Delivering Breakthrough Science through High-Performance Computing: Relevance to Additive Manufacturing Computational End Station (ACE)

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Research Performed within NSF-I/UCRC: Center for Integrative Materials Joining Science for Energy Applications

Outline

- Why additive manufacturing?
  - Definition, Perspective & Potential Advantages
  - What is the relevance to high performance computing?
- What are the needed science & technology breakthroughs?
  - Scope: Example: Electron Beam Melting Powder Bed Process
  - Quantum Level Modeling [energy and material interactions]
  - Physical Process Modeling [fluid & heat flow, phase transitions]
  - Spanning the Length and Time Scale Resolution [10^8 scans/m^3]
  - Experimental measurements (e.g. Neutrons & microscopy) towards Qualification
- Technology Transfer to Industries
- Summary and Conclusions

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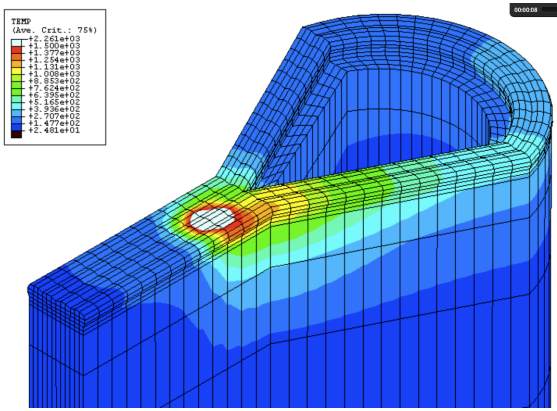
Current: Powder to Parts
Future AM: Molecule to Parts

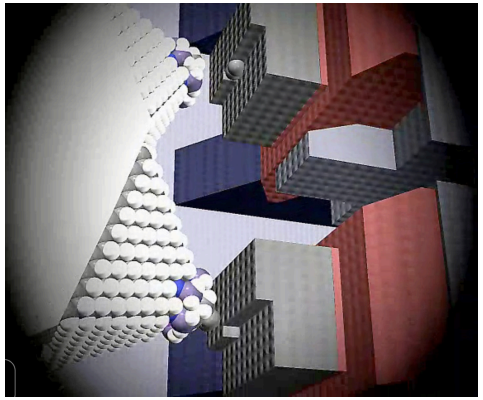
- Definition: Small lot manufacturing by addition of "basic" building blocks; Atoms, Molecules, Powders, and Laminates
- Some processes: Stereo-lithography, selective laser sintering, fused deposition modeling, Powder Metal Deposition, 3DPrinting, Multi-jet Modeling, and Laminated Object Manufacturing

Current



Laser Cladding of Nickel Alloys; From Powder to Solid
Ref: EWI

Future



Productive Nano-systems from molecules to products
Ref: NanoRex

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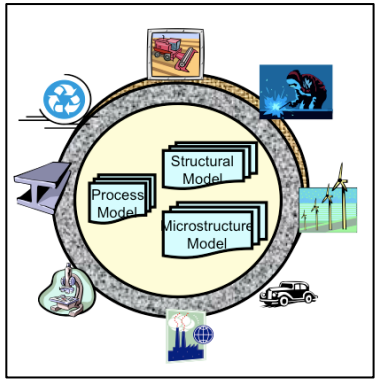
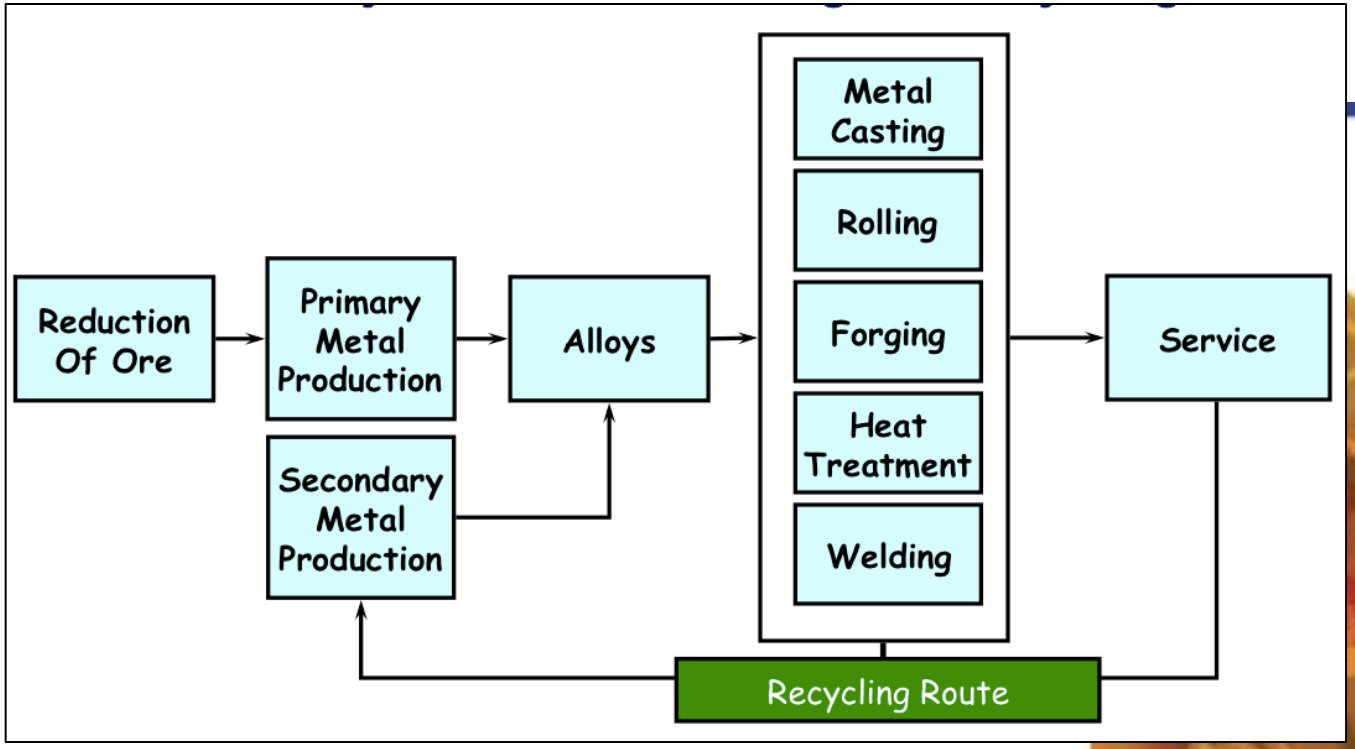
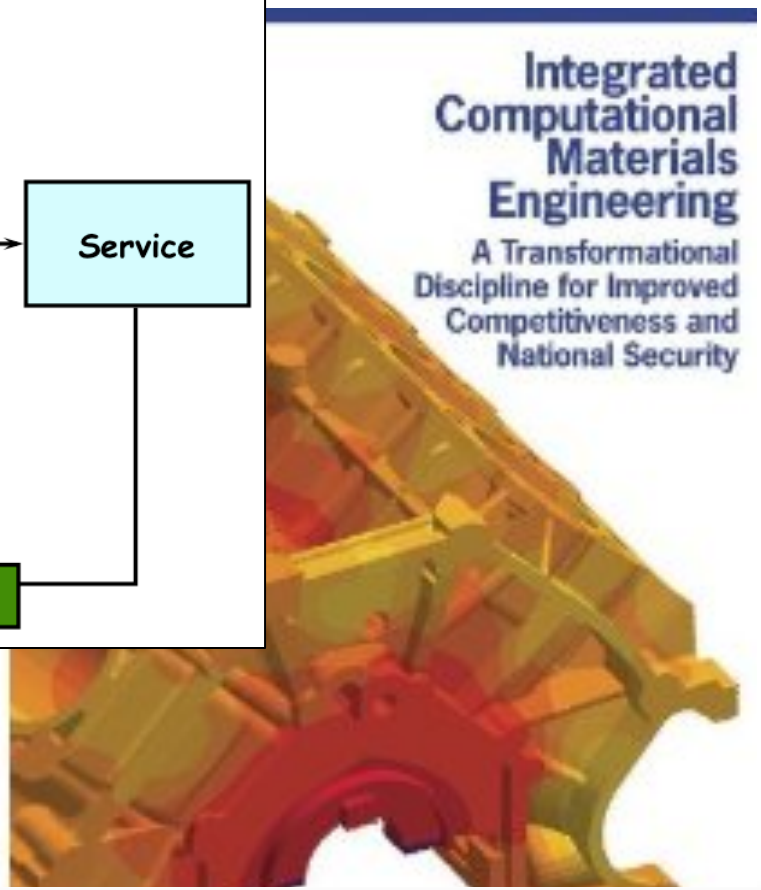
Traditional manufacturing is established and integrated computational materials engineering tools are being deployed to accelerate innovation.







- Then, what are the advantages of additive manufacturing?

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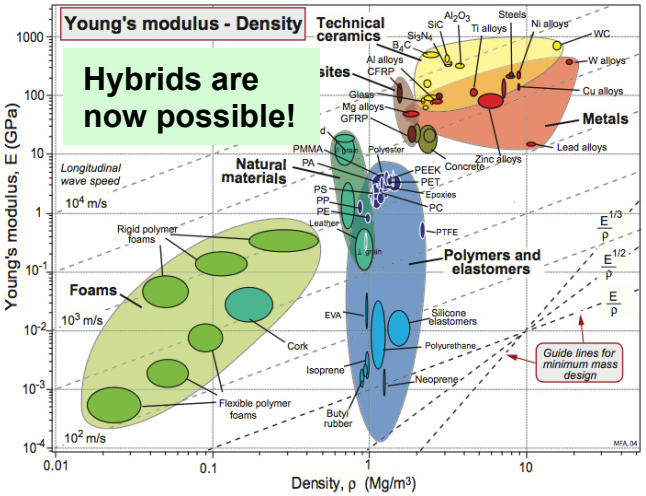
Motivation: By providing design flexibility, Additive Manufacturing is considered as the Renaissance of US manufacturing across the Small-, Medium-, and Large-Scale Industries



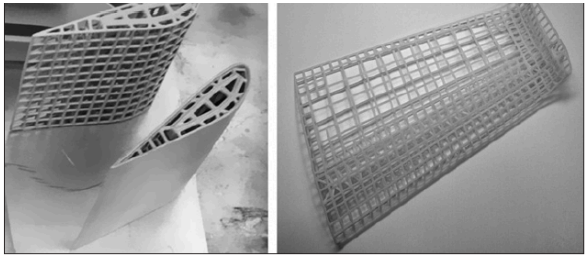
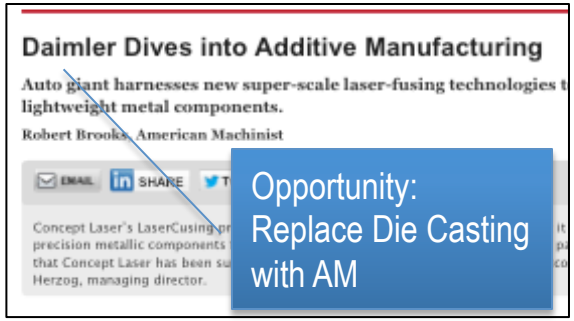
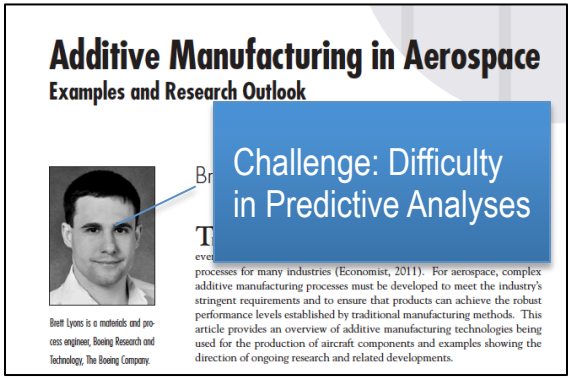


FIGURE 4 Two complex trusses suggest the difficulty of predictive analysis.





Embedded Electronics

There are many additive manufacturing processes

- Our focus: Facilitate the adoption of this technology as quickly as possible
- What are the challenges?

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Process: Laser Additive Manufacturing

- Original concept developed by Department of Energy Laboratories
- Commercial systems are available (e.g. OPTOMEC)
- Key Process Variables:
  - Laser power
  - Travel Speed
  - Powder Characteristics
  - Build path
  - Additional Processing (e.g. Hot Isostatic Pressing, Heat Treatments)

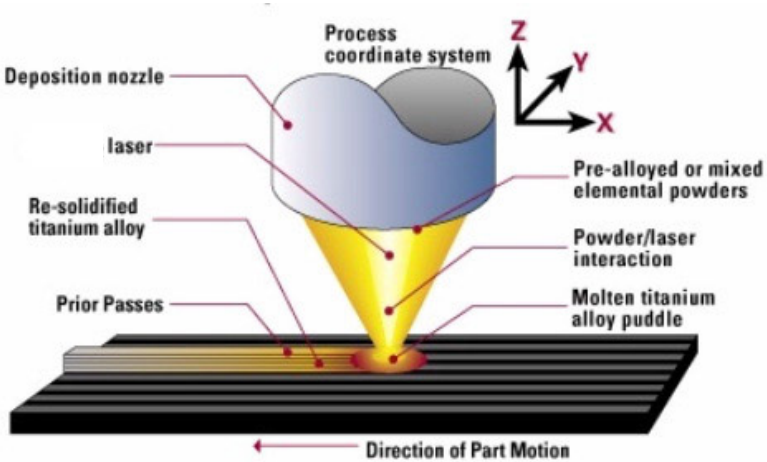

Photo courtesy of Kelly, S. (2004). Thermal and Microstructure Modeling of Metal Deposition Processes with Application to Ti-6Al-4V.

- Challenges
  - Microstructure evolution
  - Mechanical Heterogeneity
  - Poor Properties in Z-direction
  - Residual Stress
  - Distortion
  - Surface Roughness

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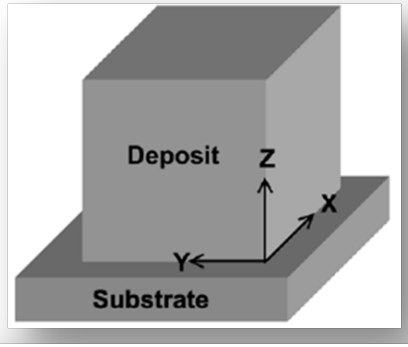
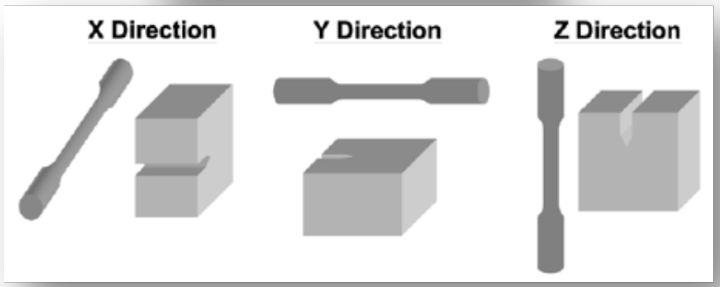
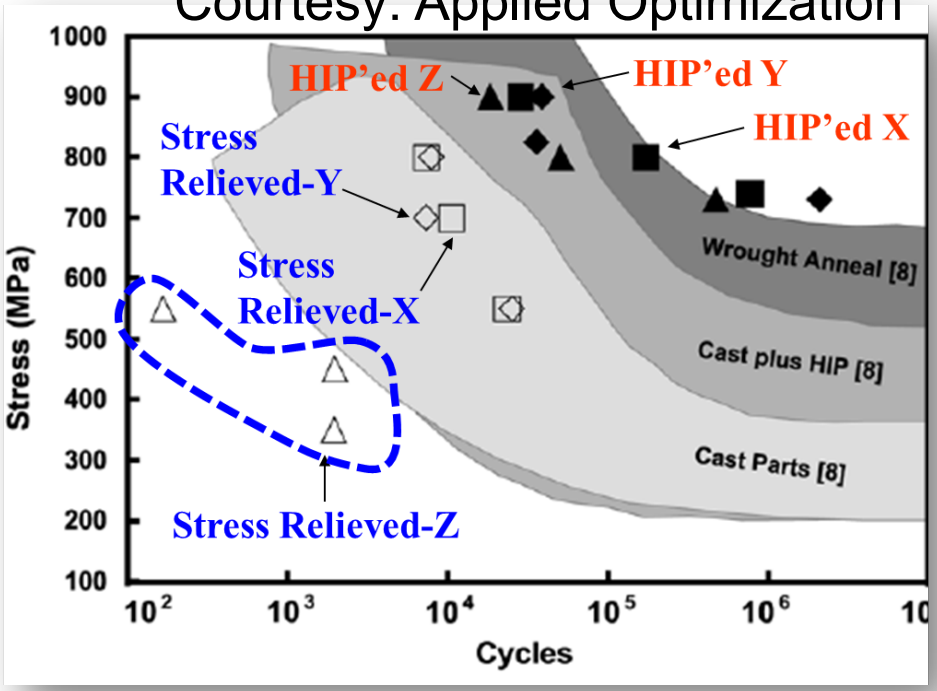
Mechanical anisotropy and poor properties are observed in z-direction

From: Kobryn, Semiatin, 2001





Courtesy: Applied Optimization



- Anisotropy is a function of material thermal path.
- Thermal path of deposit material is non-uniform
- HIP is not feasible for all additive deposits
- This poses a challenge in part qualification

Fundamental Understanding of the Property

- Trial and error optimization is not possible. However, computational optimization is feasible.

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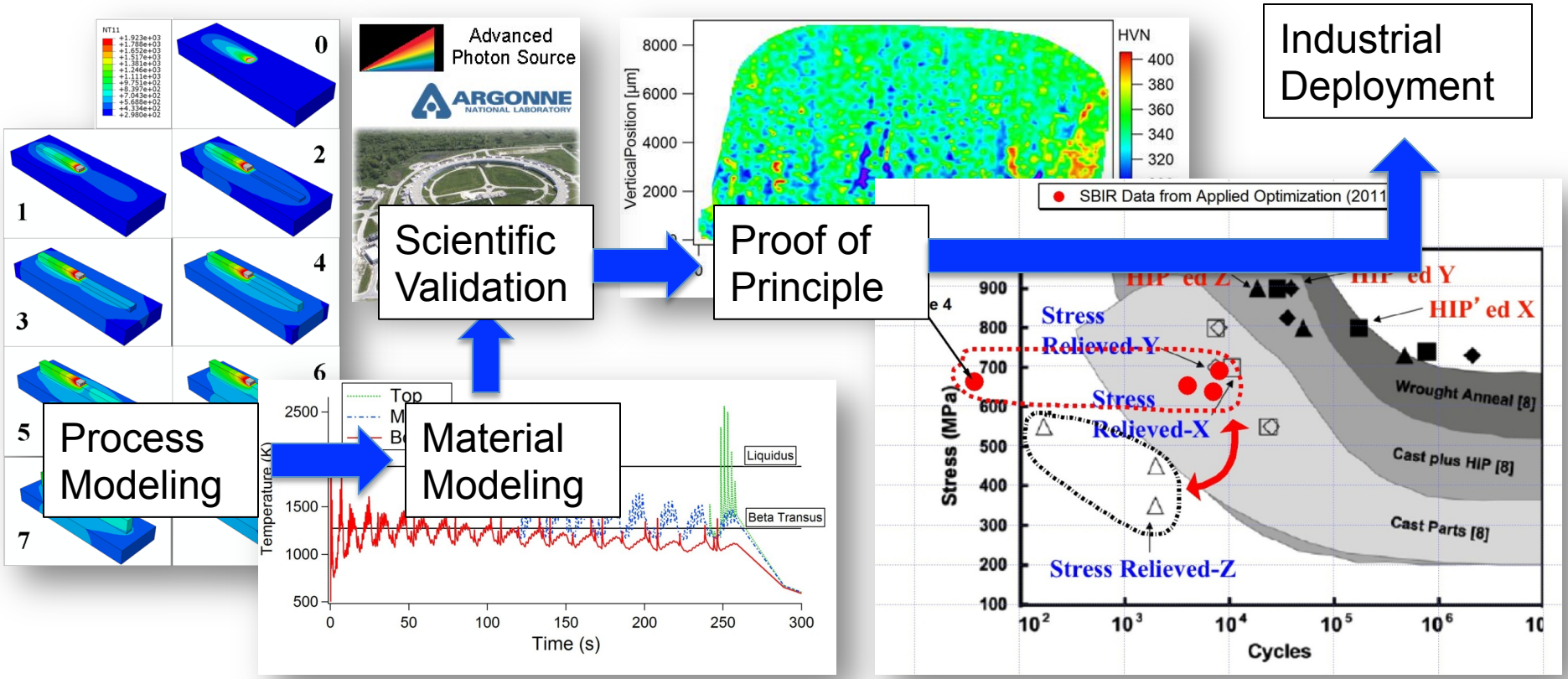
By integrating process, material modeling, in-situ, ex-situ characterizations, we have developed innovative processing routes.



- However, this engineering solution was developed after many years of research. Can we accelerate this innovation?

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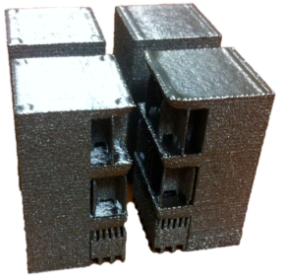
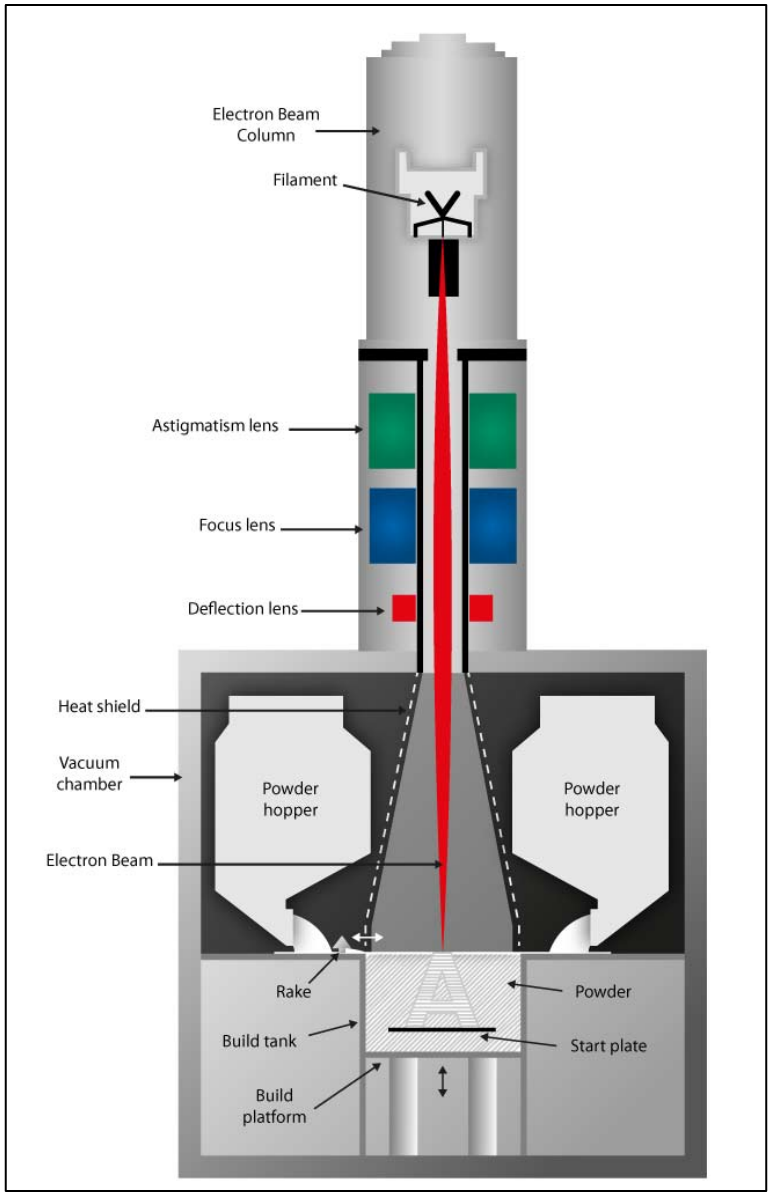
Let us take a popular additive manufacturing process: Electron Beam Powder Melting Process (ARCAM)

In-situ imaging of electron beam raster





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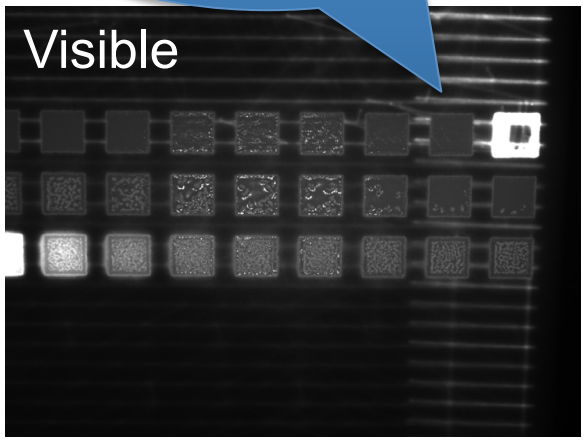
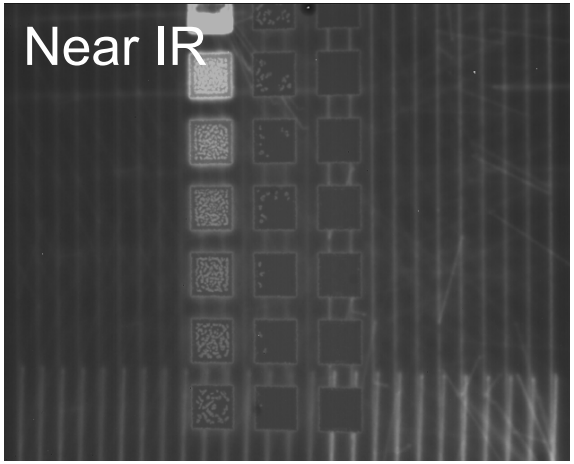
Details of Technical and Scientific Challenges:

- Thermal Conditions
  - Coupling of Energy Source with Feed Stock
  - Wide Range of δT/δx & δT/δt ➔Microstructural & Residual Stress Gradients
- Microstructural Heterogeneity
  - Solidification – Crystal Orientation ➔ Anisotropy
  - Solid-State Phase Transformation ➔ Heterogeneous Microstructure
- Mechanical Heterogeneity
  - Due to different precipitation kinetics ➔Residual Stress
  - Locked in Residual Stresses ➔ Pre-existing Cracks
  - Fatigue Properties ➔ Inferior to Traditional Manufacturing
  - Unreliable mechanical properties ➔Need for Secondary Process

Typical data showing spatial variations of temperature within a layer





Basic Steps of Computational Transient Thermo-Mechanical Modeling

Heat and Mass Transfer Predicts the molten shape and thermal cycles
- Energy
- Speed
- Materials

→

Liquid to Solid Transformation
- Shape
- Temperature gradient
- Liquid Solid Interface Velocity

→

Solid to Solid Transformations
- Thermal and Mechanical Transients
- Chemistry
- Properties

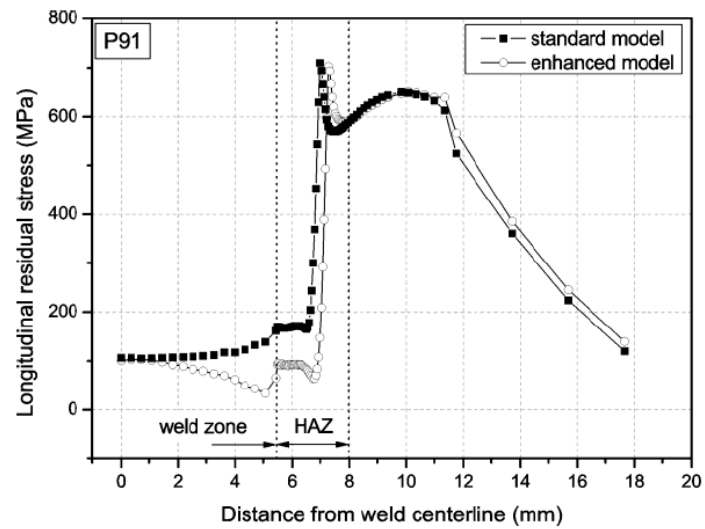
→

Residual Stress and Distortion
- Restraints
- Post-Process Heat Treatments

$$\frac{\partial T}{\partial t} = \frac{\lambda}{\rho c}\left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right] = a\left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right]$$

$$\rho\nabla(V.V) = -\nabla P + \mu\nabla.(\nabla V) + (S_V - \rho\nabla.(U_s V))$$

$$\rho\nabla(V.h) = \nabla.\left(\frac{k}{C_p}\nabla h\right) + S_l + S_h - \rho\nabla.(U_s h)$$



Let us evaluate individual steps

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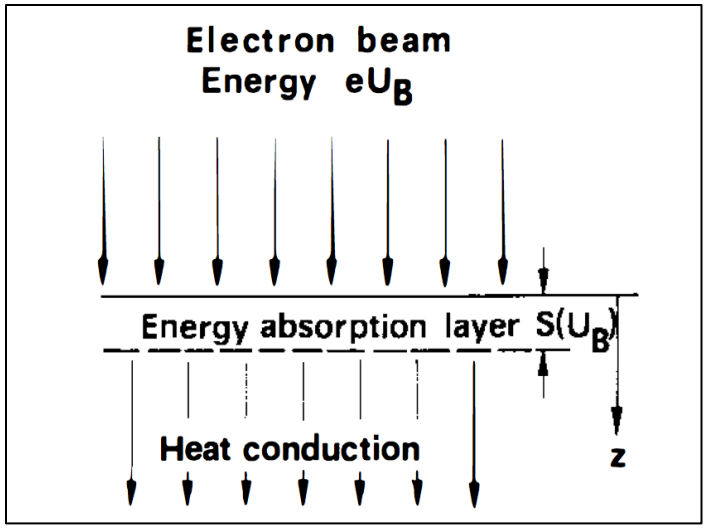
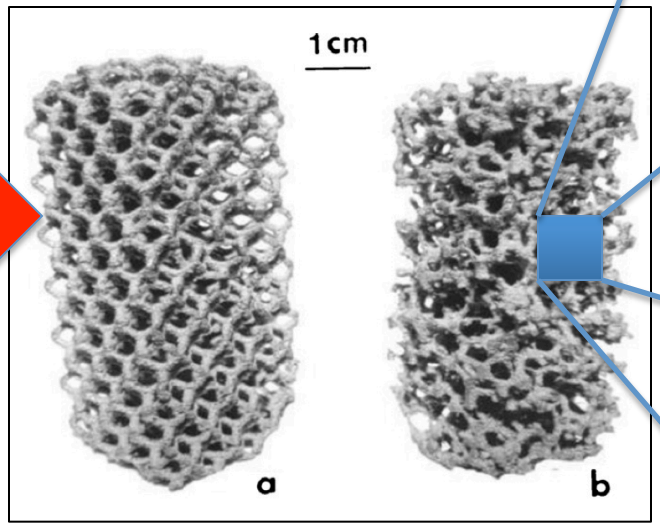
Electron and Materials Interactions

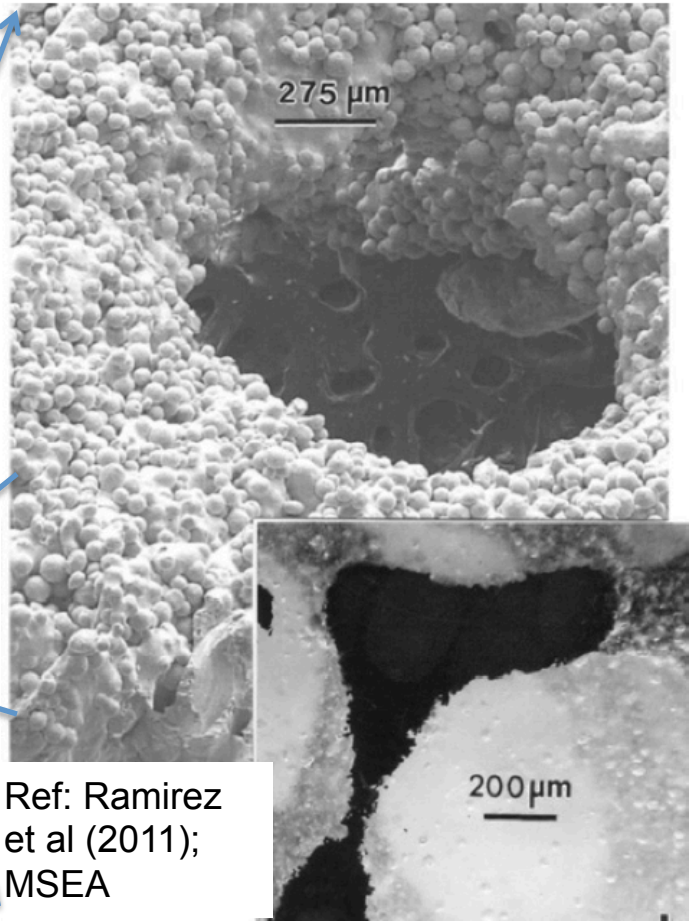
Ref: Schiller and Panzer, 1988



- **Electron energy transfer**
- **Thermal equilibrium lag time**
- **Heat Transfer in a transient porous media**

- Beam interaction may lead to partial sintering, full sintering, partial melting and full melting!

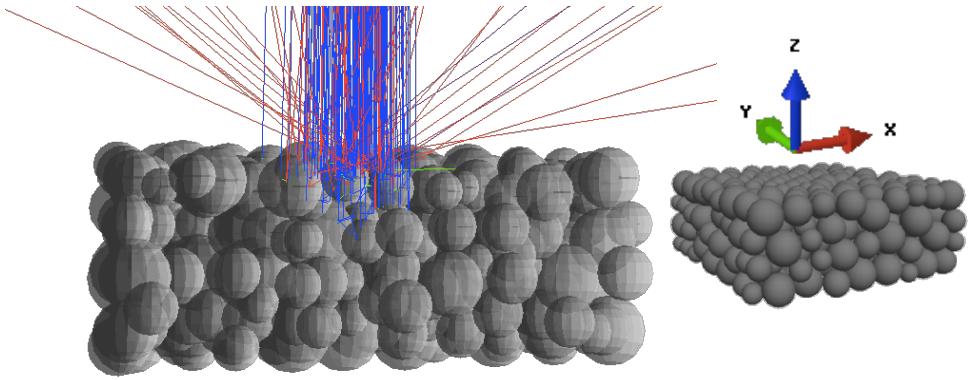




Ref: Ramirez et al (2011); MSEA

Electron-Particle Interaction Sub-model

Ref: J. Chen et al (2012)



Goal: Obtain the energy input required in the heat transfer model

Theory: (Rutherford & Mott)

- Primary electrons
- Secondary electrons
- Back-scattered primary electrons
- Back-scattered secondary electrons

Approach: 3D Monte Carlo simulation

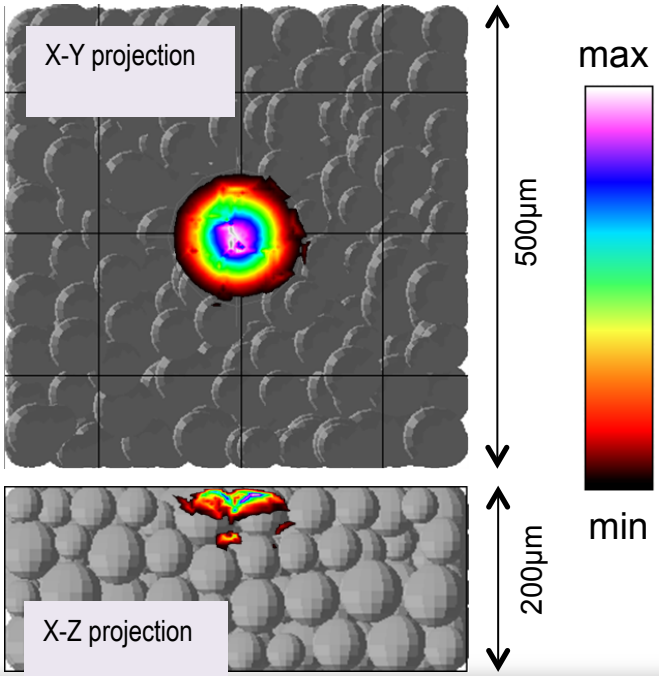
Input:

- Particle amount: 354
- Particle diameter: 40-70 μm randomly distributed
- Pack density ≈ 65~85%
- Electron beam diameter = 150 μm
- Electron energy = 20 KeV
- Amount of simulated primary electron = 5×10^6

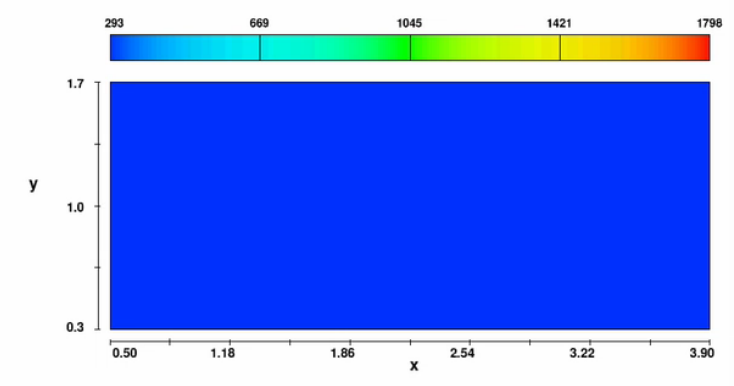
Output:

Pack density	65%	75%	85%
Predicted absorption coefficient	77.67%	77.41%	77.02%

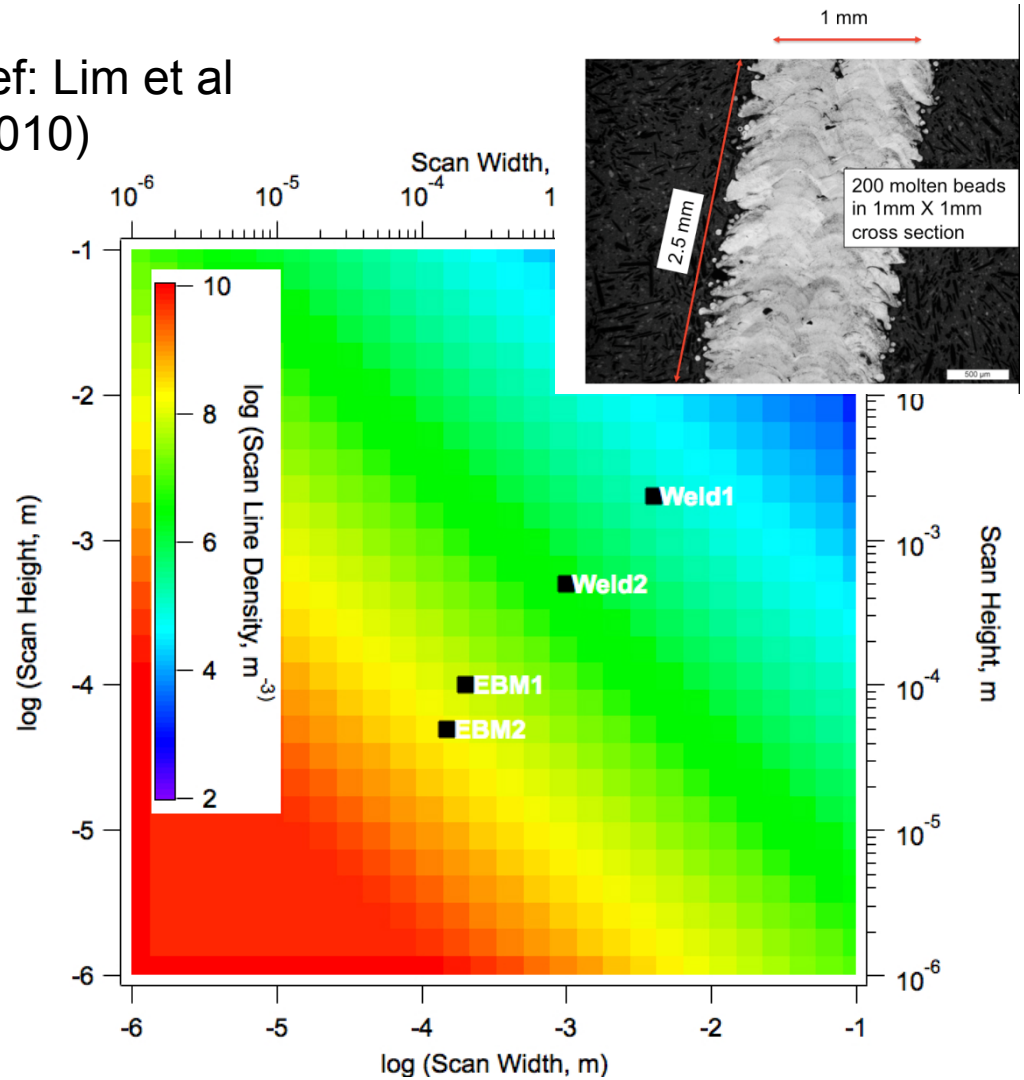
Energy distribution



Heat and Mass Transfer: Commercial Softwares are not Scalable for Additive Manufacturing (10^{10} scans per m^3)



Ref: Lim et al (2010)

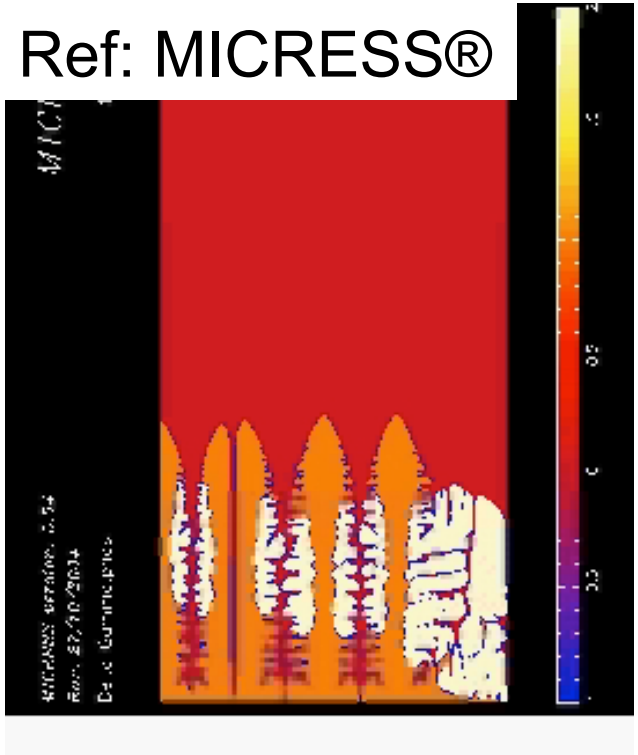


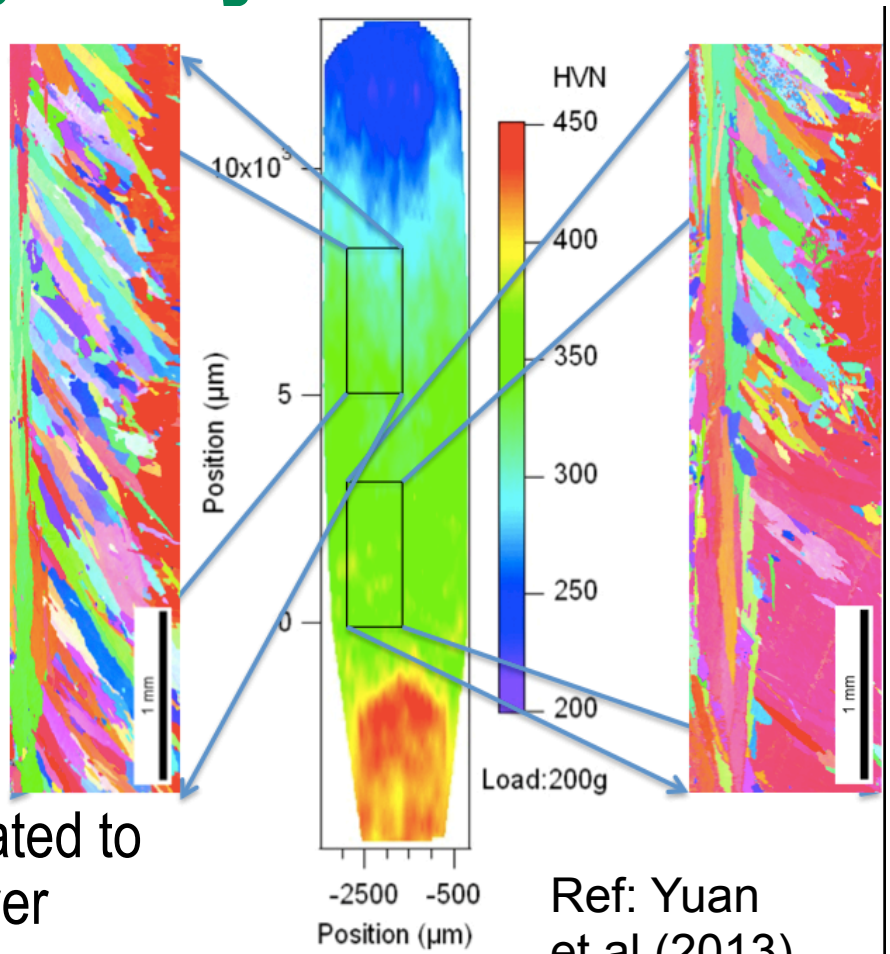
3-mm weld pool motion simulation takes more than 48 hours in a high-end computer using a commercial fluid dynamics software!

- We need to develop a radically advanced HPC model for the AM process using innovative mathematical algorithms for up scaling (e.g., TRUCHAS)

Solidification conditions, high- temperature gradients ($\Delta T/\Delta x=10^5$ K/m) and velocities ($\Delta x/\Delta t$= 3 m/s), lead to crystallographic and microstructure heterogeneity.

Ref: MICRESS®





Ref: Yuan et al (2013)

- Phase field models have to be accelerated to capture these small-scale transients over large build volumes.

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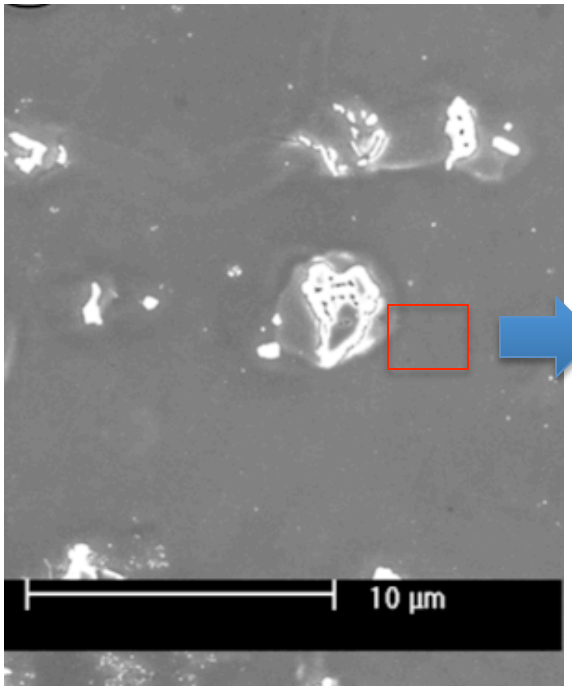
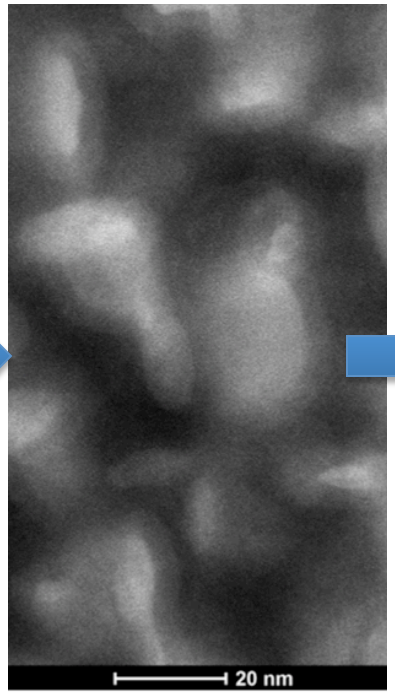
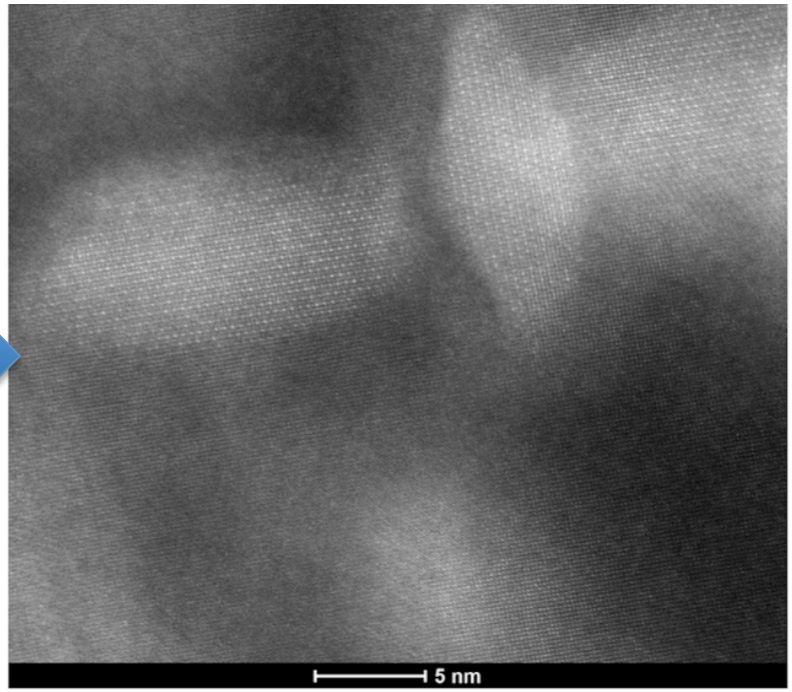
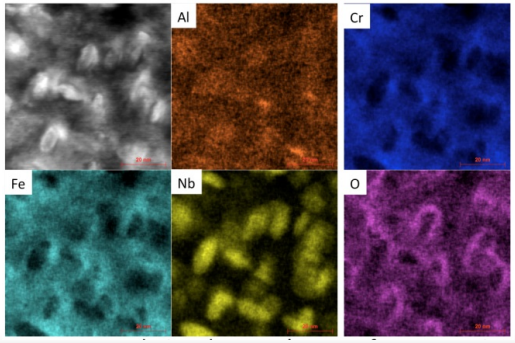
Solid-state transformations are affected by repeated thermal cycling; Leads to µm- and nm- scale heterogeneities









- Existing material models, can consider either µm-scale or nm-scale changes; Seamless integration across the scale appears to be elusive!

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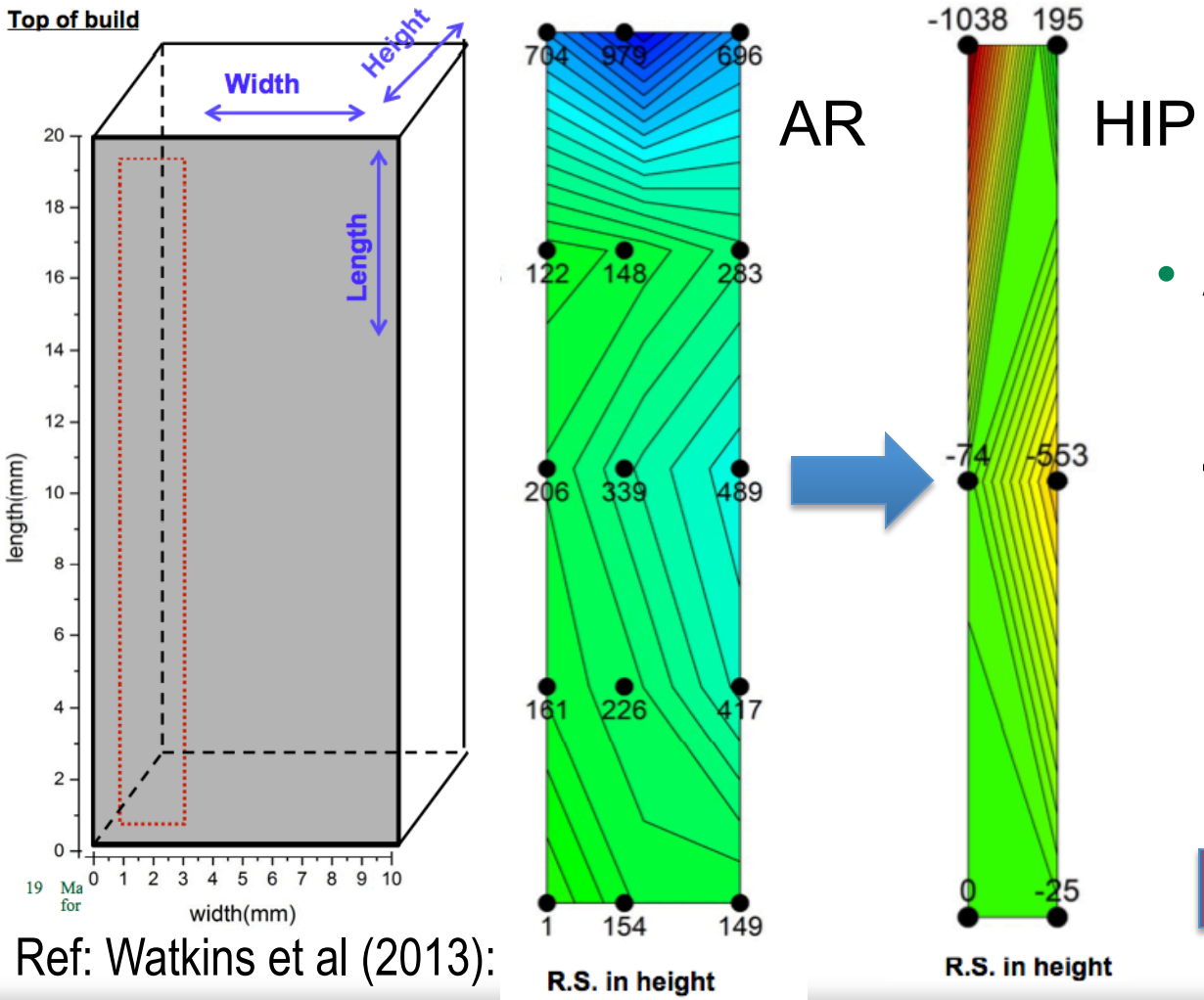
Residual stress distribution in IN718 build are compressive after Hot Iso-static Pressing.

HB-2B/NRSF2 area: overhead crane for mounting large specimens or accessories



- Ref: Watkins et al (2013):

- **Ability to process the measured data and analyze with reference to mathematical models still is manual and often time consuming!**

Compressive

Tensile

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Vision and Proposed Approach

Thermography Experiments from MDF

Adopt HPC TRUCHAS Model

Adopt HPC AMP Model

Describing Energy Interaction with Powder Particles → Calculation of Heat and Mass Transfer in HPC Models → Calculation of Thermo-Mechanical Transients in HPC Models → Calculated Distortion and Spatial Distribution of Residual Stress

Adopt OSU/ UTK Phase Transformation Models

Verify and Validate Residual Stress Distribution Ni-Alloys using HFIR and SNS

- Deliverable: Develop and Deploy a framework for scalable, verified, and validated HPC model for emerging AM user and application base within ORNL's "Additive Manufacturing Computational End Station"

Why open source HPC software?

TRUCHAS Users Manual

- Example: Adaptation of TRUCHAS-Solving for conservation of mass-momentum and energy + Thermo/Kinetics for powder bed manufacturing
- "TRUCHAS" software can be modified to simulate Thermo-Fluid-Mechanical-Material Interactions by coupling with AMP and Material Models
- Significance: Coupling of heat and mass transfer, elastic and plastic deformation, verification methodologies

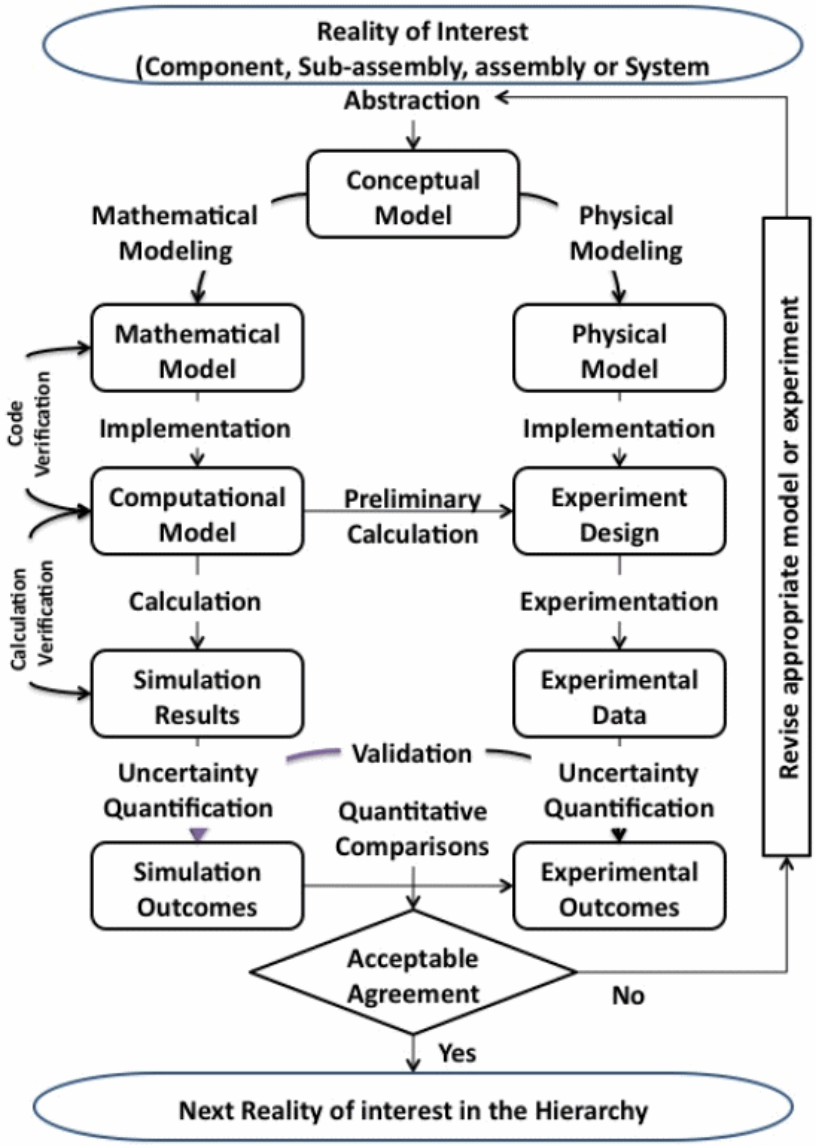

Figure 1—Verification and Validation Activities and Products (*Source:* Reprinted, with permission, from ASME, *V&V 10-2006,* New York: ASME, Figure 1 (page 6).

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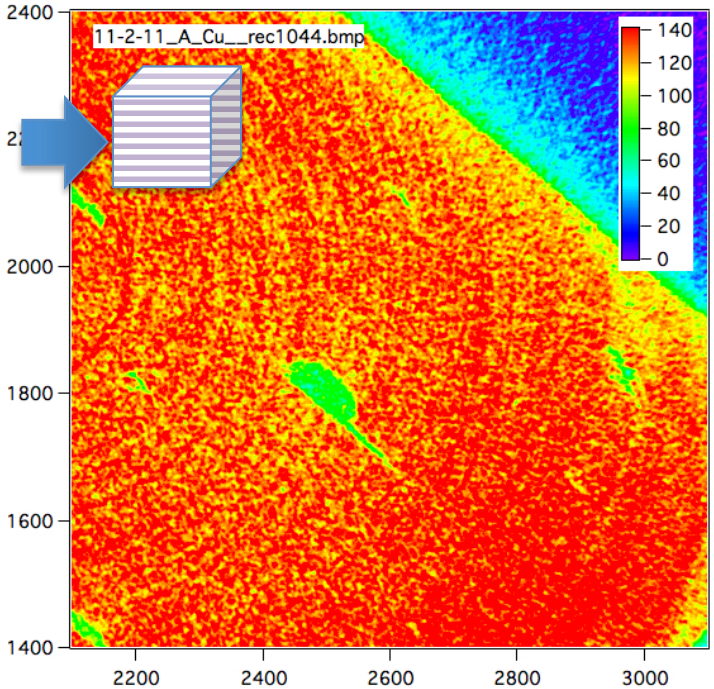
Step 1: Scientific Impact: HPC Model development in conjunction with rapid qualification of parts by probing in 3D with multi-scale resolution

Example Tomography data from UAM part

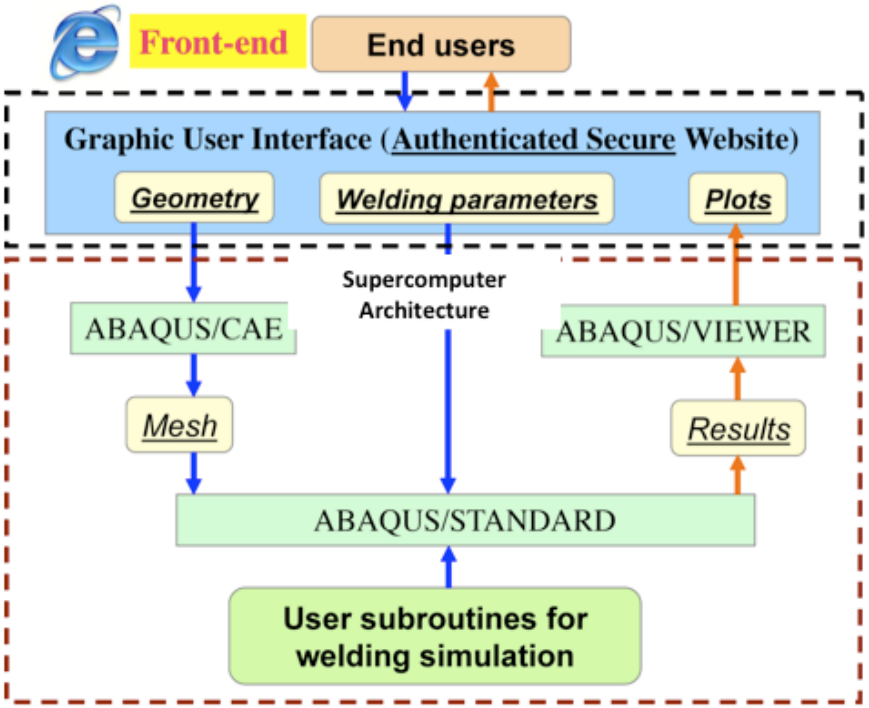


Can we qualify the parts within 48 hrs?

- Residual Stress, Microstructure & Mechanical Heterogeneity
- ORNL (e.g. SNS, HTML, ShaRe) & Joint Institute for Advanced Materials

Undergraduate Student Training
Graduate Student Research

Step 2: Industrial Impact: Deploy calibrated models for all additive manufacturing processes through cloud based services



Can we optimize the processes within 24 hrs?

Undergraduate Student Training
Graduate Student Research

- **E-WeldPredictor® architecture – EWI/OSU/OSC Research:**
- **Ref: US Patent: 8,301,286B@: Babu et al., (2012) Remote High Performance Computing Materials Joining and Material Forming Modeling System and Method**

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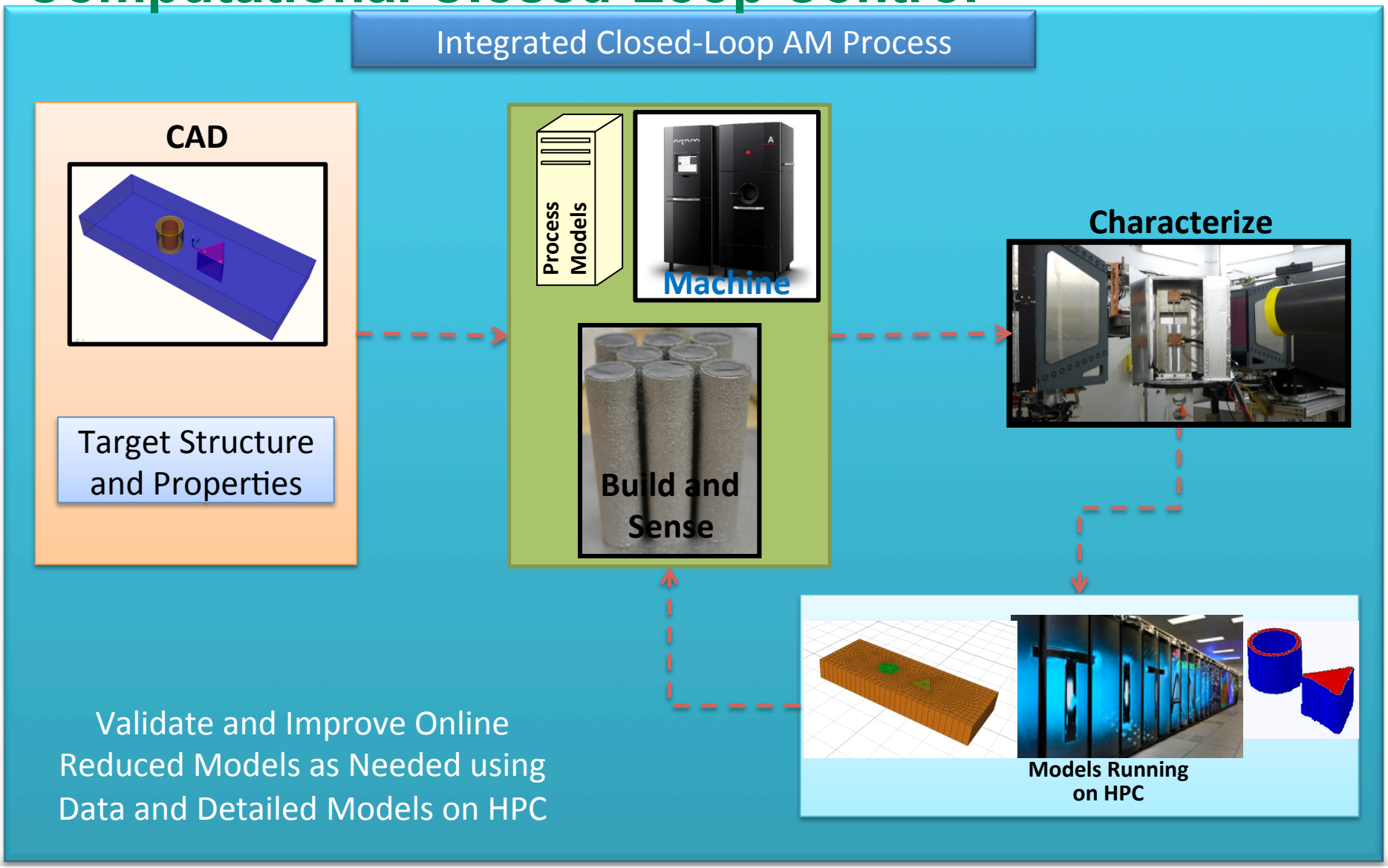
Step 3: Phased Development for AM Computational Closed-Loop Control



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OAK RIDGE NATIONAL LABORATORY
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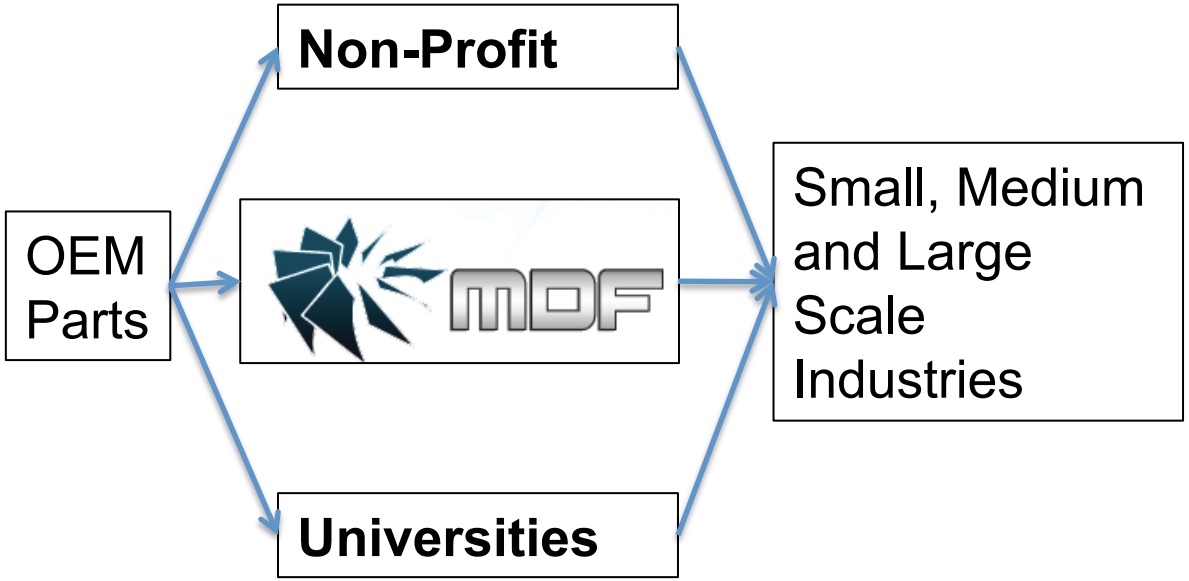
Step 4: Deploy the additive manufacturing processes to large number of small-scale manufacturers



Can we deploy AM process within 1 month?

High School
Community Colleges
Undergraduate Student Training
Graduate Student Research

- Suit of Additive Manufacturing Tools Demonstration within one building exists now in Tennessee
- MDF can act as a bridge between OEM and Small businesses

Summary and Conclusions

- Additive manufacturing: Potential to accelerate the dream-design-create-deploy innovation life-cycle
- Scientific Challenges: Mechanical heterogeneity due to spatially (μm to nm) and temporally ($<10^{-4}$ s to 1 min) varying chemical, thermal and mechanical gradients
- Vision & Steps: Develop and deploy verified and validated open domain HPC models
- Expected Breakthrough: Fundamental understanding of heterogeneity in all additive manufacturing processes, as well as, innovation to eliminate the same

Process Centric Developments

Design Centric Developments

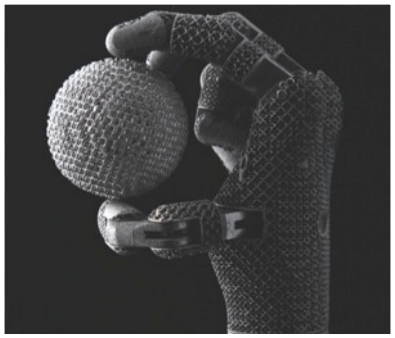
MDF Thrust Area

Additive Manufacturing

MDF Manufacturing Demonstration Facility

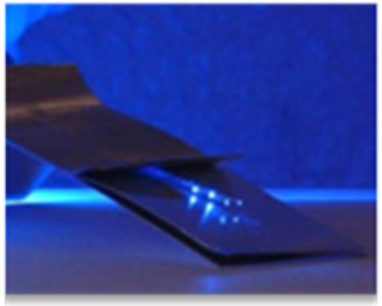
Metal

Electron Beam Melting



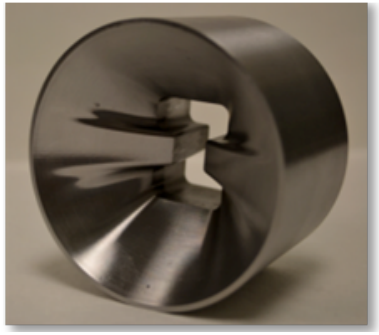
- Developing in-situ characterization, feedback and control
- Precision melting of powder materials
- Processing of complex geometries not possible through machining

Ultrasonic Additive Manufacturing



- Simultaneous additive and subtractive process for manufacturing complex geometries
- Solid-state process allows embedding of optical fibers and sensors

Laser Metal Deposition



- Site-specific material addition
- Application of advanced coating materials for corrosion and wear resistance
- Repair of dies, punches, turbines, etc.

Polymer

Fused Deposition Modeling

- Development of high-strength composite materials for industrial applications
- Precision deposition of thermoplastic materials

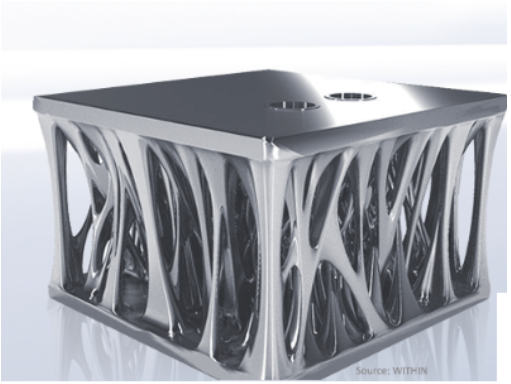
Working with AM equipment providers to develop high-performance materials, low-cost feedstock, processing techniques and in-situ characterization and controls to enable broad dissemination of technologies

We have wide range of processes to make 3D metallic parts.

e-Manufacturing Solutions

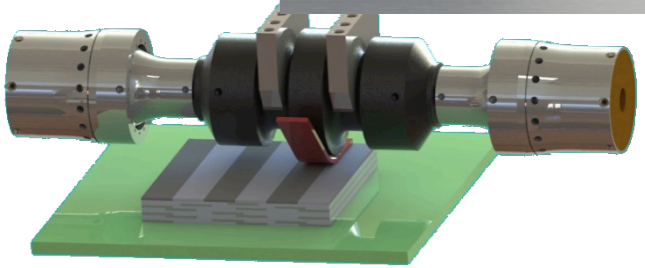
CAD TO METAL®
Arcam AB®

OPTOMEC®
Additive Manufacturing Systems—from NANO to MACRO™



Low Pressure Turbine blade in γ-titanium aluminide.
Courtesy of Avio S.p.A.

FABRISONIC
Solid State Additive Manufacturer of Metals



- Based on Feedstock & Energy Source
  - Powders, Wires, & Tapes
  - Laser, Electron Beam, Arc, and Ultrasonic
- Are they mature? Do we have scientific and technical challenges?