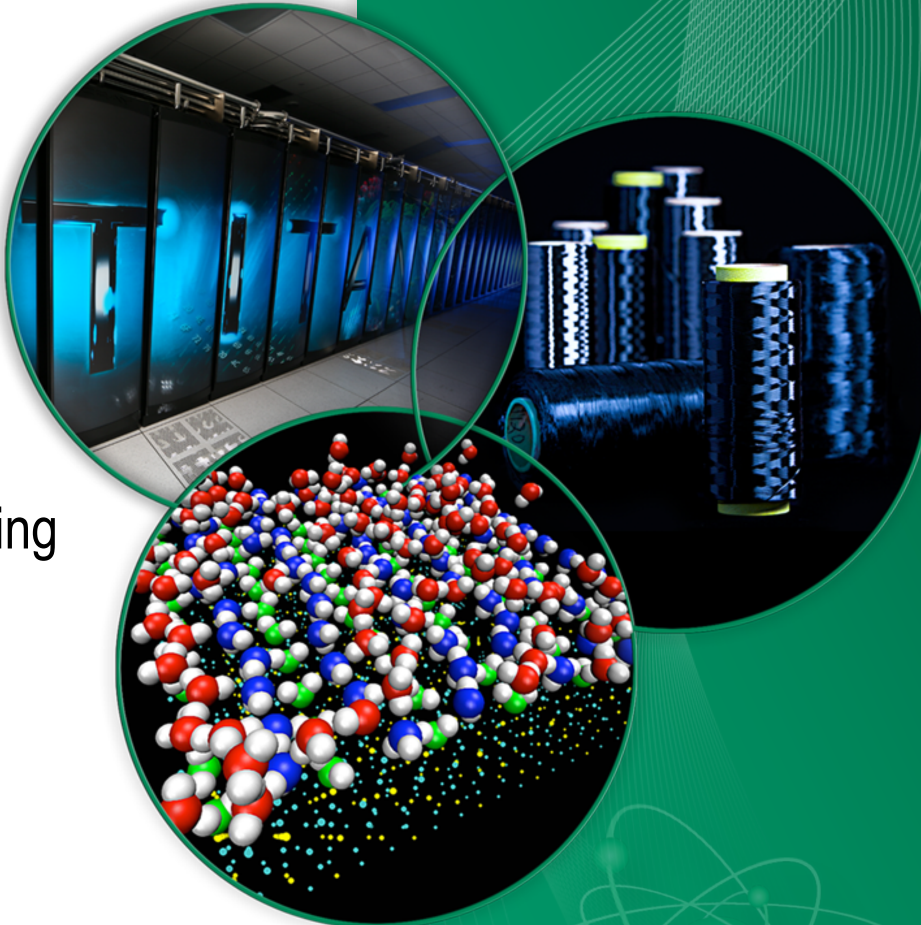
Computational Simulations for Additive Manufacturing



The Sixth AICS International Symposium

Plans and future for international Collaborations on extreme scale computing

February 22-23/2016, Kobe, Japan

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Neil Carlson
Los Alamos National Laboratory

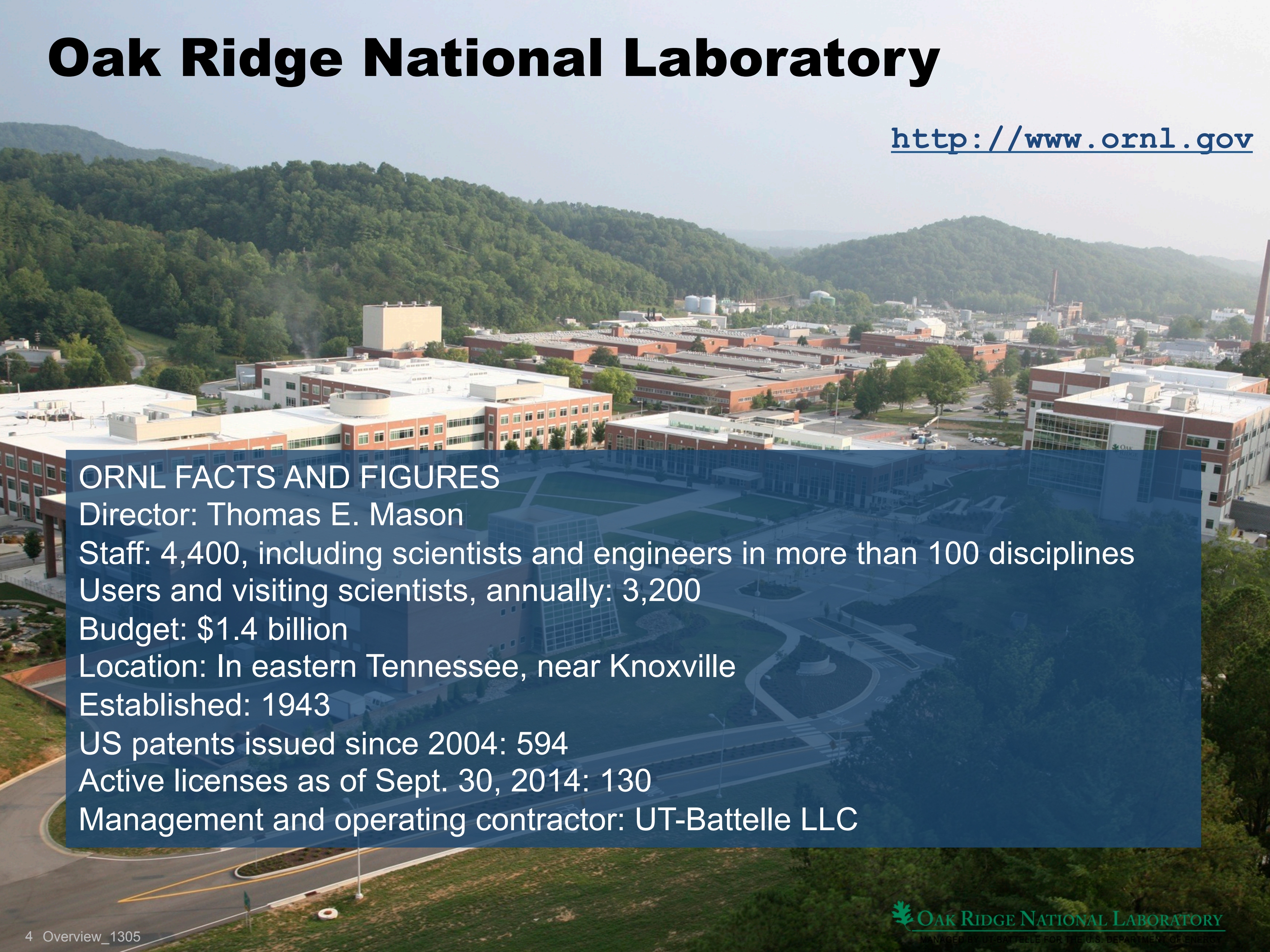
… and many more

Outline

- Introduction to computing at ORNL
- Scientific and computational modeling challenges of AM processes
  - Metal powder AM
  - Reinforced polymer AM
- Opportunities for collaboration
- Summary

http://energy.ornl.gov/

Oak Ridge National Laboratory



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ORNL FACTS AND FIGURES

Director: Thomas E. Mason

Staff: 4,400, including scientists and engineers in more than 100 disciplines

Users and visiting scientists, annually: 3,200

Budget: $1.4 billion

Location: In eastern Tennessee, near Knoxville

Established: 1943

US patents issued since 2004: 594

Active licenses as of Sept. 30, 2014: 130

Management and operating contractor: UT-Battelle LLC

The Oak Ridge Leadership Computing Facility is one of the world's most powerful computing facilities

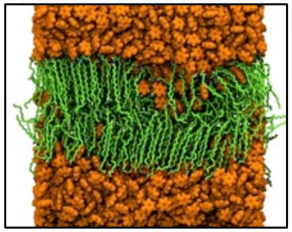
- 27.1 PF/s peak performance
- 17.6 PF/s sustained perf. (LINPACK)
- 18,688 compute nodes, each with:
  - 16-Core AMD Opteron CPU
  - NVIDIA Tesla "K20x" GPU
  - 32 + 6 GB memory
- 710 TB total system memory
- 200 cabinets (4352 ft^2)
- 8.9 MW peak power

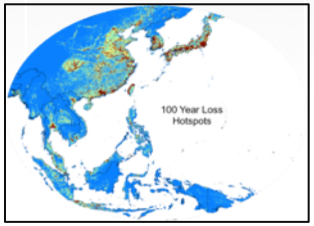

Spallation Neutron Source

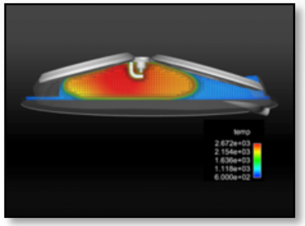
- The ecosystem surrounding the machine – file systems, visualization resources, expertise – is where science really happens.
- Experimental validation, data analysis, and visualization are the steps in the scientific workflow that lead to insight.

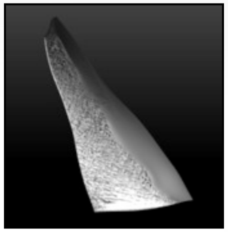
Growing Industrial Partnerships

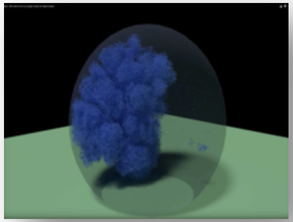
P&G	KatRisk	Ford	United Technologies Research Center	GE	CAT
Human skin barrier	**Global flood maps**	**Engine cycle-to-cycle variation**	**Fuel efficient jet engines**	**Wind turbine resilience**	**Welding Software**
Demonstrated small molecules can have large and varying impact on skin permeability depending on their molecular characteristics—important for product efficacy and safety	Developed fluvial and pluvial high resolution global flood maps to enable insurance firms to better price risk and reduce loss of life and property	Developing novel approach to using massively parallel, multiple simultaneous combustion cycle simulations to address cycle-to-cycle variations in spark ignition engine	Conducting first-of-a-kind high-fidelity LES computations of flow in turbomachinery components for more fuel efficient, next-generation jet engines	First time simulation of ice formation within million-molecule water droplets is expanding understanding of freezing at the molecular level to enhance wind turbine resilience in cold climates	Evaluating large-scale HPC and GPU capability of critical welding simulation software and further developing & testing weld optimization algorithm





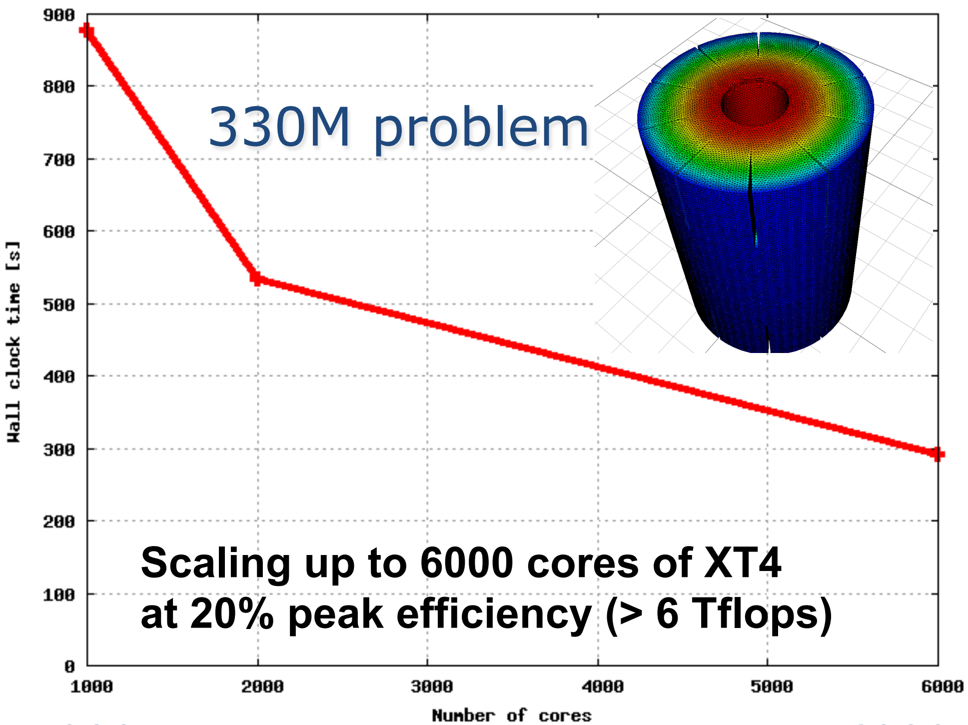




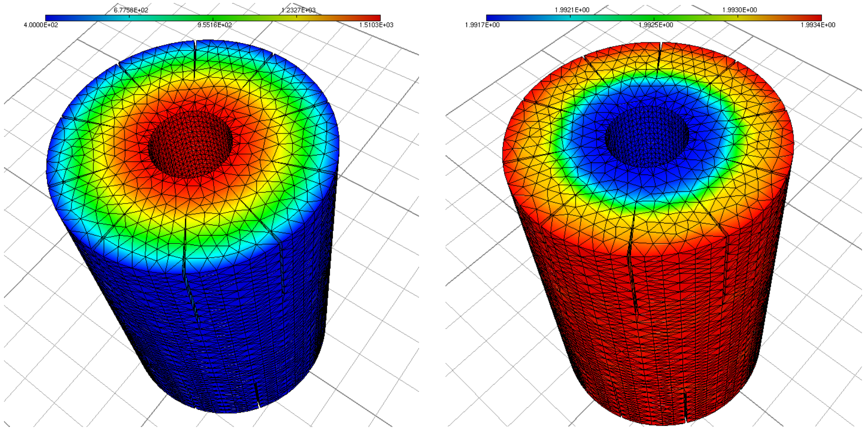


Previous Informal Collaboration on HPC with Japan Researchers

- Based on ADVENTURE system developed in Japan for Earth Simulator project

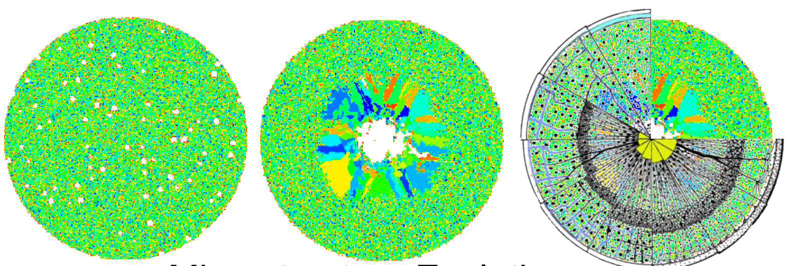


1000 Number of cores 6000



Temperature Oxygen/Metal

- Demonstration of HPC for nuclear fuel simulations.
- Coupling of multi-physics and multi-scale models

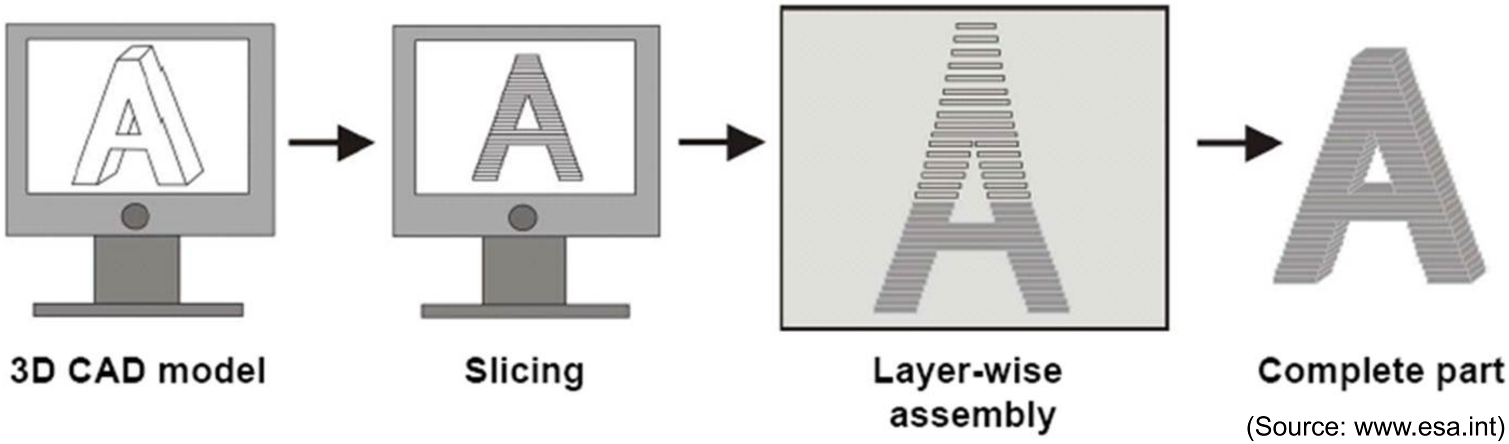


Microstructure Evolution

http://energy.ornl.gov/

MEET Oak Ridge National Laboratory, where scientists take on the toughest basic and applied research challenges. INTERESTS: Materials research, high-performance computing, energy efficiency, biofuels, nuclear science, adorable sports cars. IN THIS PHOTO: This reproduction of a Shelby Cobra two-seater was 3-D printed at ORNL to demonstrate additive manufacturing's industrial potential. #NationalLabs #LabsRoadShow

Additive Manufacturing in a Nutshell



(Source: www.esa.int)

Advantages of AM:

- Ability to fabricate complex structures
- Low buy to fly ratio
  - Significant reduction in raw material cost
- Shorter Lead Time
- Low Carbon Emissions†
- Part Consolidation
  - GE fuel nozzle: 25 welded parts to 5
- Lattice structures are possible
  - Weight reduction

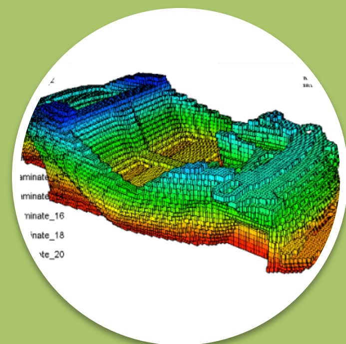
† GUO, J. (2012). *FEATURE BASED COST AND CARBON EMISSION MODELLING* . CRANFIELD UNIVERSITY.

R&D to Enable Broader AM Application

ORNL is working to resolve challenges and accelerate AM technology implementation

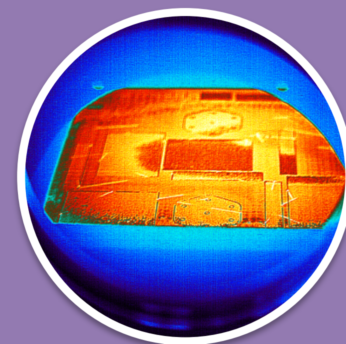
Improved and AM-Specific Materials Development

- High Temperature Applications
- Light Weighting
- Bio Derived Materials
- Functional Materials



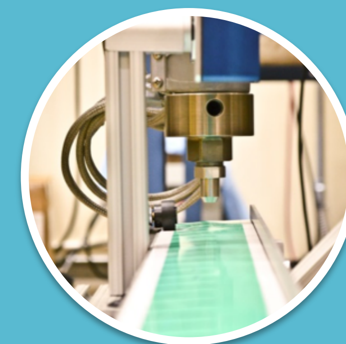
AM Process Science

- Material Property Dependency on Process Inputs
- Computational Framework for Data Visualization and Analytics
- Topology optimization for AM



Process Characterization for Qualification

- In-Situ Non-Destructive Evaluation
- Neutron Diffraction and Imaging
- Coupling to National Laboratory Network



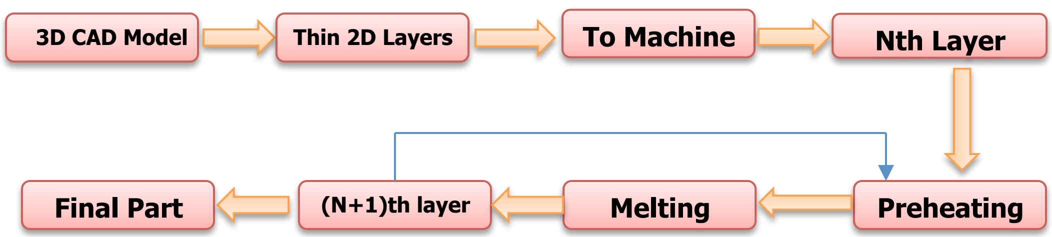
Exploring Next-Generation Systems

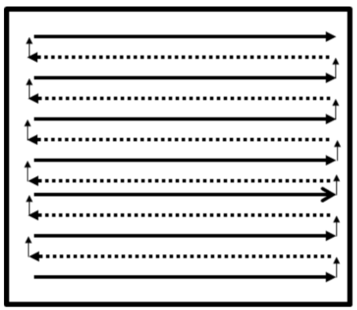
- Bigger, Faster, Cheaper, & Better
- Integrating the Supply Chain
- Working with Current and Future Equipment Developers

Computational Modeling and HPC are the Key Enabling Technologies

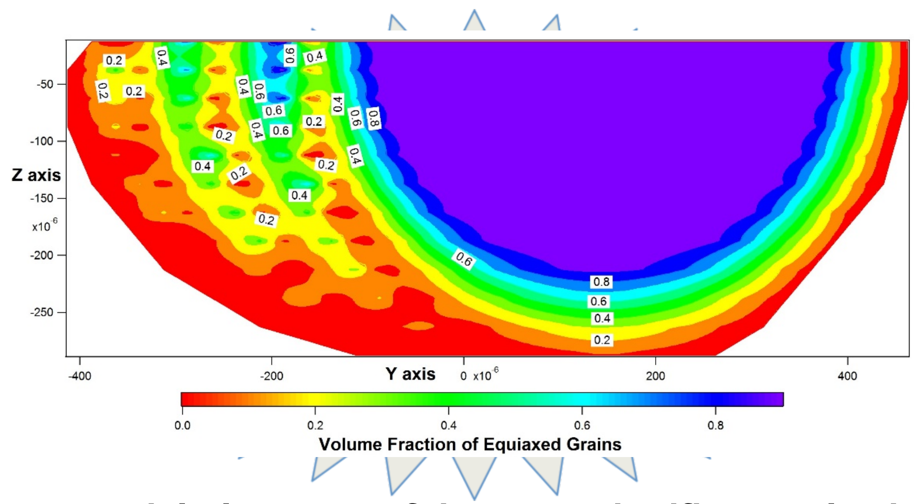
http://energy.ornl.gov/

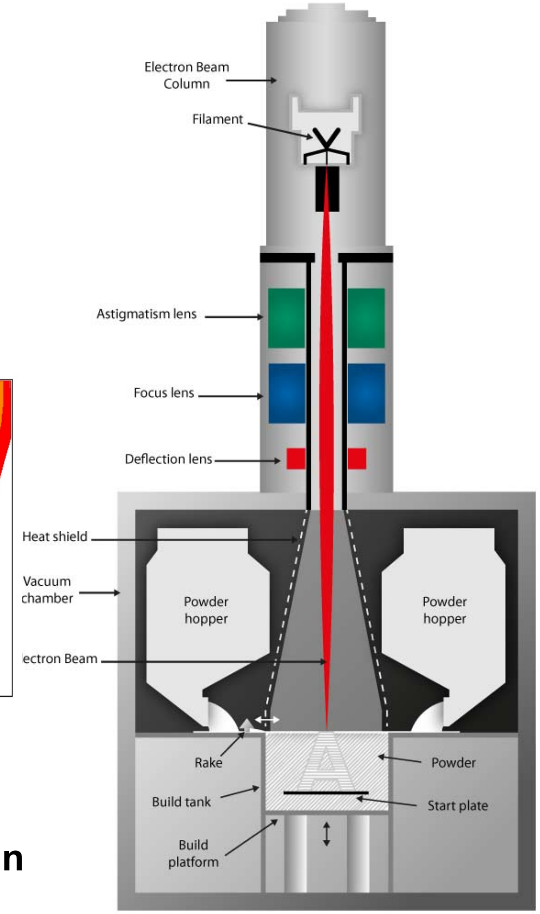
Overview of Electron Beam Additive Manufacturing (Arcam®)





Conventional Raster Melt sequence





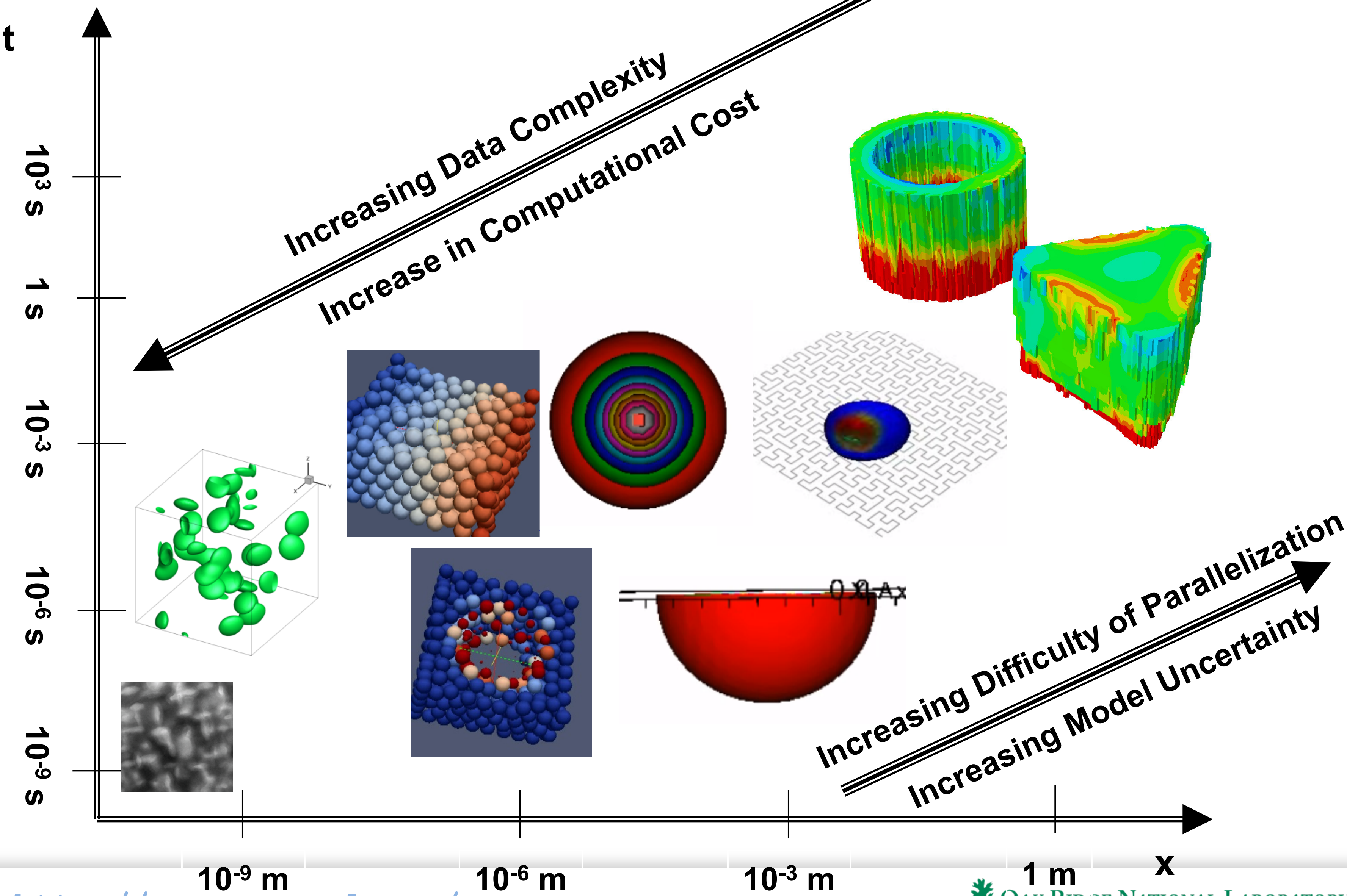
Source: http://www.arcam.com/technology/electron-beam-melting/hardware/

- **Microstructure of the material plays one of the most significant roles in determining the mechanical properties of the part.**
- **Feasibility of manipulating the microstructure and composition via additive manufacturing adds additional dimensions to the process.**
- **Can we achieve the goal of Crystallographic Texture Engineering with AM?**

Multiple computational challenges must be addressed for AM simulations.

- 1 m^3 ~ 10^{12} particles ~ 10^9 m of "weld" line (assuming 50μm particles) and build times of hours (HPC)
  - Brute force approaches will fail
- Large temperature gradients, rapid heating/cooling, melting and solidification (HPC)
  - necessary / sufficient coupling between thermomechanics and melt/ solidification, high resolution of computational mesh
- Heterogeneous and multi-scale problem (HPC)
  - resolution of energy sources and effective properties of powder for continuum simulations
- Path optimization is needed for part build feasibility and performance (HPC)
- Large number of parameters and missing understanding of correlations (HPC)
  - uncertainties with key parameters and propagation of those uncertainties

Complex coupled multiscale physics processes control additive manufacturing



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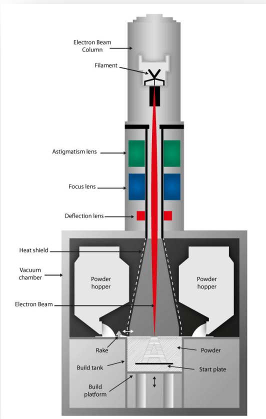
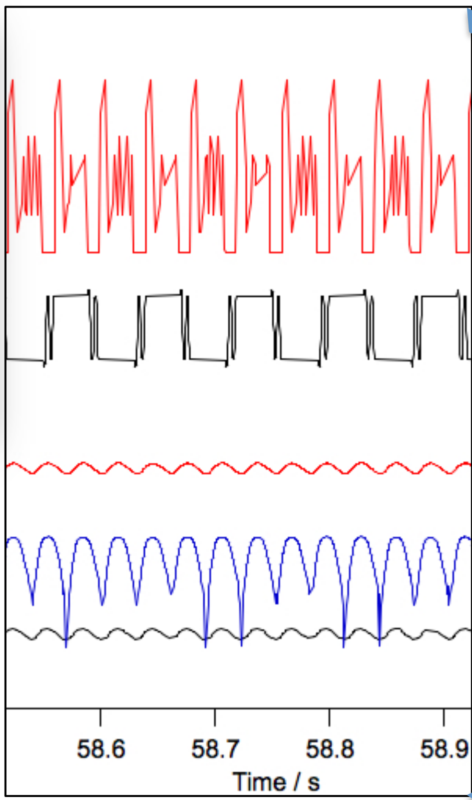
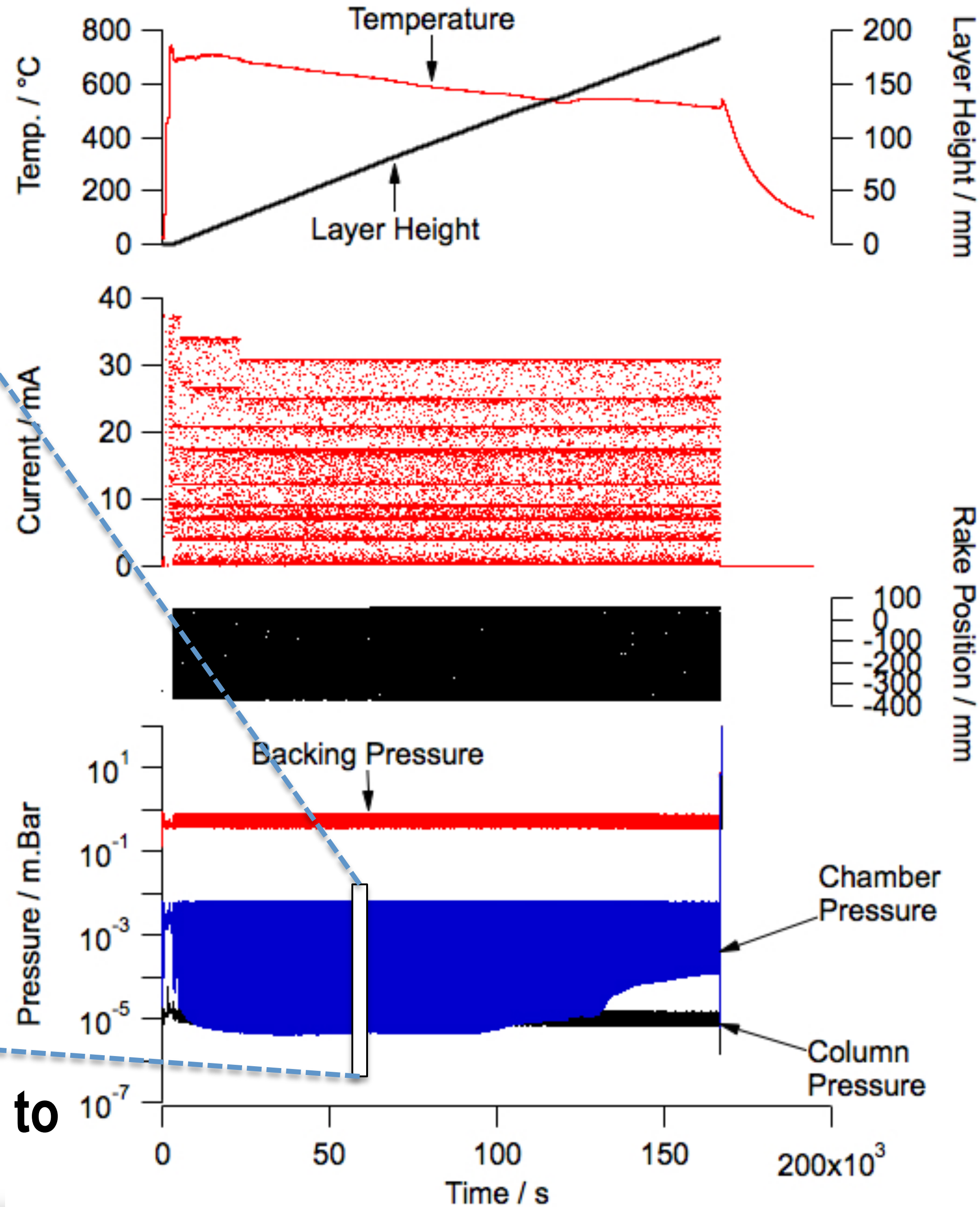
Data from numerous sensors is available.



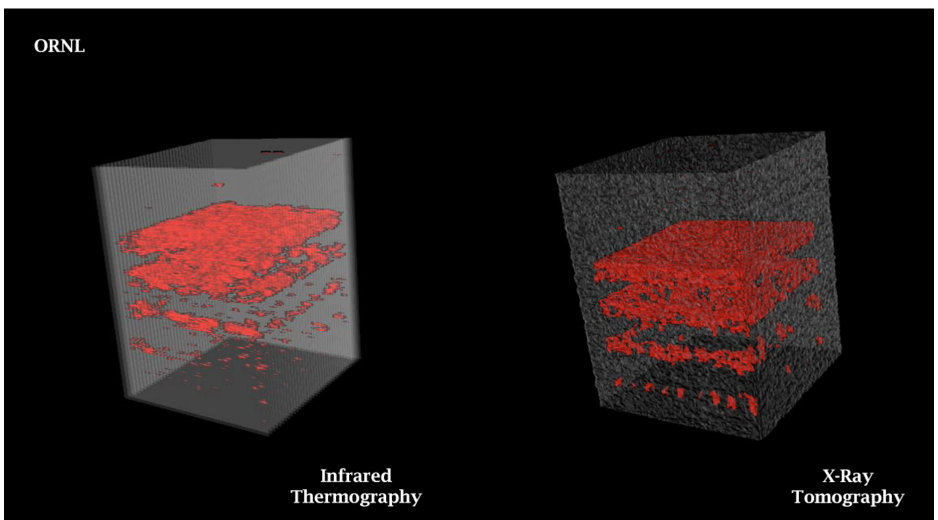




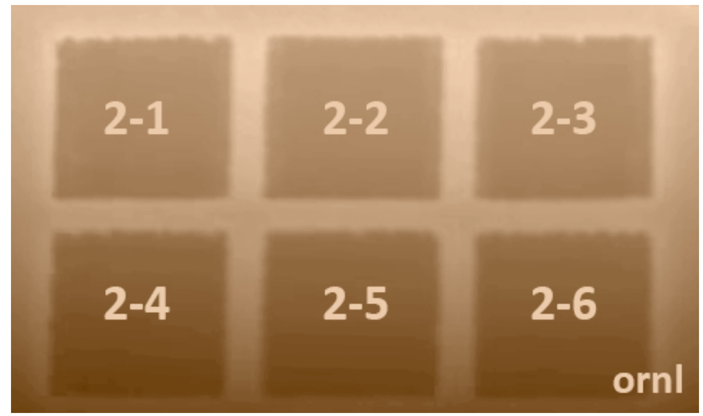
- **Can we couple the sensor data to computer models?**

In-situ Monitoring: High-Infrared Imaging for Defect Detection and Understanding of Thermal History

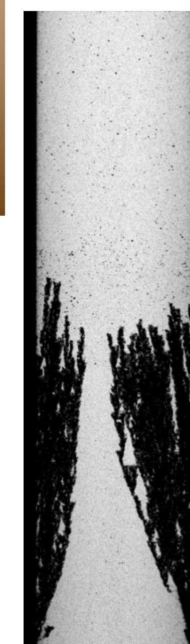
- **Preliminary correlation has been performed showing porosity detection correlation to X-ray computed tomography. The process is currently being automated.**



Dehoff et al (2015)
Image stack of sample showing vertical porosity from focus offset changes

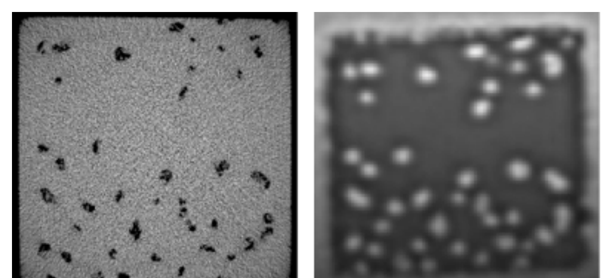


X-ray CT Minimum Projection



Side View

Correlation between xXray CT and in-situ identified porosity

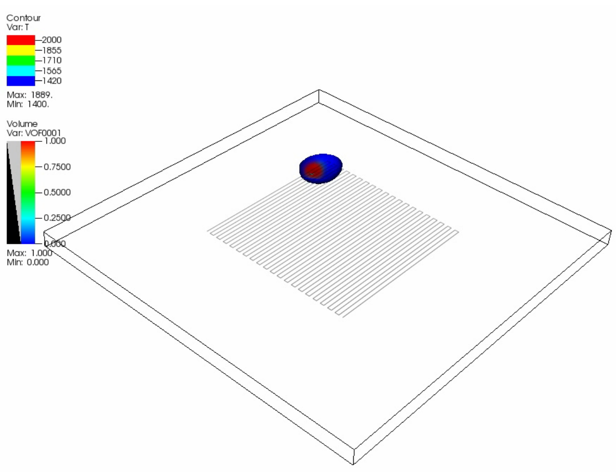


Top View slice projection

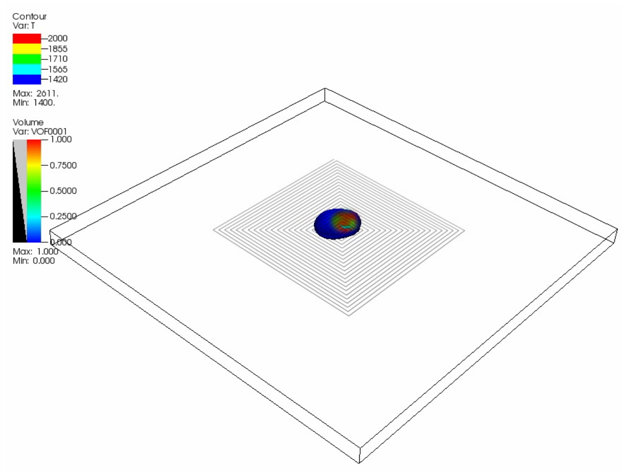
http://energy.ornl.gov/

HPC for Macro-Microscale Melting/Solidification

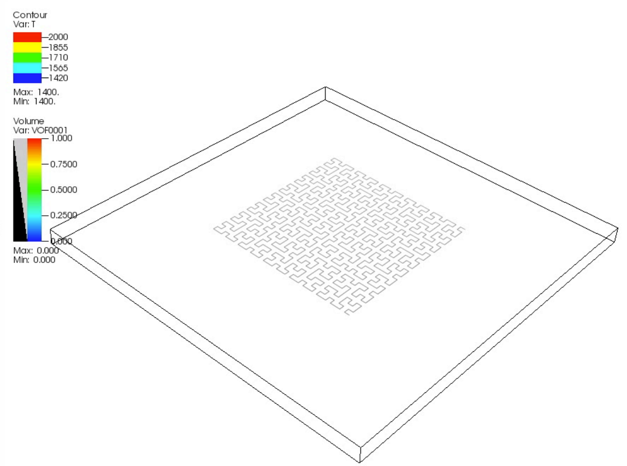
- Truchas was developed at LANL for modeling metal casting processes
  - Heat conduction, convection, radiation, multi-component advection-diffusion
  - Incompressible, multi-material, free-surface fluid flow with VOF interface tracking
- Adapted by LANL and ORNL for AM applications and ORNL HPC systems



Oxen Path



Spiral Path



Hilbert Path

Temperature and Liquid Volume Fraction

Beam moving at 4 m/s and 30 mA current
Sides: Adiabatic Boundary Conditions
Bottom: Pre-heat temperature (1400K)
Top: Radiation to the ambient at 1000K with 0.5 emissivity

- What about the microstructure aberrations at various scales?

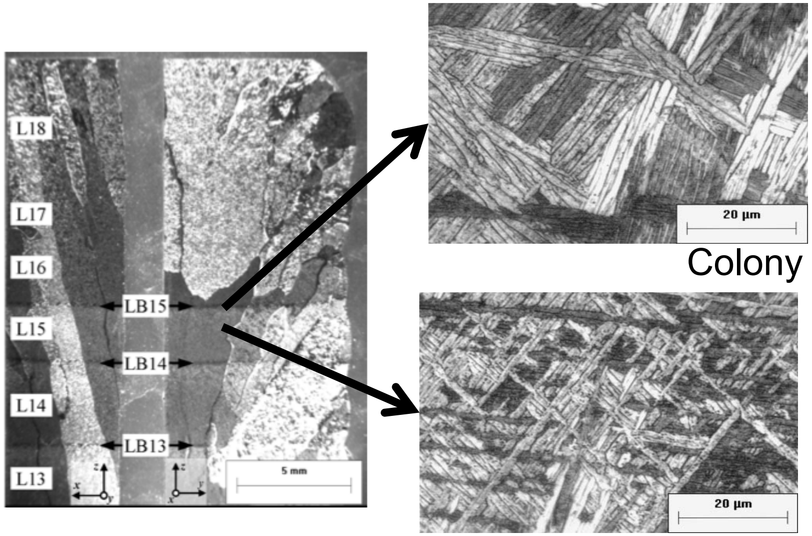
Phase Field Simulations on HPC for Understanding Microstructural Evolution during LAM of Ti-6Al-4V

Features of Phase Field Model

- Fully integrated with system thermodynamics
- System energy includes contributions from anisotropic interfacial energy, and elastic energy due to transformation strains
- Governing equations solved using Fourier spectral method exploiting P3DFFT library in Titan (large runs with thousands of processors)
- Unique composite nucleation model that allows growth of specific variants assisted by local strain field

Fundamental question addressed

- Why do layer bands form during solid-state transformation of pre-solidified material?
  - Intra-granular nucleation of colony structure?



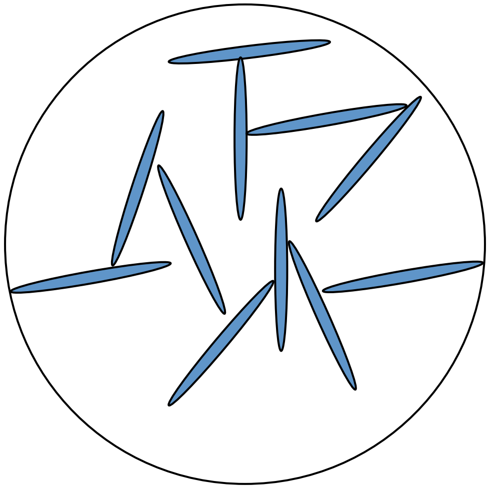
Kelly and Kampe, 2004

Basket weave

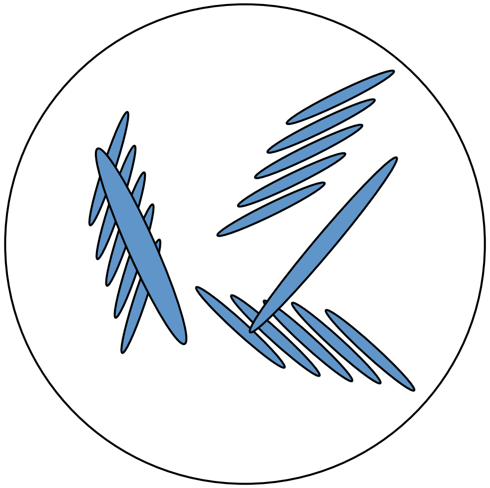
Length scale of prior β grains is much larger than packet size of the colony structure.

Alternate hypothesis for basket weave to colony structure transition in bands

- High thermodynamic driving force and high nucleation rates
  - multiple variants nucleate and grow in a complex strain field giving rise to basket weave structure (same as before)
- Low thermodynamic driving force and low nucleation rates
  - Low energy variants nucleate first
  - Formation of subsequent nuclei only after previously nucleated variants have grown to a large size
  - Subsequent nucleation influenced by the strain field of pre-existing α variants
- Isothermal simulations under above conditions were used to validate the hypothesis



Basket weave



Colony

Nucleation rate identified as the main factor responsible for formation of colony structure

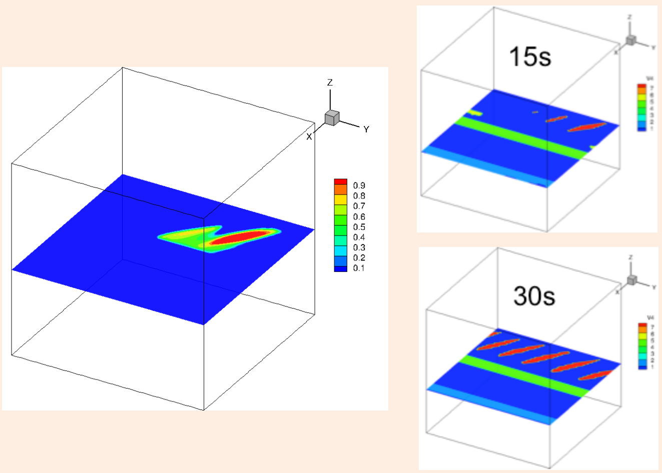
Parametric studies performed using HPC phase field simulations

- Two levels of thermodynamic driving force: low (1000K) and high (950K).
- Two levels of nucleation rate: low (0.5 s^{-1}) and high (5 s^{-1})

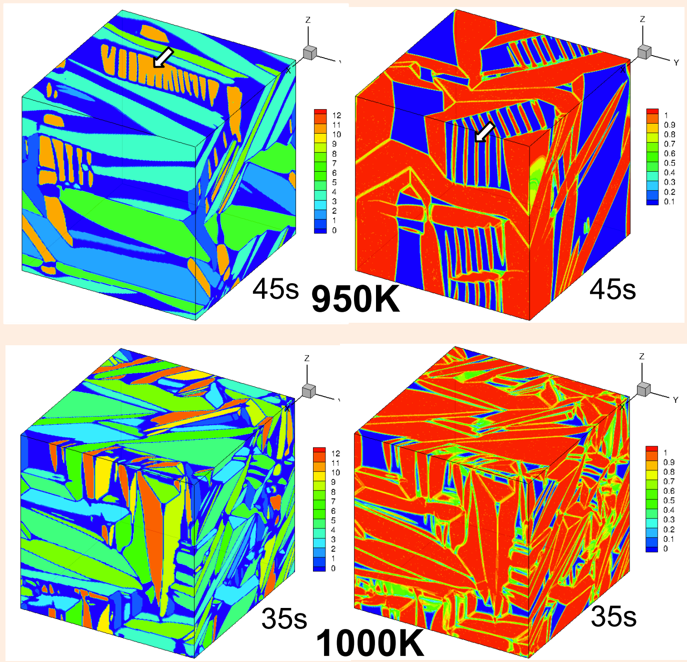
Crucial Findings

- Low nucleation rate promotes colony when a new nucleus sees well developed strain field from a nearby variant
- High nucleation rate promotes basket weave when all nuclei see complex strain field due to multiple, evolving nuclei

Auto-catalytic colony nucleation

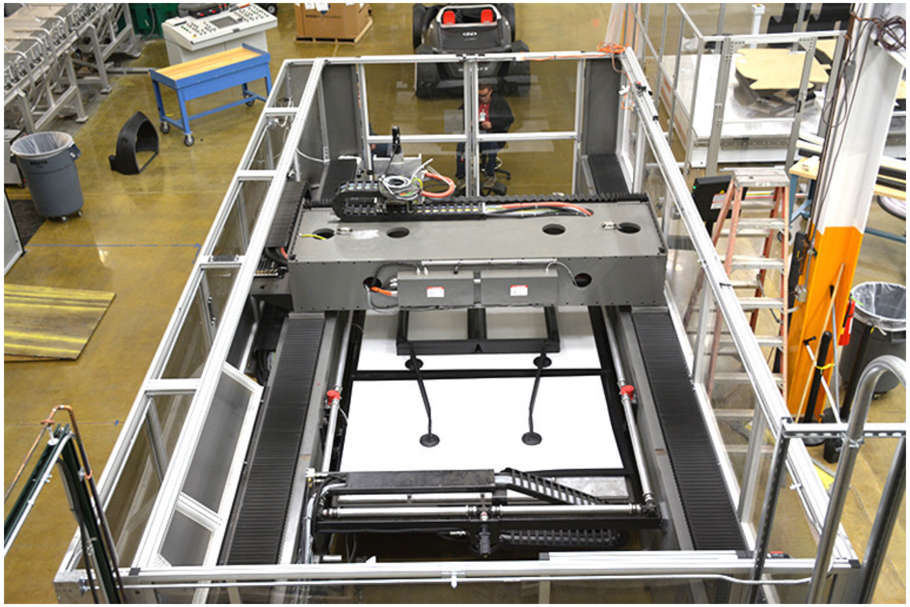


B. Radhakrishnan, S.B. Gorti and S.S. Babu, PTM 2015: International Conference on Solid-Solid Phase Transformations in Inorganic Materials, Whistler, Canada (Invited)



Polymer Composites Big Area Additive Manufacturing

- New direction for manufacturing with composites
- How large can we print?



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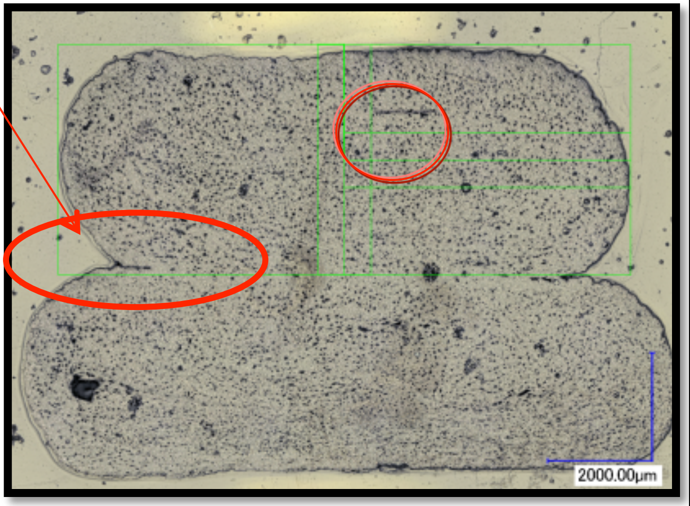
Technological Problem Description

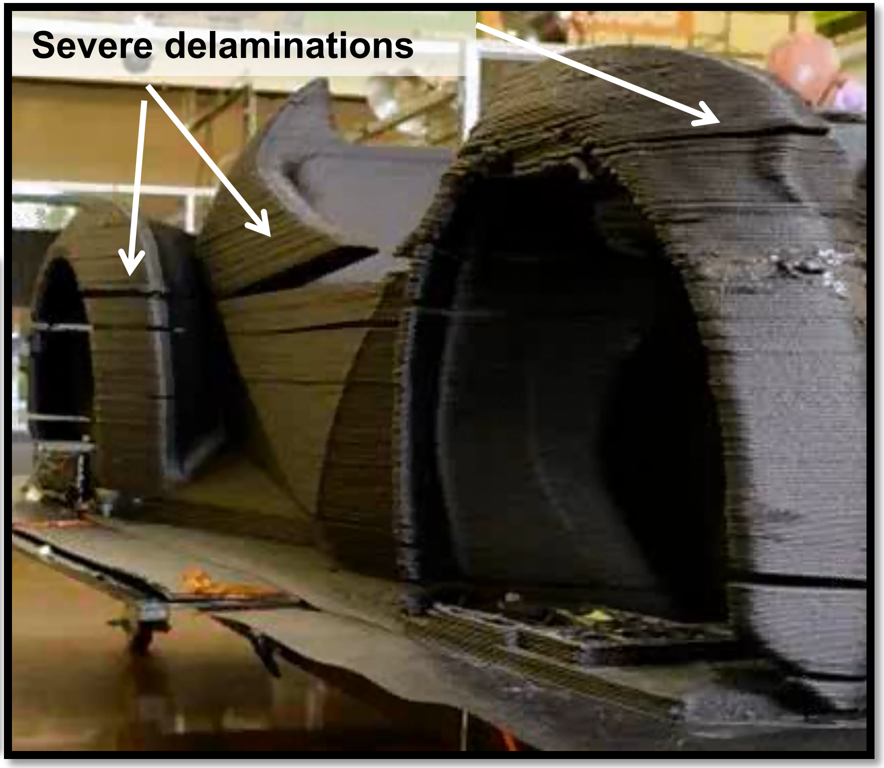
- Thermal history induces delaminations.

The variation of thermal loading and differential cooling induces shear stresses and imperfections that result in delaminations in the product.

Initial cracks between the beads



Cross section of consecutive beads



Delaminated product after production

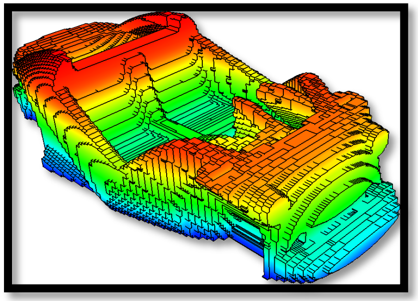
Computational Problem Description

• Simulate manufacturing process and detect crack behavior

Objective:

- Simulate **carbon-ABS** chopped fiber 3D printing manufacturing process
  - include **crack formation** due to thermal history
- Simulation should include:
  - **physical parameters** that can be altered to improve the production process to minimize the crack formation problem during production.
- The analysis time should not exceed **24 hrs**
- A software should be delivered that fully **automates**:
  - **Material characterization:** thermoplastic chopped fiber
  - Model generation
  - Post processing
  - Damage and fracture evolution
- An example of successful industry – lab partnership and technology transfer

Production process of the printed car (ORNL)



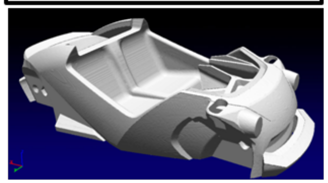
Numerical model generated by GENOA GUI

Determine when, why and where failure/fracture occurs

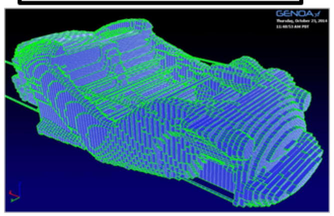
Solution Approach

- Integrated approach: generate model; characterize fibers; progressive damage/fracture analysis
- R&D 100 Winner for 2015

Read STL Machine Code File → **GENOA® GUI Mesh Generator** → **Solution Types** → **Model Validation**



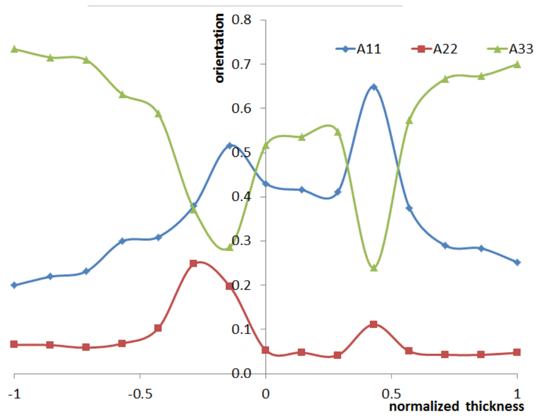
Import from STL file to generate G-Code



STL to FEM Mesh Model

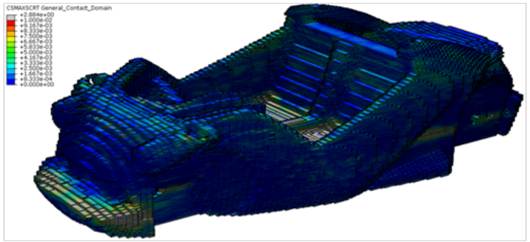
Solution Types:
- Uncoupled Heat Analysis
- Sequential Coupled Solution
- Coupled Heat-Stress (Plot)
- Coupled Heat-Stress (Predictive)

Material Characterization → **Solution Types**



Tensor orientation

Model Prediction

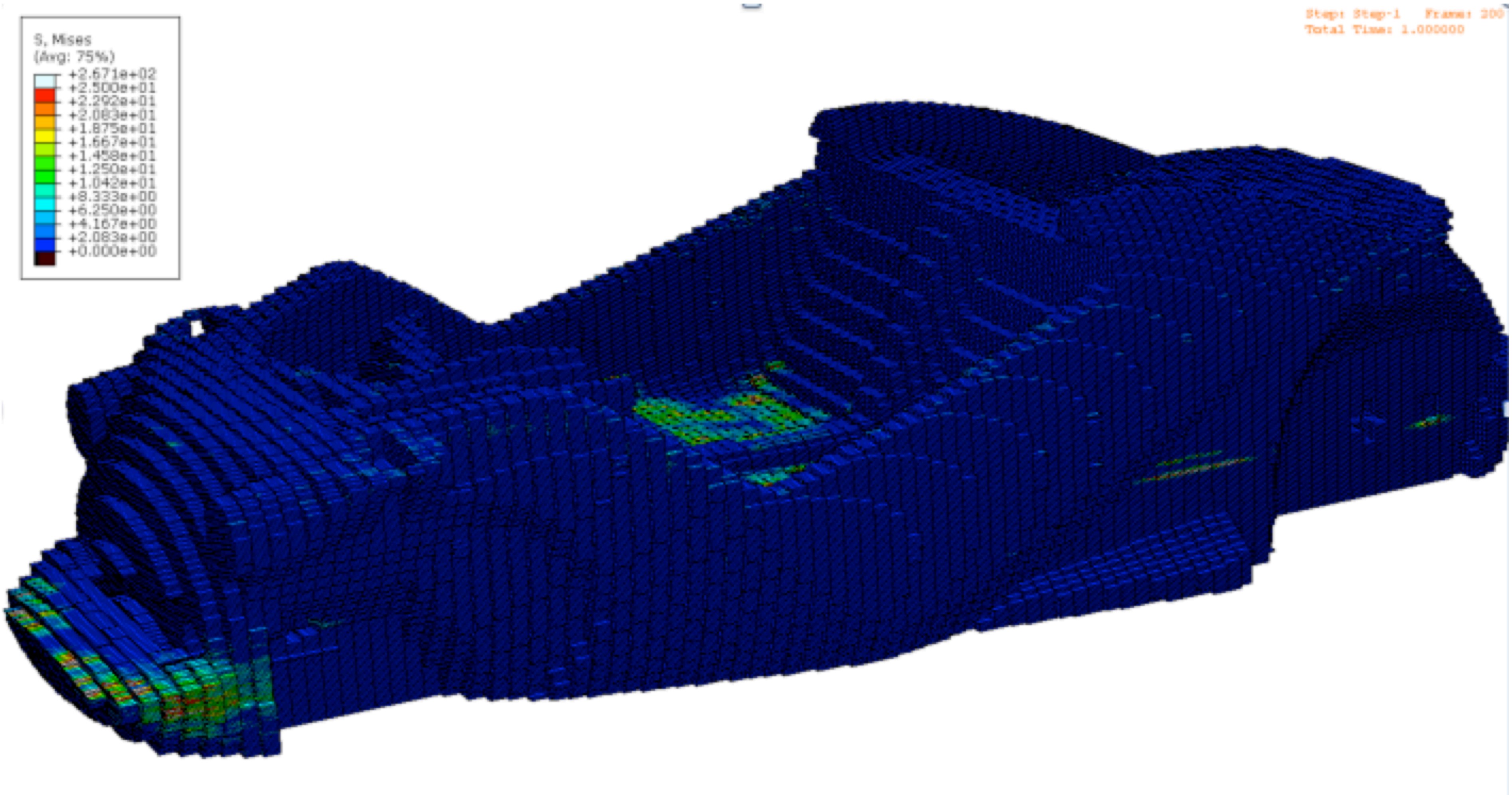


Delamination initiation and damage contour plot

Multiple solution strategies have been considered

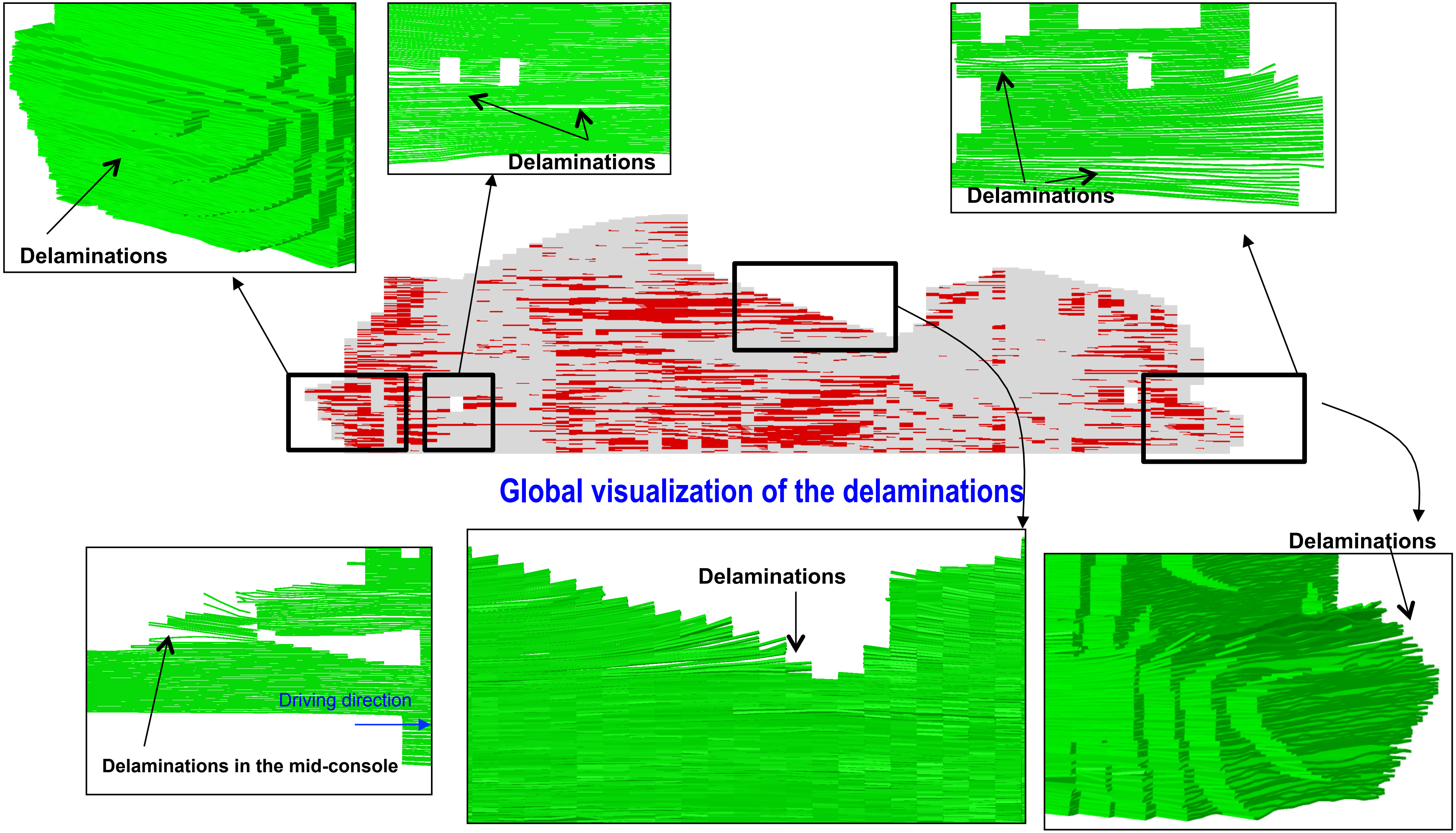
Residual Stress Development

BAAM 3D Process Modeling



Highlights

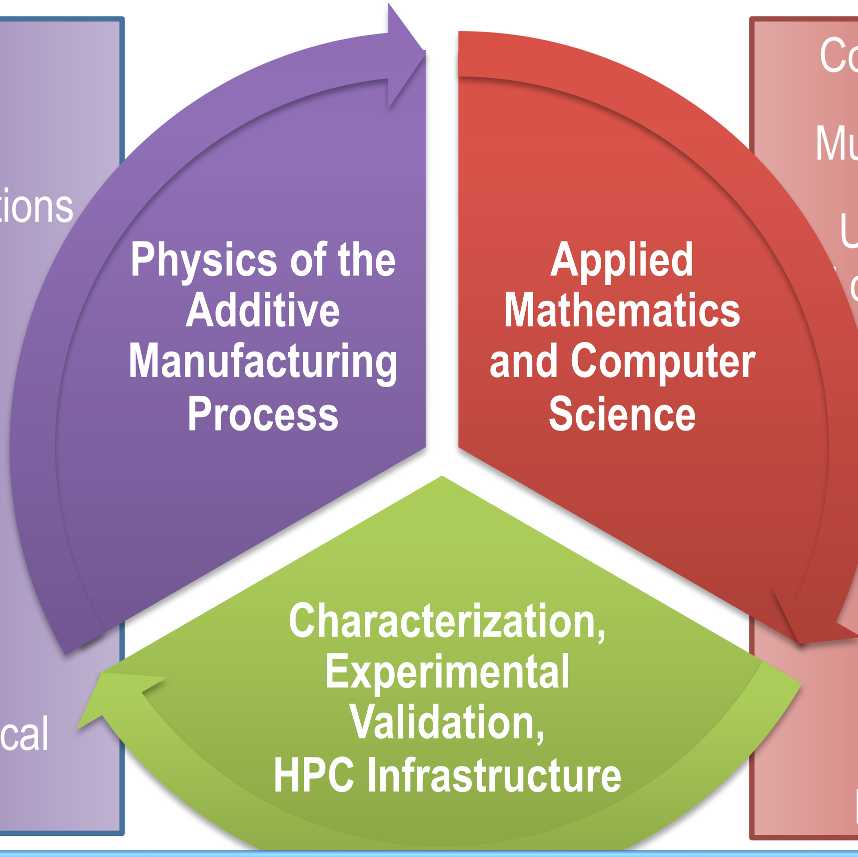
- Potential delaminated areas can be identified



Local visualization of the delaminations (scaled displacements for the sake of visualization (x3))

A broad spectrum of computational science is required to fully realize the potential of additive manufacturing.

- Energy Interaction with Porous Materials
- Gas-Liquid-Solid Reactions
- Rapid Melting, Solidification & Crystallography
- Elastic / Plastic Strain Evolution
- Solid-Solid Phase Transformation Under Thermomechanical Cycling



- Coupled large-scale PDEs
- Multiscale coupled physics
- Uncertainty quantification design under uncertainty
- Scalable software
- Advanced parallel solvers and time integrators.
- Large-scale inverse problems
- Large-scale optimization

Tools exist that provide some combinations of the required computational capabilities, but few (none?) are scalable to HPC.

Recap of Physics Models and HPC Numerics Needs

Physical Processes

- Conductive, convective, and radiative heat transfer
- Melting and solidification
- Solid-solid phase transformations
- Fluid flow with surface tension
- Solid mechanics
- Energy deposition in porous and powder materials

Numerical Methods

- HPC enabled finite volume and finite element methods
- Coupled nonlinear PDEs
- HPC multiscale methods
- Particle and discrete element methods
- HPC viewfactor radiation models for large assemblies
- HPC Phase field methods
- Multi objective optimization
- Bridging data and physical sciences
- Uncertainty Quantification

Opportunities for Collaboration

- Developing methods and computational algorithms for coupling physics models at different time and space scales.
- Collaboration on HPC frameworks for coupling models and programs.
- Methods for fusion of big data and computational models.
- Porting and performance tuning.
- Demonstration projects for targeted applications.

Questions?

e-mail: simunovics@ornl.gov

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