Critical Issues and Potential Applications of Computational Materials in Qualification and Certification of Process Intensive Metallic Materials

Part 2

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Presented by:

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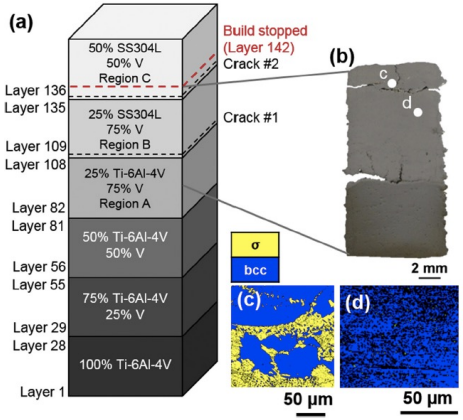


Outline

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

Increasing Complexity of AM Parts

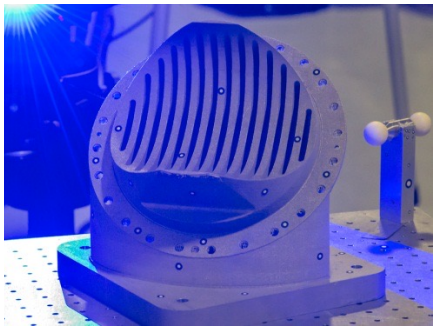




Graded Materials
Image: JPL*



Topology Optimized Bracket
Image: AutoDesk



Pogo Z-Baffle
Image: NASA

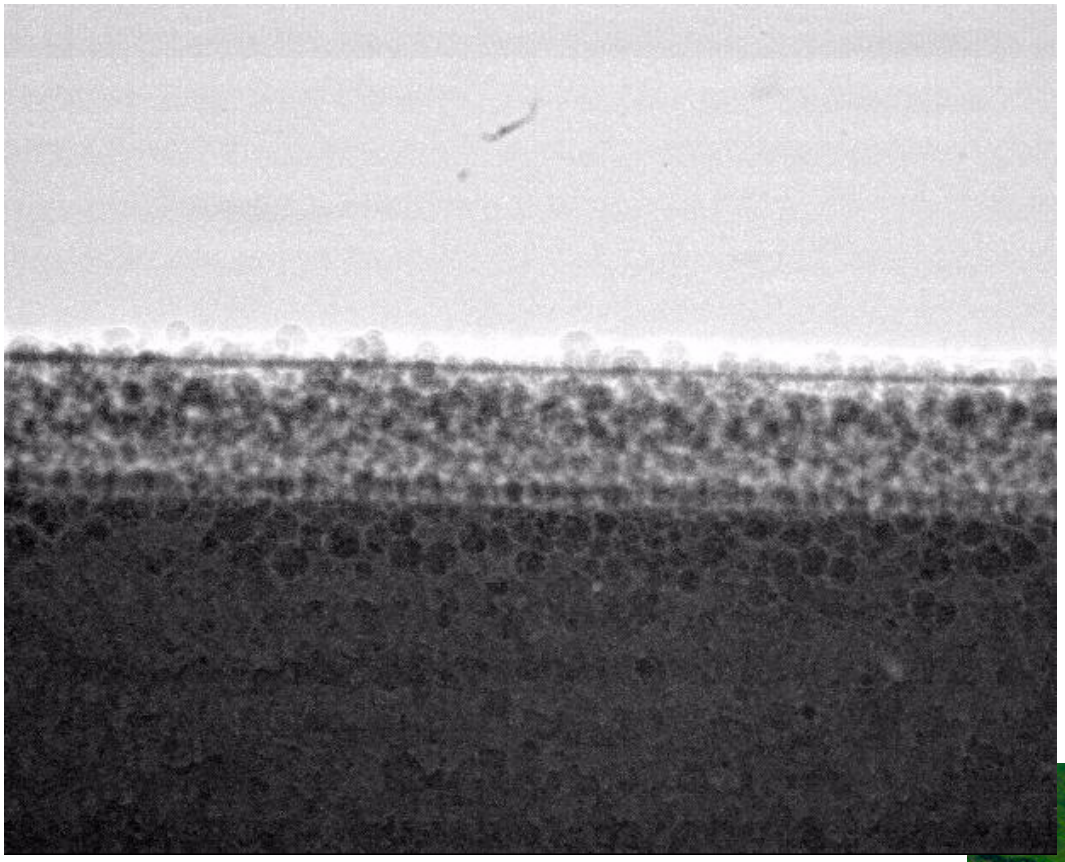


Fuel Injector
Image: GE

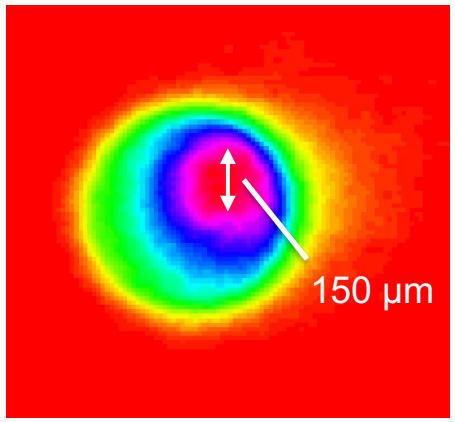
Increasing Complexity

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

Laser - Powder Bed Fusion (L-PBF) Process



Dynamic X-Ray Radiography of L-PBF



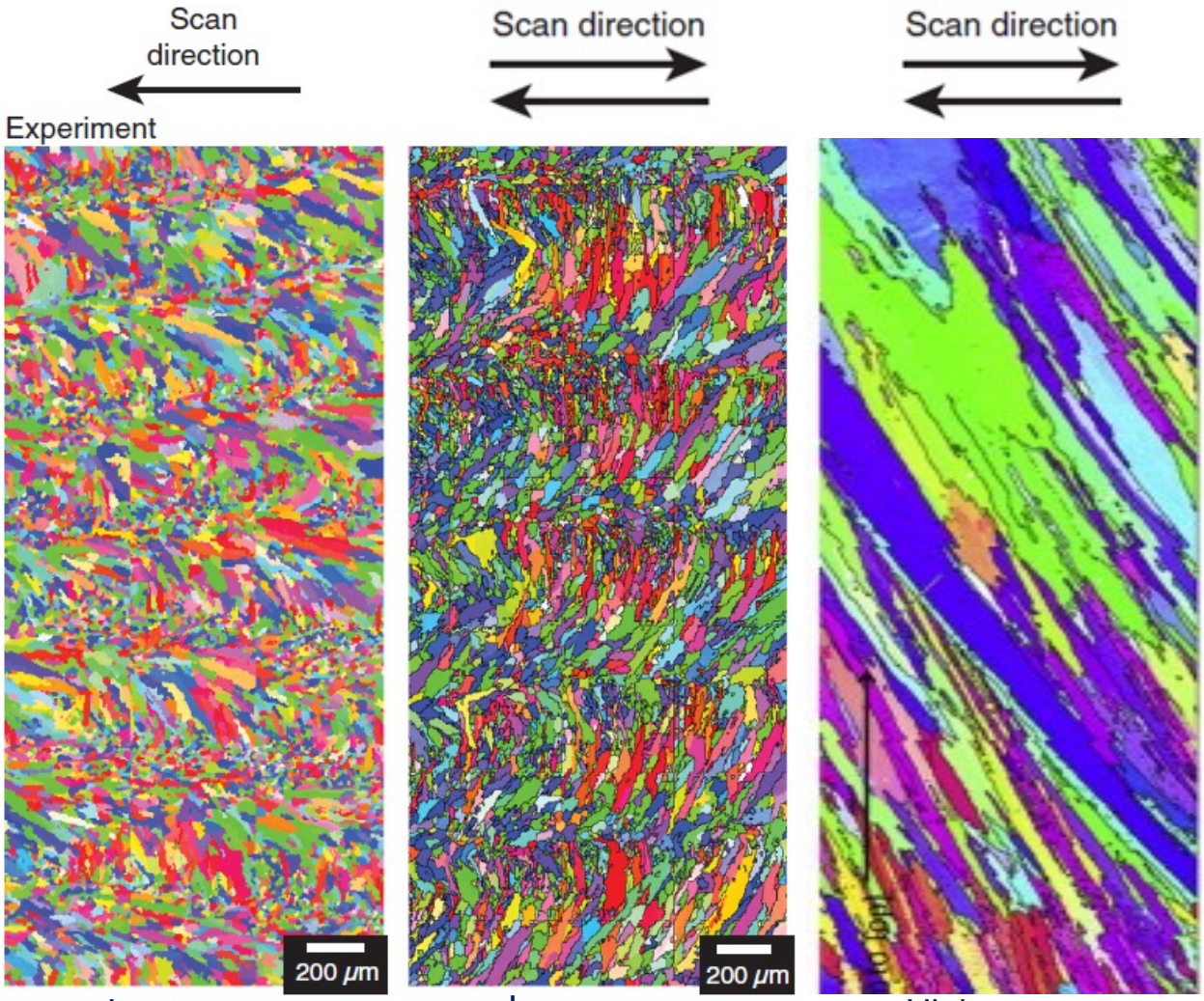
In-situ Thermal Image
of Melt-Pool



Advanced Photon Source (APS) at
Argonne National Laboratory

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

Complex/Variable AM Microstructure*



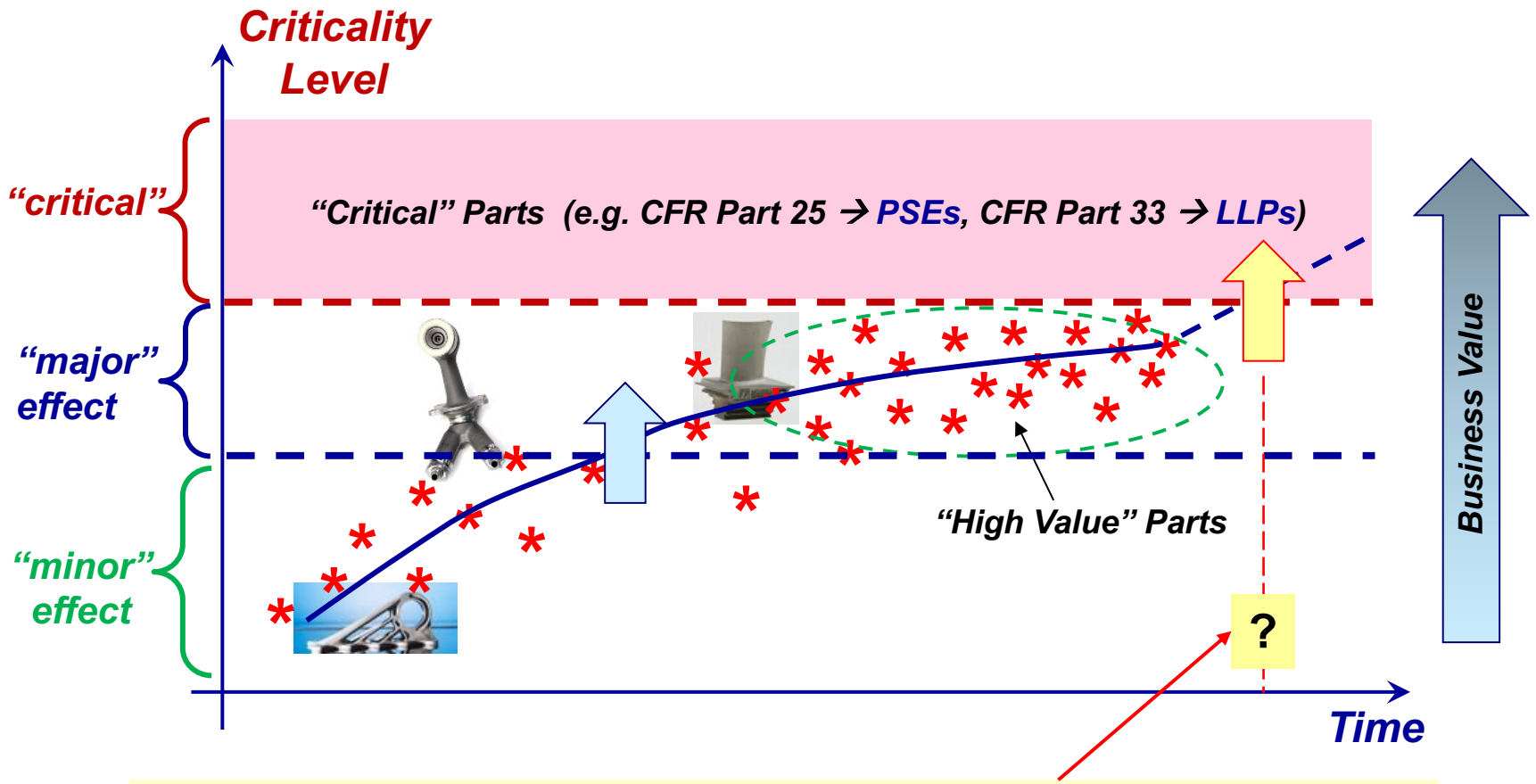
Low-power unidirectional scan

Low-power bidirectional scan

High-power bidirectional scan

*Parimi et al. (2014) Materials Characterization 89:102

Evolution of Criticality of AM Parts*



Transition to "safety-critical" applications in aviation will occur sooner than initially expected

* Adapted from Michael Gorelik, FAA

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**


Image: NASA

- 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"**


Image: NASA

* Adapted from Michael Gorelik, FAA

Input from the Aerospace Community



NASA/CR—2018-219771

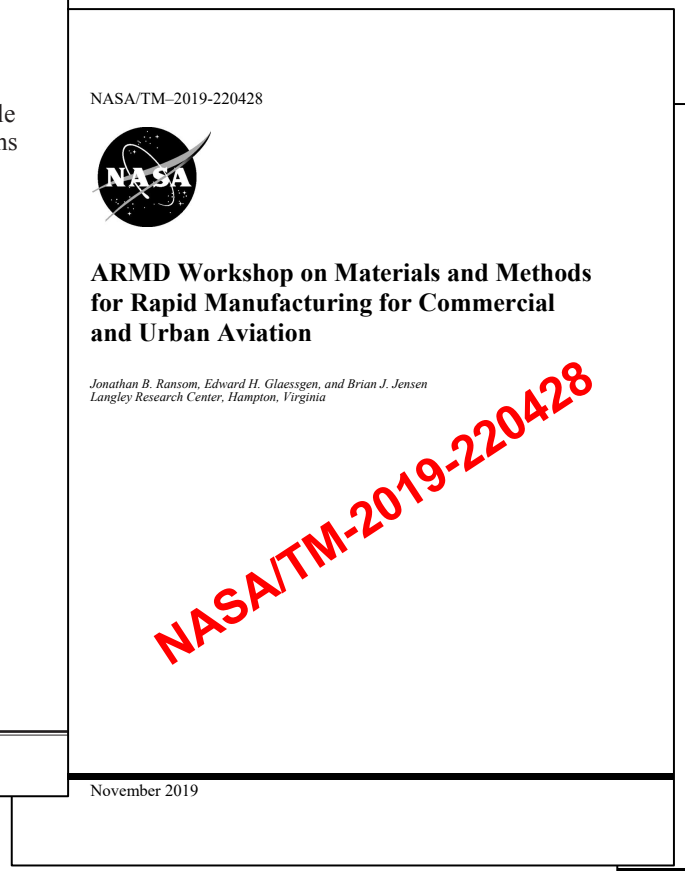
Vision 2040: A Roadmap for Integrated, Multiscale Modeling and Simulation of Materials and Systems

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

Jared Kosters and Jack Holmes
Nexight Group, Silver Spring, Maryland

March 2018

NASA/CR-2018-219771



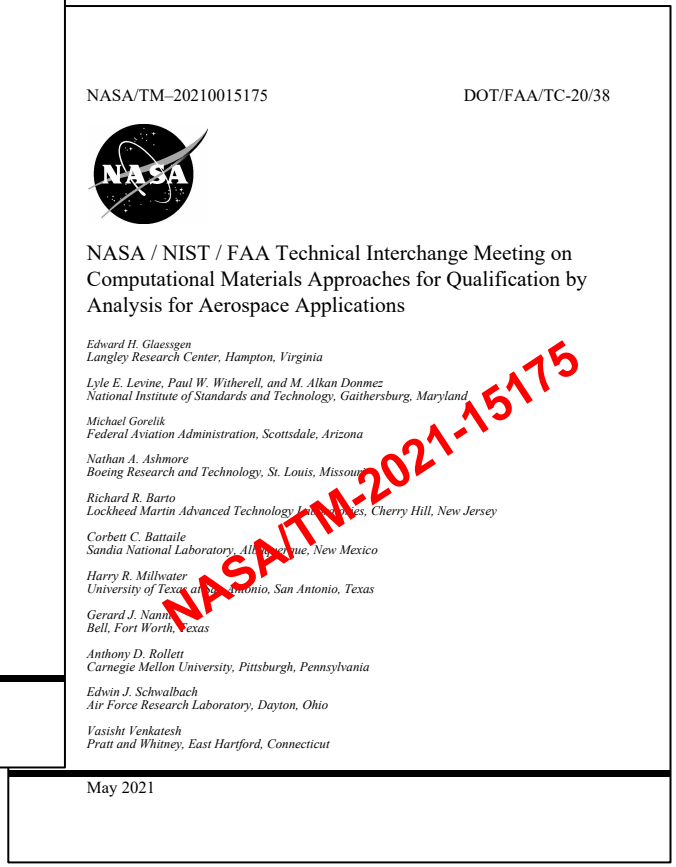
NASA/TM–2019-220428

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

November 2019

NASA/TM-2019-220428



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



- 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 Capabilities That Should be Developed (Process-Microstructure)

Question 9: 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?

All years

- Provide robust data for validation of simulations.
- Develop both physics-based and data driven simulation approaches.
- Develop an understanding of the inherent sources of variability – not just with machines, but in the feed stock and the AM process itself.
- Develop improved mechanisms and guidance for acquiring and sharing both data and metadata.

5 years

- Provide guidance for measurements needed to validate basic sets of process parameters to support qualification of process parameters and machines.
- Make the connection between the complete set of process parameters and the local state of the material for a narrow set of materials and conditions.
- Develop a framework for defining and implementing model maturity levels including specifications for Verification and Validation.
- Work with standards organizations to address the problem of material specifications for AM feedstocks.

Some Comments Related to Capabilities That Should be Developed (Process-Microstructure), cont.

10 years:

- Connect the set of process parameters to the local state of the material for a wide range of materials and conditions.
- Develop best practice guides for achieving a specific material state by adjusting the qualified build parameters.

20 years:

- Develop specifications that will lead to build characteristics that are consistent between multiple machines, multiple machine models and multiple machine vendors. Provide statistically valid data to demonstrate this consistency.

Some Comments Related to Capabilities That Should be Developed (Microstructure-Performance)

Question 9: 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?

- Develop new durability and damage tolerance capabilities:
- Micro-structure sensitive defect-mediated durability and damage tolerance.
- Simulation and characterization of microstructurally small crack initiation and propagation.
- Accelerated high-cycle fatigue tests and models.
- Develop capabilities for quantitative in-situ micro-structure characterization and evolution.
- Develop non-standard characterization and testing methods.
- Increase investment in probabilistic and UQ methods.

- Focus on computational-based design for inspectability integrated into the design process.
- Enhance capabilities for non-destructive evaluation of thick additive parts (e.g., high-z, complex configurations).

Some Comments Related to Capabilities That Should be Developed (Microstructure-Performance), cont.



- Develop appropriate standards for computational materials approaches.
- Increase disciplinary workforce training and development.
- Use research experience to help to mentor industry in best practices for computational materials.

- Create an industry group to develop requirements for a computational materials framework including V&V and UQ.
- Develop a broader joint roadmap for technology developers, educators, end users, and regulators with focus on incremental progress and demonstrable deliverables.

Computational Materials for Qualification and Certification (CM4QC) Steering Group

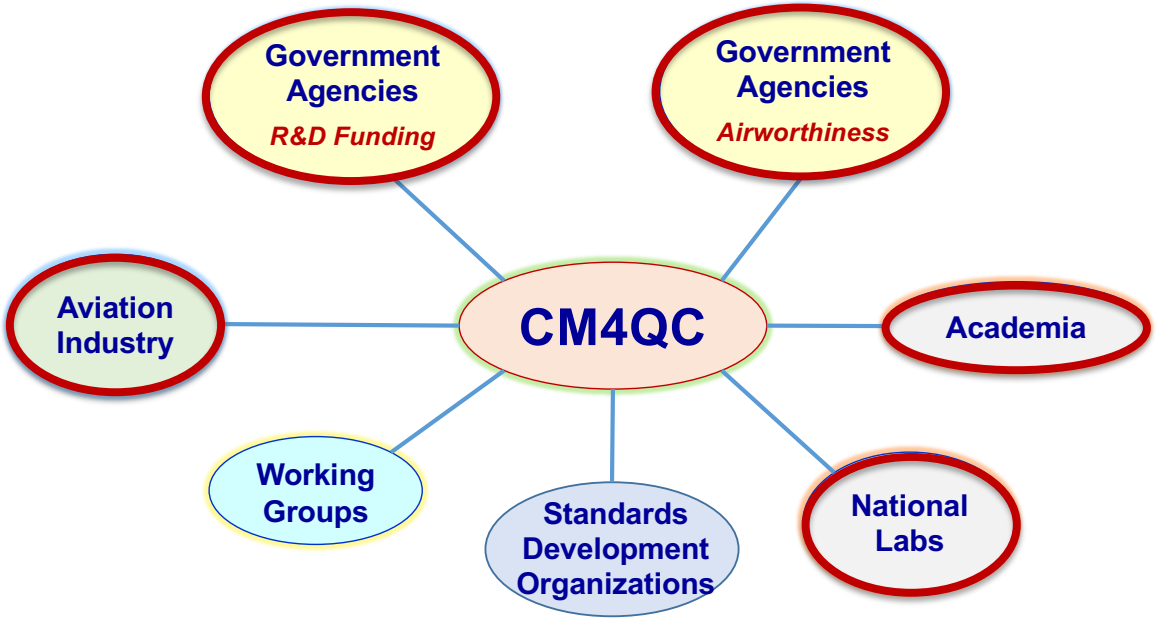
The ***primary goals*** of this Steering Group are to

- 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)

CM4QC Membership

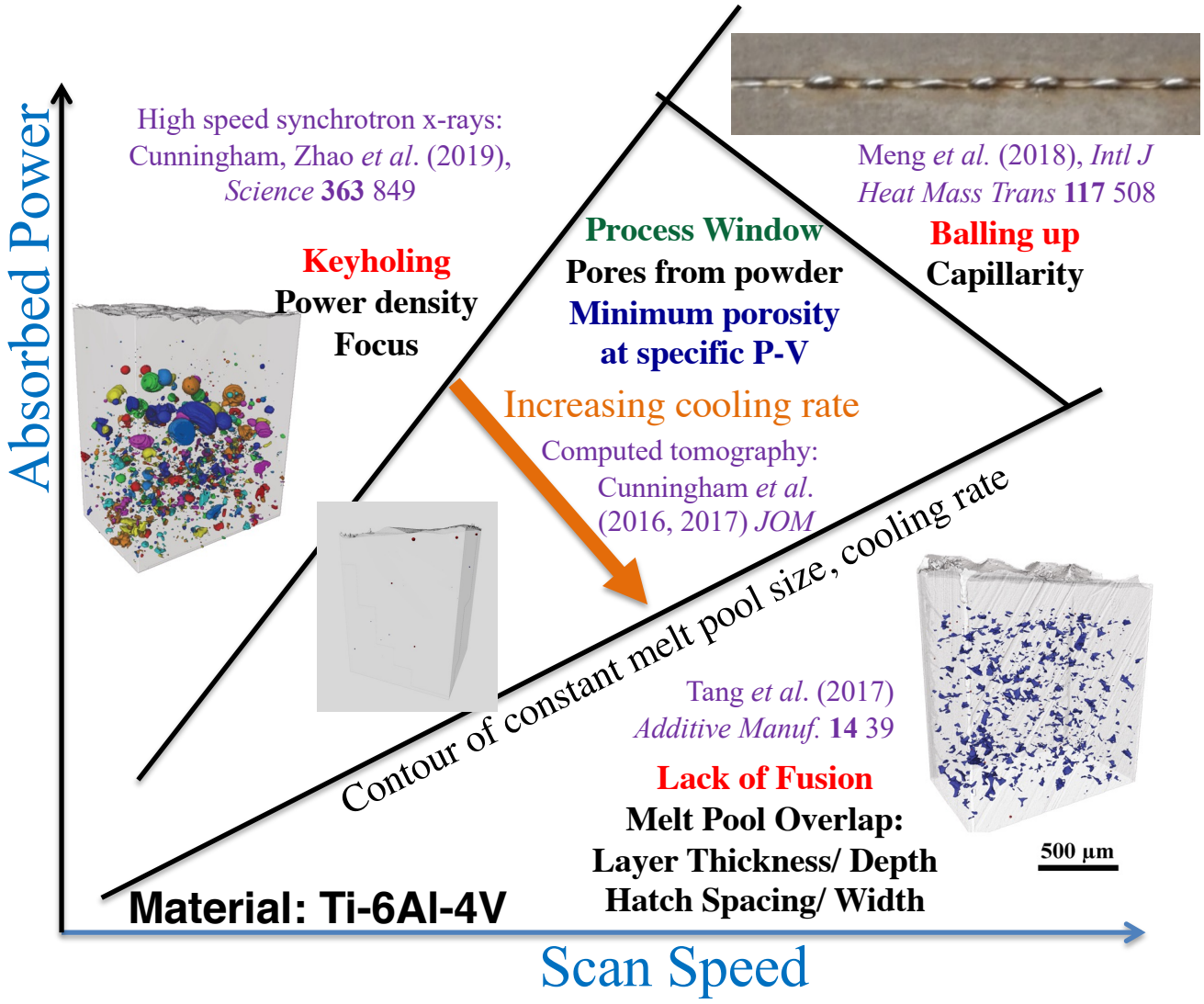
Complementary Investments

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*

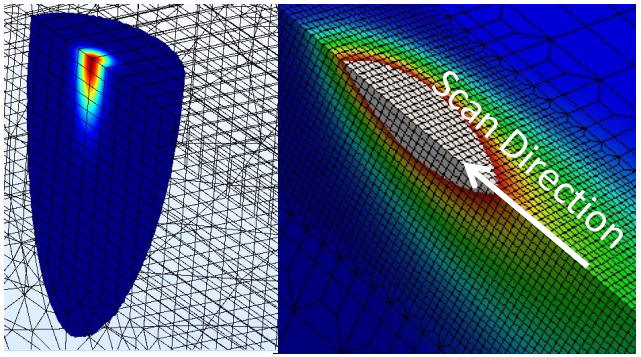
- Key-holing: excessive power density
- Lack-of-fusion: geometry of melt pool relative to layer depth & hatch spacing
- Capillarity causes “balling up”; complicated by fluid flow behind the heat source
- Note the sharp increase in porosity predicted in the lower right (lack of fusion) and upper left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

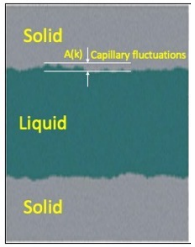
Simulation of AM Processes



Thermal Modeling

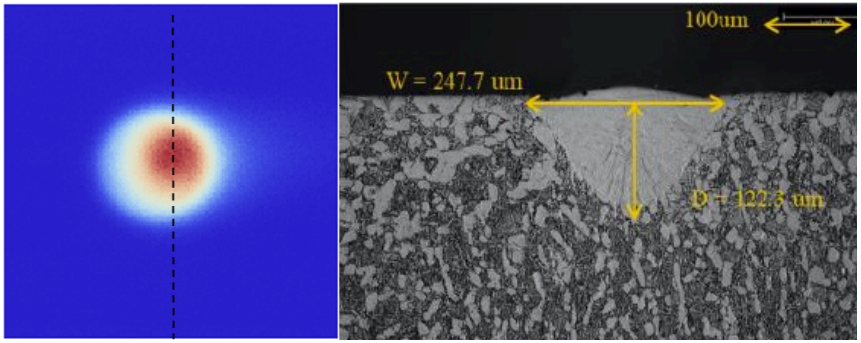


Simulation of Microstructure & Defect Evolution

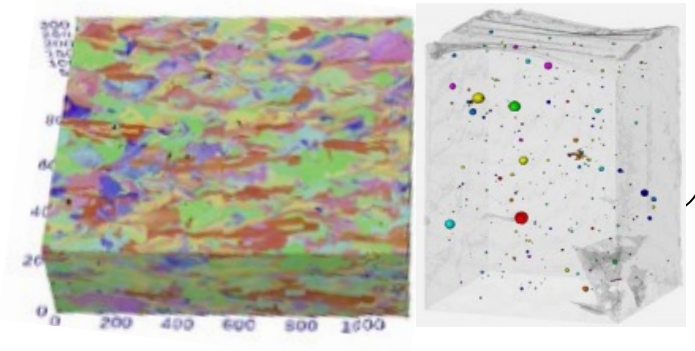


Input Parameters from MD Simulation

Measurement and Characterization



Examination of the Melt Pool



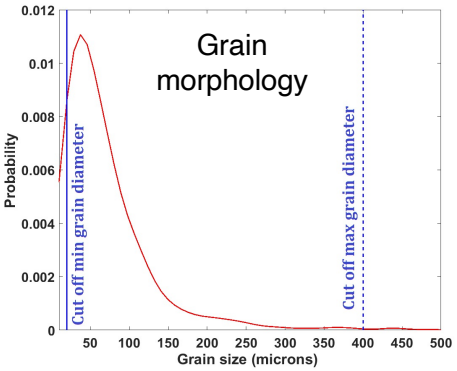
Microstructure & Defects

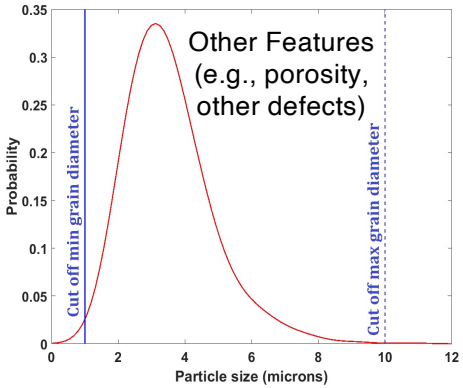
Physics-based simulation and high-fidelity characterization of AM processing provide input to microstructure performance simulations

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

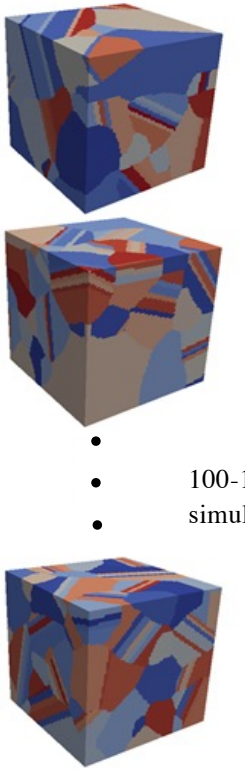
FEA Simulations Consider Representative Microstructures Developed from Processing Simulation and Characterization Data – Capture Microstructural Details and Responses

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



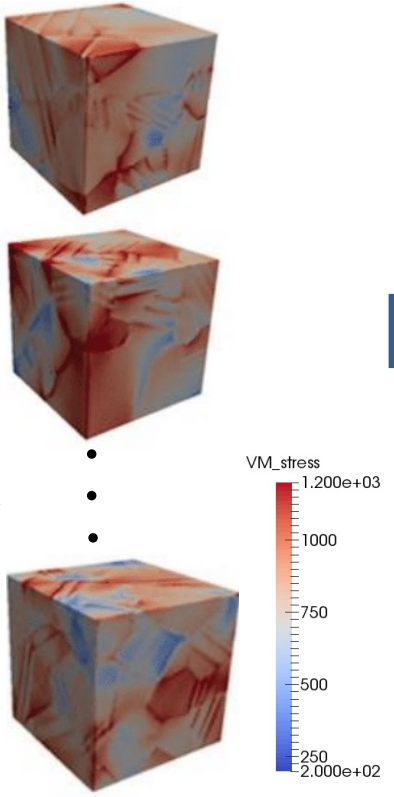


*Microstructure instantiations for FEA**



100-1000 independent simulations

*FEA Simulations**



Finite element simulations account for variability in microstructure

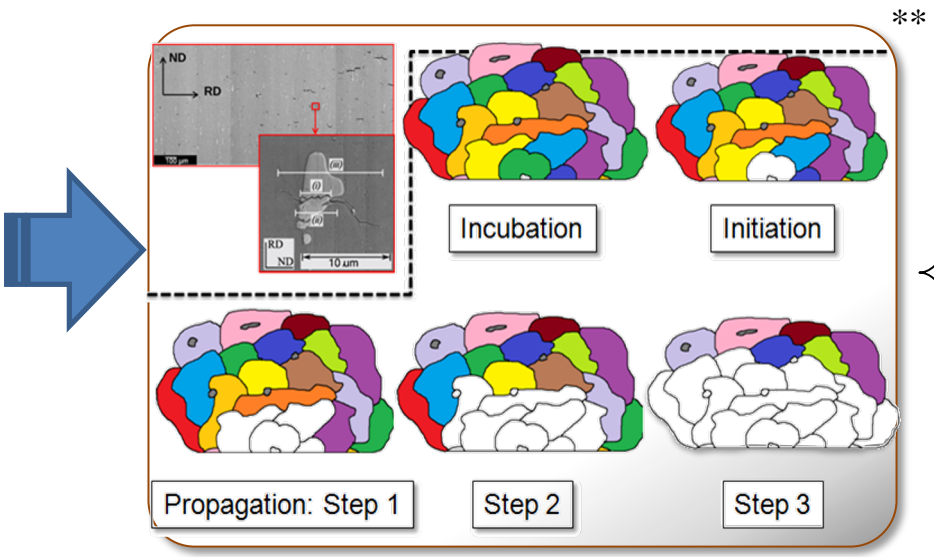
*Yeratapally, et al., NIA

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

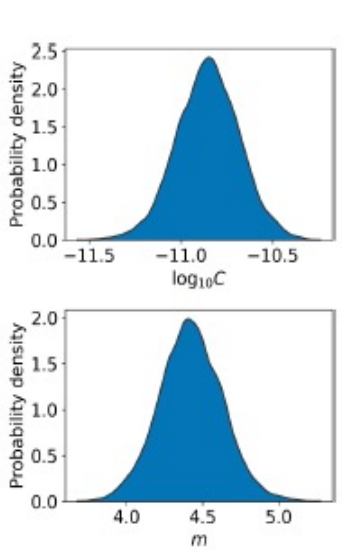
Development of Microstructurally-Informed D&DT (3/4)

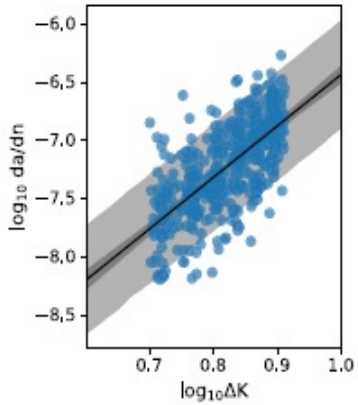
Transition from Microstructurally Small Crack Growth Estimates to Engineering Codes

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



*Fatigue Crack Growth Material Parameter Distributions****





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

Nondeterministic prediction of fatigue life considering effects of microstructure

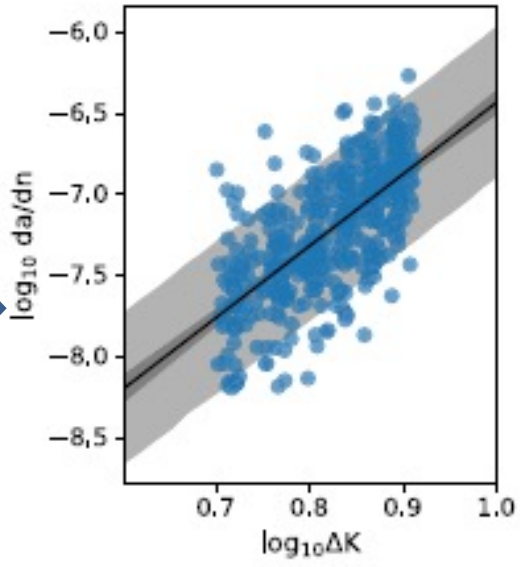
**Sum of the cycles to incubation, initiation, microstructurally small crack growth and microstructurally large crack growth*

***McDowell, et al, GaTech* ****Hochhalter, Yeratapally, Leser, et al., LaRC*

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

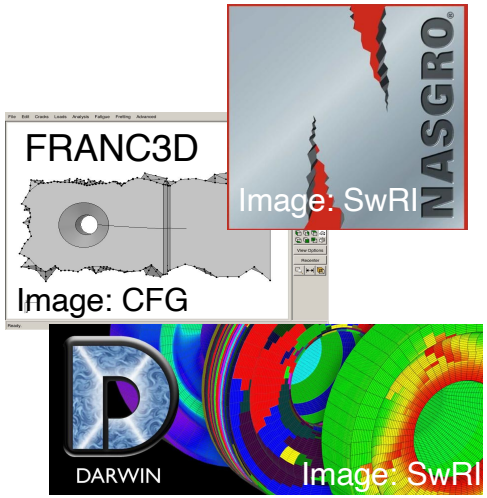
Microstructurally-Informed D&DT of Fracture-Critical Components

Microstructure-Informed Variability in Crack Growth Rates

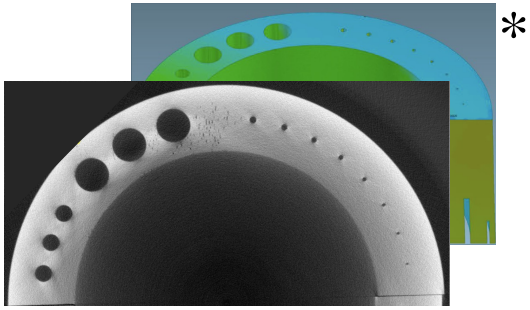


$$\frac{da}{dN} = C(\Delta K)^m$$

Embed these Relationships within Engineering Codes



Component Level Inputs



*

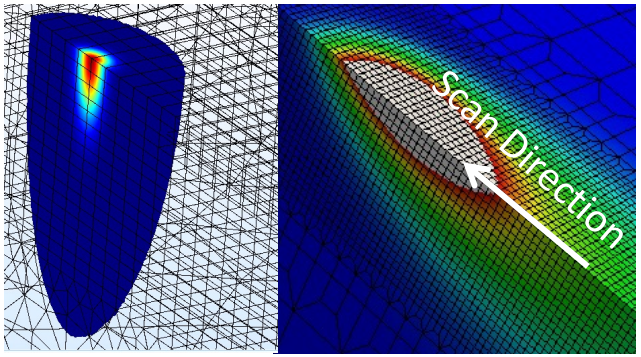
Microstructurally-informed D&DT simulation applied to determine distribution in fatigue life of fracture-critical AM components with variable microstructures

→ 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.*

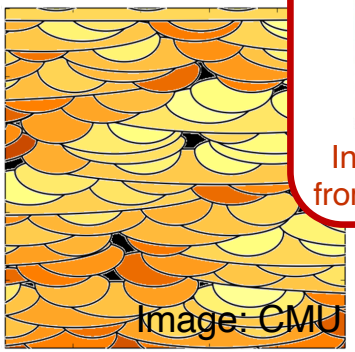
Development of Microstructurally-Informed Durability and Damage Tolerance (D&DT)

Simulation of AM Processes

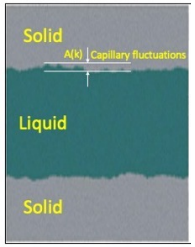


Thermal Modeling



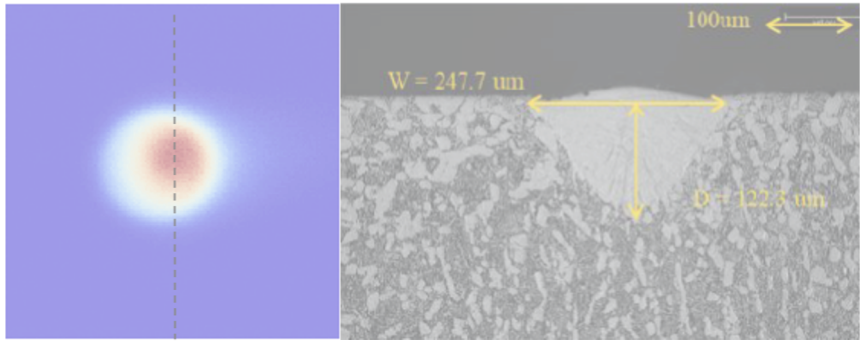


Simulation of Microstructure & Defect Evolution



Input Parameters from MD Simulation

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

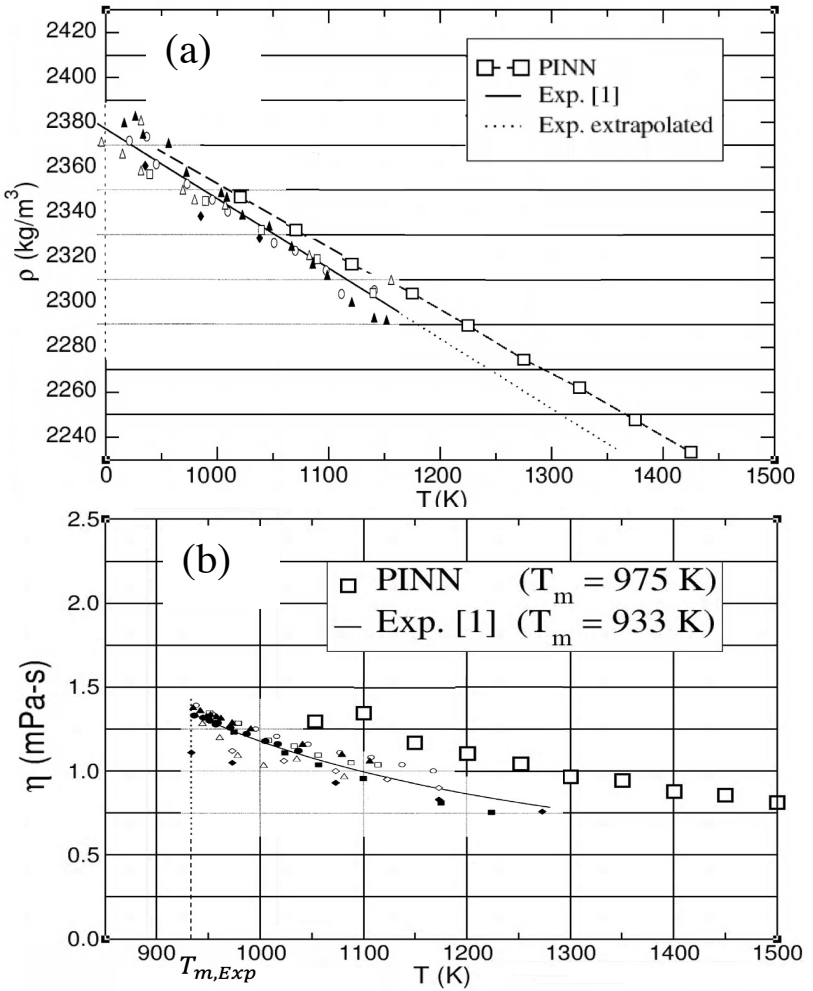
- Al system simulated using physically-informed neural network (PINN) potential. Ti system simulated using state-of-the-art embedded-atom method (EAM) empirical potential.
  - PINN potential trained using density functional theory (DFT) and achieves high accuracy (~ 1meV/atom).
  - Melt properties calculated 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 (~ 10^4-10^5 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

Probabilistic Calibration and Validation of Simplified AM Thermal Process Model

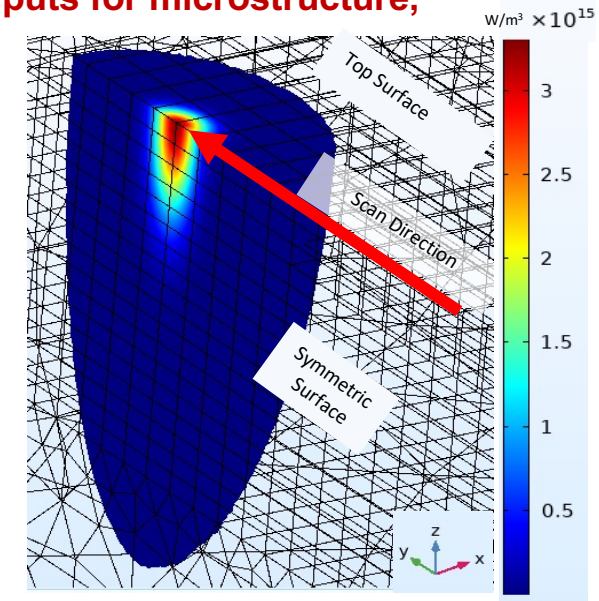
Automated calibration and validation of a single scan track thermal process finite element model to build a data driven rapid predictor of local scale thermal inputs for microstructure, defect, and part scale models.

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, α_{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.



Volumetric Heat Source (Symmetric Cross Section)

- Gaussian Process Regression for probabilistic calibration using scant data.
- Iterative validate-calibrate adaptive learning algorithm employed to converge after minimal FEA model calls.

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

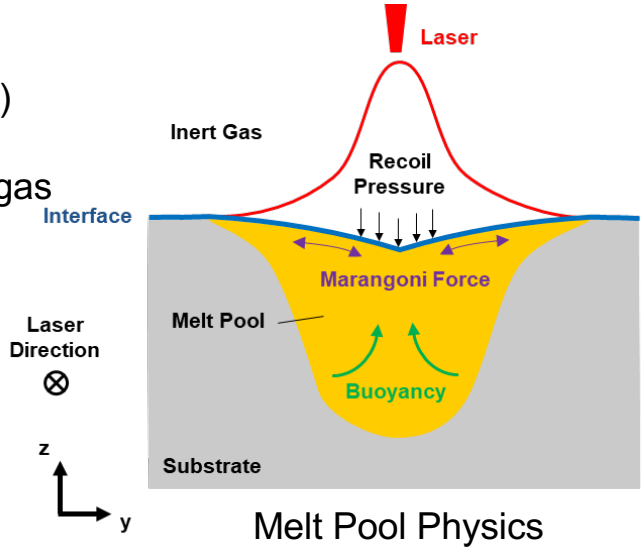
- Solve the coupled Energy, Mass, and Momentum (Naiver-Stokes) conservations equations.
- Sharp interface: use the levelset method to evolve the substrate/gas interface according to the fluid velocity.
- Incorporate melt pool physics:
  - Fluid Flow
  - Buoyancy
  - Surface Tension
  - Recoil Pressure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

RECENT ACCOMPLISHMENTS and IMPACT

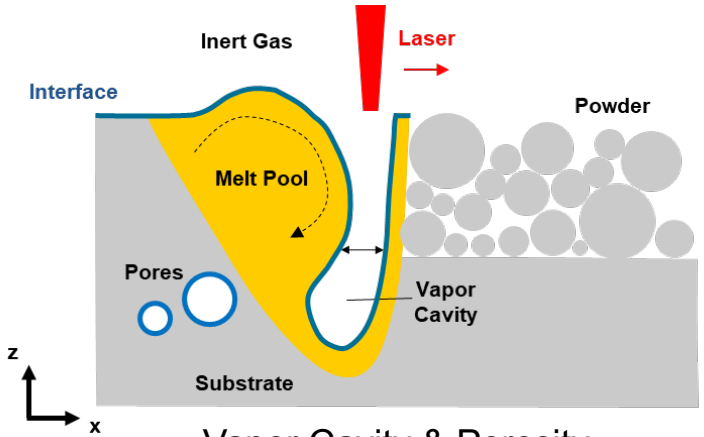
- Recent accomplishments
  - Diffuse interface implemented.
  - Spot weld analysis completed with comparison to a transient thermal analysis.
- Impact.
  - High-fidelity solution capability for process parameter linkage.
  - Predict porosity formation at root of vapor cavity for impact to property and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

NEXT STEPS

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



Melt Pool Physics



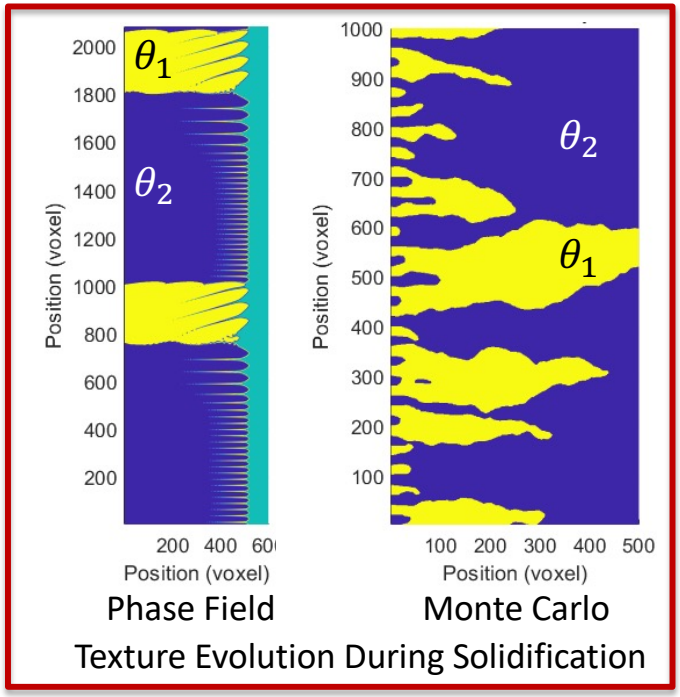
Vapor Cavity & Porosity

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 2nd order conserved and isotropic spatial derivative formulations.



RECENT ACCOMPLISHMENTS and IMPACT

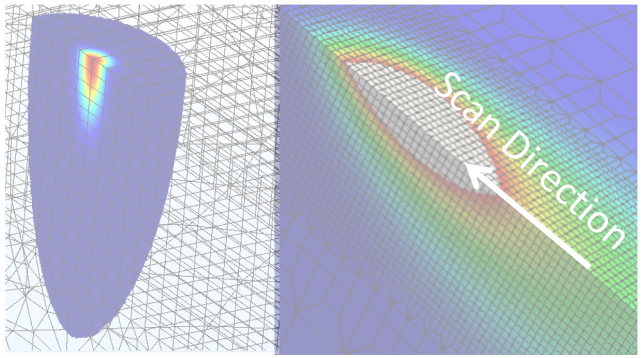
- Implemented quantitative binary-alloy phase-field model with support for multiple grains of various orientations.
- Performed large phase-field and Monte Carlo study on texture development comparing rate of grain overgrowth vs. input grain orientation.

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.

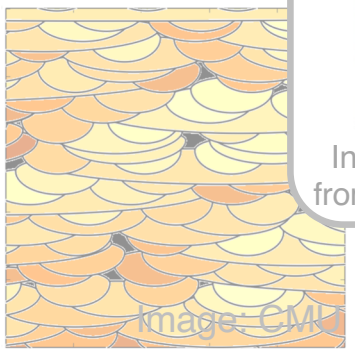
Development of Microstructurally-Informed Durability and Damage Tolerance (D&DT)

Simulation of AM Processes

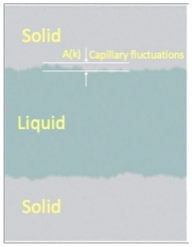


Thermal Modeling



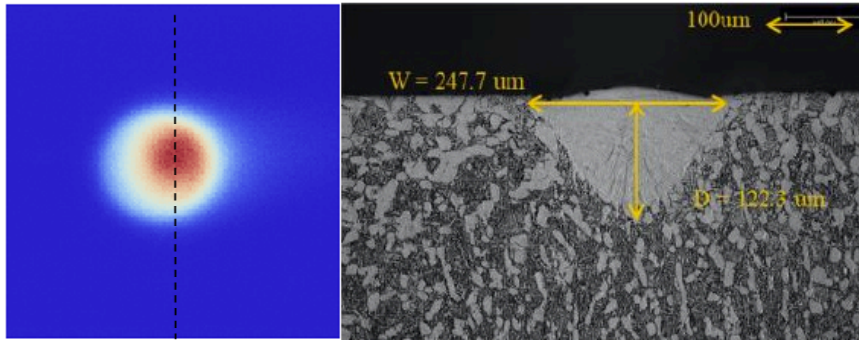


Simulation of Microstructure & Defect Evolution

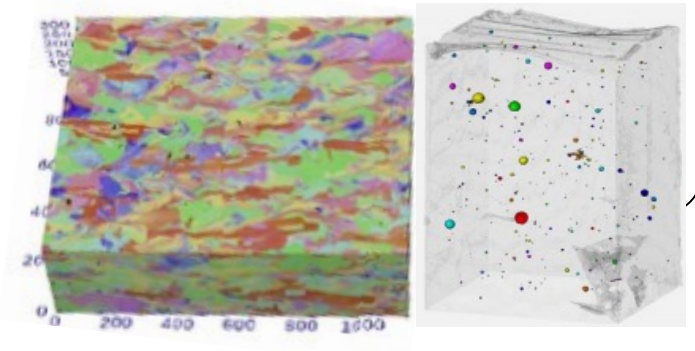


Input Parameters from MD Simulation

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

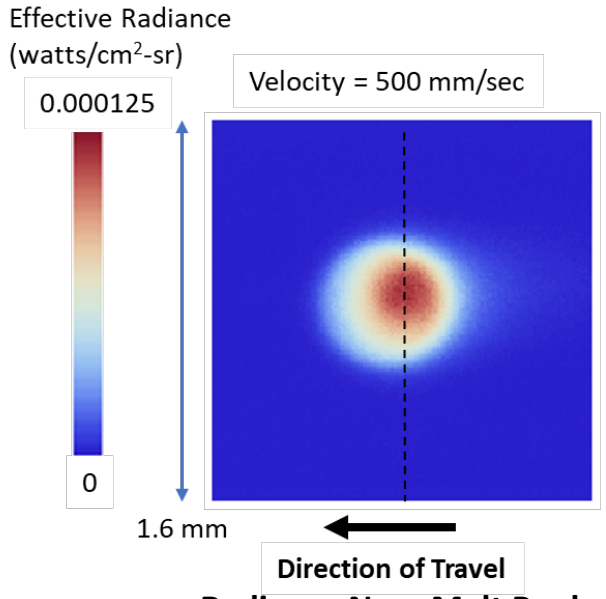
Reliable and traceable in-situ inspection techniques are needed to identify process anomalies and material defects.

APPROACH

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

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

- λ is the wavelength variable, T is temperature, *c1 and c2 are* functions of the speed of light, Plank'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.



Radiance Near Melt Pool

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

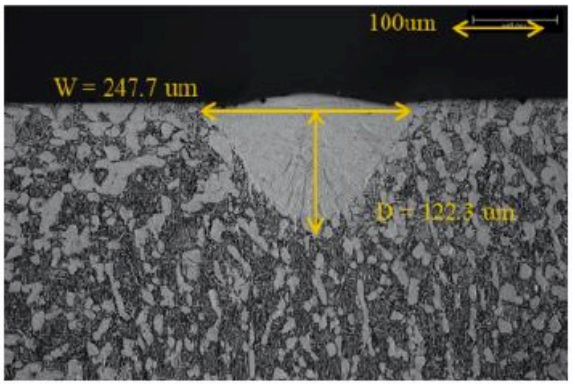
- Implement full build tomography with cross-correlation analyses of in-situ measurements with ex-situ measurements. Quantify measurement uncertainty and identify measurement requirements.

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.



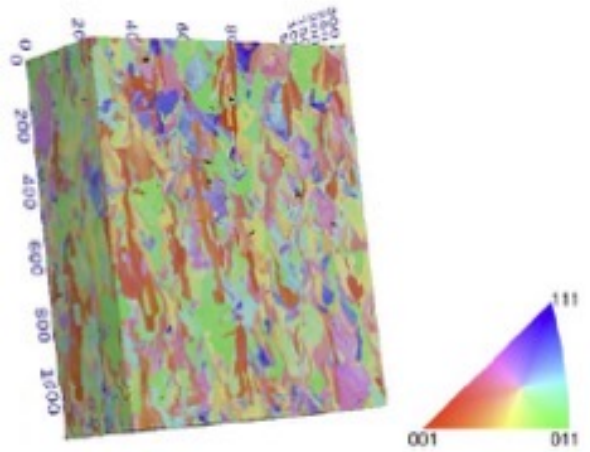
Single Track Melt Pool Measurement

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

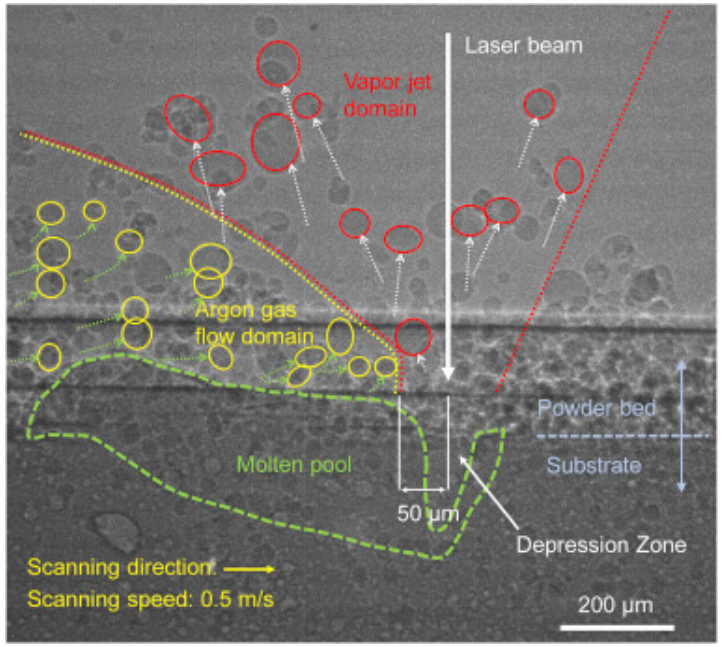
Rowenhorst, et al. *Current Opinion in Solid State and Materials Science* 24.3 (2020): 100819.

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.



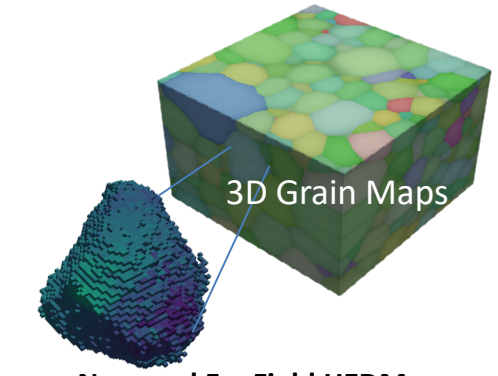
Dynamic X-ray Radiography

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

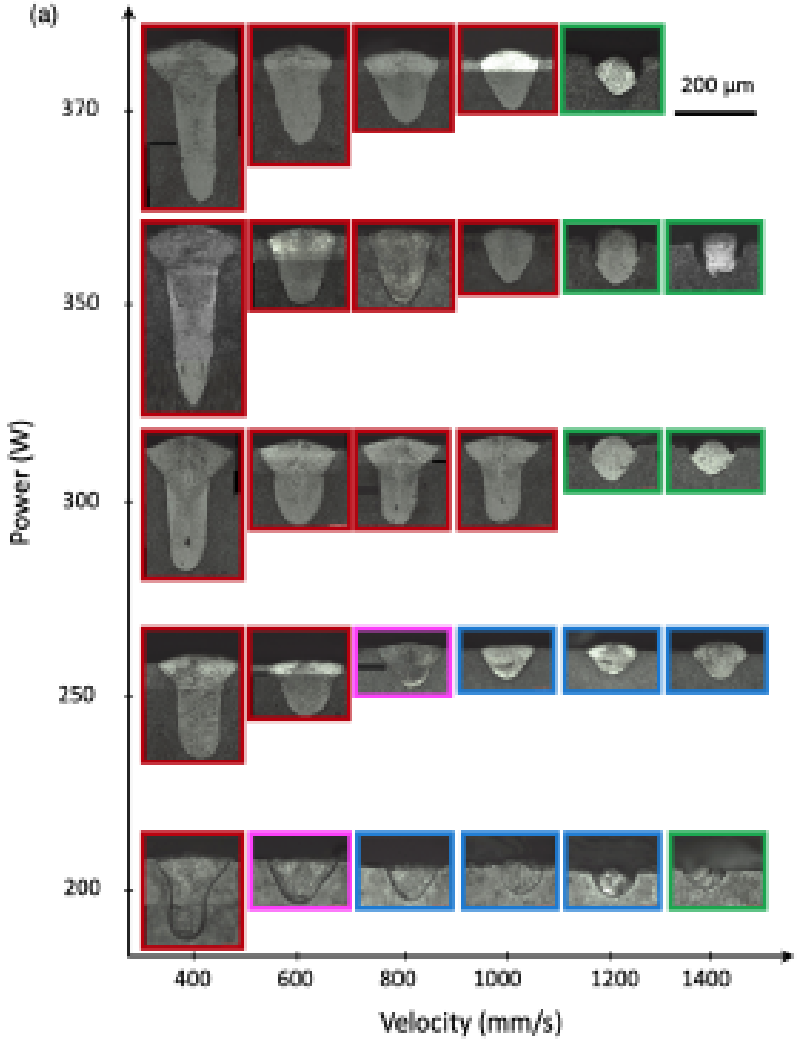
- Calibrated process models are needed to predict temperature history and enable simulation of melt pool dimensions, deformation, residual stresses and microstructure.
  - Development of deep learning and recommender system methodologies, to include generative models, to predict and generate microstructure 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

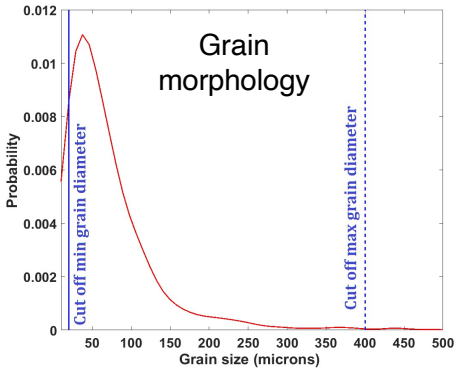
- Application of a conditional generative adversarial network (C-GAN) to incorporate thermophysics variables as input features.

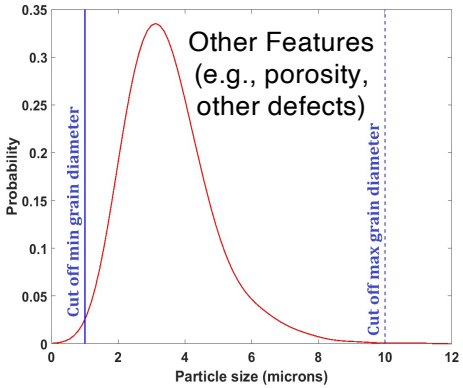


Development of Microstructurally-Informed D&DT

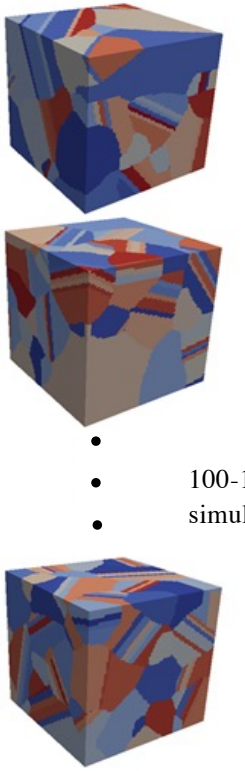
FEA Simulations Consider Representative Microstructures Developed from Processing Simulation and Characterization Data – Capture Microstructural Details and Responses

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



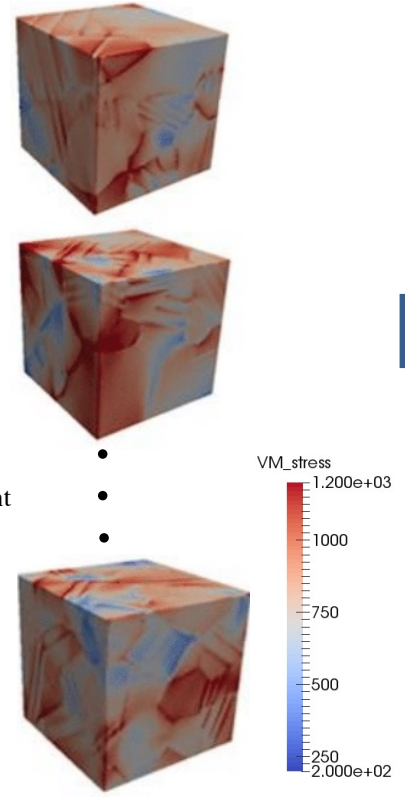


*Microstructure instantiations for FEA**



100-1000 independent simulations

*FEA Simulations**



Finite element simulations account for variability in microstructure

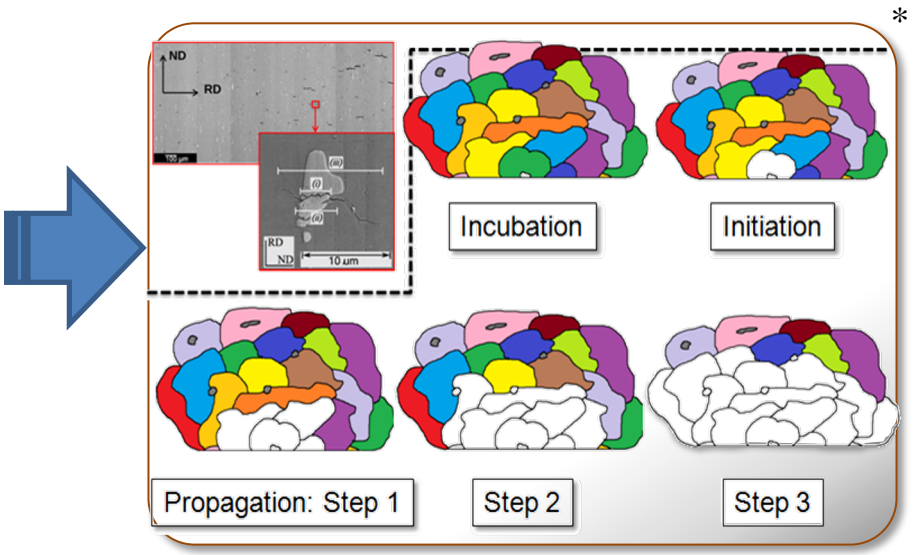
*Yeratapally, et al., NIA

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

Development of Microstructurally-Informed D&DT

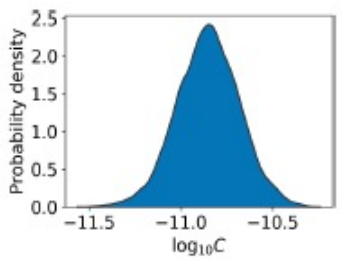
Transition from Microstructurally Small Crack Growth Estimates to Engineering Codes

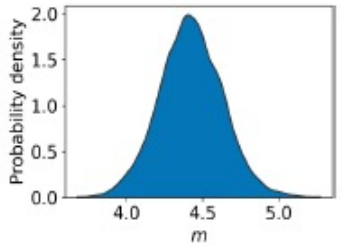
$$N_{failure} = N_{incu} + N_{init} + N_{MSC} + N_{MLC}$$

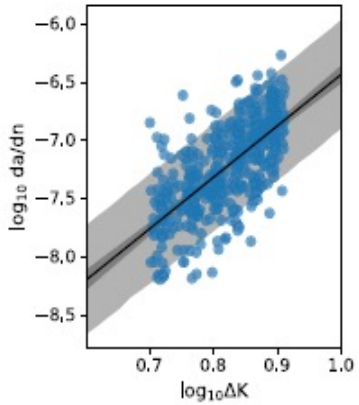


*

*Fatigue Crack Growth Material Parameter Distributions***







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

Nondeterministic prediction of fatigue life considering effects of microstructure

*McDowell, et al, GaTech

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

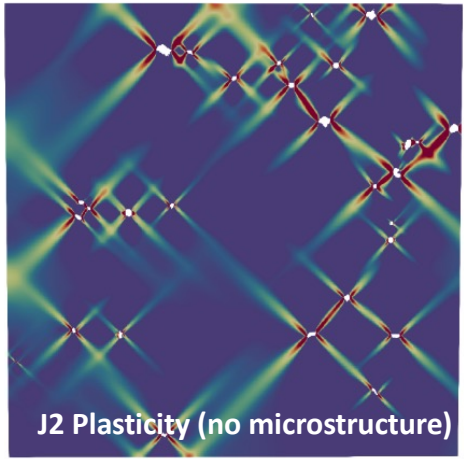
Investigation of Effect of Defect Distributions on the Localization of Plastic Strain

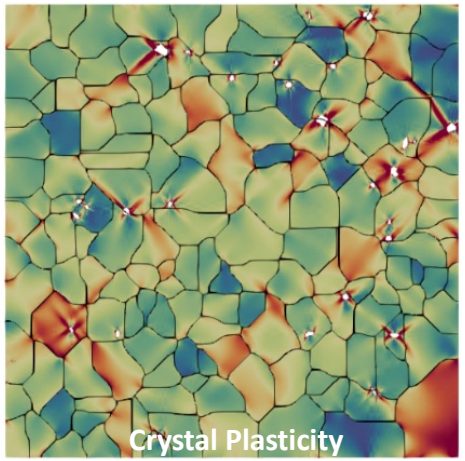
Use microstructure-based high-fidelity computational models to understand the effect of process-specific defects on the accumulation of damage and debit in mechanical performance.

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 (Γ): $\sum_{s=1}^{N}|\gamma^s|$; γ^s is slip on slip system, *s*.
  - Fatigue indicator parameter on slip plane *p*, $FIP^p = \int_0^t \Gamma\left(1+\frac{\sigma_p^n}{\sigma^Y}\right)dt$

    σ_p^n is normal stress on slip plane p and σ^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.





Equivalent 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.

Mechanical Testing of AM Ti-6Al-4V

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

APPROACH

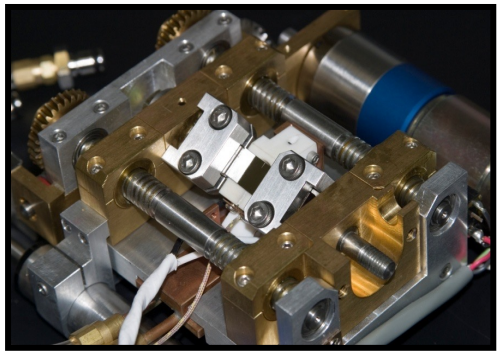
- Fatigue crack initiation / growth are often the dominant life-limiting failure mechanism; effect of AM processing defects not well understood.
- Perform fatigue crack initiation / growth testing on AM Ti-6Al-4V material under nominal, high-power (keyhole defects likely), and low-power (lack-of-fusion 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

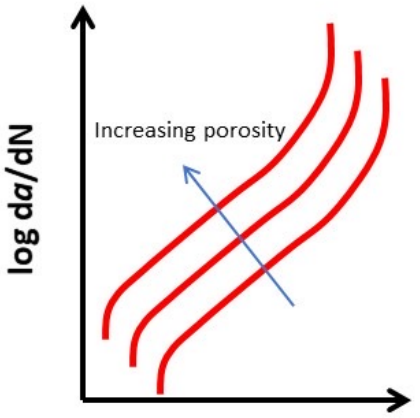
- Capabilities coming back on-line.
- Understanding the first-order variables that affect fatigue and fatigue crack growth behavior are critical for next-generation Qualification and Certification.

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



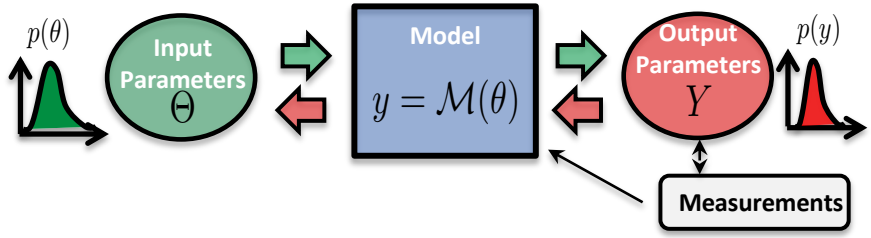
Anticipated Effect of Porosity on Crack Growth Rate

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).



Uncertainty Quantification and Propagation

- Estimating n^{th}-order statistical moments (e.g., mean, $n = 1$) of a quantity of interest (e.g., fatigue life) involves integration:

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

- Joint probability density function of model inputs, θ, is $f(\theta)$. c is value about which the moment is estimated.
- Integral is over the entire parameter space Θ 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.

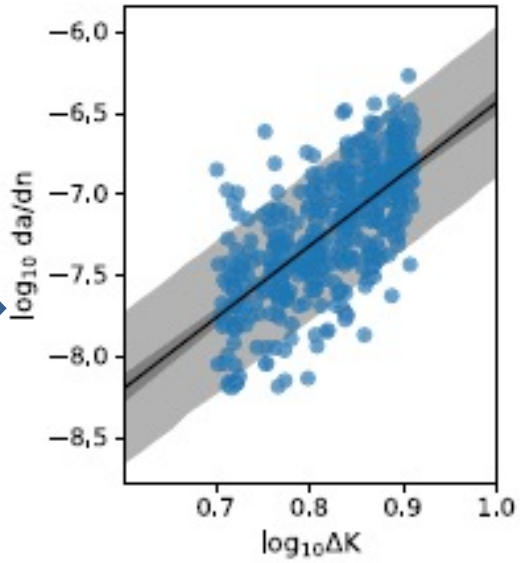
NEXT STEPS

- 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

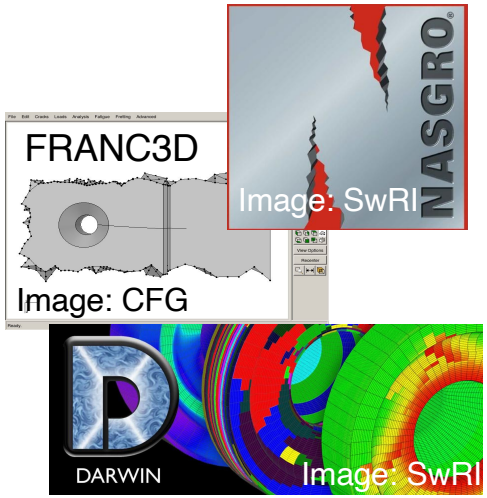
Microstructurally-Informed D&DT of Fracture-Critical Components

Microstructure-Informed Variability in Crack Growth Rates

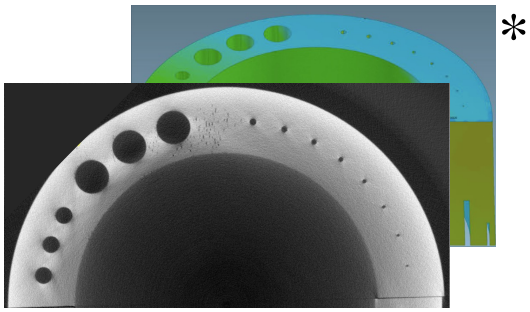


$$\frac{da}{dN} = C(\Delta K)^m$$

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.*

Concluding Remarks



- 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

TTT Computational Materials for Qualification & Certification of AM Group

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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



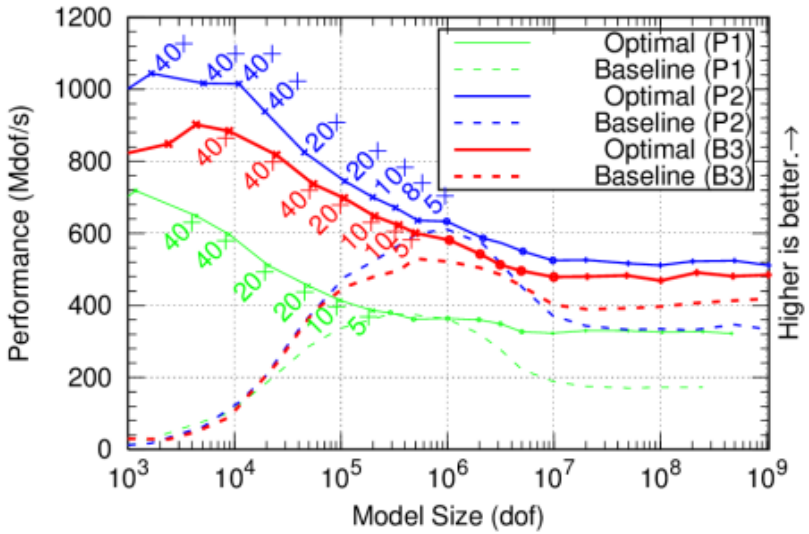
e.h.glaessgen@nasa.gov

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

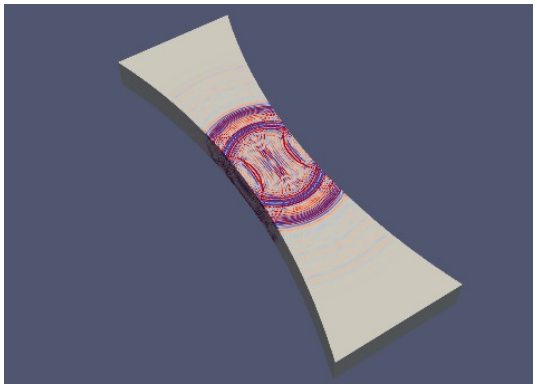
- Demonstrate alternative workflows and document best practices that reduce or eliminate the pre-processing bottleneck and improve analysis throughput.
- Continue to integrate and mature elements of the code; applications to computational materials simulation (e.g., crystal plasticity FEA).

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

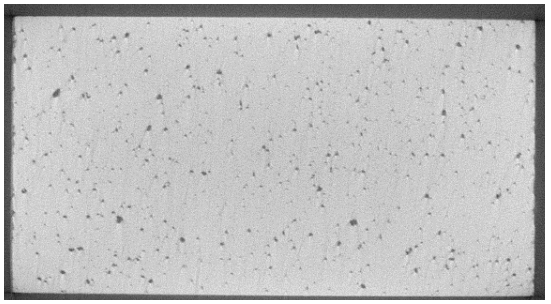
- Physics-based simulation of ultrasound propagation and wave-defect interaction in AM Ti-6Al-4V parts under varying porosity conditions.
- Gold standard flaw data extracted from high resolution (5 μm) X-Ray CT. Extracted pore metrics used to develop a simulation case generator; results will be validated 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 5μm 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.