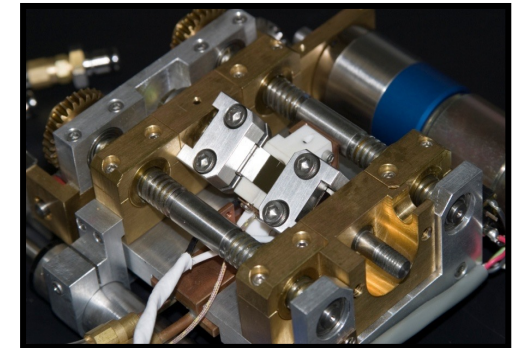
- Fatigue crack initiation / growth are often the dominant life-limiting failure mechanism; effect of AM processing defects not well understood.
- Perform fatigue crack initiation / growth testing on AM Ti-6Al-4V material under nominal, high-power (keyhole defects likely), and low-power (lack-of-fusion defects likely) conditions.
- Examination of crack surfaces to reveal information about the interaction between the crack tip and defects.
  - Scanning electron microscopy to characterize defects that interact with the crack tip.
  - Determine role of various attributes of defects (e.g., size, shape, position, orientation) on fatigue crack performance.

## RECENT ACCOMPLISHMENTS and IMPACT

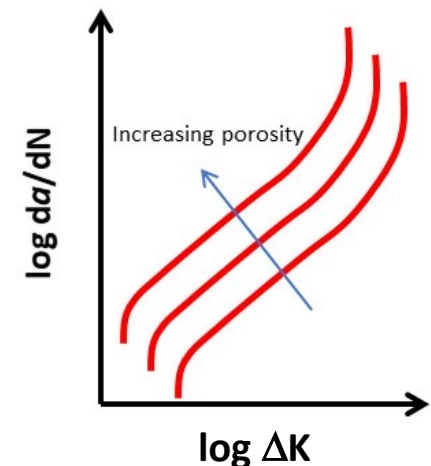
- Capabilities coming back on-line.
- Understanding the first-order variables that affect fatigue and fatigue crack growth behavior are critical for next-generation Qualification and Certification.

## NEXT STEPS

- Conduct fatigue crack growth experiments including smooth-bar fatigue testing to study natural crack initiation at defects.
- Testing within scanning-electron microscope will allow real-time monitoring of damage evolution during service-like loading.



**In-Situ Testing**



**Anticipated Effect of Porosity on Crack Growth Rate**

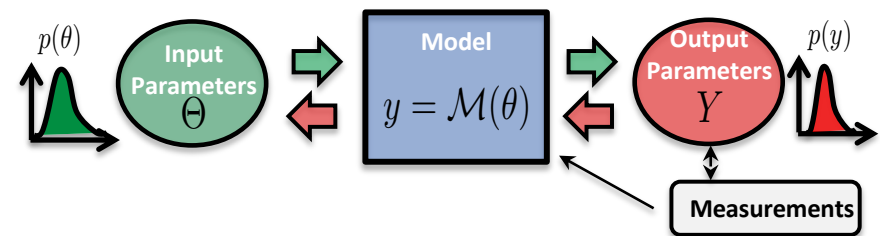
# Quantification and Propagation of Uncertainty for Qualification & Certification of AM Parts



Variability in part performance due to processing conditions is predicted using a high-fidelity, multi-scale simulation pipeline where uncertainties are quantified and propagated at each scale.

## APPROACH

- Probabilistic analysis to capture inherent variability:
  - Quantify uncertainties at each simulation scale through elicitation or inverse methods (red arrows).
  - Propagate uncertainties to the subsequent scale (green arrows).
- Address computational expense:
  - Quantifying uncertainty often involves an expensive inverse problem (red arrows).
- Estimating  $n^{th}$ -order statistical moments (e.g., mean,  $n = 1$ ) of a quantity of interest (e.g., fatigue life) involves integration:



Uncertainty Quantification and Propagation

$$\mu_n = \int_{\Theta} (\theta - c)^n f(\theta) d\theta$$

- Joint probability density function of model inputs,  $\theta$ , is  $f(\theta)$ .  $c$  is value about which the moment is estimated.
- Integral is over the entire parameter space  $\Theta$  for all models, making it *expensive* to estimate
- High performance computing (HPC) and multi-fidelity (MF) Monte Carlo methods to **overcome** expense but **maintain** fidelity/accuracy.

## RECENT ACCOMPLISHMENTS and IMPACT

- Developed Python framework for performing automated Monte Carlo analysis using NASA HPC.
- Accounting for inherent variability in the AM process is essential for next-generation Q&C of AM.

## NEXT STEPS

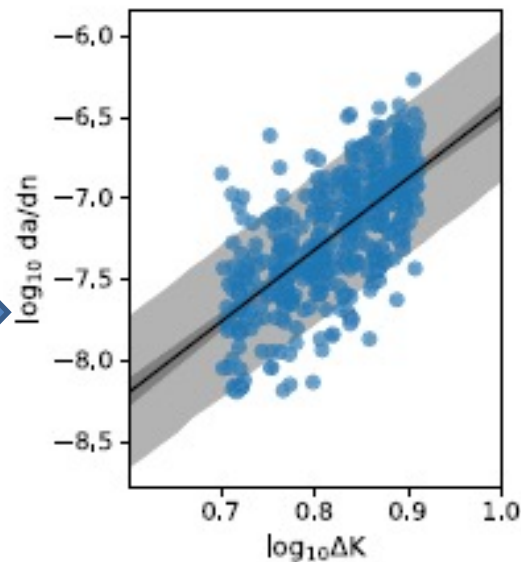
- Continue testing of the HPC capabilities in preparation for first proof-of-concept analysis using uncertainties propagated from a calibrated process model.

# Development of Microstructurally-Informed D&DT



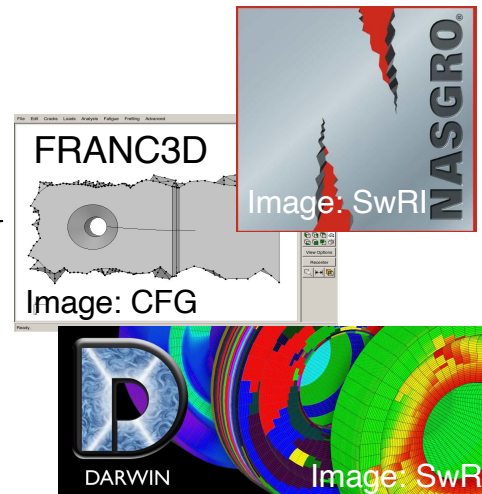
## Microstructurally-Informed D&DT of Fracture-Critical Components

Microstructure-Informed Variability in Crack Growth Rates

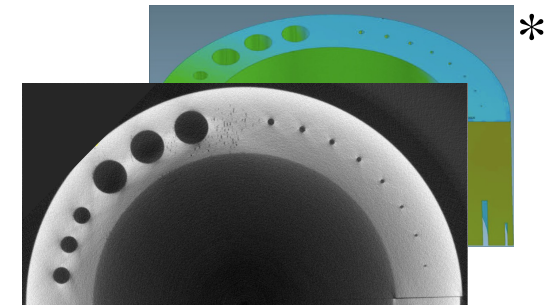


$$\frac{da}{dN} = C(\Delta K)^m$$

Embed these Relationships within Engineering Codes



Component Level Inputs



**Microstructurally-informed D&DT simulation applied to determine distribution in fatigue life of fracture-critical AM components with variable microstructures**  
**→ Maturing Computational Materials Science to Solve Engineering Problems**

\*Beshears, R., "Computed Tomography Inspection and Analysis for Additive Manufacturing Components," ASNT Annual Conference, November 2, 2017. 38

# Concluding Remarks

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- Additive manufacturing (AM) offers unprecedented design flexibility and enormous potential economic impact but with increased material variability
- Use of AM parts in critical applications is evolving rapidly and necessitates new approaches to Q&C
- FAA requirements provide entry points for computational materials simulation if supported by testing
- Continued extensive engagement with the community across the TRL scale
- NASA research is aimed at development of needed capabilities to support next-generation Q&C

# Extended Team

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## TTT Computational Materials for Qualification & Certification of AM Group

Devin Burns

Josh Fody

Erik Frankforter

Elizabeth Gregory

Samuel Hocker

Elora Kurtz

Chris Lang

Pat Leser

Paul Leser

Gretchen Murri

Andy Newman

Andy Ramlatchan

Brodan Richter

Peter Spaeth

Wes Tayon

David Wagner

Vesselin Yamakov

Sai Yeratapally

Joe Zalameda

Prof. Tony Rollett and the ARMD ULI on Development of an Ecosystem for Qualification of Additive Manufacturing Processes and Materials in Aviation

Prof. Caglar Oskay and Prof. Mike Sangid (grantees via STMD ESI)

Prof. Somnath Ghosh and Prof. Kevin Hemker (new grantees via ARMD NRA)

Dr. Michael Gorelik and the Computational Materials for Qualification and Certification Steering Group

National Aeronautics and  
Space Administration



NASA Langley Research Center 1917-2017

*A Storied Legacy, A Soaring Future*

**e.h.glaessgen@nasa.gov**

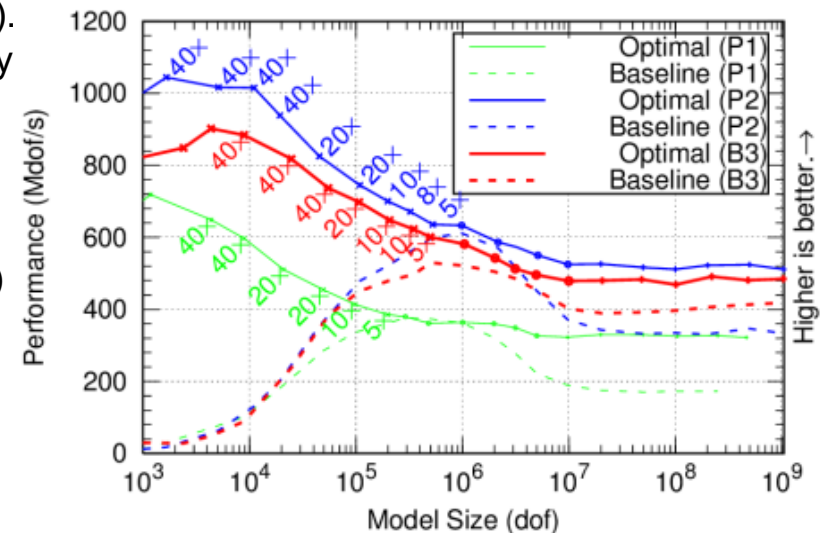
# Matrix-Free Finite Element Analysis - Femera



**Femera is a high-performance tensor-based matrix-free finite element analysis (FEA) code.**

## APPROACH

- Matrix-free solver (i.e., solve without building a system matrix).
  - Traditional FEA solver performance is limited by the memory and bandwidth needed for the sparse system matrix.
  - Matrix-free tensor train evaluation reduces memory needed by 90% and large 3D unstructured mesh elasticity solution time by 75-80%.
- Flexible data handling (i.e., read/write a variety of file formats)
  - FEA applications for elasticity typically require input data to be pre-processed into a specialized format unique to the application.
  - Open-source libraries allow Femera to read and write a variety of data formats and enable on-demand meshing to reduce or eliminate pre-processing.



**Femera Mini-app v0.1 solver performance (Nx concurrent models)**

## RECENT ACCOMPLISHMENTS and IMPACT

- Femera Mini-app v0.2 developed and baseline tests conducted.
- Baseline tests identify data handling bottlenecks that limit analysis throughput; mitigations being developed.

## NEXT STEPS

- Demonstrate alternative workflows and document best practices that reduce or eliminate the pre-processing bottleneck and improve analysis throughput.
- Continue to integrate and mature elements of the code; applications to computational materials simulation (e.g., crystal plasticity FEA).

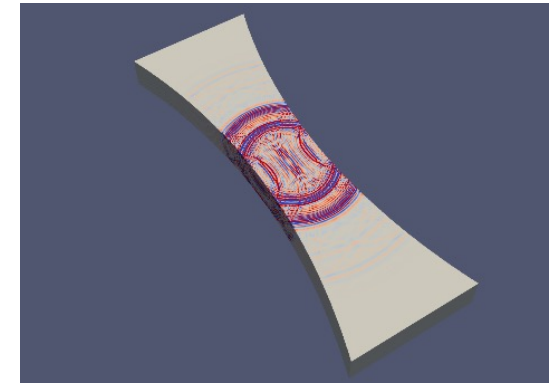
# Ultrasonic NDE Simulation of Porosity Characteristics



**Physics-based simulation of ultrasonic NDE for AM parts, assessing flaw-signal relationships and advancing towards simulation-based inspection guidance.**

## APPROACH

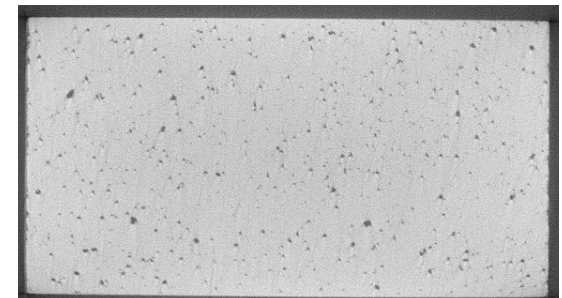
- Physics-based simulation of ultrasound propagation and wave-defect interaction in AM Ti-6Al-4V parts under varying porosity conditions.
- Gold standard flaw data extracted from high resolution (5  $\mu\text{m}$ ) X-Ray CT. Extracted pore metrics used to develop a simulation case generator; results will be validated using ultrasonic immersion scan data.
- Three-dimensional elastodynamic equations solved using a rotated staggered grid (RSG) finite difference algorithm.
  - HPC algorithm well-suited for simulation of ultrasound propagation in heterogeneous, anisotropic media.



**Elastic wave simulation in AM dog bone specimen.**

## RECENT ACCOMPLISHMENTS and IMPACT

- Performed image segmentation on X-Ray CT data, extracting pore metrics (e.g., shape, size, location >10,000 individual pores).
- Built a case generator that incorporates pore feature distribution into inspection domain.
- incorporating pore characteristics into HPC simulation, we can explore connections between defect features and inspection methodologies/results. This is a fundamental step towards strategic capabilities (e.g., development of simulation-based inspections).



**Cross-sectional slice from 5 $\mu\text{m}$  resolution X-Ray CT inspection of high laser power build.**

## NEXT STEPS

- Complete validation studies via empirical-simulation comparison of key metrics (e.g., velocities, attenuation).
- Employ parametric exploration methodologies, iterating over flaw features to explore connections with inspection results.