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Linking Process, Structure, Property, and Performance for Metal-based Additive Manufacturing: Computational Approaches with Experimental Support

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Workshop on Quantification of Uncertainties in Material Science
NIST, Gaithersburg, MD, January 14-15, 2016
Organized by Maria Emelianenko (GMU), Igor Levin (NIST) and Qiang Du (Columbia)

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A Quotation from NAE President Dan C. Mote

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Quotation from "**Making a World of Difference: Engineering Ideas into Reality (An NAE Report)**"

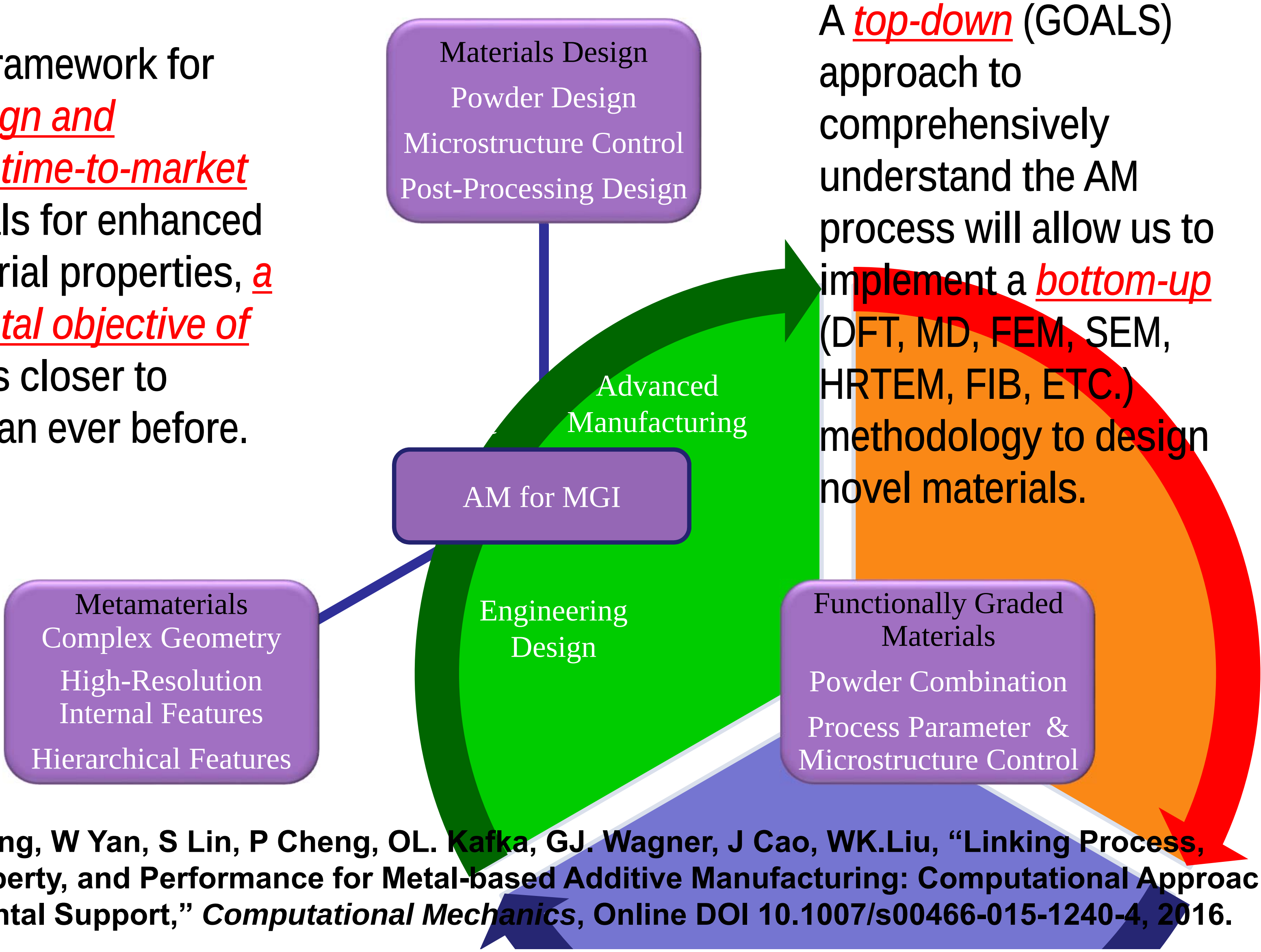
"Technological advances made over just a few decades are boosting economies, feeding the hungry, and healing the sick. ….. New vaccines hold out the promise for tackling scourges like malaria and some cancers, while doctors save lives by replacing diseased heart valves—in some cases without open-heart surgery. ….
All these advances have come through engineering carried out in companies, universities, and national laboratories. Those efforts have created new materials like nanotubes and ***high-strength alloys, manufacturing technologies like 3-D printing, software and algorithms for harnessing the power of supercomputers and mining vast stores of data,*** and countless other innovations. ***Yet these examples barely scratch the surface of the remarkable changes wrought over the last quarter century."***

On October 7-9, 2015, the U.S. National Committee on Theoretical and Applied Mechanics (USNC/TAM) held a Workshop on ***Predictive Theoretical and Computational Approaches for Additive Manufacturing*** in the ***US National Academies, Washington, DC.*** The three-day workshop featured 24 presentations from speakers in academia, industry, and government labs. 50 experts attended the workshop in person, 200 joined through the webinar and over 2,000 viewers have already watched the video sessions. Please noted that the 190+ online viewers of the workshop was the highest viewing audience for the National Academies in-house video webcasting to date. We welcome you to visit the USNC/TAM site (**http://sites.nationalacademies.org/pga/biso/IUTAM/**) where you will be able to access the speakers' session slides and videos.

Additive Manufacturing (AM) for Materials Genome initiative (MGI)

A stable framework for *rapid design and improved time-to-market* of materials for enhanced bulk material properties, *a fundamental objective of the MGI*, is closer to fruition than ever before.

A *top-down* (GOALS) approach to comprehensively understand the AM process will allow us to implement a *bottom-up* (DFT, MD, FEM, SEM, HRTEM, FIB, ETC.) methodology to design novel materials.



Materials Design
Powder Design
Microstructure Control
Post-Processing Design

Advanced Manufacturing

AM for MGI

Engineering Design

Metamaterials
Complex Geometry
High-Resolution Internal Features
Hierarchical Features

Functionally Graded Materials
Powder Combination
Process Parameter & Microstructure Control

J Smith, W Xiong, W Yan, S Lin, P Cheng, OL. Kafka, GJ. Wagner, J Cao, WK.Liu, "Linking Process, Structure, Property, and Performance for Metal-based Additive Manufacturing: Computational Approaches with Experimental Support," *Computational Mechanics*, Online DOI 10.1007/s00466-015-1240-4, 2016.

The materials system

The equation

$$\text{Materials system properties} = A(\text{Building blocks}, \text{Interactions}, \text{Structure})$$

$$\downarrow$$

$$\text{Materials system genomes} = A(\text{Archetypes}, \text{Interactions}, \text{Conformation})$$

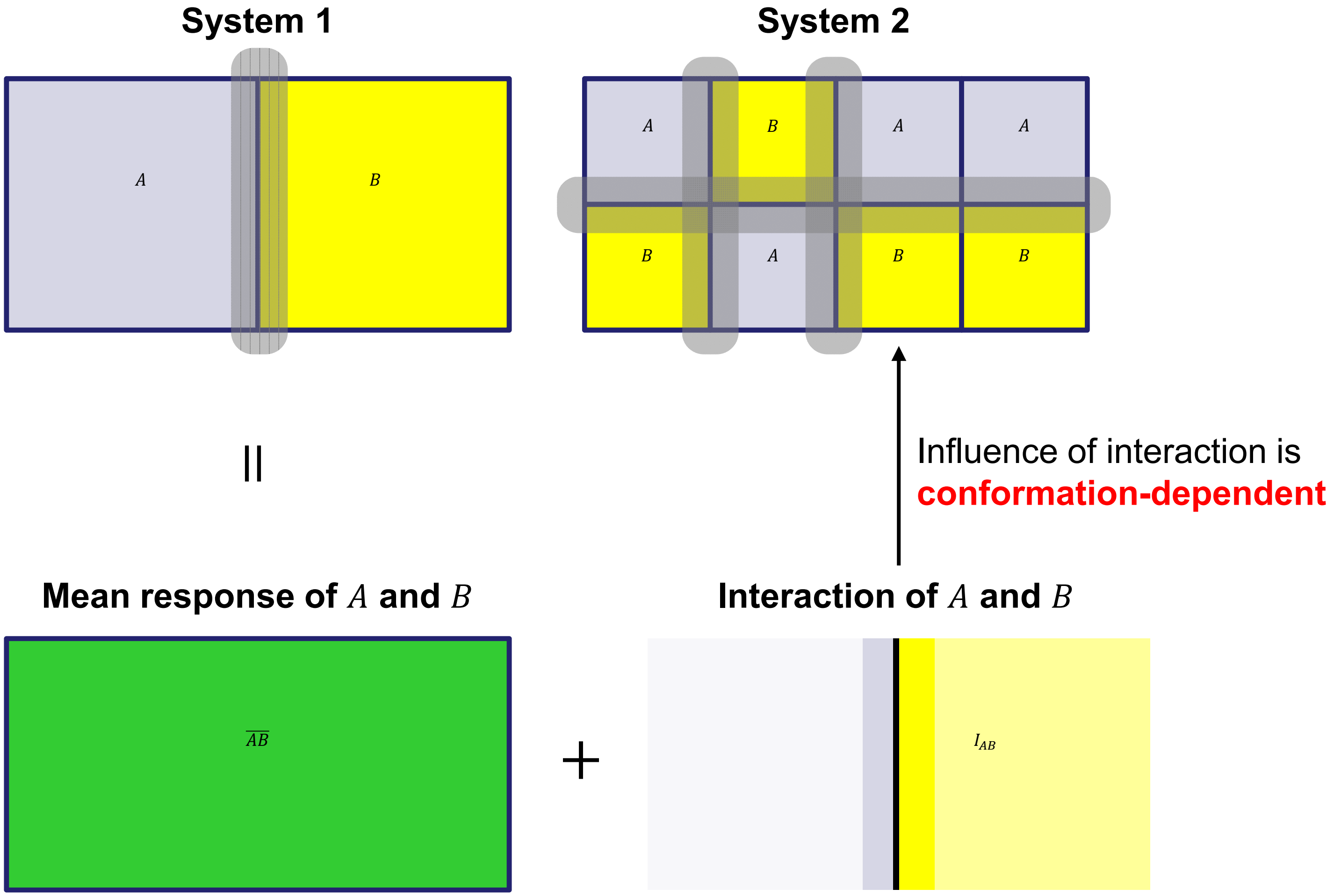
Materials system property is the entirety of the apparent property information that the material contains

Takeaways: the materials system depends on

- Building blocks of the material (individual components, phases),
- Interactions of the archetypes (e.g. chemistry, friction),
- The structural configuration of the archetypes
- The *assembly function* A, which includes material/structure processing
- **Write a design theory with uncertainty quantification to wrap around the above**

Greene, M., Y. Li, W. Chen, and W.K. Liu. The **archetype-genome exemplar** in molecular dynamics and continuum mechanics. *Computational Mechanics,* 2014.
KI Elkhodary, MS Greene, S Tang, T Belytschko, WK Liu. **Archetype-blending continuum theory.** *Computer Methods in Applied Mechanics and Engineering*, 2013

Decomposition of systems



System 1

System 2

Influence of interaction is **conformation-dependent**

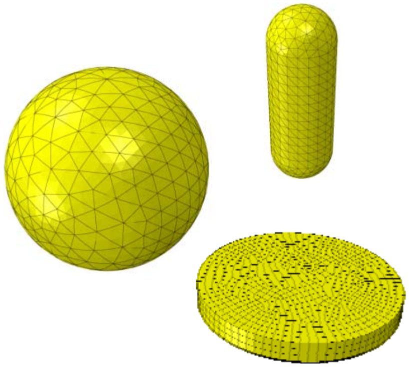
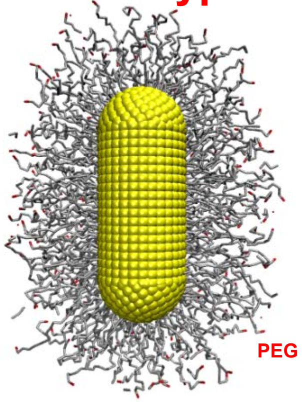
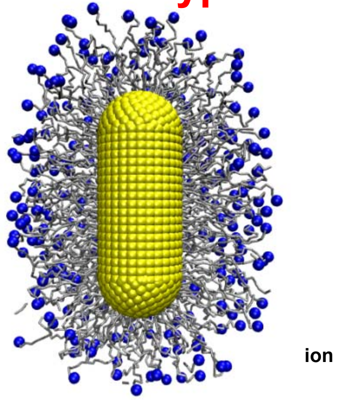
Mean response of A and B

Interaction of A and B

Evolution of Nanoparticles Design

Selection of archetypes via molecular simulation and from data base

Genome: targeted delivery of drugs

	First generation **Archetypes**	**Second generation** **Archetypes**	**Third generation** **Archetypes**
			
Nano-Materials	• Material design • Water solubility • Biocompatibility	• Maximize delivery • Stealth (passive) • Active targeting	• Environment-response • Dynamics properties • Biological or external cues • Theranostic abilities
Biological challenges	• Unstable • Removal by MPS • Poor tumor targeting	• Overreliance on EPR effect • No “universal” antigen • Active targeting is disappointing • <10% dose in tumor	• No “universal” design principle

Evolution of nanoparticle design, highlighting the interplay between evolution of nanomaterial design and fundamental nano-bio studies.
Abbreviations: Ab, antibody; EPR, enhanced permeation and retention; MPS, mononuclear phagocyte system; **PEG, poly(ethylene) glycol**.

Bao, Liu et al. 2014, Journal of The Royal Society Interface 11 (97), 20140301

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Archetype-Genome: Nanoparticle-mediated drug delivery

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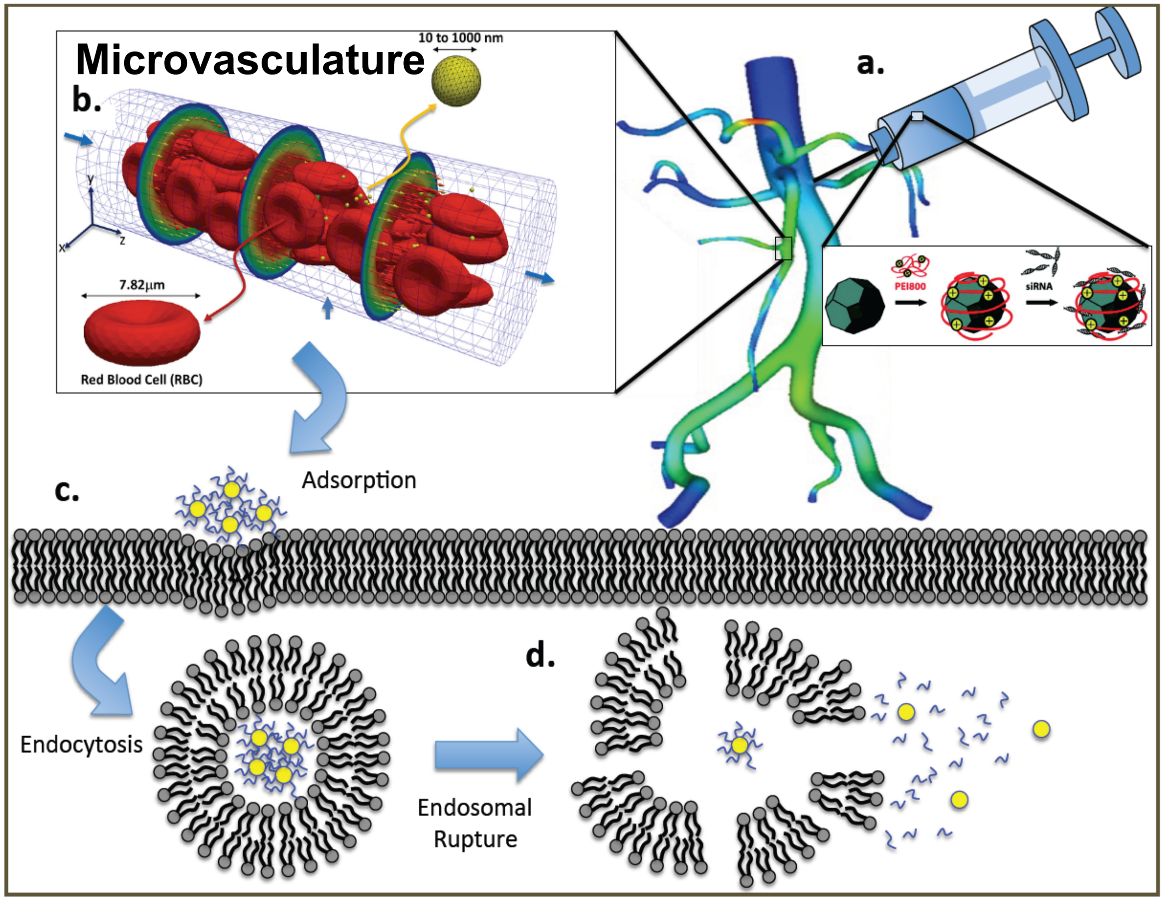


(b) Nanoparticles are segregated from red blood cells, increasing their interaction with the endothelium, leading to their removal from circulation. **(Modeling and Simulation)**

(c) Nanaparticles diffusion through the extracellular matrix;

adsorbing onto the surface of a target cell;

nanoparticles are then endocytosed from the lipid membrane. **(Modeling and Simulation)**

(a) A solution containing nanoparticle delivery platforms is injected into a patient's circulatory system. **(Building Blocks or Archetypes)**

(d) The endosome containing the drug-delivery complex ruptures, releasing the therapeutic agents into the cytoplasm.

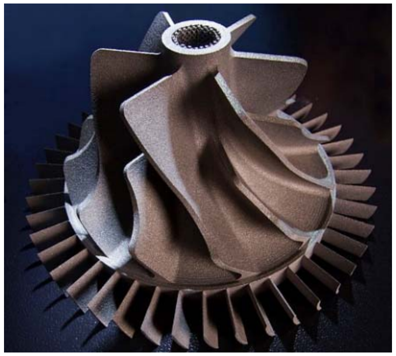
When released from the endosome, the nanoparticle cargo may be dissociated due to the pH environment change. **(Modeling and Simulation)**

(*Genome*)

Y.Li, W Stroberg, TR Lee, HS Kim, H, Man, D. Ho, P. Decuzzi, WK Liu, "Multiscale Modeling and Uncertainty Quantification in Nanoparticle mediated Drug/Gene Delivery," *Computational Mechanics on Nanomedicine*, (2014). **TR Lee, AM Kopacz, WK Liu, P Decuzzi,** "On the near-wall accumulation of injectable particles in the microcirculation: smaller is not better," Scientific Reports, 2013. **TR Lee, WK Liu, et al.,** "Quantifying uncertainties in the microvascular transport of nanoparticles," Biomechanics and Modeling in Mechanobiology, 2014. **Y Li, Y Lian, LT. Zhang, WK Liu,** "Cell and Nanoparticle Transport in Tumor Microvasculature: the role of size, shape and surface functionality of nanoparticles," *Interface Focus*, 6 (1), 20150086, 2015.

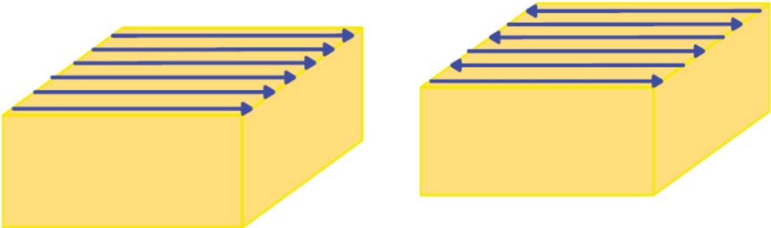
What is the Archetype-Genome Exemplar for AM?

1.Complex geometry



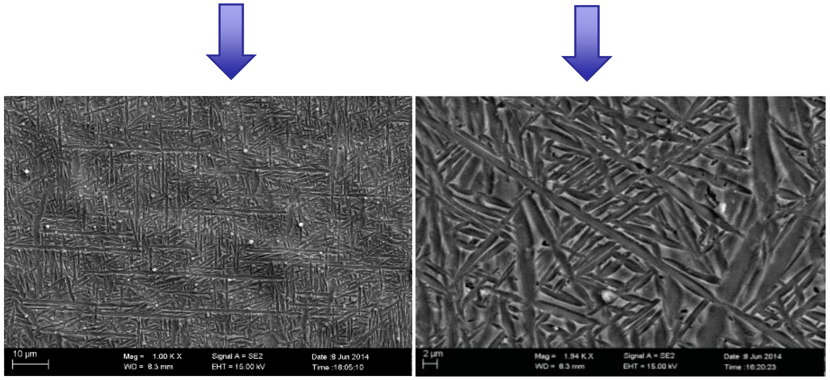
2.Control microstructure

W Ge et al,.2014.SFF



(a) Z-shaped scan line

(b) S-shaped scan line



3.Design materials

%Powder #1 + %Powder #2 + %Powder #3

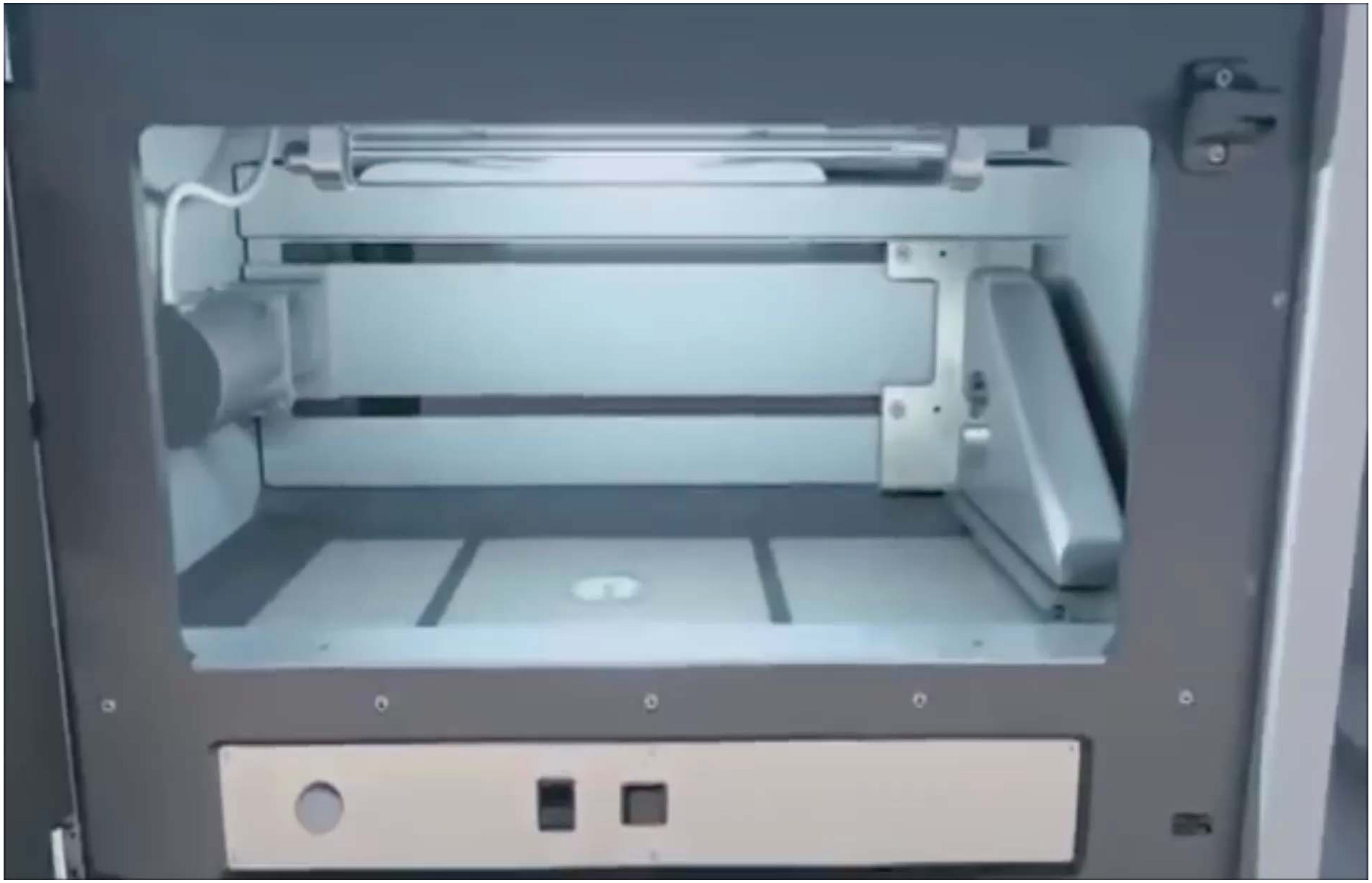
=

Unique Powder Combination

Archetypes are the powders and chemistry

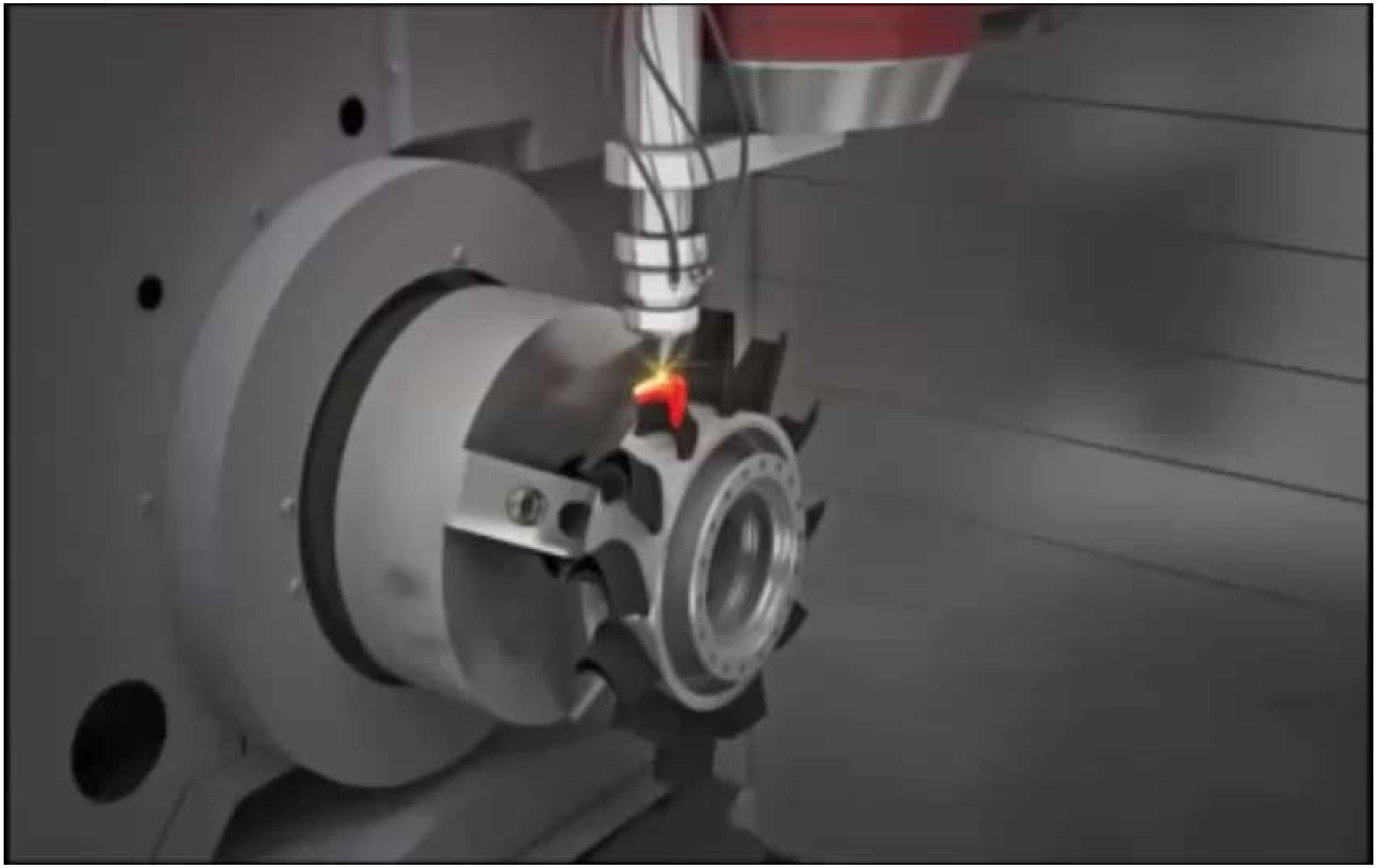
Genomes: metrology, properties and performance

Powder Bed Fusion



Walls, Sheraton. (2012, August 22). *Direct Metal Laser Sintering* [Video file]. Retrieved from https://www.youtube.com/watch?v=cRE-PzI6uZA

Direct Energy Deposition



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Directed Energy Deposition Industrial Application

Hybrid Additive and Subtractive Machining

Prototypes and small series production of complex lightweight and integral parts for:

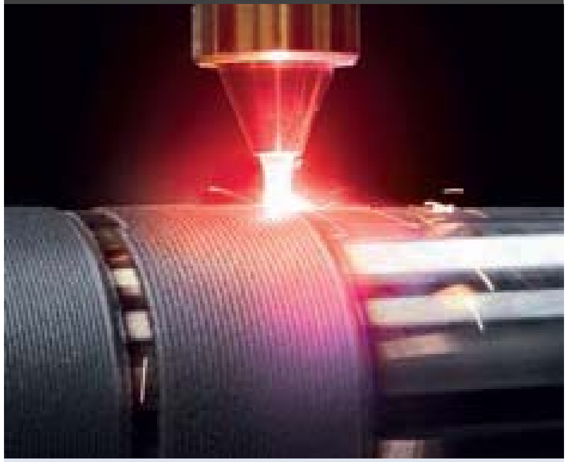
1) Die & Mold
2) Aerospace
3) Automotive
4) Medical

Repair of Turbine and Die & Mold Components

Repair of damaged and worn components for:

1) Medical
2) Die & Mold
3) Aerospace
(e.g. Blade Tip Repair)

Corrosion and Wear Resistant Coatings



Partial coatings and complete part coatings (corrosion and wear resistant):

1) Mould Making
2) Off Shore Drilling
3) Machine Tool
4) Medical

Used with permission from DMG Mori

Hybrid AM Processes

Under construction

ARPI

Additive Rapid Prototyping Instrument at Northwestern University

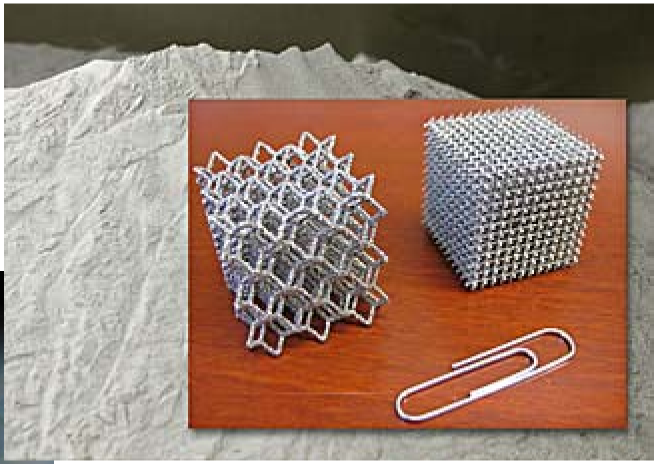
- **Primary Additive Processing**
  - Laser Engineered Net Shaping (LENS) Module
  - Powder Bed Fusion (PBF) Module
  - CW Laser 1 kW
- **Secondary Surface Operation**
  - Electric Field Module
  - Magnetic Field Module
  - Pulsed Laser
- **In-Situ Metrology**
  - Pulsed laser
  - Interferometer
  - IR Camera

What is involved in Process-Structure-Property Design?

Typical engineering applications incorporate multiscale phenomena

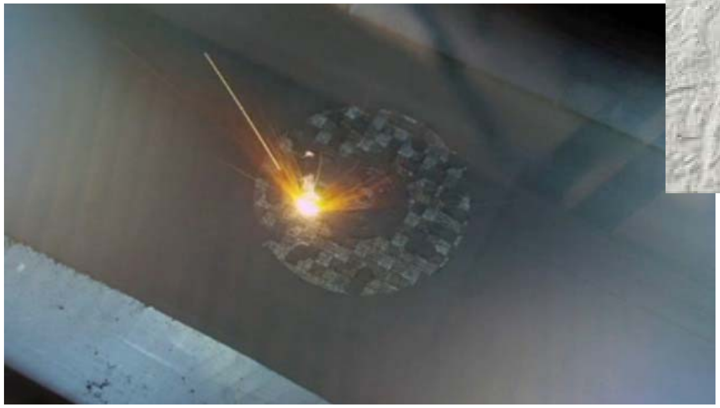
EXAMPLE: Additive Manufacturing

Final part



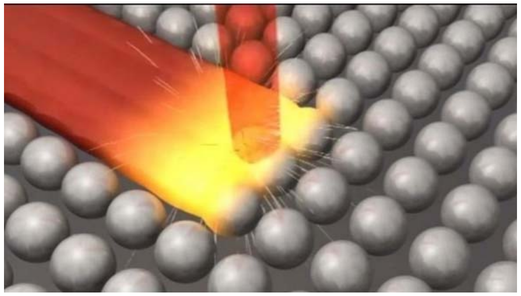
Structural property

Solidified layers



Surface roughness

Cyclic melting/re-melting on power scale



Microstructure evolution

Critical Problems (uncertainty source) for AM alloys

- Extremely fast heating and cooling rates
- Involving remelting and numerous low temperature reheating cycles
- Segregation & Phase distributions
- Long columnar grains along z-axis
- Impossible (at this time) to refine microstructure via deformation

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Introduction to Selective Laser/EB Melting

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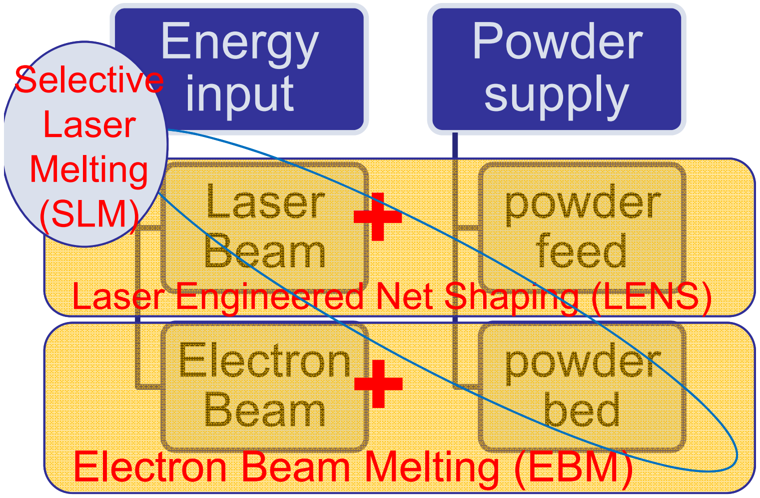
Additive manufacturing


Energy input

Powder supply

Selective Laser Melting (SLM)

Laser Beam + powder feed

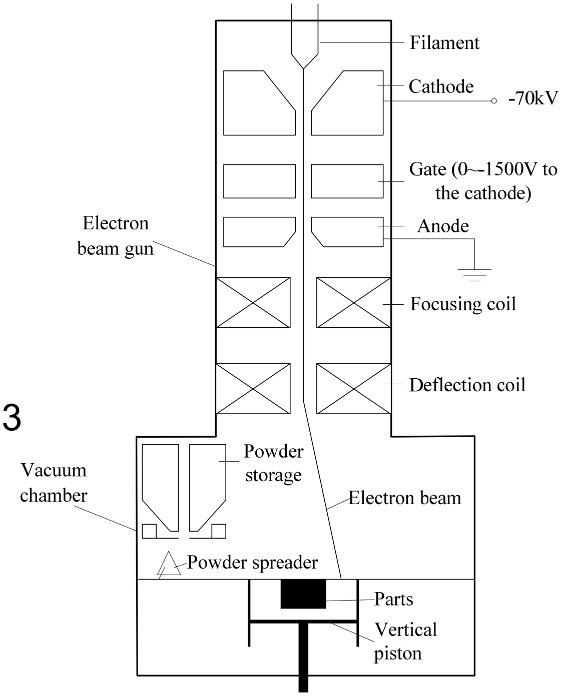
Laser Engineered Net Shaping (LENS)

Electron Beam + powder bed

Electron Beam Melting (EBM)

Electron Beam Melting

1. Spread powder bed
2. preheat: use defocused electron beam
3. melt: use focused electron beam
4. lower platform and repeat 1~3



- The advantages

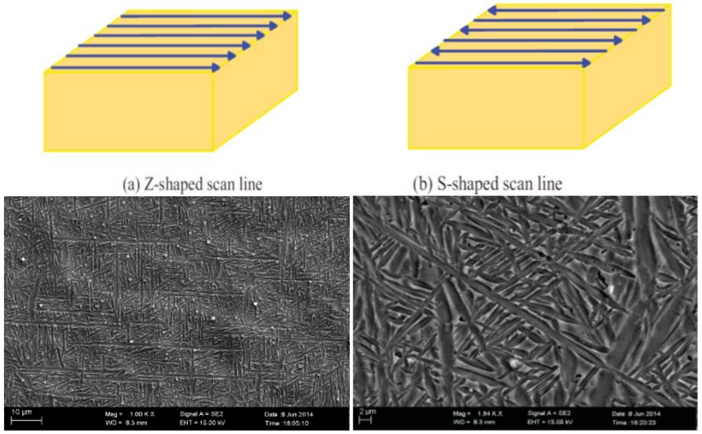
1. Complex geometry

2. control microstructure

3. Design materials

William 3D .

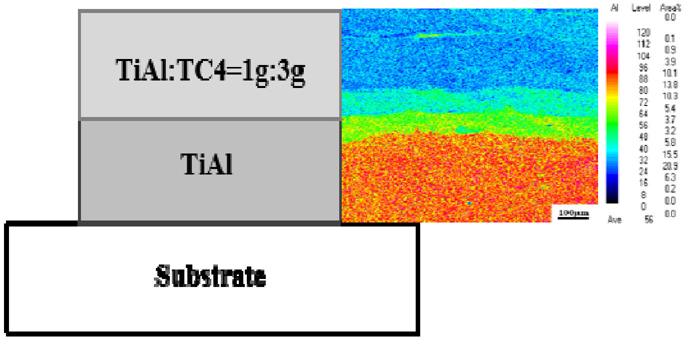
W Ge et al,. SFF, 2014.


(a) Z-shaped scan line

(b) S-shaped scan line

Functional Gradient material

W Ge et al,. SFF, 2015



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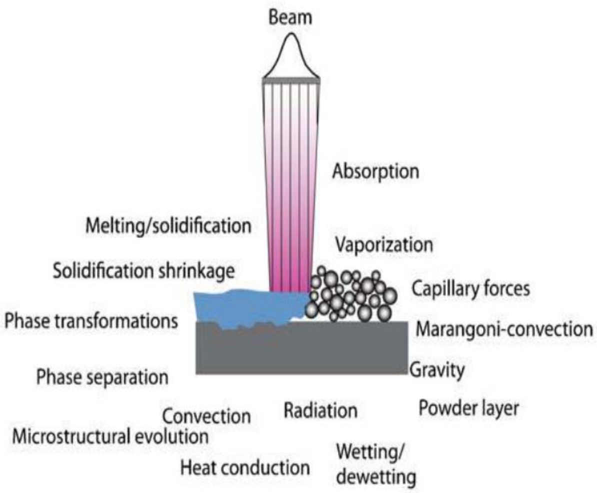
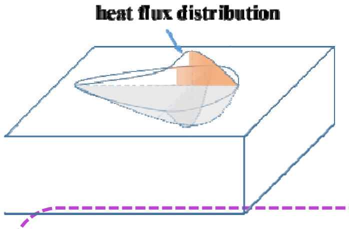
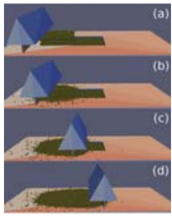
Framework of Predictive AM Modeling

LENS: Laser Engineered Net Shaping

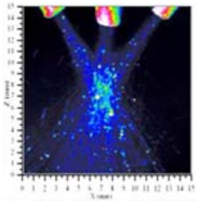


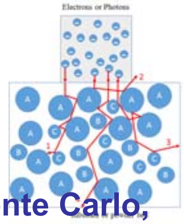


Multiple powders falling/powder-gas interaction

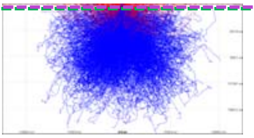


Powder bed formation (SLM/EBM)
powder feed (LENS)

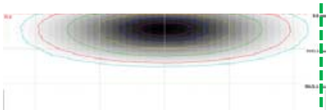




Beam-powder interactions



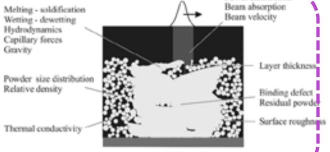
Heat source model



Monte Carlo,
Raytracing,
Development of Heat Source Models

Micro & Macro
Heat Transfer &
Phase
Transformation:

Powder transformation model
coupling of heat transfer, melting, flow, evaporation
solidification



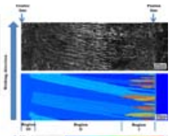
Solidification,
Phase Changes:
Materials Characterization
Constitutive
Modeling, etc

Thermo-elastic-plastic model

Thermal stress & distortion prediction

Phase evolution model

Microstructures prediction



Micro voids and pores prediction

Surface roughness and dimensional accuracy prediction

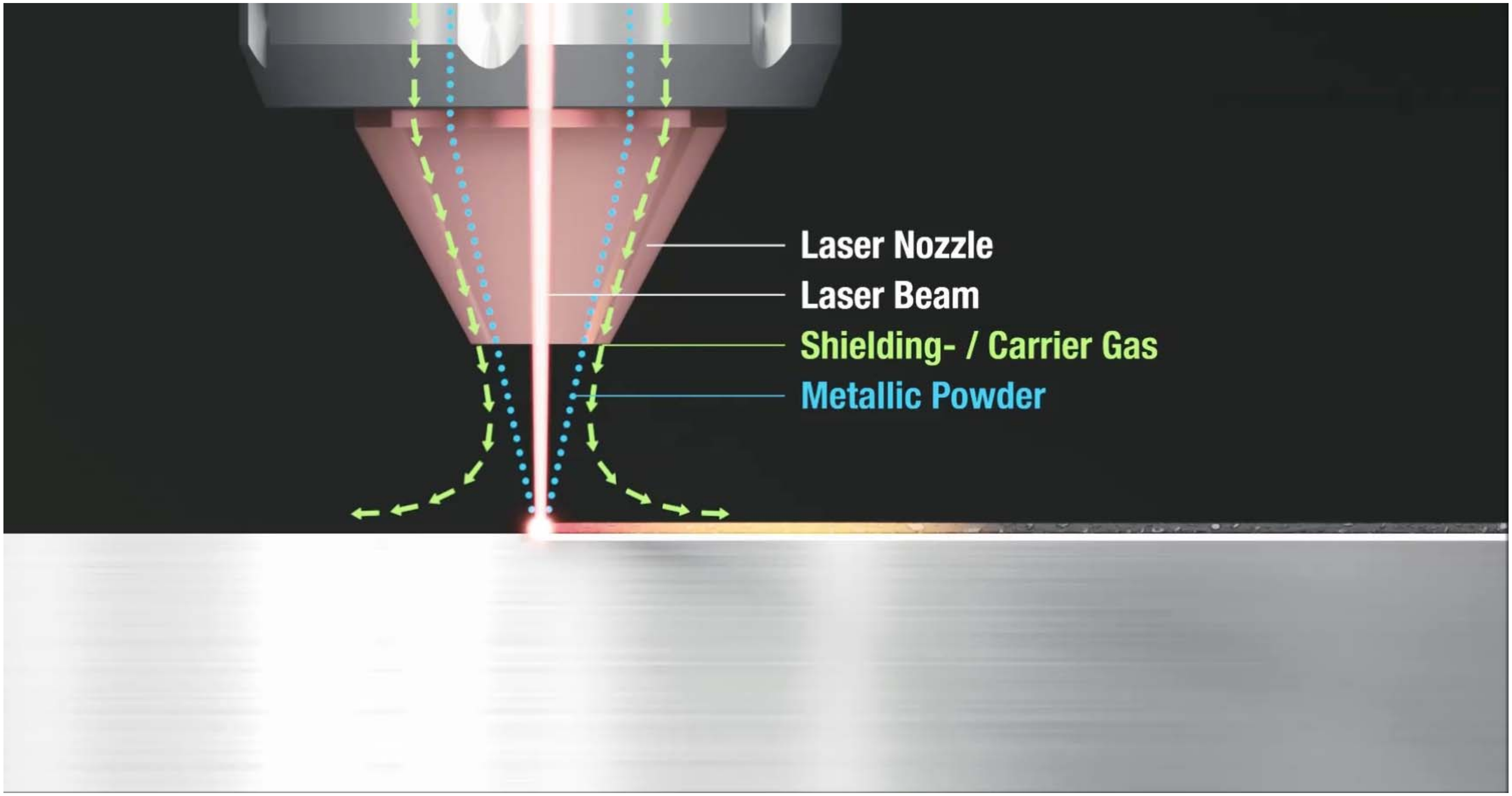
Archetypes

APL Integration

Genome

Working performance prediction

Laser Engineered Net Shaping (LENS)



Movie; Used with permission from DMG Mori

What is involved in Process-Structure-Property Design?

- **Metal-Based Processes**
  - **Accumulation and Energy Input (HEAT SOURCE) Methods**
  - **Computational Process Modeling for Microstructures Nucleation and Evolution (To make life easier or harder: Uncertainty Propagation)**
    -- Micro heat source modeling
    -- Macro heat source modeling and its microstructure evolutions
- **Experimental (Statistical) Materials Characterization**
  - The Role of Microstructure
- **Informatics-Driven (with UQ) Design Methodologies: Linking of Process-Structure-Property**
  - Image-Based Data Collection
  - Reduced Order Microstructural Modeling
  - Image-based Mechanistic Plasticity
  - Multiscale Fatigue Modeling
  - Image-Based materials behavior modeling (Constitutive Law Development)

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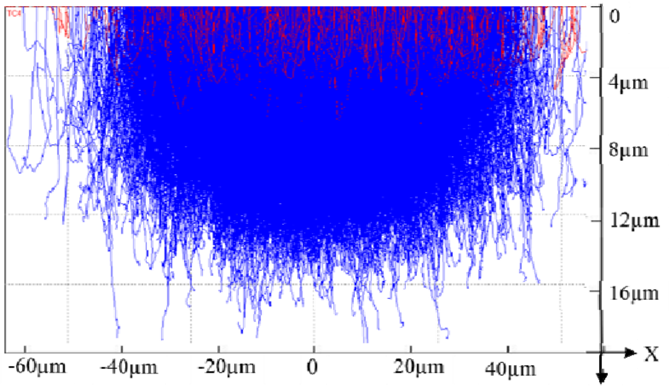
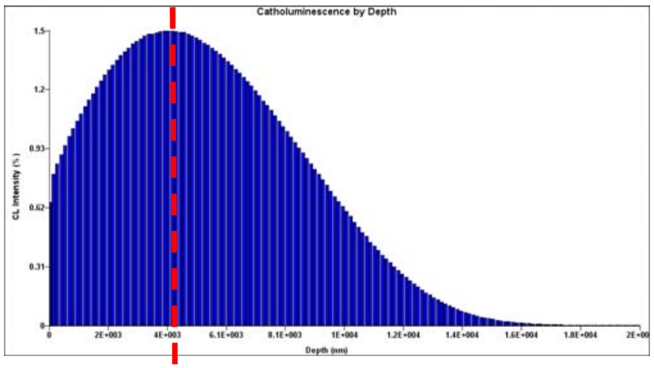
Microscale model

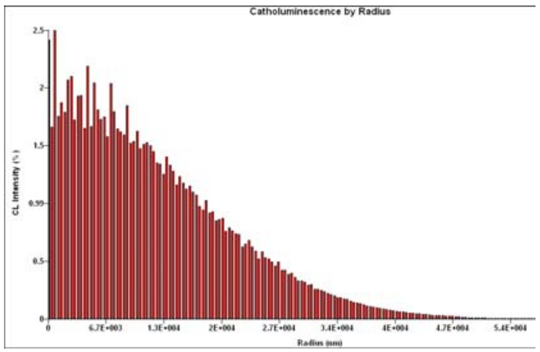
New heat source model established



Trajectories

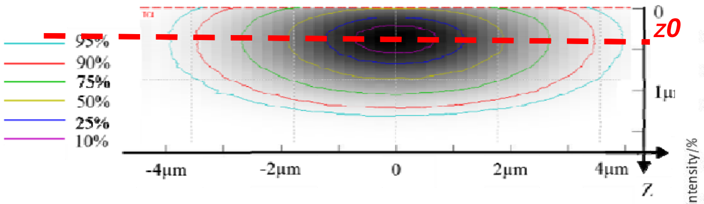


Energy Distribution in Z

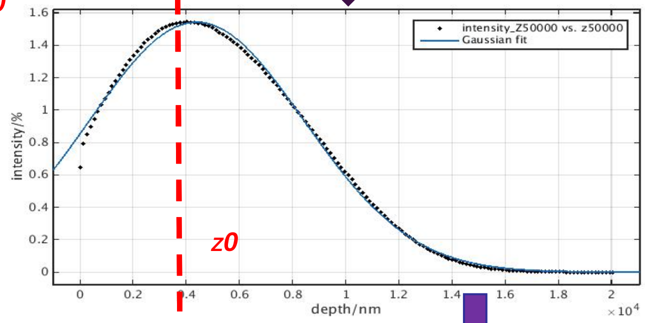


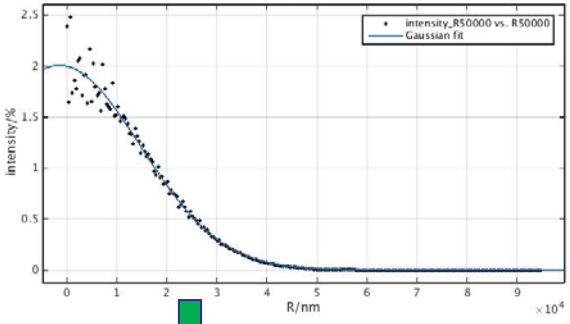
Energy Distribution in R

Curve fitting



Absorbed energy distribution in XZ plane





New heat source model

Z_0: depth with highest energy density
δ: characteristic depth

$$q(x,y,z) = Q * \left[\frac{1}{\delta \cdot \int_{-\frac{z_0}{\delta}}^{+\infty} \exp(-t^2)dt} \exp\left(-\frac{(z-z_0)^2}{\delta^2}\right) \right] * \left[\frac{N}{\pi R_b^2} \exp\left(-N \cdot \frac{(x-x_s)^2+(y-y_s)^2}{R_b^2}\right) \right]$$

Energy distributed through depth
determined by the speed of the electron and the material

Energy distributed across cross section
determined by the electron distribution

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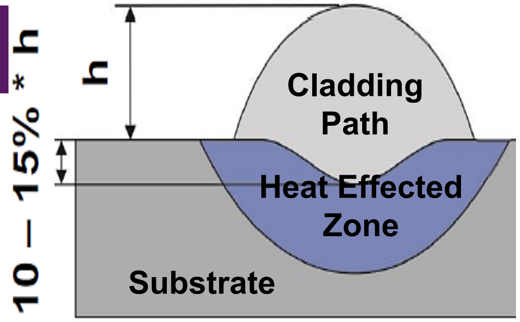
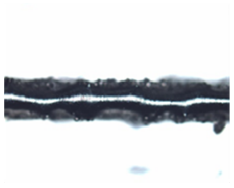
Prediction of Surface Finish

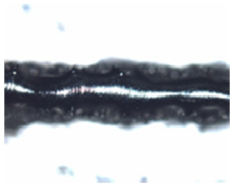


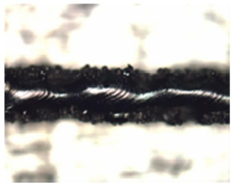
Single track formation process

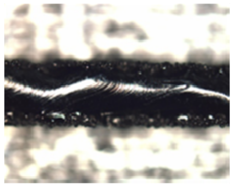
Experiments by Electron Beam Melting

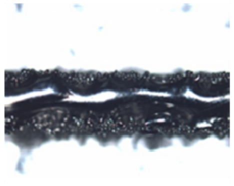
Electron beam scans straightly, but the solidified tracks are not straight.


I=1mA, V=0.05m/s


I=1.5mA, V=0.05m/s


I=2mA, V=0.1m/s


I=3mA, V=0.1m/s

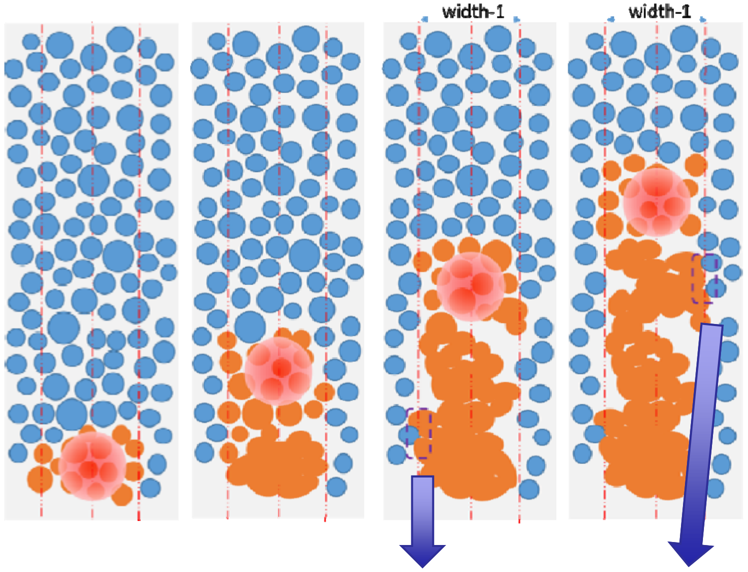

I=6mA, V=0.3m/s


I=9mA, V=0.3m/s

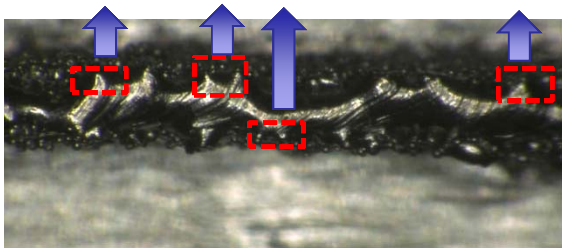
v↑, quality↓

How to predict?

Mechanism view

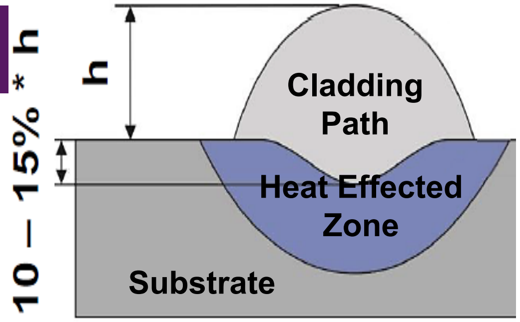


Random arrangement of powder bed



McCormick
Northwestern Engineering

Prediction of Surface Finish



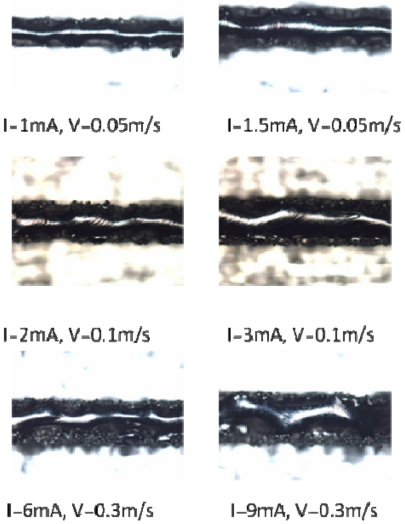
Comparison of experimental and simulated results

width-1 (μm) [experiments/simulations]

P/v	1200J/m	1800J/m
0.05m/s	420/450	506/490
0.1m/s	463/480	622/570
0.3m/s	550/540	660/600

Define line power input
P/v=UI/v
P: power
v: velocity

P/v=1200J/m P/v=1800J/m


I-1mA, V-0.05m/s
I-1.5mA, V-0.05m/s
I-2mA, V-0.1m/s
I-3mA, V-0.1m/s
I-6mA, V-0.3m/s
I-9mA, V-0.3m/s

width-2 (μm) [experiments/simulations]

P/v	1200J/m	1800J/m
0.05m/s	287/310	421/420
0.1m/s	326/360	466/480
0.3m/s	383/420	502/490

- The differences are caused by the simplifications of the model, e.g. treating powder bed as continuum and neglecting the molten pool flow.
- However, the simplified model could act as a useful tool for the fabrication parameter selection.

Experimental results come from our collaborators in Tsinghua University, China

Thermo-Calc Software

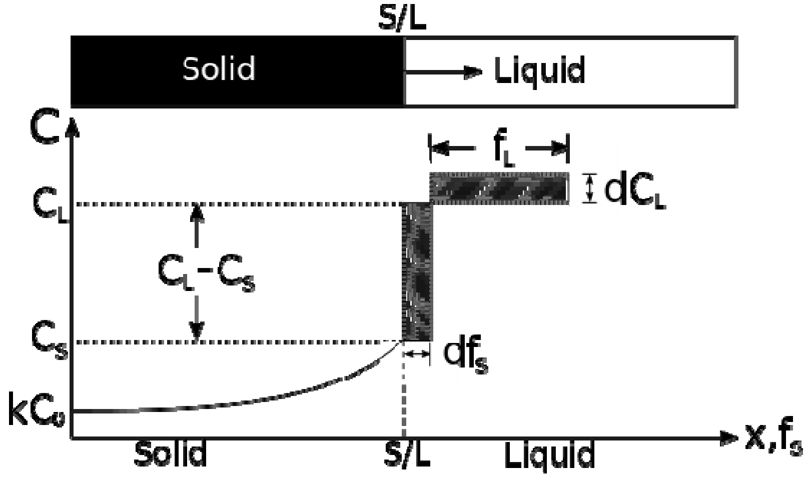
Thermo-Calc Software

❖ Powerful software package for a variety of thermodynamic calculations with <u>composition</u> and <u>temperature</u> as inputs including :

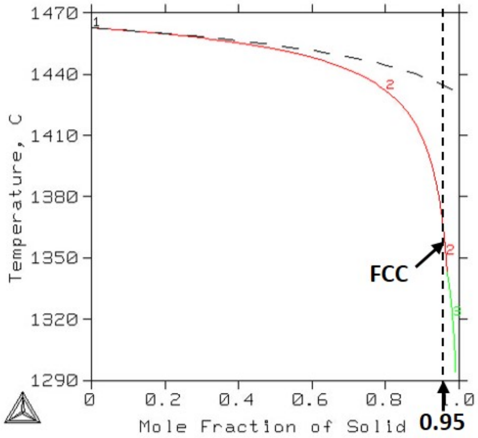
- ❑ Stable and meta-stable heterogeneous phase equilibria
- ❑ Amounts of phases and their compositions
- ❑ Thermochemical data such as enthalpies, heat capacity and activities
- ❑ Transformation temperatures, such as liquidus and solidus
- ❑ Driving force for phase transformations
- ❑ Phase diagrams (binary, ternary and multi-component)
- ❑ Solidification applying the Scheil-Gulliver model
- ❑ Thermodynamic properties of chemical reactions
- ❑ And much, much more…

Solidification: Scheil Model

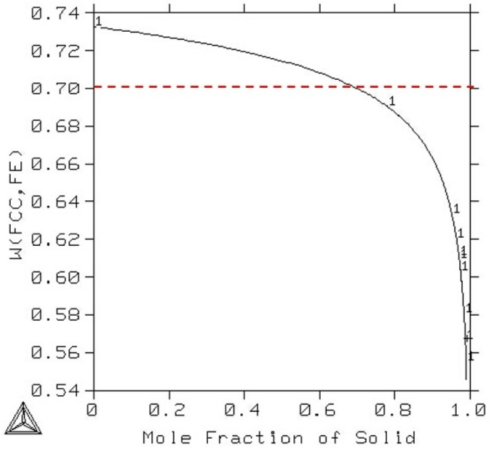
Solute redistribution by assuming local equilibrium at solid/liquid interface



Solid Fraction vs. Temp



Composition vs. Solid Fraction

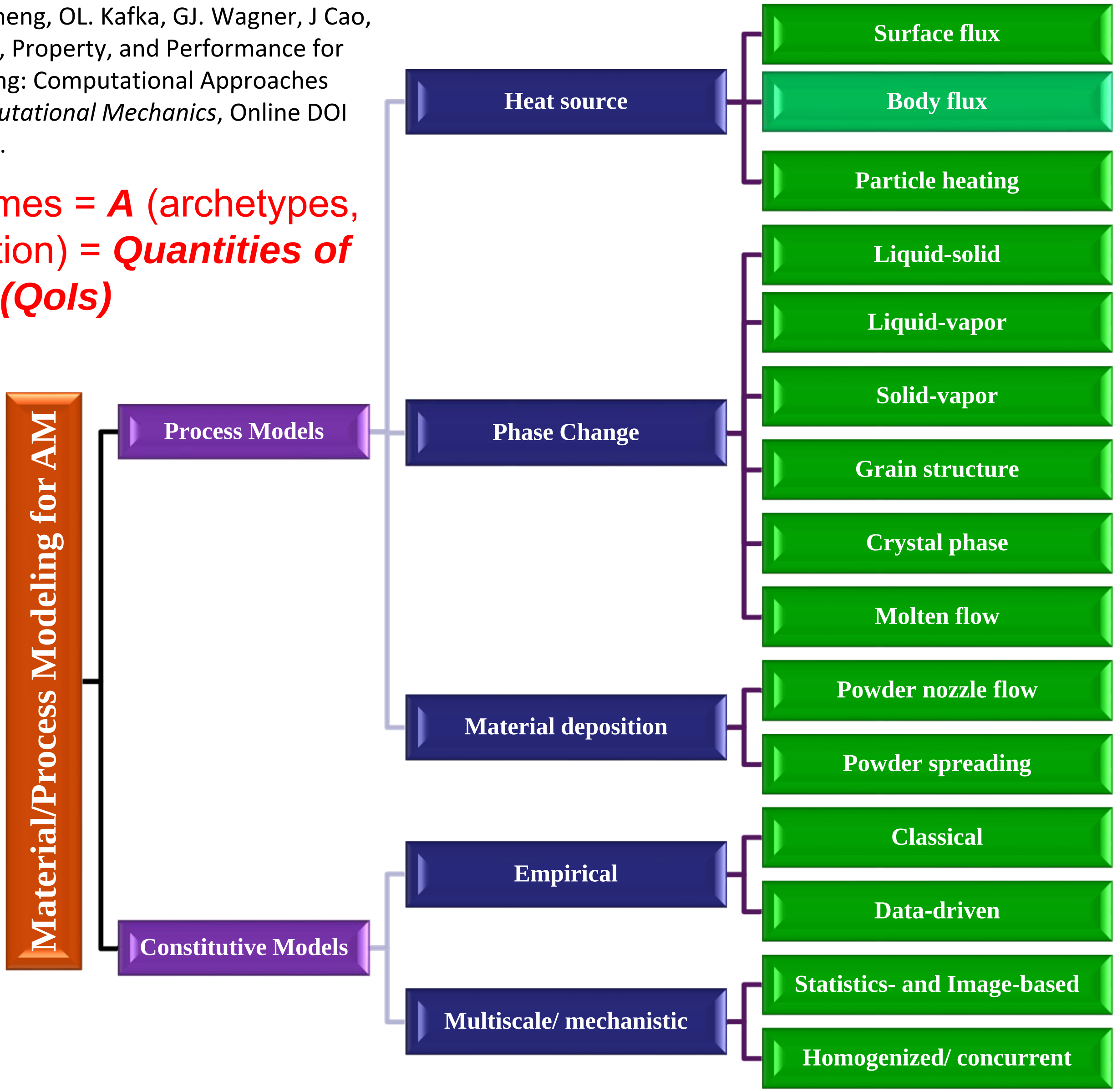


Multiscale Multiphysics Methodologies

J Smith, W Xiong, W Yan, S Lin, P Cheng, OL. Kafka, GJ. Wagner, J Cao, WK.Liu, “Linking Process, Structure, Property, and Performance for Metal-based Additive Manufacturing: Computational Approaches with Experimental Support,” *Computational Mechanics*, Online DOI 10.1007/s00466-015-1240-4, 2016.

Materials system genomes = ***A*** (archetypes, interactions, conformation) = ***Quantities of Interest (QoIs)***

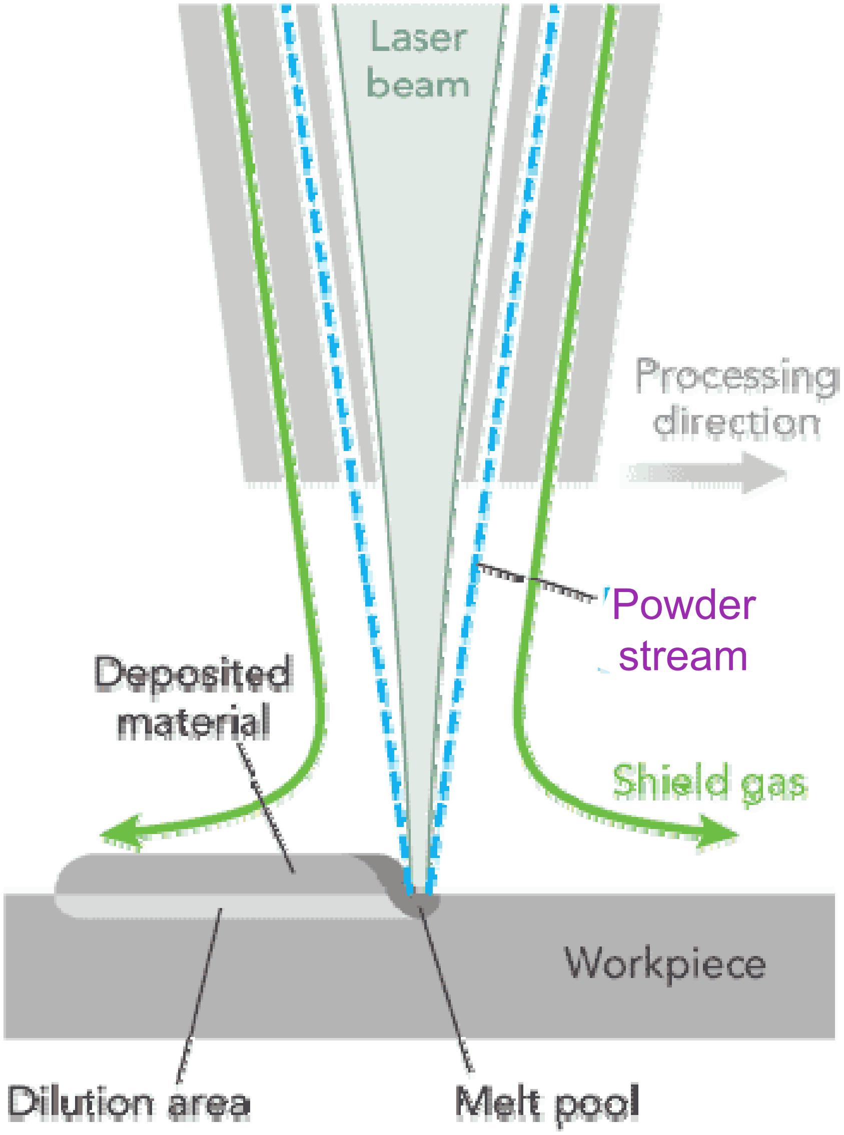
- Various sources of uncertainties
- Quantification of uncertainties
- Uncertainties propagation
- Uncertainty quantification (UQ) is the quantifying of the uncertainty in predicted ***QoIs***



- **Material/Process Modeling for AM**
  - **Process Models**
    - **Heat source**
      - **Surface flux**
      - **Body flux**
      - **Particle heating**
    - **Phase Change**
      - **Liquid-solid**
      - **Liquid-vapor**
      - **Solid-vapor**
      - **Grain structure**
      - **Crystal phase**
      - **Molten flow**
    - **Material deposition**
      - **Powder nozzle flow**
      - **Powder spreading**
  - **Constitutive Models**
    - **Empirical**
      - **Classical**
      - **Data-driven**
    - **Multiscale/ mechanistic**
      - **Statistics- and Image-based**
      - **Homogenized/ concurrent**

(Statistical) Process Parameters

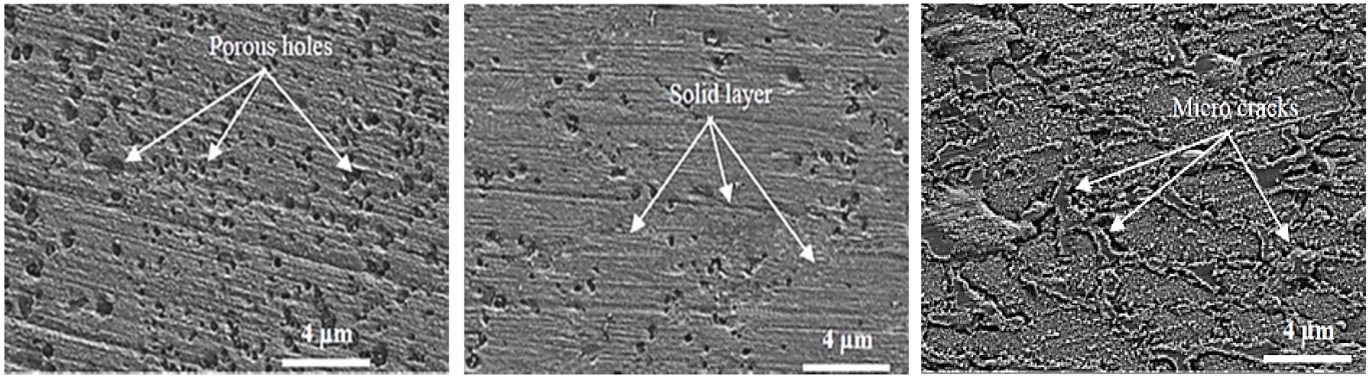
- **Powder Deposition Parameters**
  - **Powder Flow Rate**
  - **Shield Gas Flow Rate**
  - **Powder Shape/Size/Type**
  - **Nozzle Type**
- **Laser Parameters**
  - **Laser Spot Size**
  - **Laser Scanning Speed**
  - **Laser Power**
  - **Laser Type**
- **Geometric Parameters**
  - **Hatch Spacing**
  - **Layer Height**
  - **Build Geometry**
  - **Build Strategy**
- **Substrate Parameters**
  - **Substrate Surface Condition**
  - **Substrate Temperature**
  - **Substrate Size**



LENS Process to Microstructure

Question: $\text{Materials system } genomes = A(Archetypes, Interactions, \text{Conformation})$

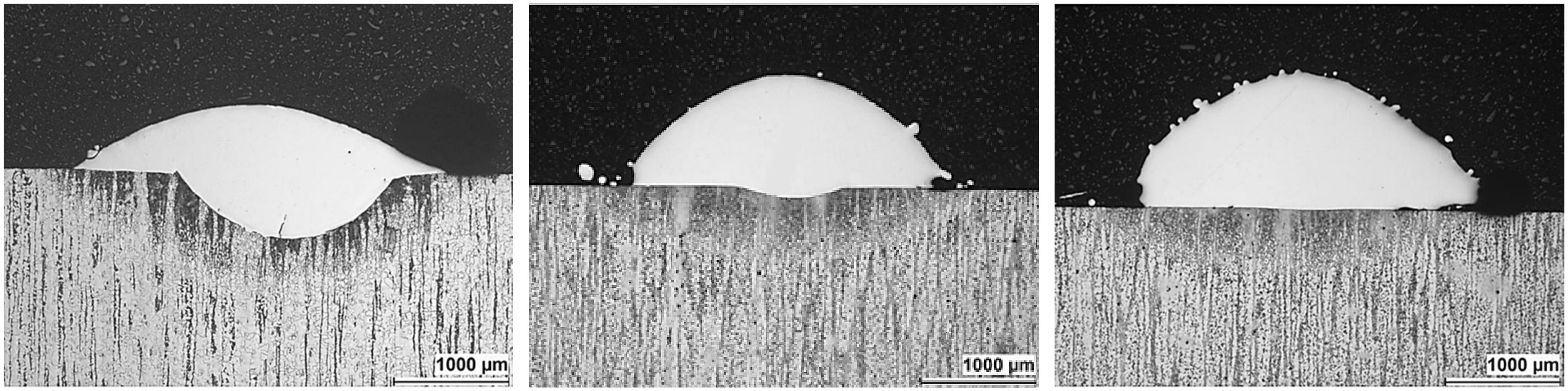
Effect of Powder Mass Flow Rate on Microstructure[1]



0.8 g/min 1.58 g/min 3.15 g/min

[2]

Effect of Powder Mass Flow Rate on Clad Quality



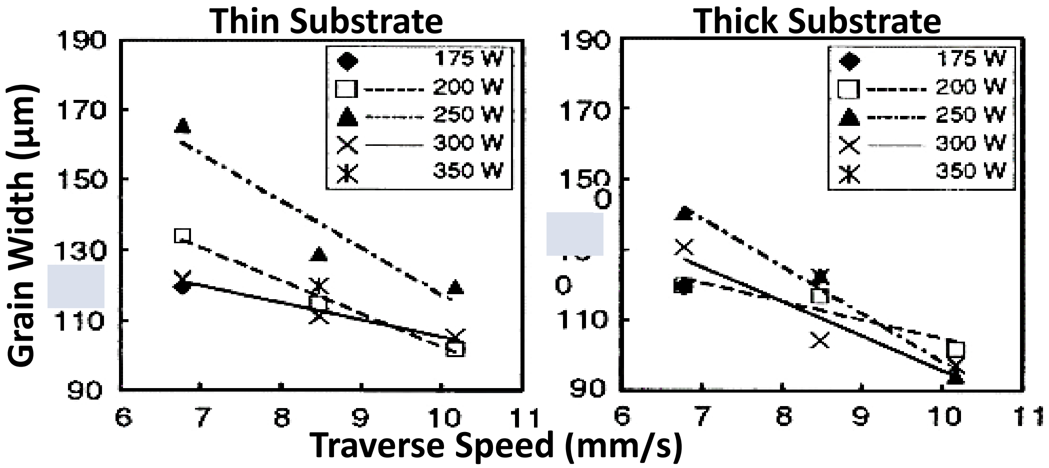
20 g/min 50 g/min 80 g/min

[1] Influence of Process Parameters in the DMD of H13 Tool Steel on Cu Alloy Substrate, Imran et al., Proceedings of the World Congress on Engineering Vol III, 2010
[2] Used with permission from DMG Mori

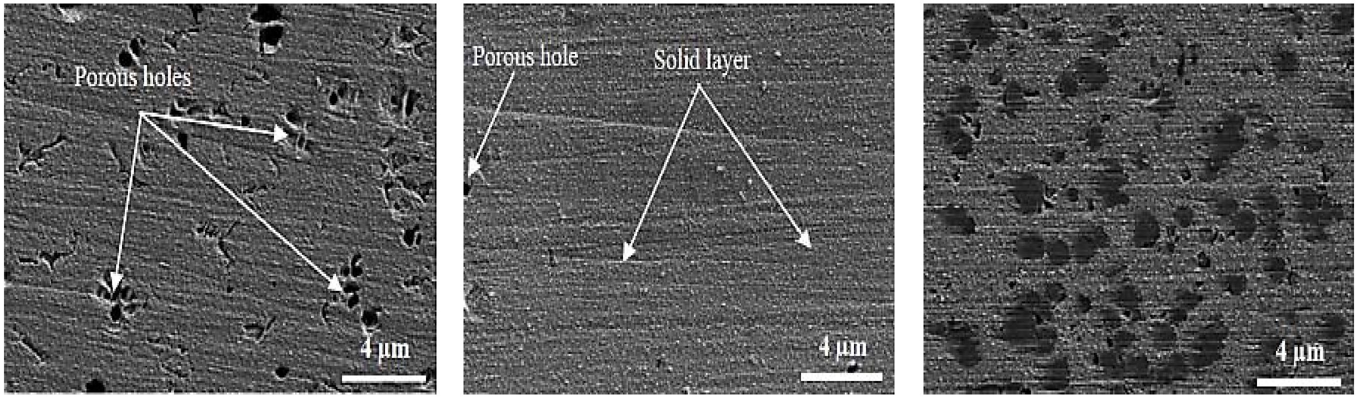
LENS Process to Microstructure

Question: $\mathbf{Materials\ system}\ \boldsymbol{genomes} = \boldsymbol{A}(\boldsymbol{Archetypes}, \boldsymbol{Interactions}, \mathbf{Conformation})$

Effect of Scan Speed and Laser Power on Ti-6Al-4V Build Microstructure



Effect of Laser Power on Microstructure [2]



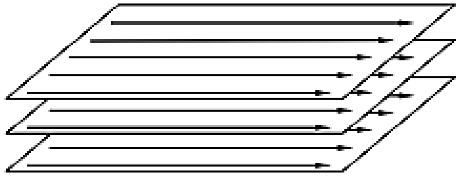
4 kW **3 kW** **2 kW**

[1] *The effect of laser power and traverse speed on microstructure, porosity and build height in laser-deposited Ti-6Al-4V, Kobryn, Scripta Materialia, 2000*
[2] *Influence of Process Parameters in the Direct Metal Deposition of H13 Tool Steel on Copper Alloy Substrate, Imran,* Proceedings of the World Congress on Engineering, *2010*

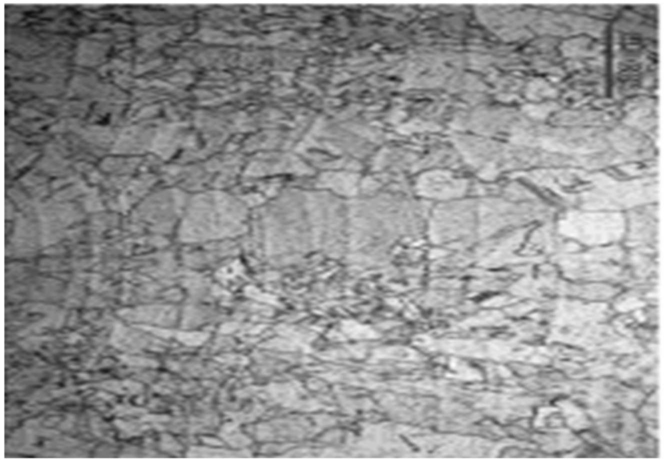
LENS Process to Microstructure

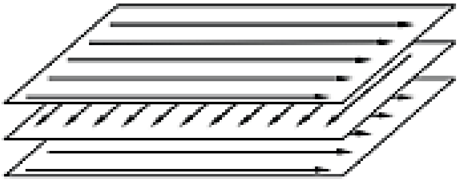
Question: Materials system $genomes = A(Archetypes, Interactions, \mathrm{Conformation})$

Effect of Deposition Direction on Microstructure

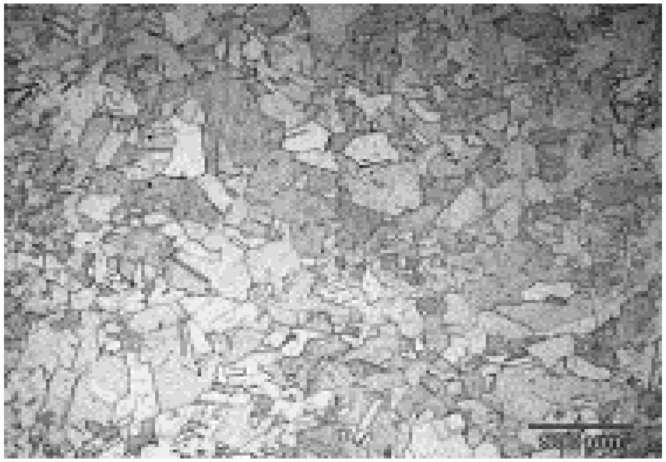


Single Direction Scanning



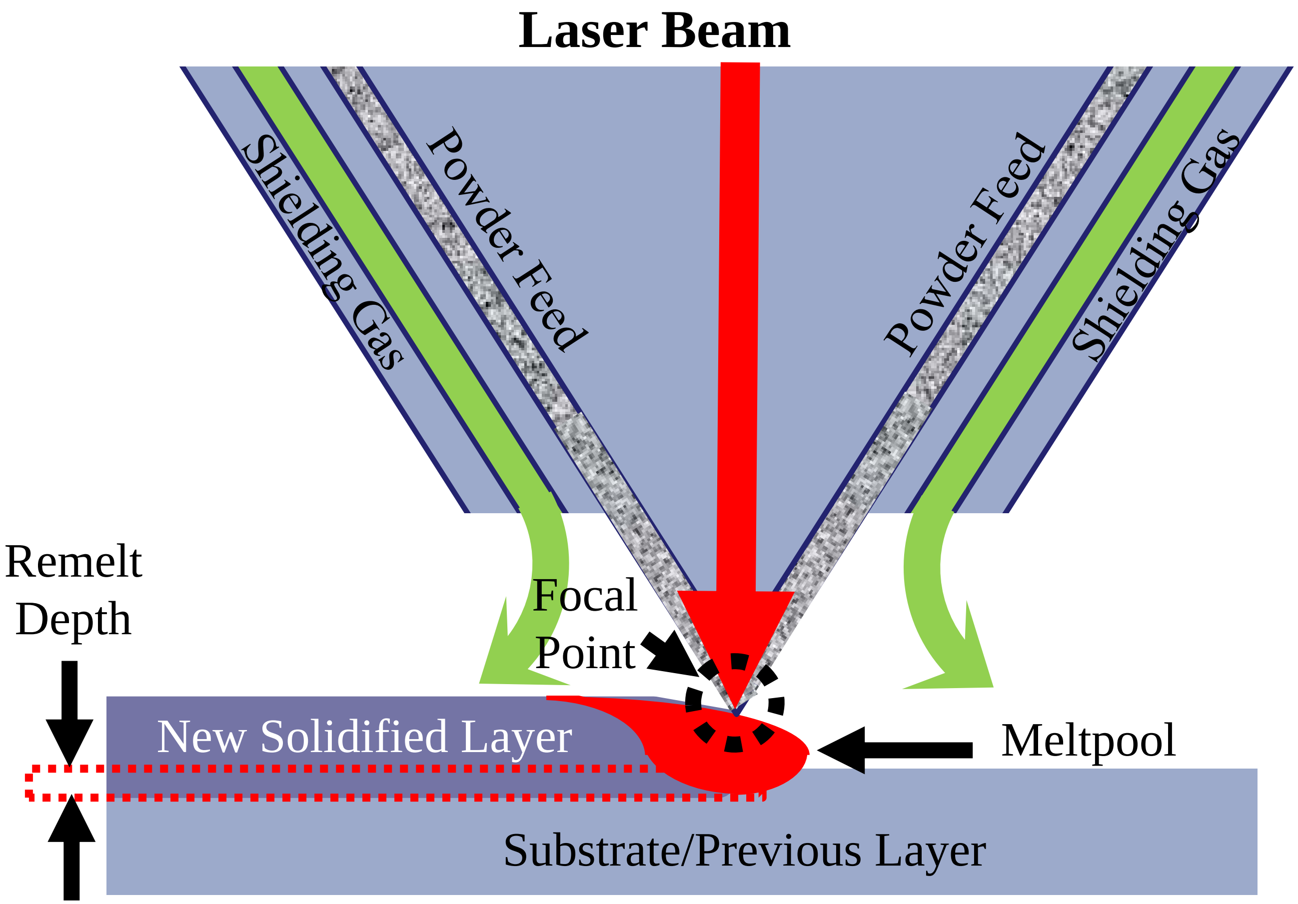


Cross Direction Scanning



The effect of laser scanning path on microstructures and mechanical properties of laser solid formed nickel-base superalloy Inconel 718, Liu, Journal of Alloys and Compounds, 2011

Laser Engineered Net Shaping



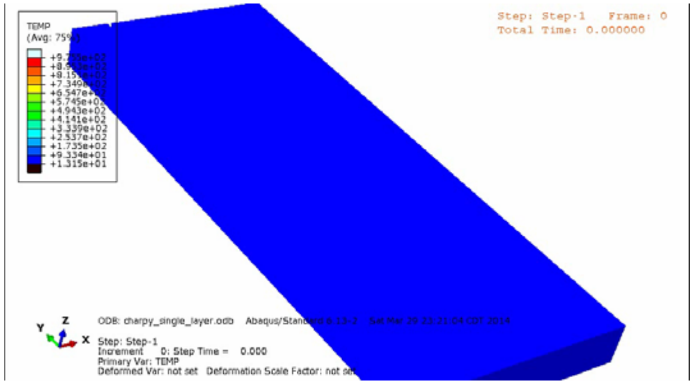
J Smith, W Xiong, W Yan, S Lin, P Cheng, OL. Kafka, GJ. Wagner, J Cao, WK.Liu, "Linking Process, Structure, Property, and Performance for Metal-based Additive Manufacturing: Computational Approaches with Experimental Support," ***Computational Mechanics*****, Online DOI 10.1007/s00466-015-1240-4, 2016.**

Integration of toolpaths into the Thermal modeling

Combining experimental toolpath with thermal analysis

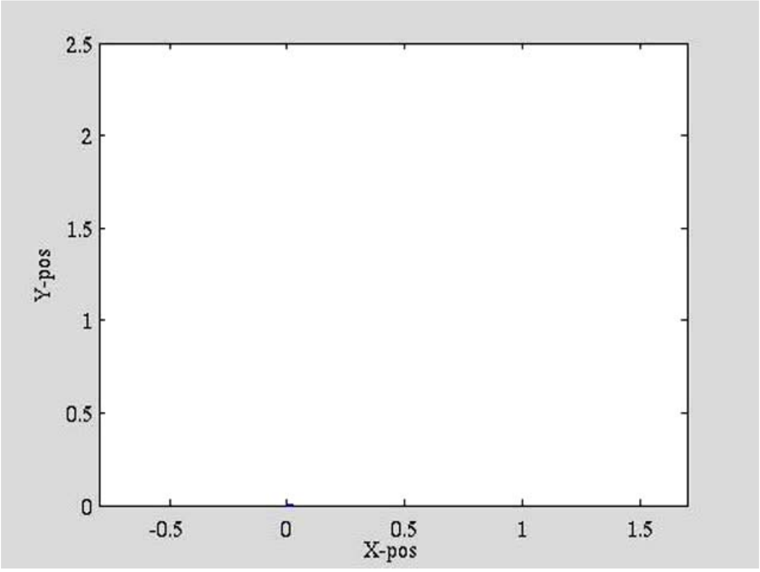
- Arbitrary toolpaths
- Better cooling rate prediction
- Reduction of preprocessing time for simulations

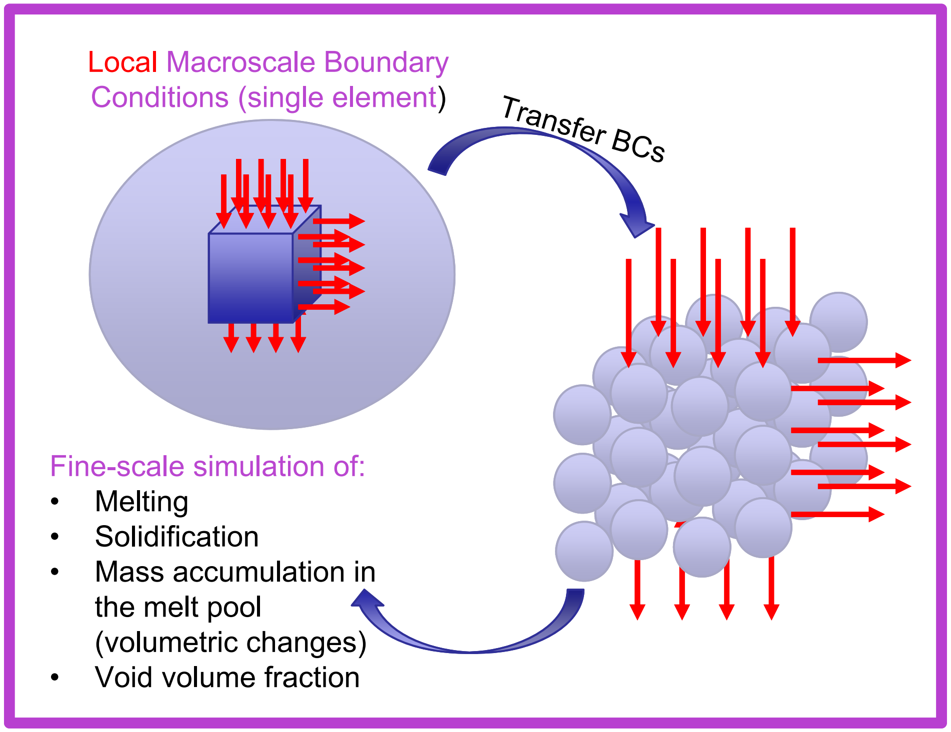
Thermal Model w/ Experimental Toolpath



Extracted Toolpath from LENS Machine Syntax

Laser On
Laser Off





Local Macroscale Boundary Conditions (single element)

Fine-scale simulation of:

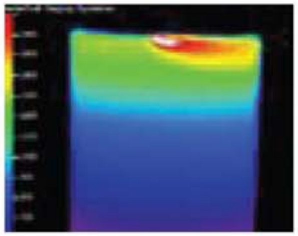
- Melting
- Solidification
- Mass accumulation in the melt pool (volumetric changes)
- Void volume fraction

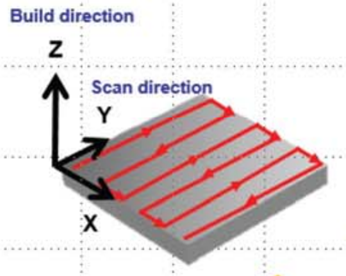
Integrated computational toolset approach

Integrated computational toolset approach for understanding process-structure-property relations for AM processes.

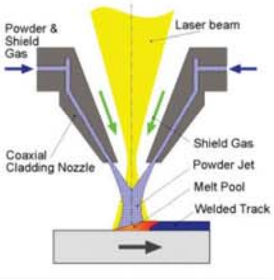
Calibration of Thermal Response

Thermal/Energy History:
IR Camera, Calorimeter, Thermocouple



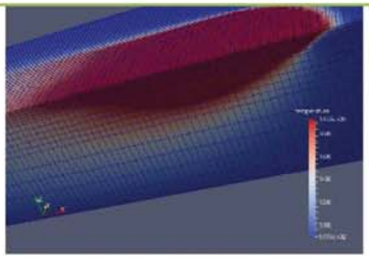


Process Parameters:
Laser Power, Laser Speed, Particle Flowrate, etc.



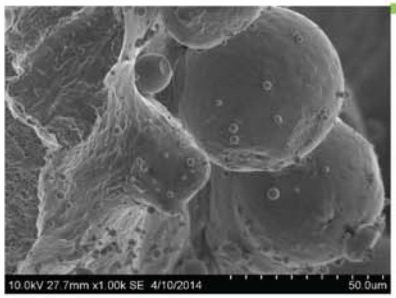
Experimental Interface and Analysis Input Parameters

Macroscale Thermal Modeling



Microstructure Evolution Analysis

Microstructure:

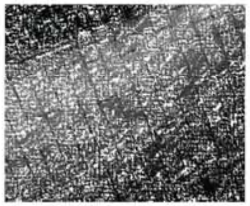


Microstructure Prediction Software:
- Interface tracking
- Particle interaction
- Melting/Resolidification
- Fluid-structure interaction

Predicted Properties:
- Elastic Properties
- Ultimate Tensile Strength
- Ductility
- Residual Stress

Predicted Microstructure:

Local non-equilibrium solution

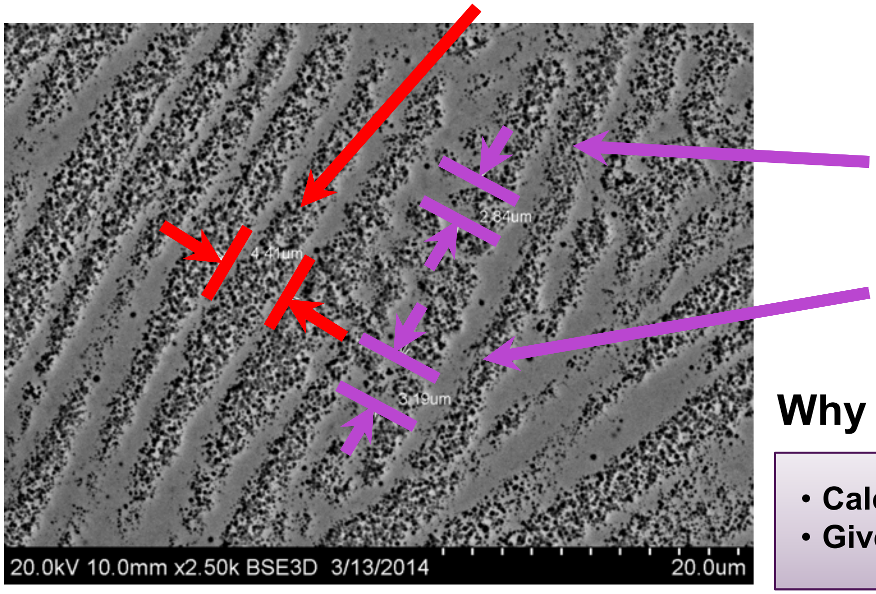


- Porosity
- Anisotropy
- Surface Roughness

Analysis Outputs

Microstructure Conformation

Primary Dendrite Spacing (4.41um)



Secondary Dendrite Arm Spacing

$$\lambda = 80\underbrace{\dot{T}^{-0.33}}_{\text{From thermal model}}$$

λ_1 = 2.84 μm
Cooling rate ~ 2.47×10^4 K/s

λ_2 = 3.19 μm
Cooling rate ~ 1.74×10^4 K/s

Why 2nd Arm Dendrite Spacing?

- **Calculate cooling rate**
- **Gives sense of mechanical properties**

Now, Process Parameters Drive Microstructure and Material Behavior

Cooling Rate Calculation

- **Latent heat during solidification**
- **Input for solidification modeling**

Microstructure Control

- **Grain size**
- **Transfer columnar dendrites to equiaxed dendrites**

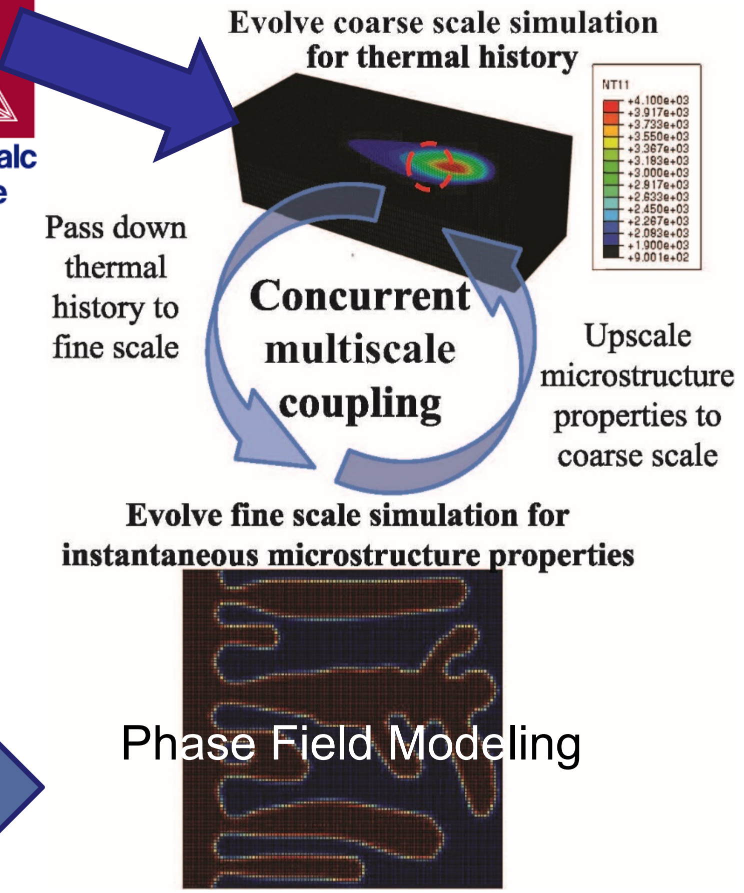
Thermodynamically Consistent Microstructure Prediction

Smith, Xiong, Cao, and Liu, "*Thermodynamically Consistent Microstructure Prediction of Additively Manufactured Materials*," *Computational Mechanics*, Online DOI 10.1007/s00466-015-1243-1, 2016.

Microstructure Evolution Analysis → **Thermo-Calc Informed Concurrent Multiscale Modeling** ← Analysis Outputs

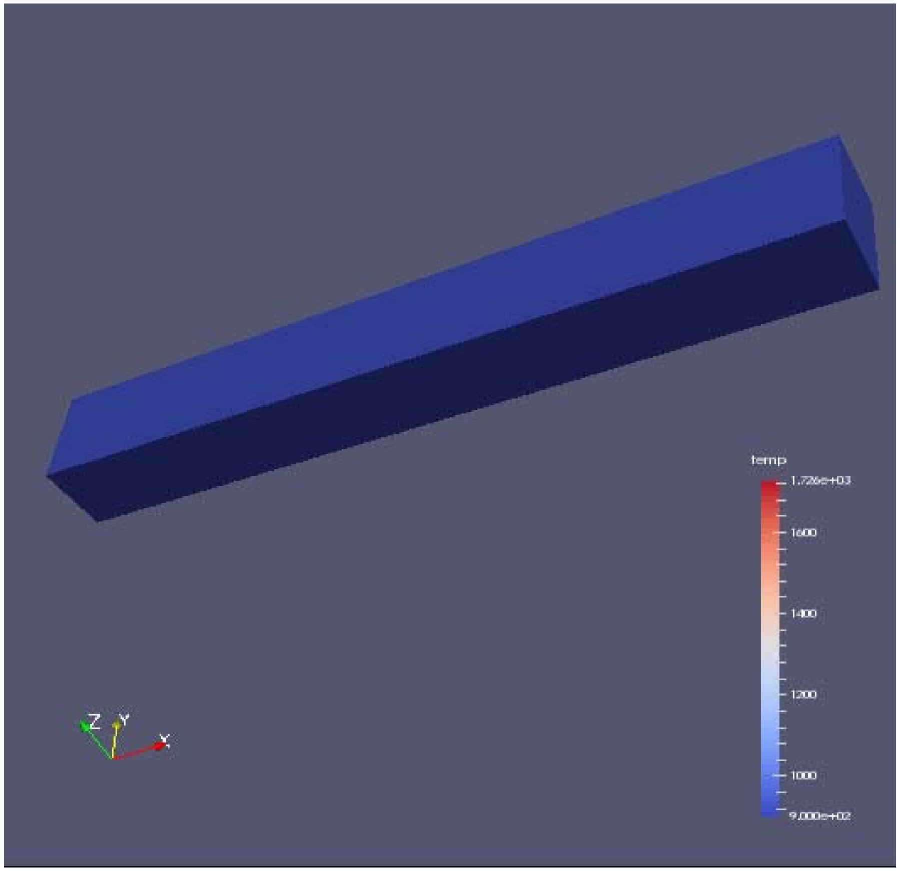
Thermo-Calc Software

- Thermodynamically Consistent Properties
- Rapid Local Microstructure Prediction
- Energetically Consistent Solution

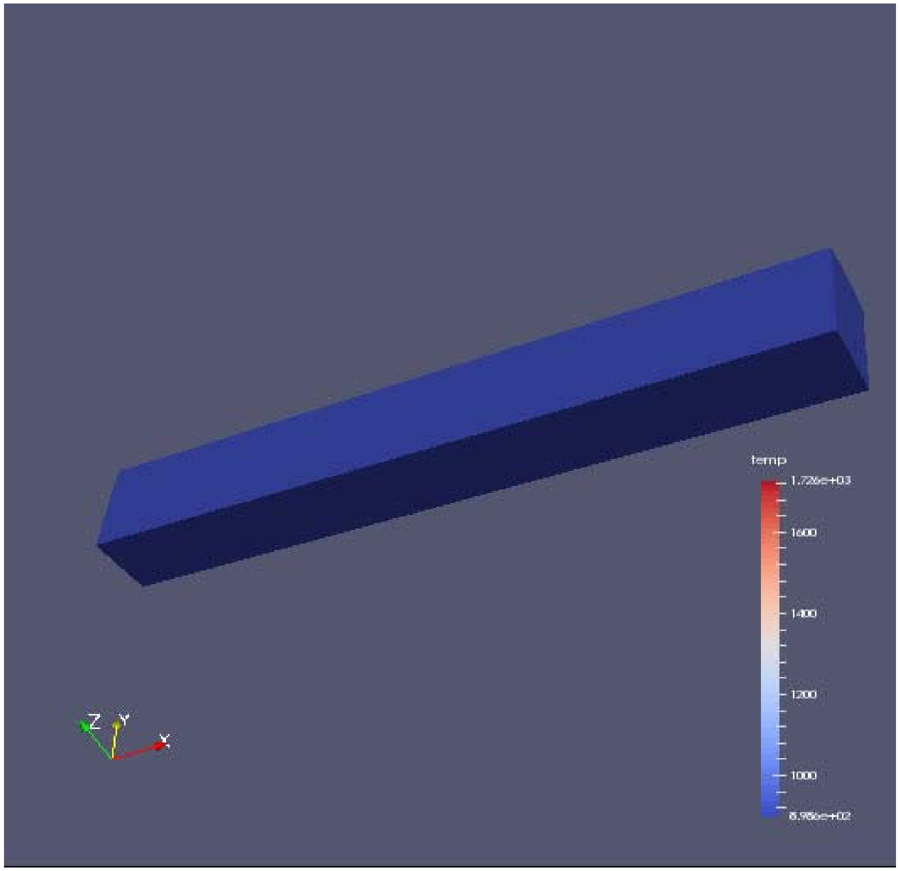


Current Simulation Efforts at Northwestern

Traditional Experimentally Derived Properties



ThermoCalc derived properties



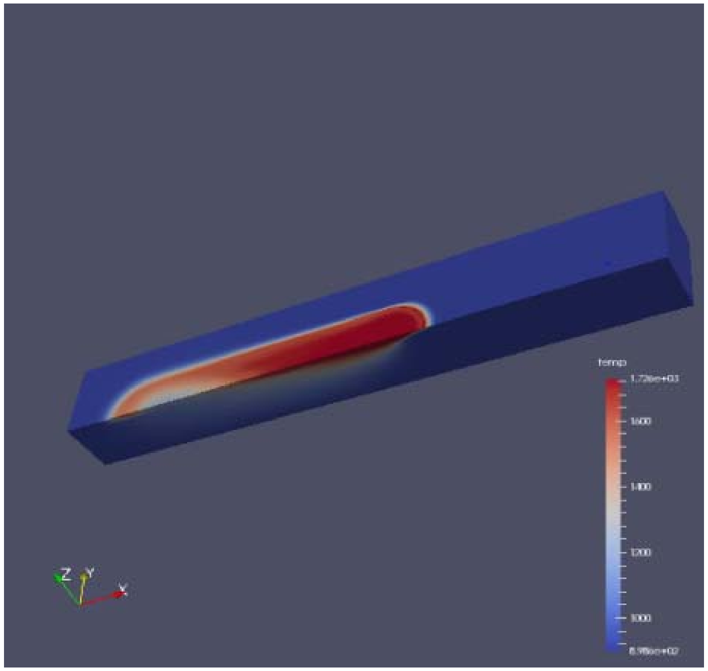
Red = Melting Region
Blue = Solid Region

Research Efforts

Thermo-Calc provides thermodynamic property and phase fraction evolution laws

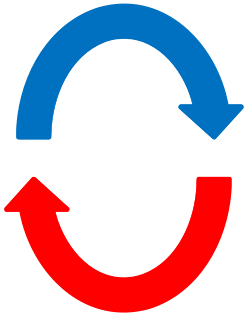
Does NOT provide a image or “snapshot” of evolved microstructure

Goal: Develop a concurrent multiscale model to capture high resolution microstructure evolution throughout AM build process

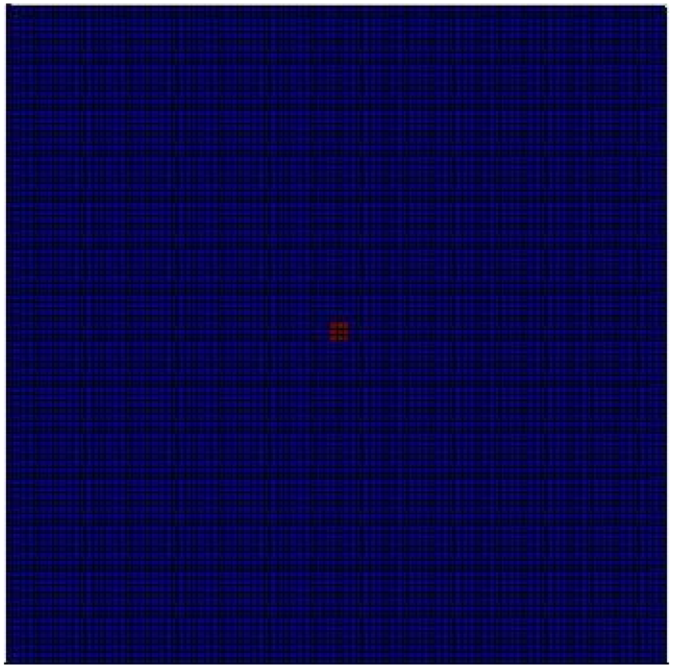


Large Scale Thermal Modeling

Thermal Information:
Cooling rate,
temperature gradient etc.



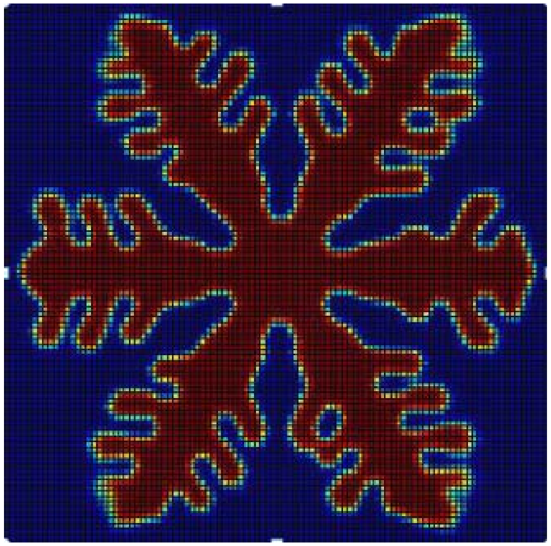
Microstructure Properties
Conductivity, latent heat
etc.



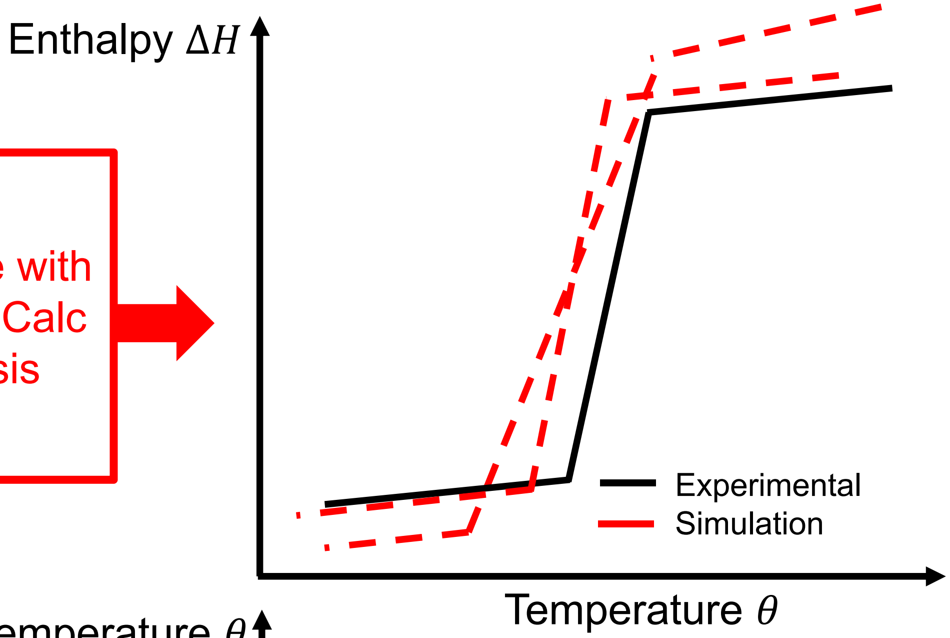
Fine Scale Phase Field Computation

Concurrent Coupling Research Efforts

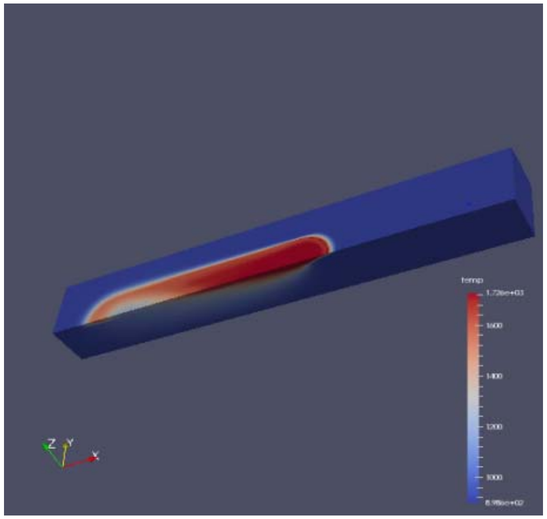
Fine Scale Phase Field



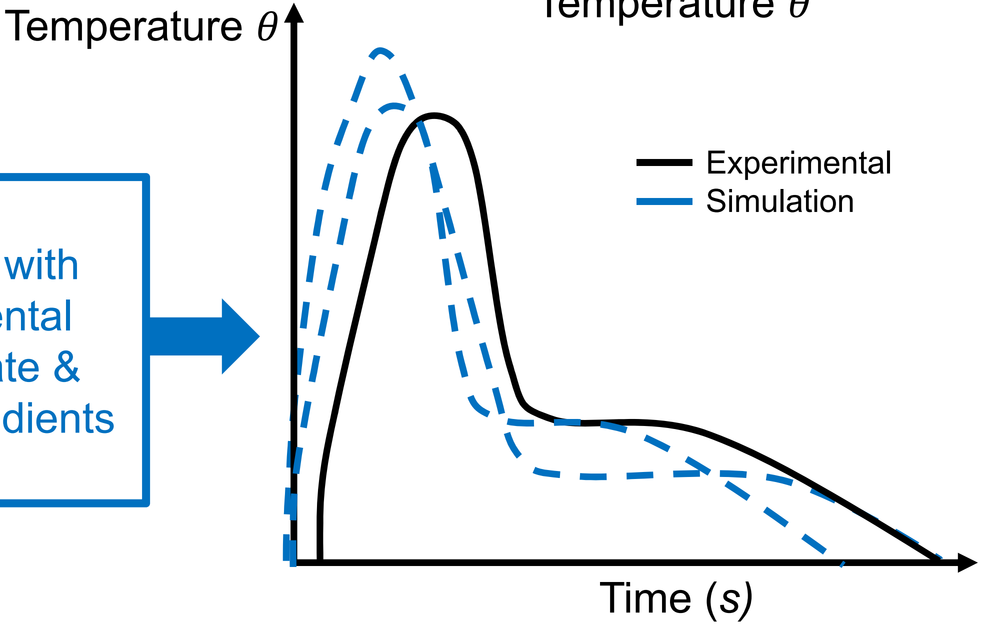
Calibrate with Thermo-Calc analysis



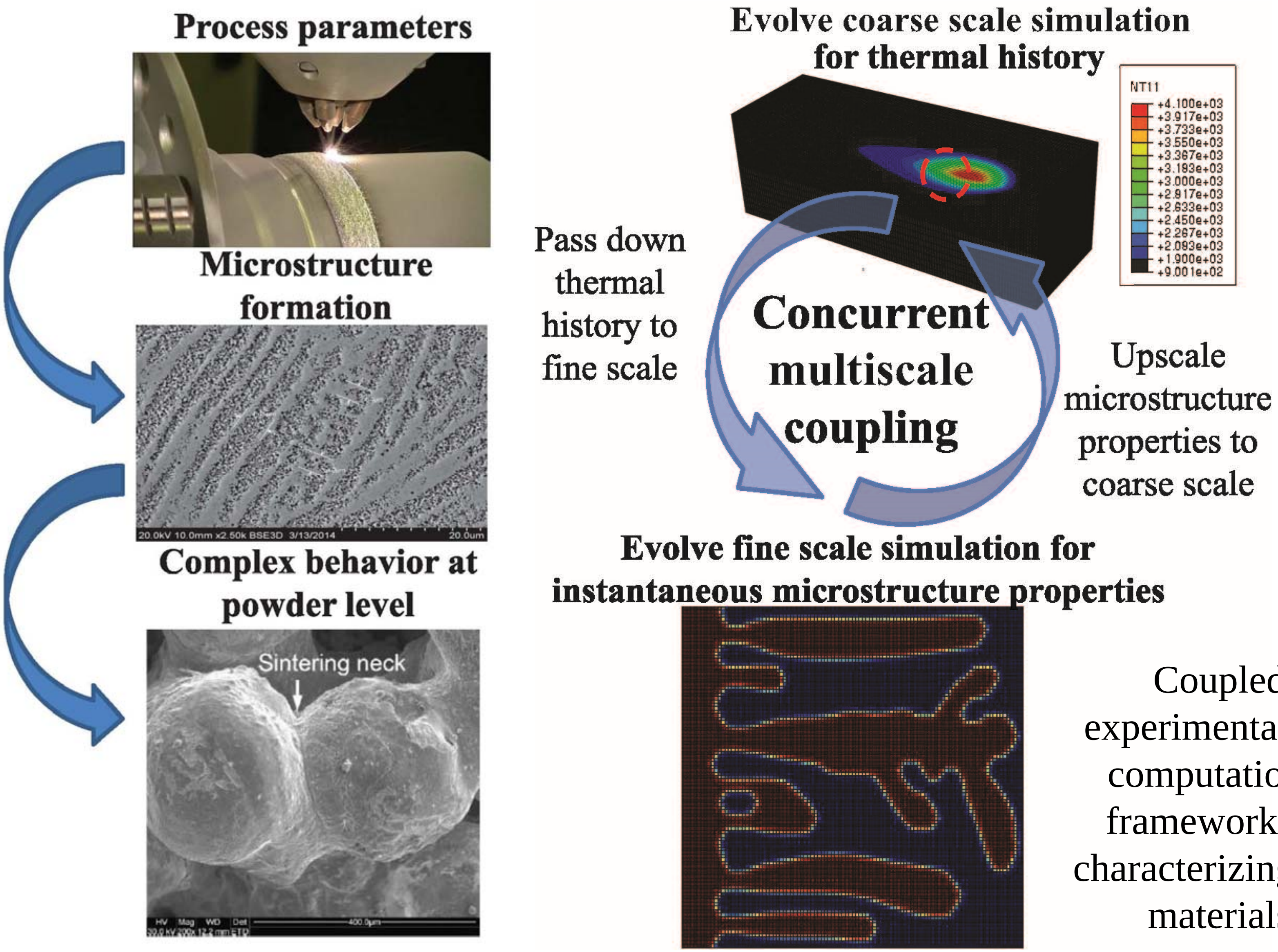
Large Scale Thermal Model



Calibrate with experimental cooling rate & thermal gradients



Coupled experimental and computational framework



Process parameters

Microstructure formation

Complex behavior at powder level

Evolve coarse scale simulation for thermal history

Pass down thermal history to fine scale

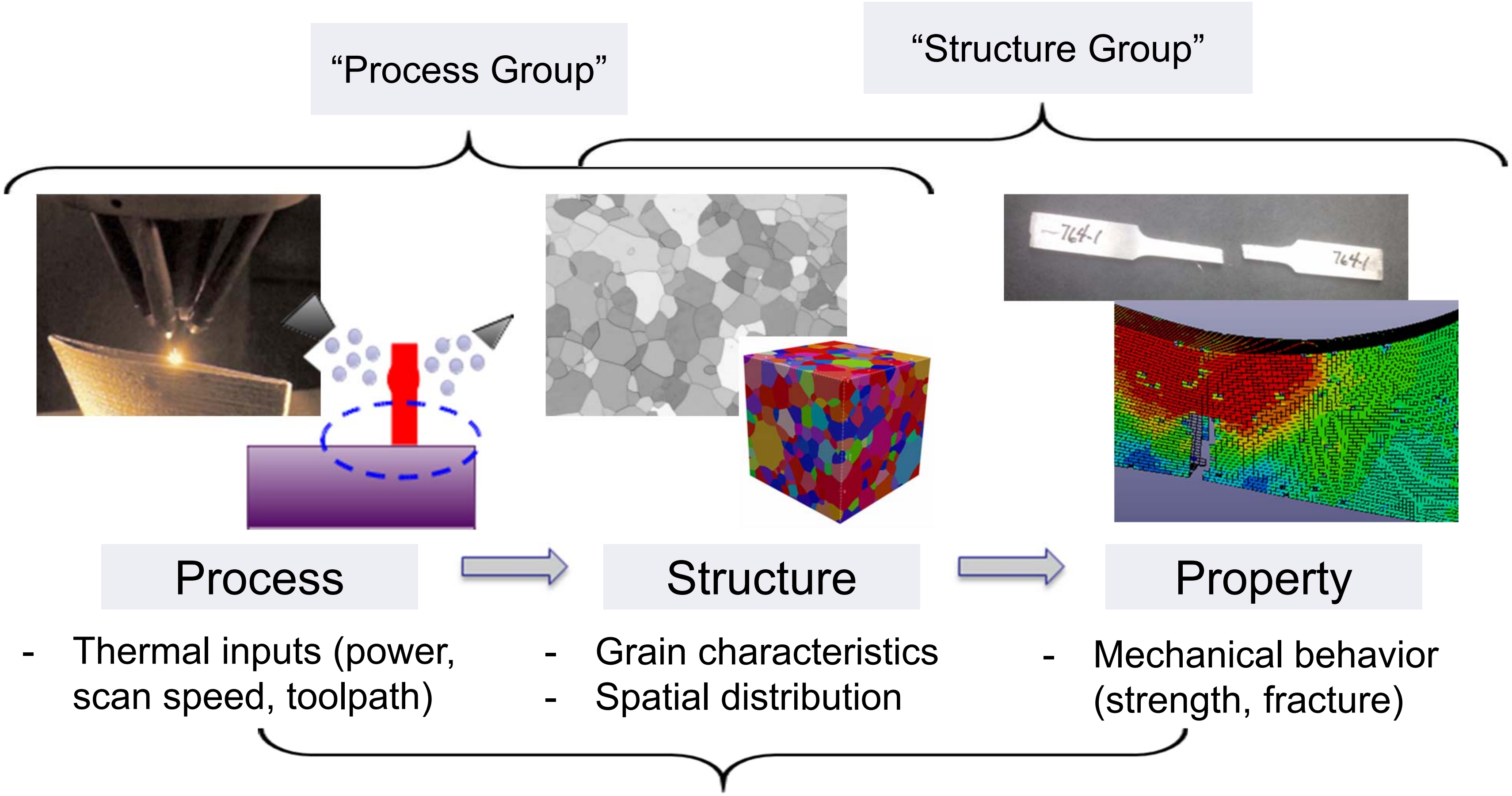
Concurrent multiscale coupling

Upscale microstructure properties to coarse scale

Evolve fine scale simulation for instantaneous microstructure properties

Coupled experimental and computational framework for characterizing AM materials

Link between Process-Structure & Structure-Property



“Process Group”

“Structure Group”

Process → Structure → Property

- Thermal inputs (power, scan speed, toolpath)

- Grain characteristics
- Spatial distribution

- Mechanical behavior (strength, fracture)

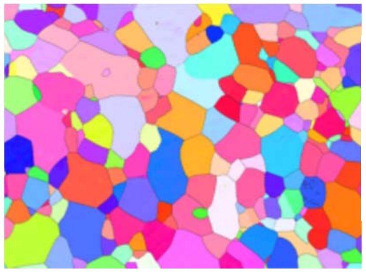
Design loop: Determine optimal processing parameters for performance

Laser Engineered Net Shaping: Manufacturing Technologies. Sandia National Laboratories.
Francois, M. Workshop on Predictive Theoretical and Computational Approaches for Additive Manufacturing, October 7-9 2015, Washington D.C.

Statistical reconstruction

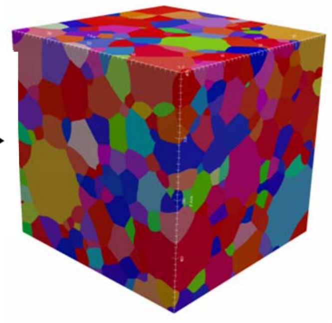
Mesoscale SVE: generate grains from images

- Construct ray of 3D SVEs from 2D images of grains
- Determine statistical relationships between **grain structure** and **mechanical properties** in SVEs through crystal plasticity



2D EBSD image data

→



Dream 3D mesocale SVE

→

What **grain characteristics** are important for the **properties** we're interested in?

Grain size
Orientations

↔

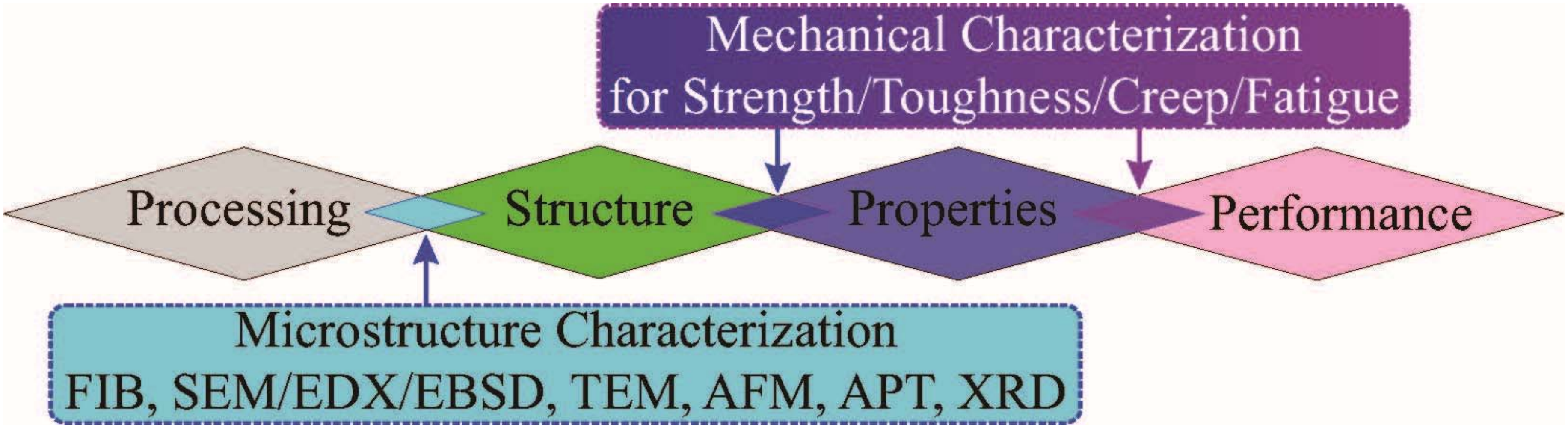
Strength
Fatigue

Sensitivity Analysis

J Smith, W Xiong, W Yan, S Lin, P Cheng, OL. Kafka, GJ. Wagner, J Cao, WK.Liu, "Linking Process, Structure, Property, and Performance for Metal-based Additive Manufacturing: Computational Approaches with Experimental Support," *Computational Mechanics*, Online DOI 10.1007/s00466-015-1240-4, 2016.

Zeliang Liu, M.A. Bessa, Wing Kam Liu, "Self-consistent clustering analysis: an efficient multi-scale scheme for inelastic heterogeneous materials," Submitted

AM Characterization Experiments



Mechanical Characterization
for Strength/Toughness/Creep/Fatigue

Processing
Structure
Properties
Performance

Microstructure Characterization
FIB, SEM/EDX/EBSD, TEM, AFM, APT, XRD

FIB: Focused Ion Beam,
SEM: Scanning Electron Microscopy,
EDX: Energy-Dispersive Xray spectroscopy,
EBSD: Electron Backscatter Diffraction,
TEM: Transmission Electron Microscopy,
AFM: Atomic Force Microscopy,
APT: Atom Probe Tomography,
XRD: Xray Diffraction.

J Smith, W Xiong, W Yan, S Lin, P Cheng, OL. Kafka, GJ. Wagner, J Cao, WK.Liu, “Linking Process, Structure, Property, and Performance for Metal-based Additive Manufacturing: Computational Approaches with Experimental Support,” *Computational Mechanics*, Online DOI 10.1007/s00466-015-1240-4, 2016.

Integration of Materials Design for Digital 3D Structures

Wing Kam Liu, et al., “Complexity science of multiscale materials via stochastic computations,” International Journal for Numerical Methods in Engineering, Volume 80, Issue 6, 5 - 12 November 2009, Pages: 932-978, 2009.

Shan Tang, Adrian M. Kopacz, Stephanie Chan, Gregory B. Olson, Wing Kam Liu, “Concurrent Multiresolution Finite Element: Formulation and Algorithmic Aspects,” Computational Mechanics, 2013, 52:1265–1279.

Shan Tang, Adrian M Kopacz, Stephanie Chan, Greg Olson, Wing Kam Liu, “Three-dimensional Ductile Fracture Analysis with a Hybrid Multiresolution Approach and Microtomography,” Journal of the Mechanics and Physics of Solids, 2013, 2108–2124.

S. O'Keeffe, S. Tang, AM Kopacz, J. Smith, DJ Rowenhorst, G. Spanos, WK Liu, GB Olson, Multiscale Ductile Fracture Integrating Tomographic Characterization and 3D Simulation, Acta Materialia, 82, (2015), 503-510.

Design Research Tools Consortium

PI: G.B. Olson

Northwestern University & QuesTek

Co-PI: Wing Kam Liu

Fracture Toughness Simulator

D 3-D digital structure

ONR

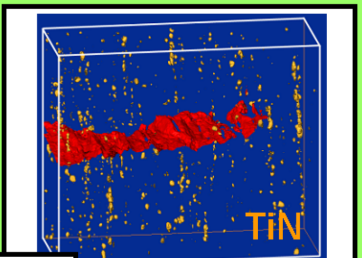
DARPA

Design Research Tools

NRL Atlas

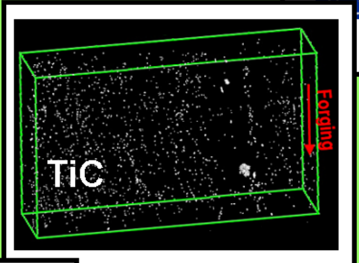
matCAT Characterization & Visualization Toolset

FSL/LOM Tomography [Pollock, Olson]
Toughness, Fatigue Strength [Olson, Kern]



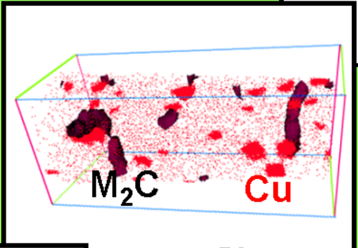
Ductile Fracture [Moran, Liu, Parks]
Fatigue Nucleation [McDowell, Olson]

FSL/FIB Tomography [Pollock]
Shear Instability [Olson, Kern]

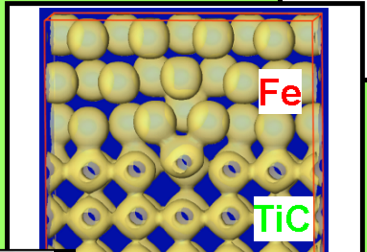


Microvoid Shear [Moran, Liu, Parks]
Fatigue Propagation [McDowell]

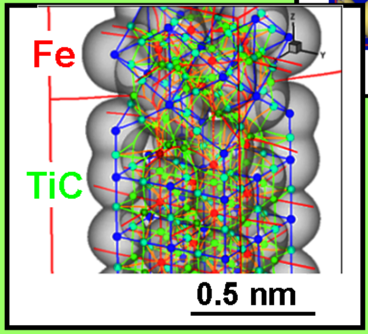
LEAP Tomography [Seidman]
Yield Strength [Olson, Kern]



Transformation Toughening [Parks, Olson]
Precipitation Strengthening [Voorhees, Wang, Jou]



Semicoherent IPB Adhesion [Freeman, Jerome, Wang]



Bond Topological S/P Relations [Eberhart]

DFrac-3D

PrecipiCalc-3D

FLAPW

TECD

iSIGHT/CMD Integration

QuesTek®
INNOVATIONS LLC

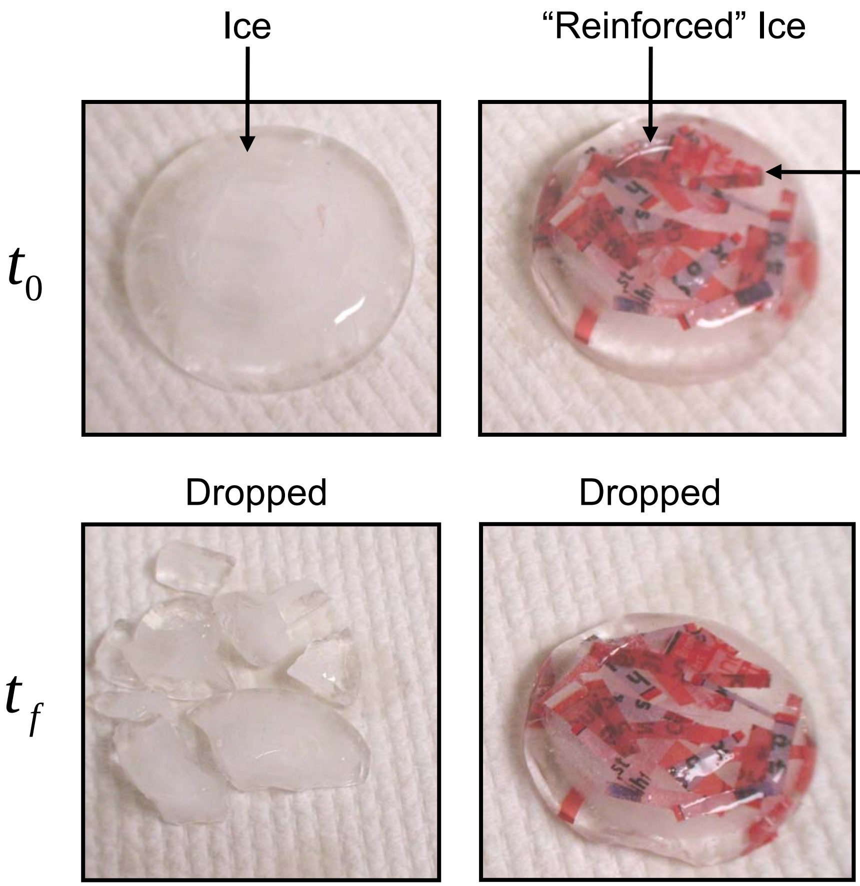
What are Genomes and Archetypes?

Why do we care?

Genome: Resistance to Breaking

Archetypes: 1) ice 2) paper

A simple demonstration



Newspaper ⟷ Random conformation

Multiscale

Reinforcement, interaction dictate the genome

Genome changes due to addition of archetypes

Experiment was performed by Professor Yip Wah Chung, Northwestern, 2003

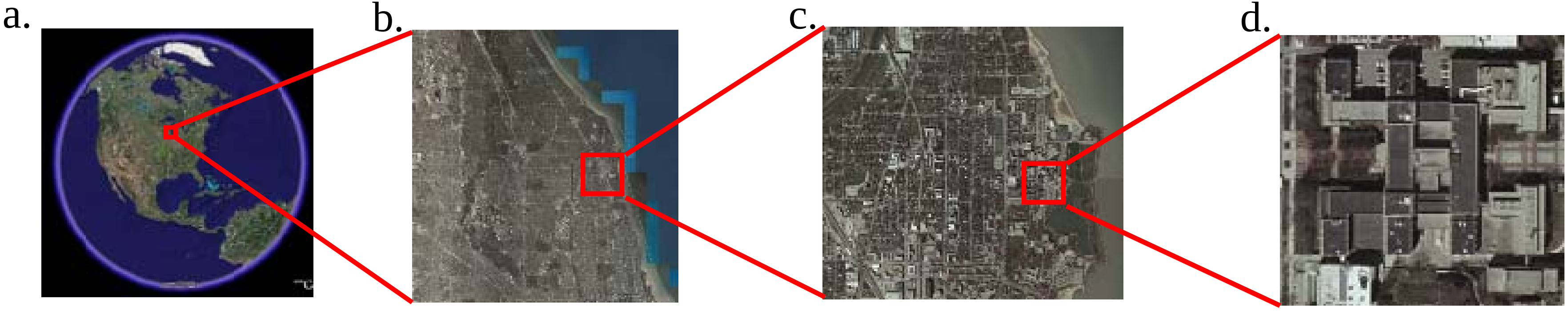
SM. Greene, Y. Li, W. Chen, WK. Liu, "The archetype-genome exemplar in molecular dynamics and continuum mechanics," Computational Mechanics, 2013.

McCormick

Northwestern Engineering

Multiresolution and Microstructure

Increasing Image Resolution



Small Number of pixels per km^2 – suitable for a global image

More resolution – cities can be observed

Increasing resolution – buildings can be observed

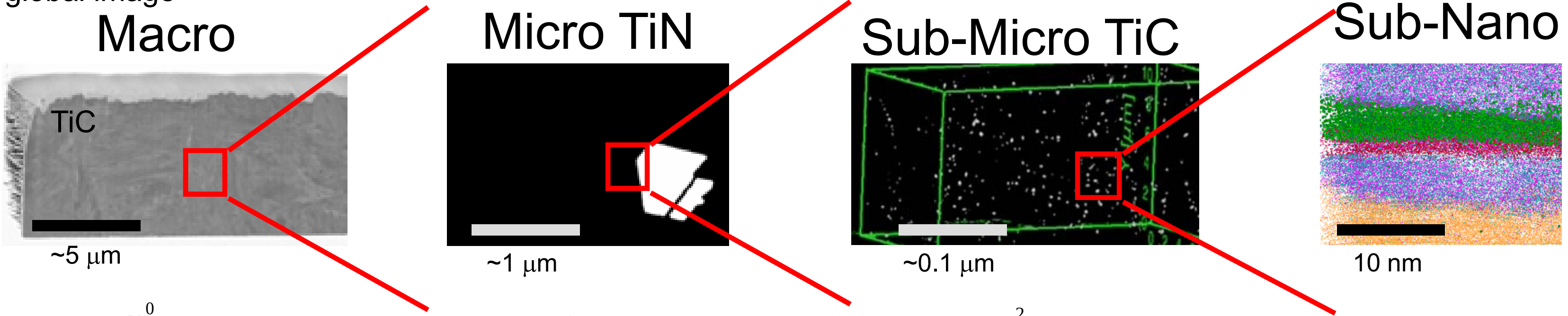
Northwestern University - a fine institution

Macro

Micro TiN

Sub-Micro TiC

Sub-Nano



~5 µm

~1 µm

~0.1 µm

10 nm

$\underline{u}^0$

Small Number of degrees of freedom – suitable for average behavior

$\underline{u}^1$

Discrete behavior of TiN primary inclusions begins to be observed

$\underline{u}^2$

Discrete behavior of TiC secondary particles is observed

$\underline{u}^3$

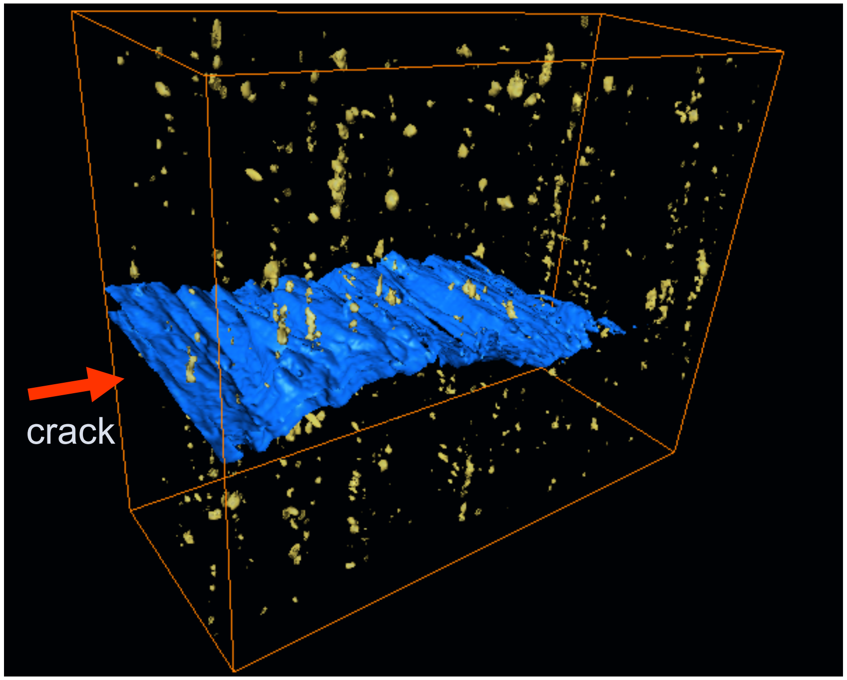
Very fine resolution – material interface is observed

Increasing Constitutive Resolution

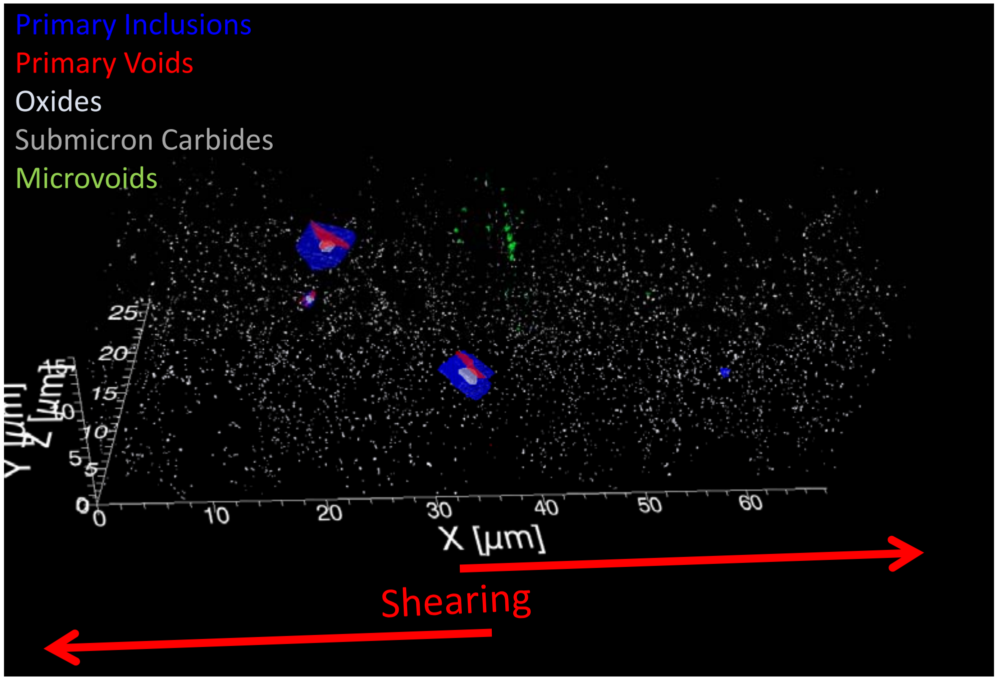
To & Liu et al., Materials integrity in microsystems: a framework for a petascale predictive-science-based multiscale modeling and simulation system, Computational Mechanics, 2008.

Liu et al., Complexity science of multiscale materials via stochastic computations,” International Journal for Numerical Methods in Engineering, 2009.

ONR/DAPRA D3D: Ultra High Strength Alloys



Mod4330 Crack tip specimen #1:
Primary particles (yellow) near crack tip
Reconstruction area: 633x516x259 μm^3
Averaged: 2.857 μm
Spacing: 16 μm
Volume fraction: 1.756%

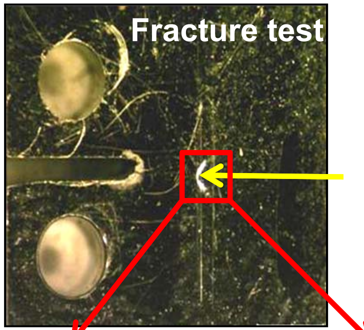


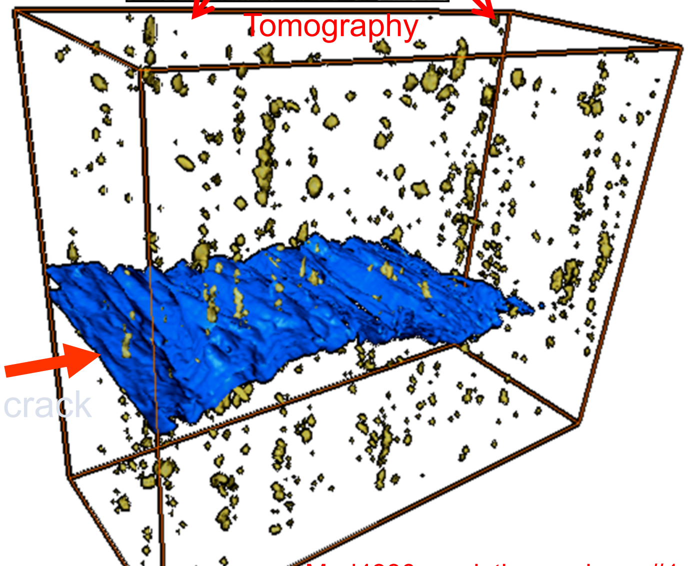
Mod4330 shear specimen:
Secondary particles (white dots) inside shear band
Reconstruction area: 70x15x28μm^3
Averaged: 0.117035 μm
Spacing: 2 μm
Volume fraction: 0.0384%

Courtesy of Stephanie Chan (Olson's group), and HJ Jou (QuesTek)

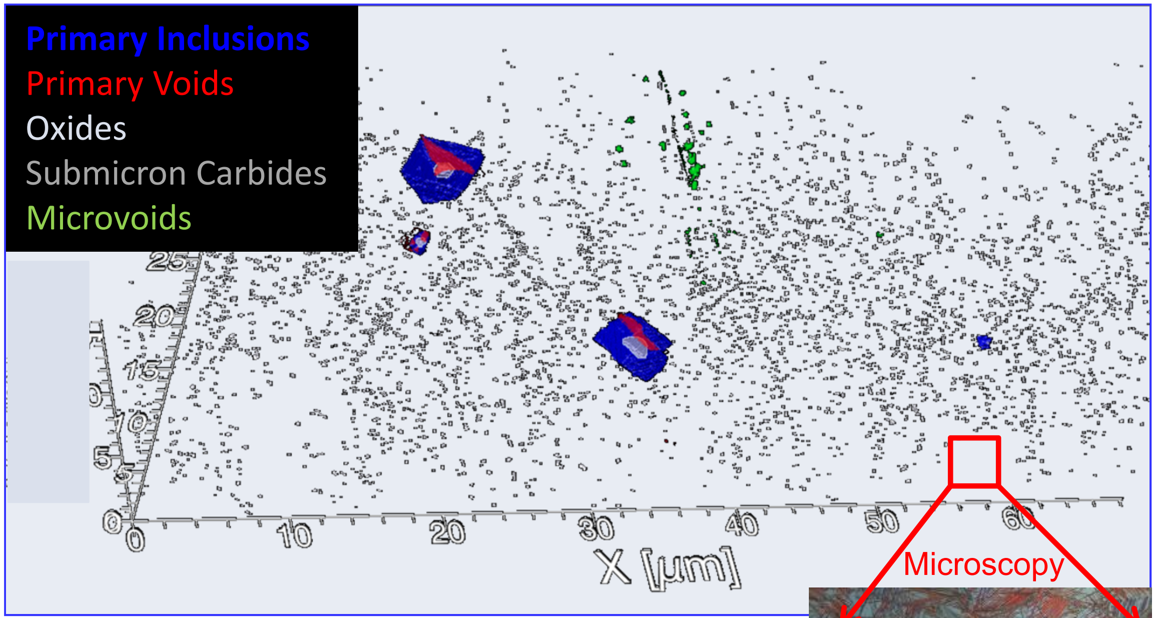
Vernervey, Moran and Liu. “Multiscale Micromorphic Theory for Hierarchical Materials, JMPS, 2603-2651, 2007
McVeigh & Liu,“Linking microstructure and properties through a predictive multiresolution continuum,” CMAME,2008
McVeigh & Liu, Multiresolution modeling of ductile reinforced brittle composites. J. Mech. Phys. Solids, 2009.
Liu et. al., Complexity science of multiscale materials via stochastic computations, IJNME, 2009.

Microstructures of Ultra High Strength Alloys





Mod4330 crack tip specimen #1:
Primary particles (yellow) near crack tip
Reconstruction area: 633x516x259 um^3
Averaged: 4.857 um
Spacing: 16 um
Volume fraction: 1.756%



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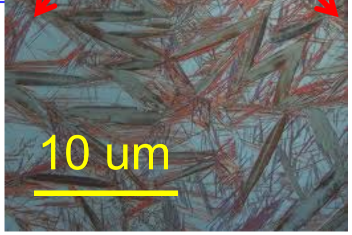
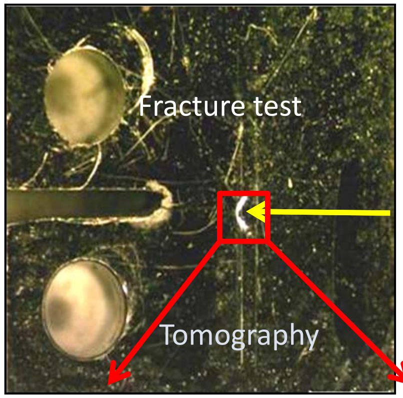
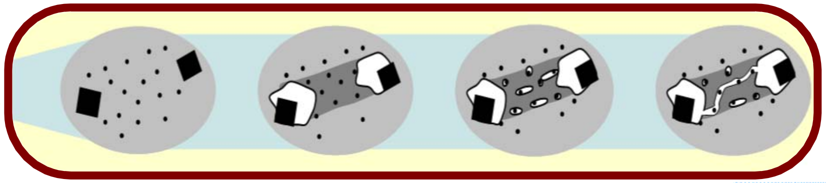


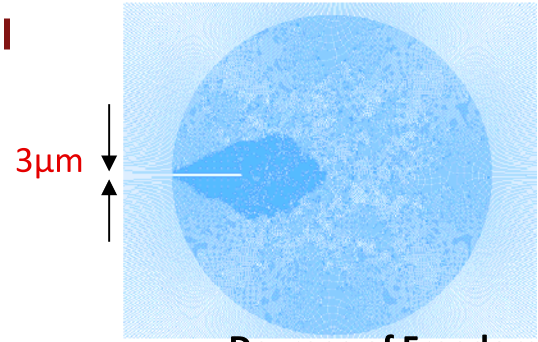
Lath martensite

Multiscale microstructures: within one grain we see
– primary particles, secondary particles, laths (too many to model explicitly)



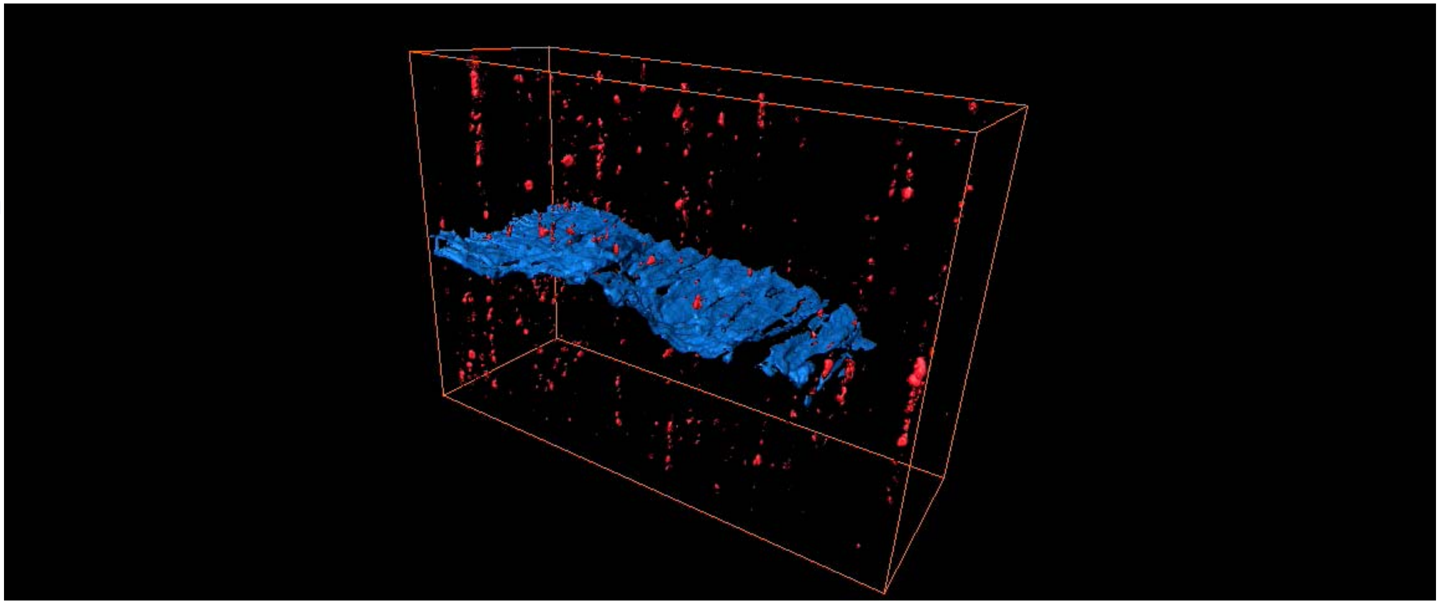


Fracture Process Model to be Validated



Mod4330 crack tip specimen #1:
Primary particles (yellow) near crack tip
Reconstruction area: 633x516x259 µm^3
Averaged: 4.857 µm
Spacing: 16 µm
Volume fraction: 1.756%

Degrees of Freedom:
30 million
(132 particles)

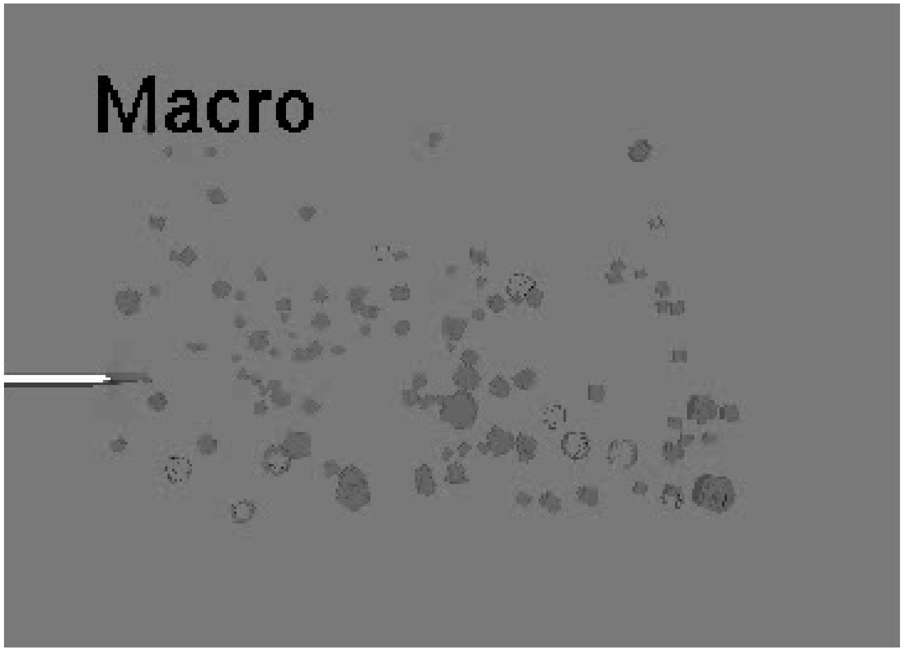


Fracture Simulation: Video

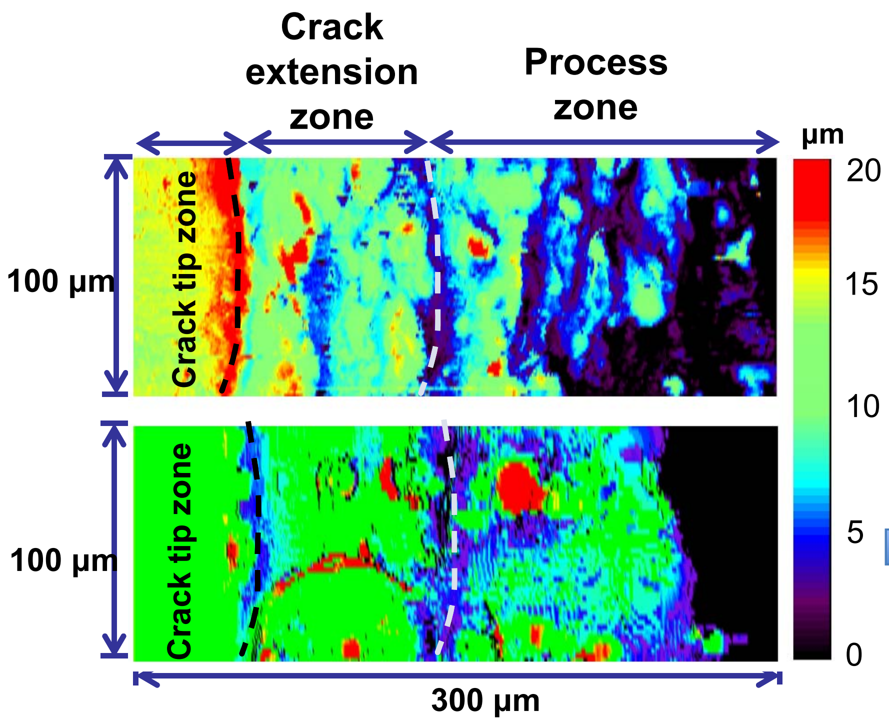
Initial Fatigue Crack Opening is about 3 microns, a load is applied gradually until the material reaches the initial and then final fracture toughness strengths followed by unloading to the final state of deformation

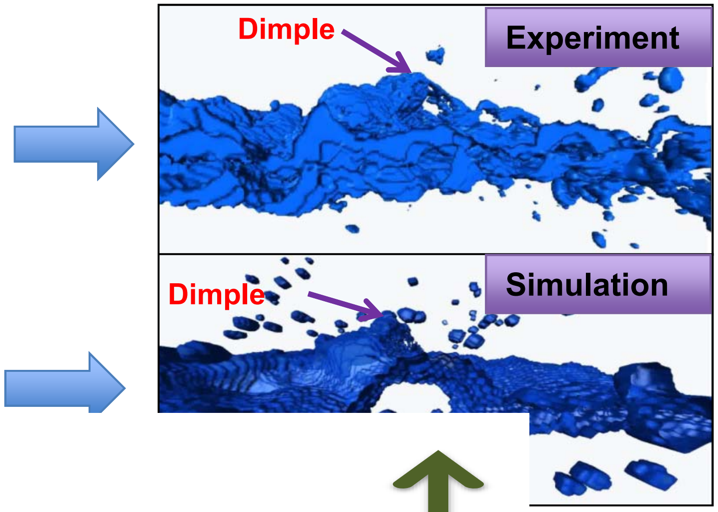
Total experimental time is one minute

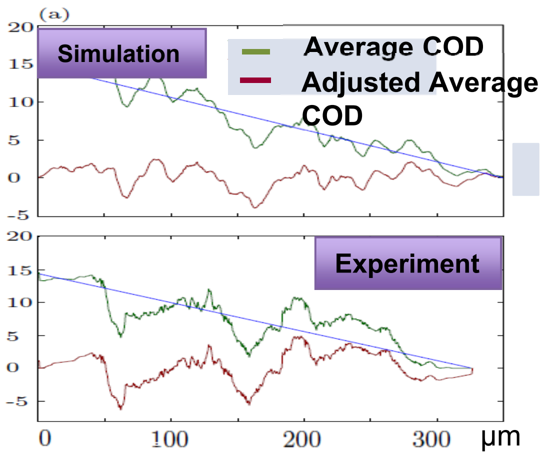
The below **MOVIE** shows the CONCURRENT interaction of macro and micro effective strains due to submicron and micron voids growth, interaction, coalescence to form Micro and macro defects (mini-cracks) that eventually define the fracture process zone

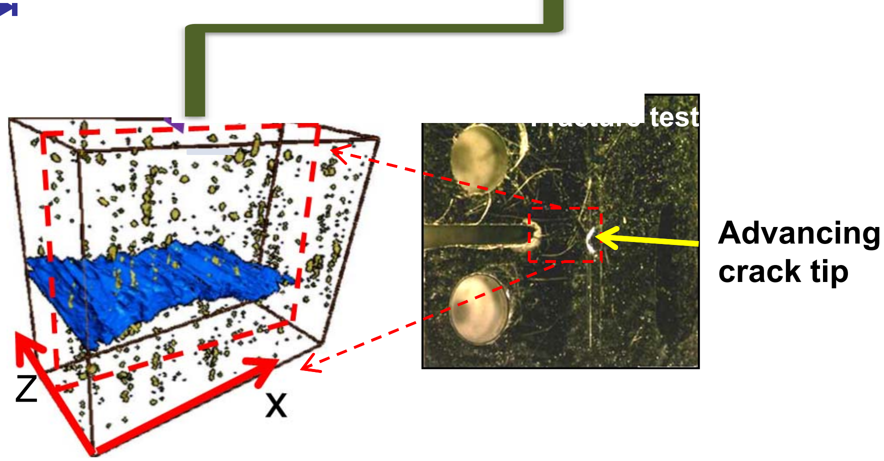


Summary of Comparison with Experimental Results

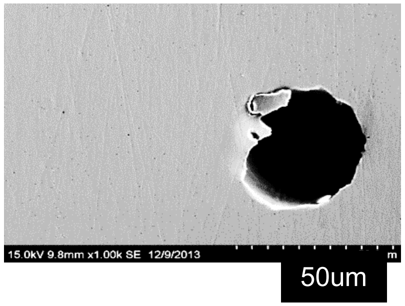


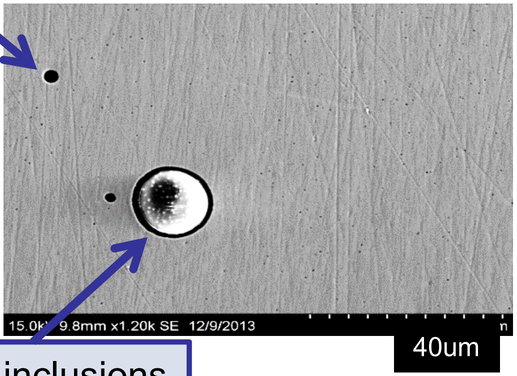


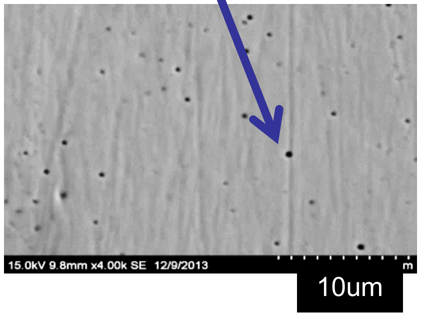




Experimental-Computational Coupling







Capturing constituencies, e.g.

- Strength
- Toughness
- Ductility
- Fatigue life

(GENOME)

}

Requires information (i.e. microstructure and conformation), e.g.

- Voids
- Inclusions
- Interfaces
- Surface properties

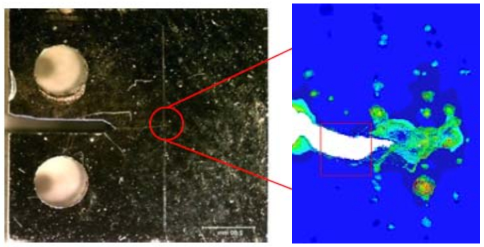
(ARCHETYPES)

Fast solution methods for hierarchical structure behavior

Development of rapid reconstruction techniques

Product-level Analysis

Mechanistic constitutive laws incorporating real microstructural data



Tian, 2010

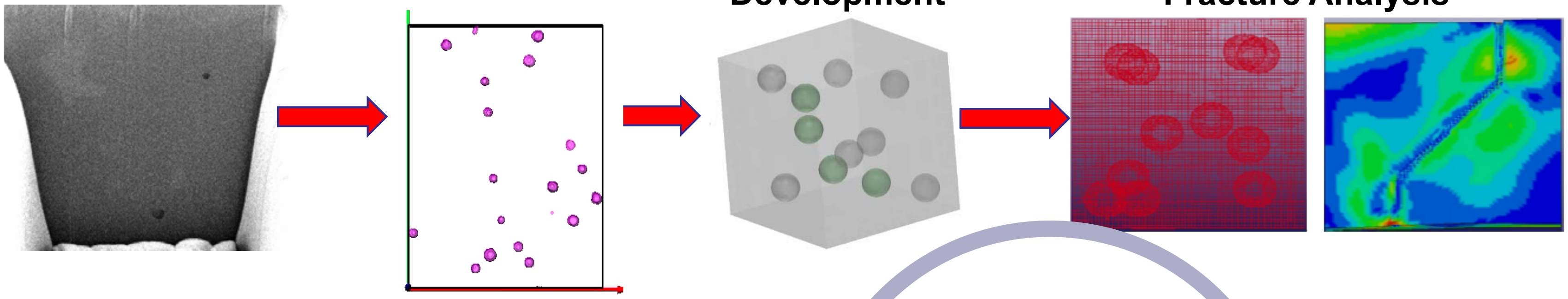
From microstructure (Archetypes) to mechanical property (Genomes) for as-built alloys

FIB Imaging

3D Reconstruction

FEA Mesh Development

Mechanical Behavior and Fracture Analysis



3D tomography

- Voids
- Microvoids
- Inclusions
- Grain structure

Microstructure Constituents

Archetypes

- Auto-polisher/OM (micron)
- Mechanical sectioning/SEM (micron)
- FIB/SEM (sub-micron)

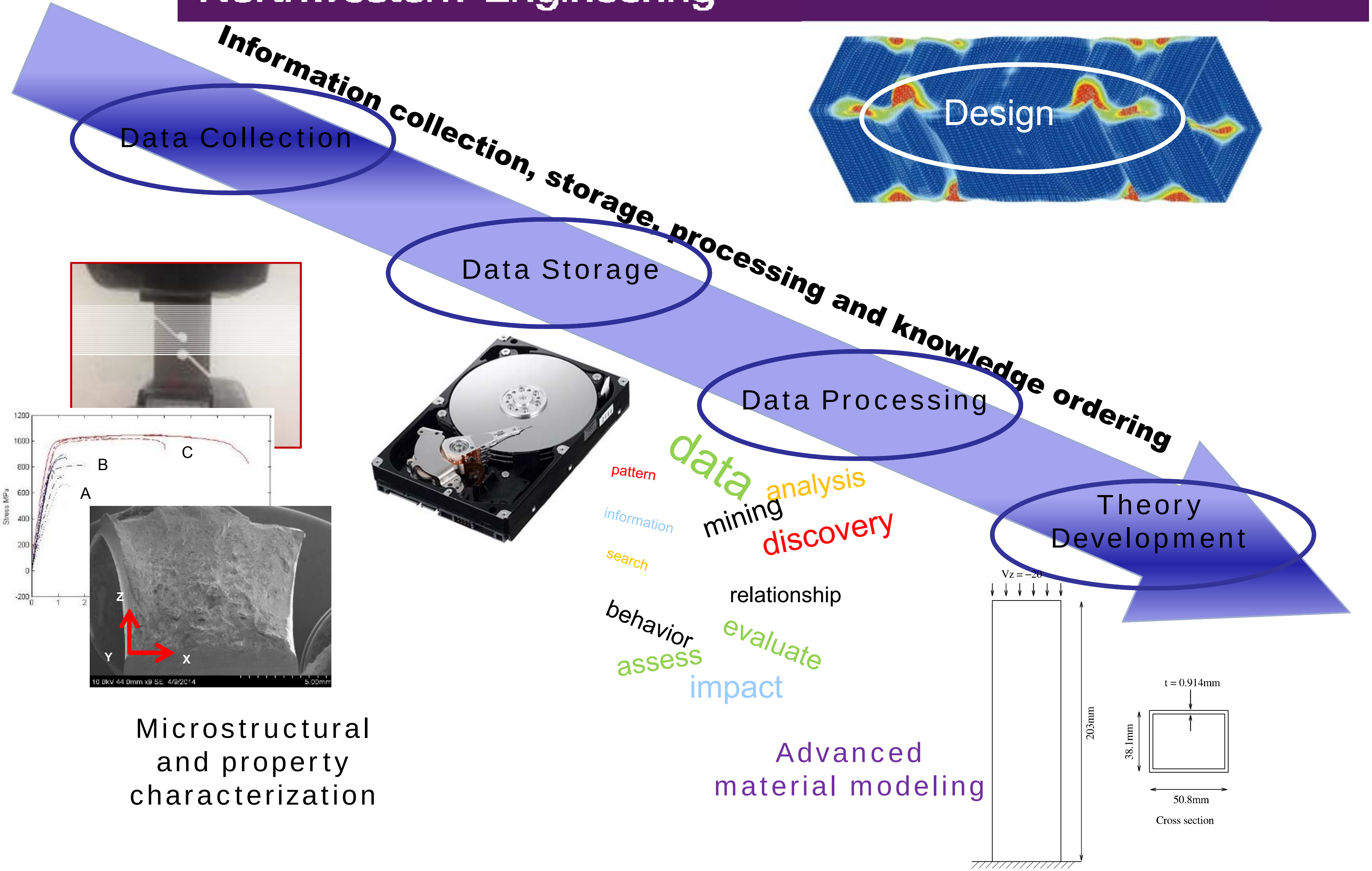
- Estimate mechanical properties (strength)

Mechanics-Based Material Model

Genome

Informatics, Data Collections, Compression, Pattern Recognition, Data Mining and Reconstruction, and Theory Development

Informatics-Driven Design: Process-Structure-Property



Information collection, storage, processing and knowledge ordering

Data Collection

Data Storage

Data Processing

Theory Development

Design

Microstructural and property characterization

data
pattern
analysis
information
mining
discovery
search
relationship
behavior
evaluate
assess
impact

Advanced material modeling

Zeliang Liu, M.A. Bessa, Wing Kam Liu, “Self-consistent clustering analysis: an efficient multi-scale scheme for inelastic heterogeneous materials,” Submitted

Selected References relevant to UQ

S. Chan O'Keeffe, S. Tang, AM Kopacz, J Smith, DJ Rowenhorst, G Spanos, WK Liu, GB Olson, Multiscale Ductile Fracture Integrating Tomographic Characterization and 3D Simulation, *Acta Materialia*, 82, (2015).

TR Lee, MS Greene, Z Jiang, AM Kopacz, P Decuzzi, W Chen, WK Liu, “Quantifying uncertainties in the microvascular transport of nanoparticles”, Biomech. Model. Mechanobiol., 2014, 13, 515-526.

Steven Greene, Ying Li, Wei Chen, Wing Kam Liu, “The archetype-genome exemplar in molecular dynamics and continuum mechanics,” Computational Mechanics, Volume 53, Issue 4 (2014), Page 687-737.

Y Li, W Stroberg, TR Lee, HS Kim, H Man, D Ho, P Decuzzi, WK Liu, “Multiscale Modeling and Uncertainty Quantification in Nanoparticle mediated Drug/Gene Delivery,” *Computational Mechanics*, (2014) 53:511–537.

Khalil I Elkhodary; Michael S Greene; Shan Tang; Ted Belytschko; Wing K Liu, “Archetype-blending continuum theory,” Comput. Methods Appl. Mech. Engrg. 254 (2013) 309–333.

Yu Liu, M. Steven Greene, Wei Chen, Dmitriy A. Dikin, Wing Kam Liu, “Computational microstructure characterization and reconstruction for stochastic multiscale material design,” Computer-Aided Design, 45, 2013.

MS. Greene, H. Xu, S. Tang, W. Chen, WK Liu, “A generalized uncertainty propagation criterion from benchmark studies of microstructured material systems,” Comput. Methods Appl. Mech. Engrg., 254, 2013, Pages 271–291.

H Xu, H Deng, C Brinson, D Dikin, WK Liu, W Chen, MS Greene, C. Burkhart, G Papakonstantopoulos, M Poldneff, “STOCHASTIC REASSEMBLY FOR MANAGING THE INFORMATION COMPLEXITY IN MULTILEVEL ANALYSIS OF HETEROGENEOUS MATERIALS,” Proceedings of ASME 2012 International Design Engineering Technical Conferences & Computers and Information in Engineering Conference, DETC2012-70668, 2012.

Greene M.S., Liu, Y., Chen, W., Liu, W.K., “Computational Uncertainty Analysis in Multiresolution Materials via Stochastic Constitutive Theory”, Computer Methods in Applied Mechanics and Engineering, (2011), **200**.

W. K. Liu, T. Belytschko and A. Mani, "Random Field Finite Elements," Int J for Numl Methods in Eng, 23, 1986.

W. K. Liu, T. Belytschko and A. Mani, "Probabilistic Finite Elements for Nonlinear Structural Dynamics," CMAME, 56, 1986.

Reduced order modelling based on clustering

Offline stage

0. Database creation

- Sampling from numerical analysis: Fine Scale, FEM, FFT-based….. methods
- Sampling from experiments SEM/TEM, X-ray …

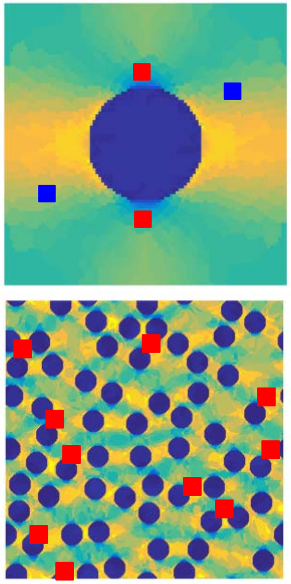
1. Data compression

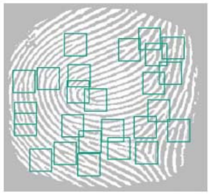
- Data type
  - Strain concentration
- Data measures
  - Distance – matrix norm
- Algorithm
  - K-means clustering

2. Micromechanics-based clustering analysis

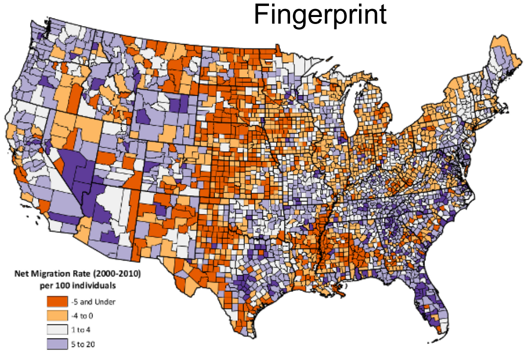
- Interaction tensors

Pattern Recognition & Clustering





Fingerprint



Migration patterns (netmigration.wisc.edu)

One-time calculation

Online stage

Inputs: boundary conditions from a point in the macro-scale continuum.

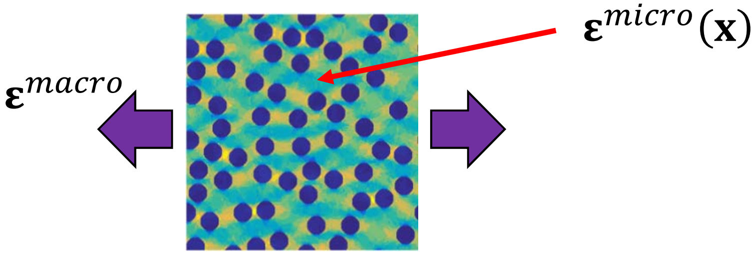
3. Reduced order Materials Modeling

- Number of DOFs is reduced.
- Arbitrary microstructure.
- Complex material behaviors.

Outputs: homogenized material response to the macro-scale continuum.

Offline Stage - **Database generation and compression**

- **Data type:** strain concentration tensor $\mathbf{A}(\mathbf{x})$ in the RVE for linear elastic material.



For 2D plane strain material, $\mathbf{A}(\mathbf{x})$ has 9 independent components, determined by *a priori* simulations under 3 orthogonal loading conditions.

$$\boldsymbol{\varepsilon}^{micro}(\mathbf{x}) = \mathbf{A}(\mathbf{x}) : \boldsymbol{\varepsilon}^{macro}$$

strain concentration tensor $\mathbf{A}(\mathbf{x})$
microscopic strain $\boldsymbol{\varepsilon}^{micro}(\mathbf{x})$
macroscopic strain $\boldsymbol{\varepsilon}^{macro}$

$$\begin{bmatrix}\varepsilon_1^{local}\\ \varepsilon_2^{local}\\ \varepsilon_3^{local}\end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & A_{13}\\ A_{21} & A_{22} & A_{23}\\ A_{31} & A_{32} & A_{33}\end{bmatrix}\begin{bmatrix}\varepsilon_1^{macro}\\ \varepsilon_2^{macro}\\ \varepsilon_3^{macro}\end{bmatrix}$$

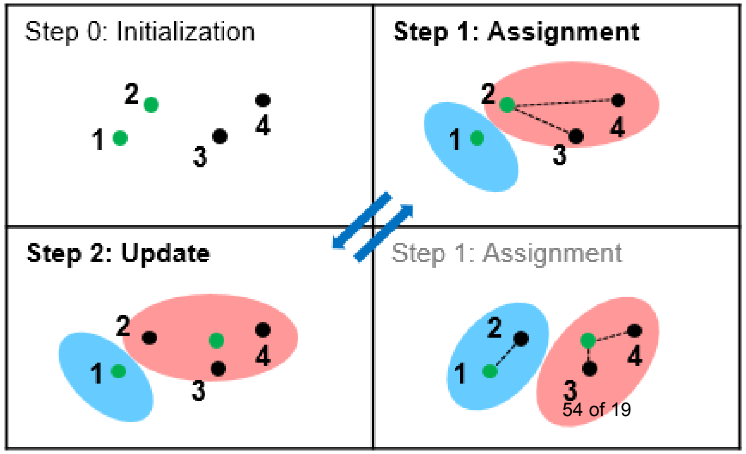
- **Data format:**

EIndex	A_{11}	A_{22}	A_{33}	A_{12}	A_{21}	A_{23}	A_{32}	A_{13}	A_{31}
1	–	–	–	–	–	–	–	–	–
2	–	–	–	–	–	–	–	–	–
⋮			⋮			⋮			⋮
N	–	–	–	–	–	–	–	–	–

* N: total number of elements (observations) in the RVE

- **Compression algorithm:**

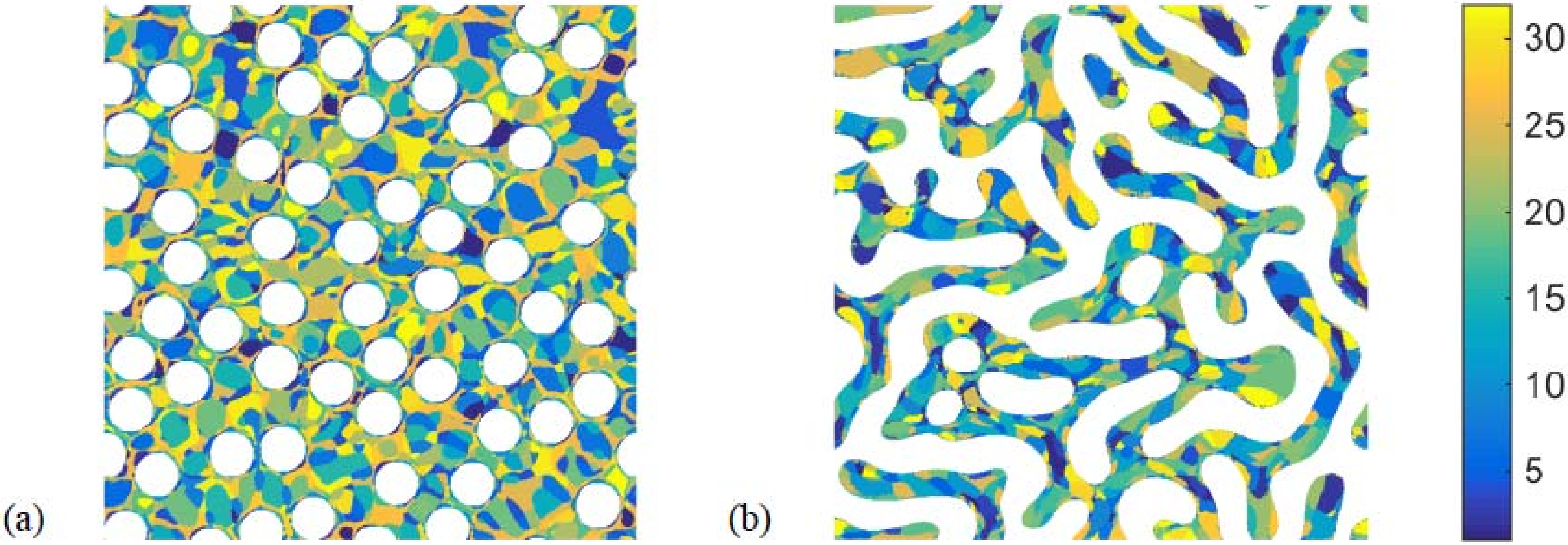
k-means clustering



Zeliang Liu, M.A. Bessa, Wing Kam Liu, “Self-consistent clustering analysis: an efficient multi-scale scheme for inelastic heterogeneous materials,” Submitted

Proposed method – offline stage

K-means clustering – results



Fiber-reinforced composite ($vf = 30\%$)

Phase-field structure ($vf = 50\%$)

DNS: 600×600

DNS: 600×600

Proposed method – offline stage

We omit the details as the paper is not published yet

Proposed method – online stage

Reduced order constitutive modeling

(1)

(2)

By substituting (2) into (1), we obtained

(3)

(4)

We omit the details as the paper is not published yet

Results and discussion

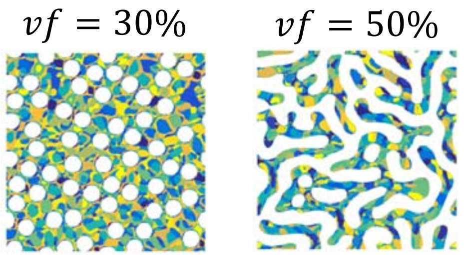
Elastic Material – The effect of number of clusters

$E_1 = 100\ \mathrm{MPa}, \nu_1 = 0.3;$ Matrix

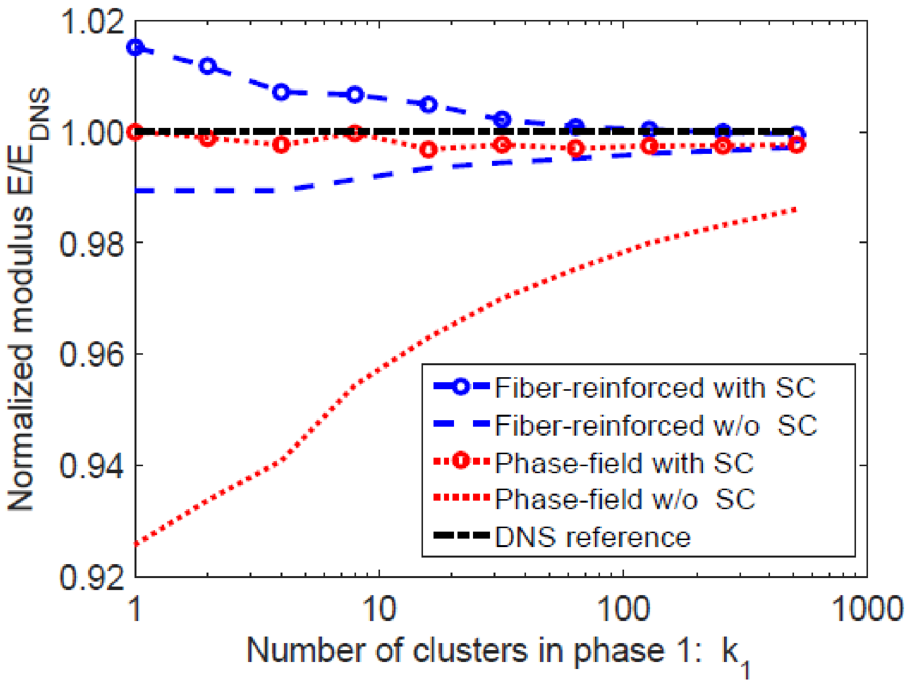
$E_2 = 500\ \mathrm{MPa}, \nu_2 = 0.19.$ Inclusion

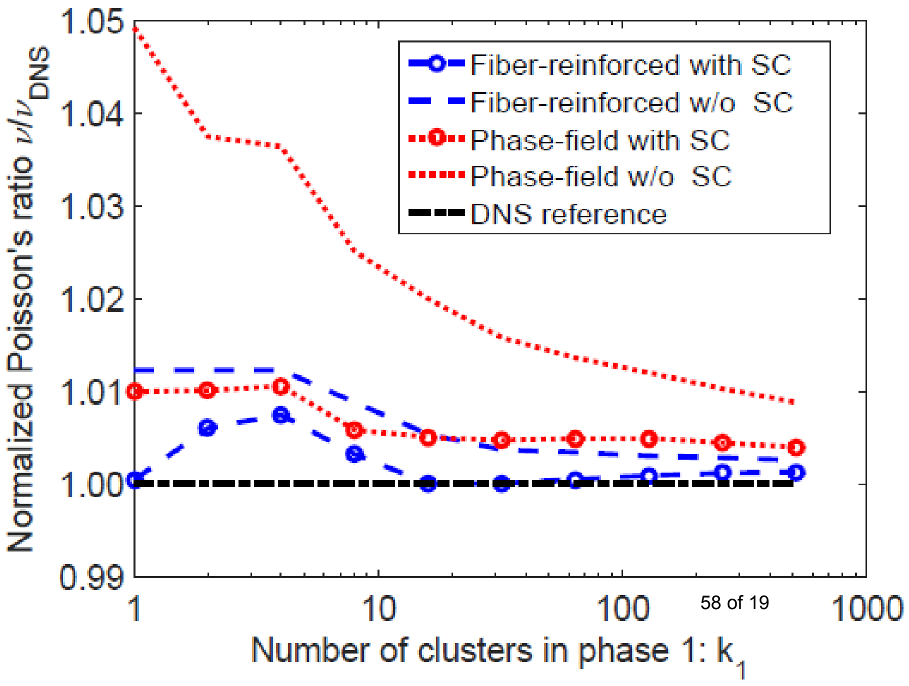
same as the ones we used for building the database

- DNS results from FE analysis with 600×600 mesh.



1. Fiber-reinforced composite: $E_{\mathrm{DNS}} = 156.43\ \mathrm{MPa}, \quad \nu_{\mathrm{DNS}} = 0.391.$
2. Phase-field material: $E_{\mathrm{DNS}} = 220.79\ \mathrm{MPa}, \quad \nu_{\mathrm{DNS}} = 0.350.$





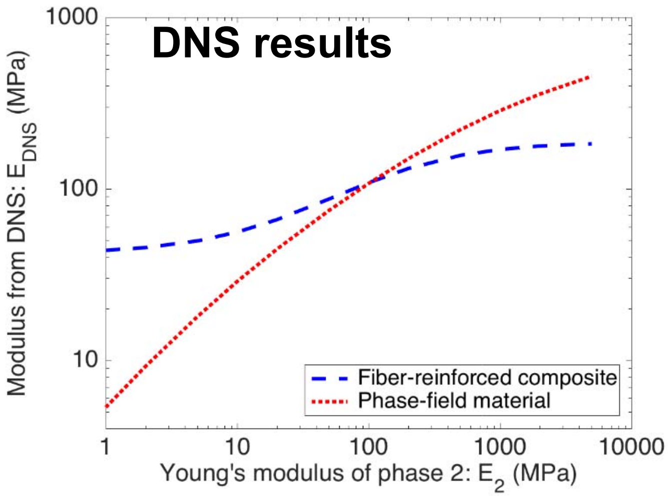
McCormick Northwestern Engineering

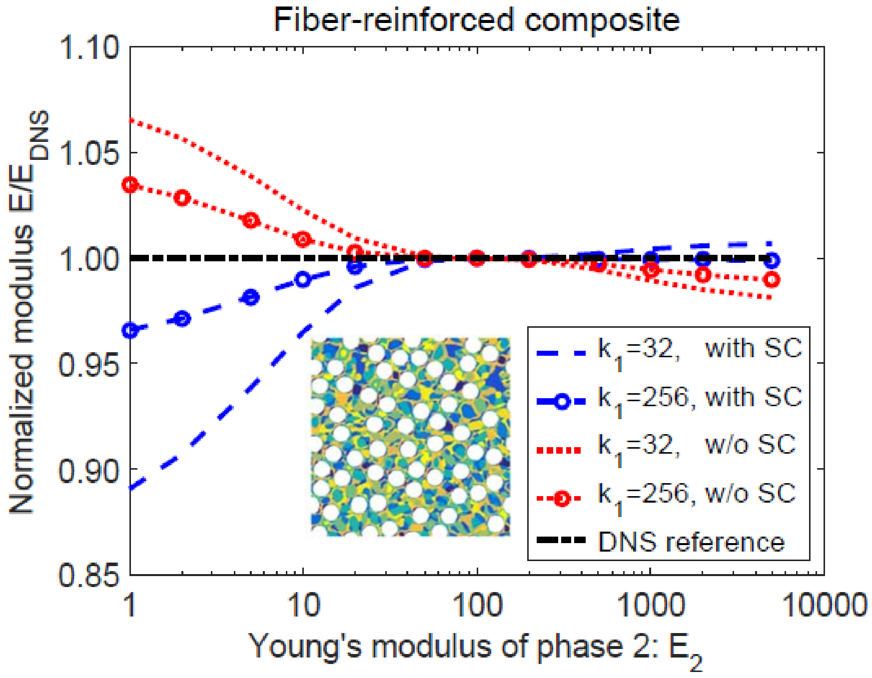
Results and discussion

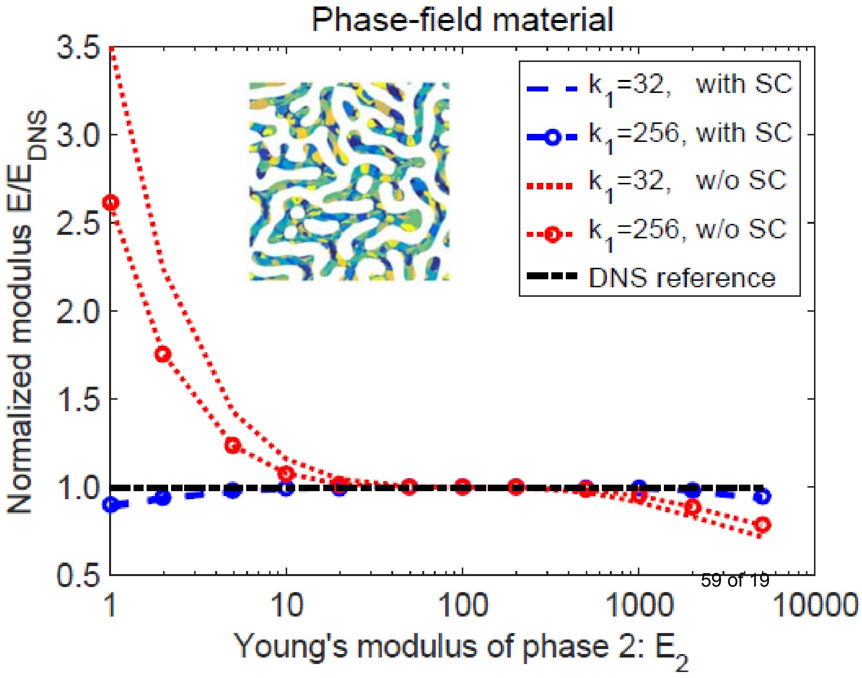
Elastic Material – the effect of phase modulus

$$E_1 = 100\ \text{MPa}, \nu_1 = 0.3; \qquad \nu_2 = 0.19.$$

Change E_2 (inclusion)







Results and discussion

Elasto-plastic Material – The importance of the self-consistent (SC) method

- Elastic domain

$$E_1 = 100\ \mathrm{MPa}, \nu_1 = 0.3; \quad E_2 = 500\ \mathrm{MPa}, \nu_2 = 0.19.$$

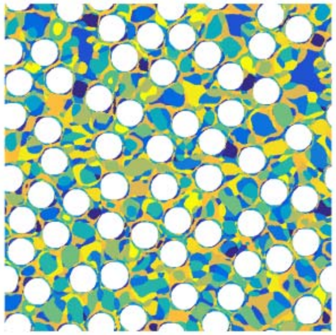
- Plastic domain: J-2 plasticity

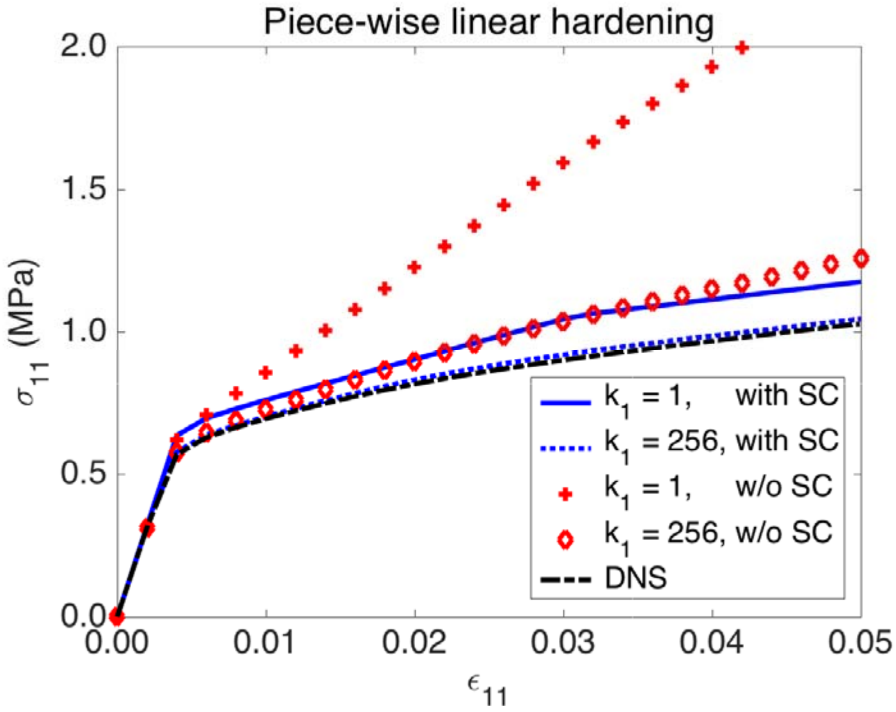
$$f = \bar{\sigma} - \sigma_Y(\bar{\varepsilon}) \leqslant 0,$$

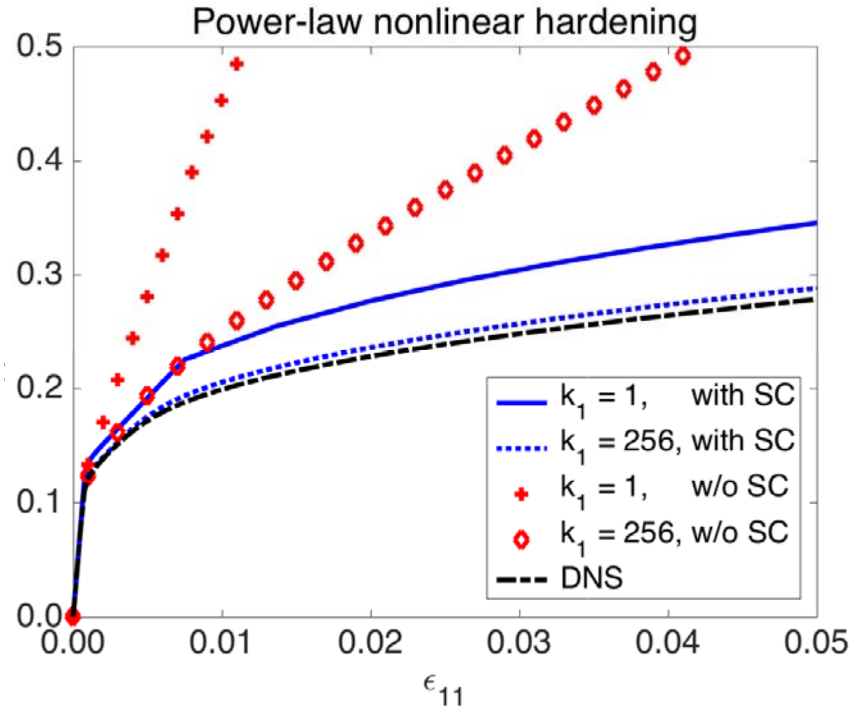
$$\sigma_Y(\bar{\varepsilon}) = \begin{cases} 0.5 + 5\bar{\varepsilon} & \bar{\varepsilon} \in [0, 0.04) \\ 0.7 + 2\bar{\varepsilon} & \bar{\varepsilon} \in [0.04, \infty) \end{cases} \ \mathrm{MPa}$$

$$\sigma_Y(\bar{\varepsilon}) = 0.1 + 0.3\bar{\varepsilon}^{0.4}\ \mathrm{MPa}.$$

Fiber-reinforced composite



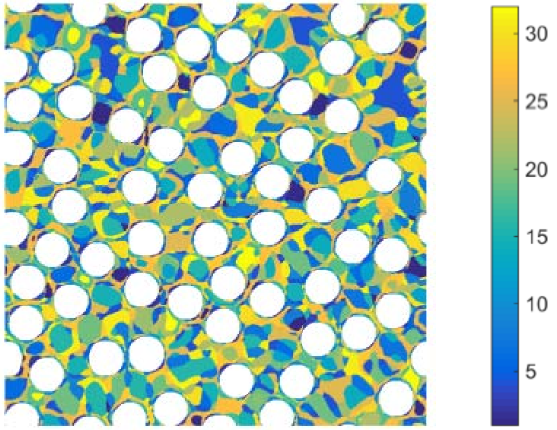




Results and discussion

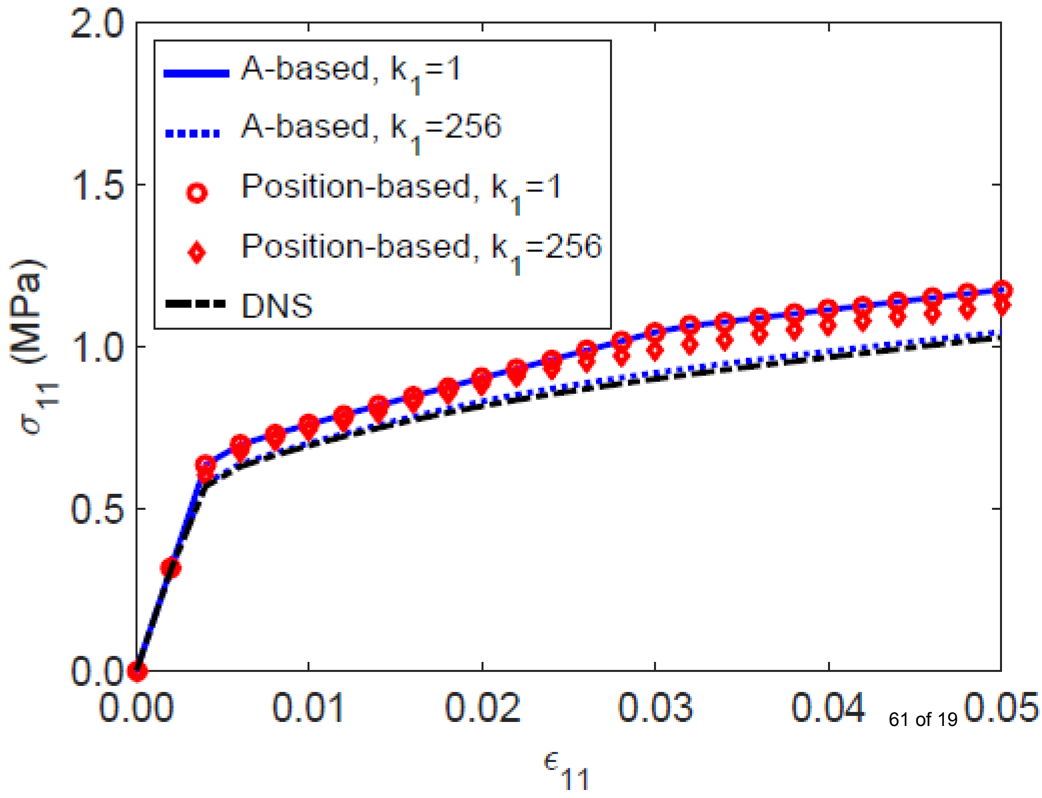
Importance of the raw data type

Strain concentration tensor: $\mathbf{A}(\mathbf{x})$



Spatial coordinates / Position: $\mathbf{x}$

- We use $\mathbf{A}(\mathbf{x})$ in order to capture the mechanical behaviors. Differently, the clustering can be also purely based on the spatial coordinates $\mathbf{x}$ of the data points, similar to the meshing in FEM…



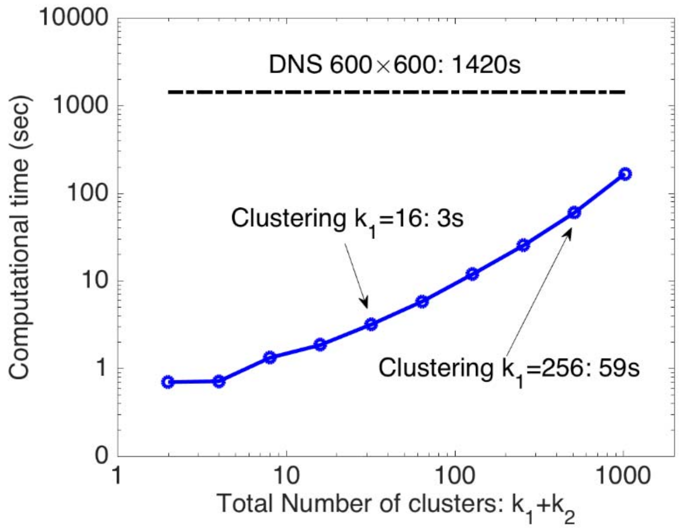
Results and discussion

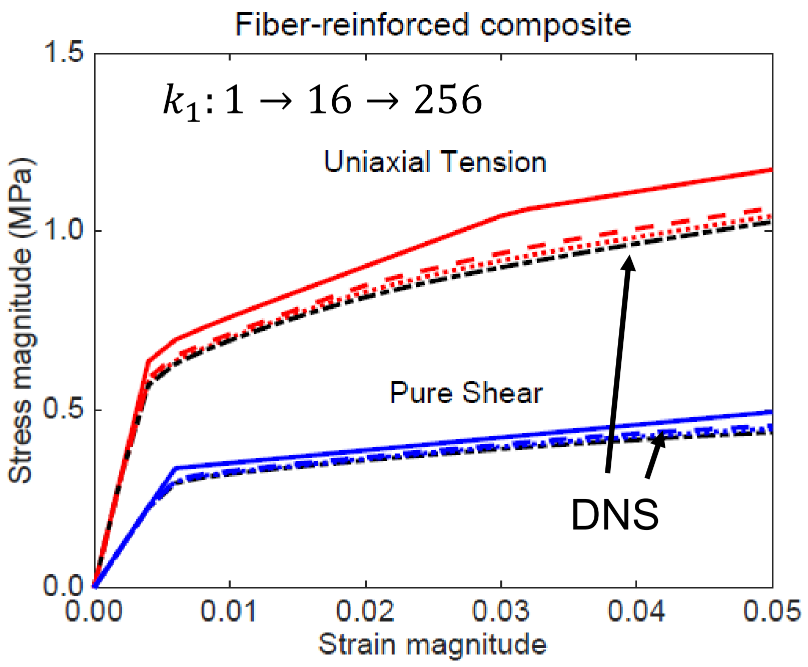
Computational time

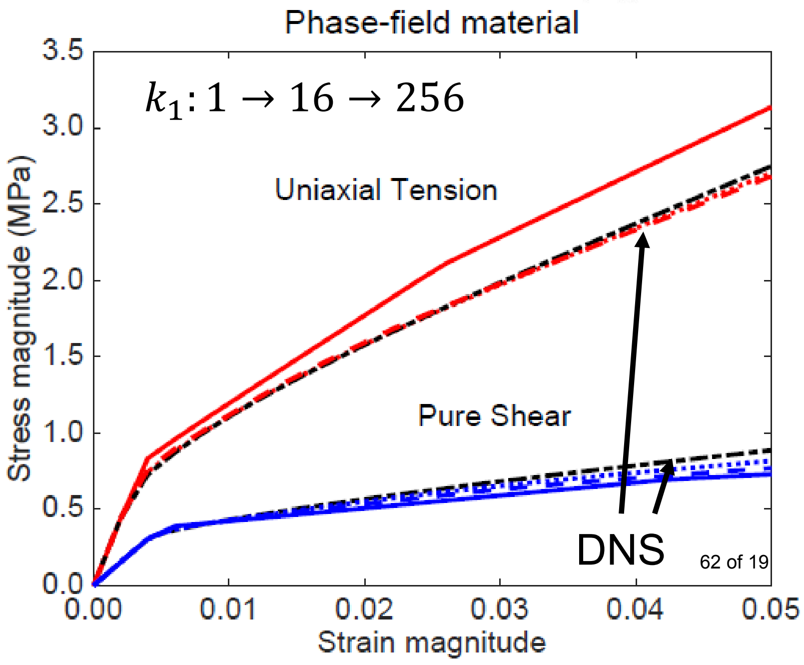
- Implicit elasto-plastic simulations with 25 incremental steps.
- Performed on one Inter® Core i7-3632QM

DNS 600×600: **Abaqus standard**

Proposed reduced order model: **Matlab**

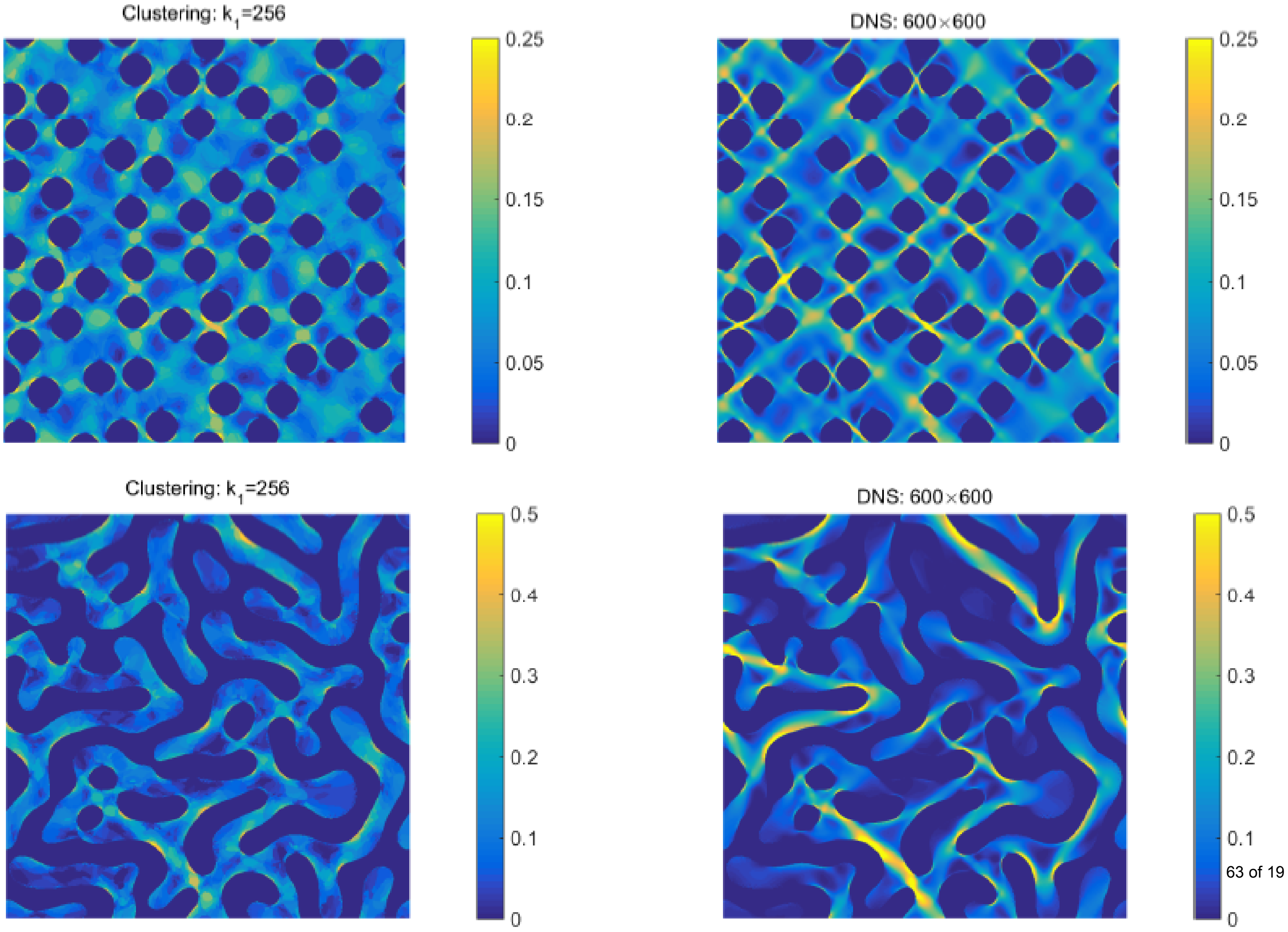






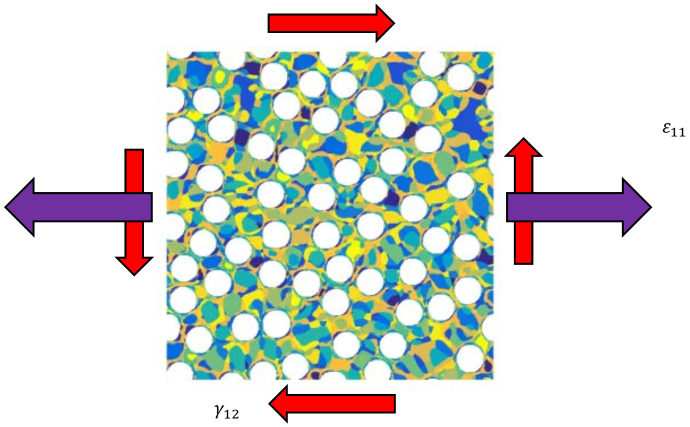
Results and discussion

Comparison of the effective plastic strain field

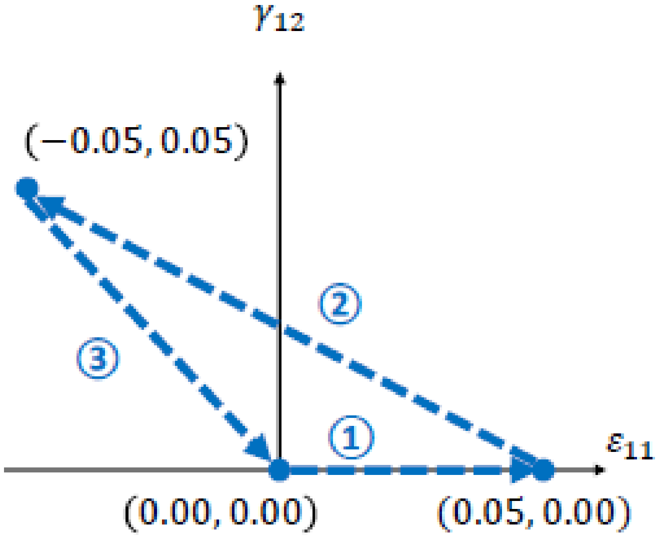


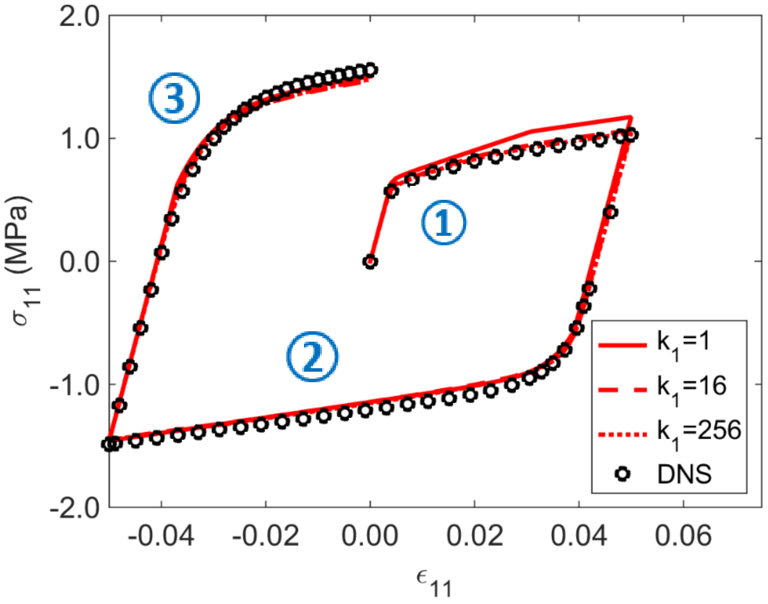
Results and discussion

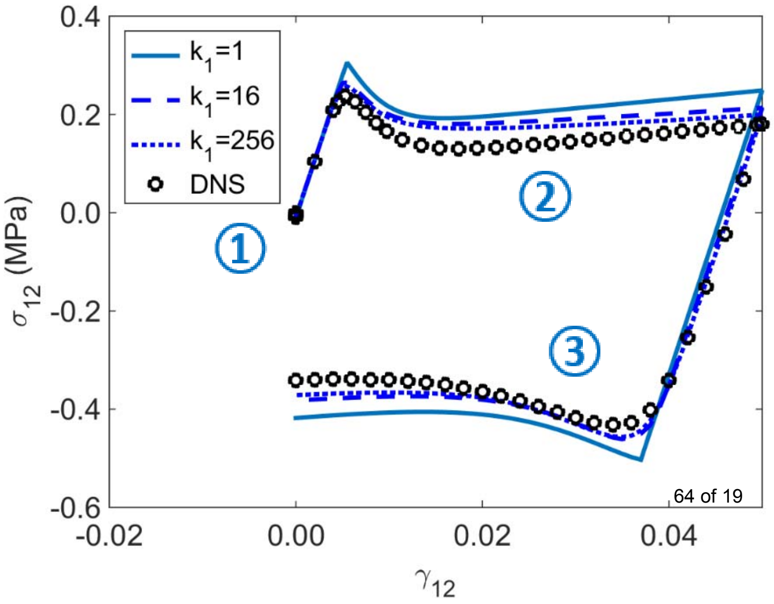
A complex loading path in 2D



- No constraint on ε_{22}

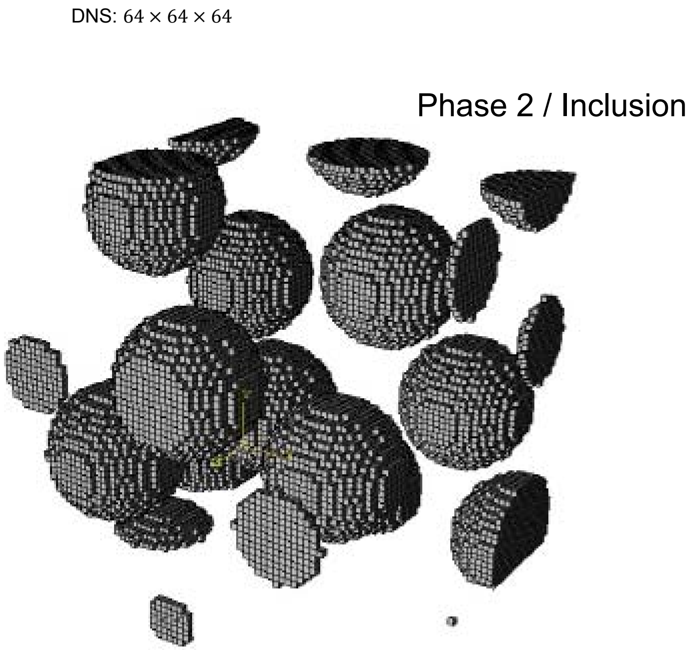


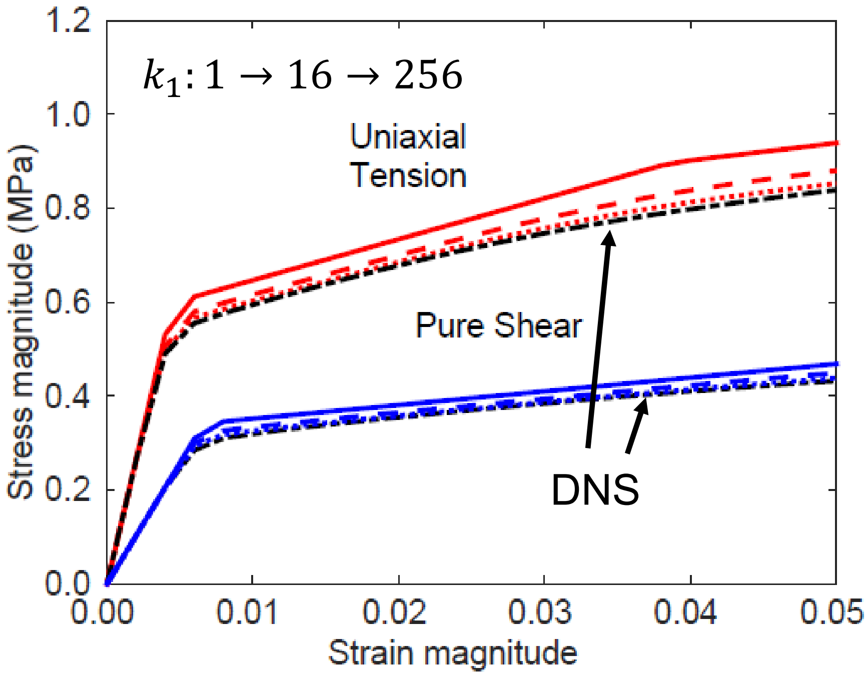




Results and discussion

3D results and the computational time





- Elastic domain

$$E_1 = 100\ \text{MPa}, \nu_1 = 0.3;$$

$$E_2 = 500\ \text{MPa}, \nu_2 = 0.19.$$

- Plastic domain: J-2 plasticity

$$\sigma_Y(\bar{\varepsilon}) = \begin{cases} 0.5 + 5\bar{\varepsilon} & \bar{\varepsilon} \in [0, 0.04) \\ 0.7 + 2\bar{\varepsilon} & \bar{\varepsilon} \in [0.04, \infty) \end{cases} \text{MPa}$$

- Implicit elasto-plastic simulations with 25 incremental steps.

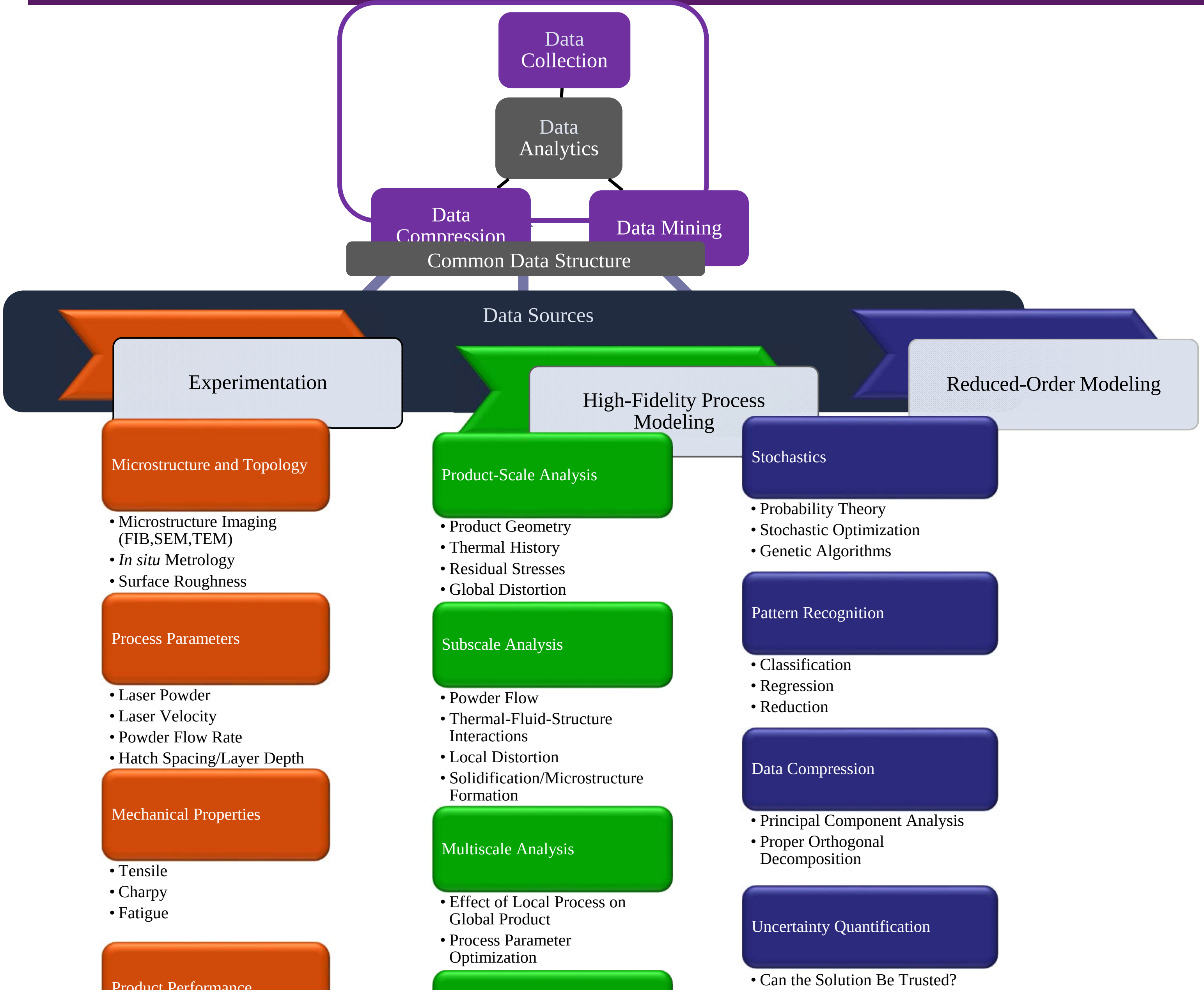
DNS: **Abaqus standard** on Hercules (32 Intel Westmere X5650 processors)

12 hours

Proposed reduced order method: **Matlab** on one Inter® Core i7-3632QM

5 sec ($k_1 = 16$); 214 sec ($k_2 = 256$)

Data analytics for AM applications



Data Collection

Data Analytics

Data Compression

Data Mining

Common Data Structure

Data Sources

Experimentation

High-Fidelity Process Modeling

Reduced-Order Modeling

Microstructure and Topology

- Microstructure Imaging (FIB,SEM,TEM)
- *In situ* Metrology
- Surface Roughness

Process Parameters

- Laser Powder
- Laser Velocity
- Powder Flow Rate
- Hatch Spacing/Layer Depth

Mechanical Properties

- Tensile
- Charpy
- Fatigue

Product Performance

Product-Scale Analysis

- Product Geometry
- Thermal History
- Residual Stresses
- Global Distortion

Subscale Analysis

- Powder Flow
- Thermal-Fluid-Structure Interactions
- Local Distortion
- Solidification/Microstructure Formation

Multiscale Analysis

- Effect of Local Process on Global Product
- Process Parameter Optimization

Stochastics

- Probability Theory
- Stochastic Optimization
- Genetic Algorithms

Pattern Recognition

- Classification
- Regression
- Reduction

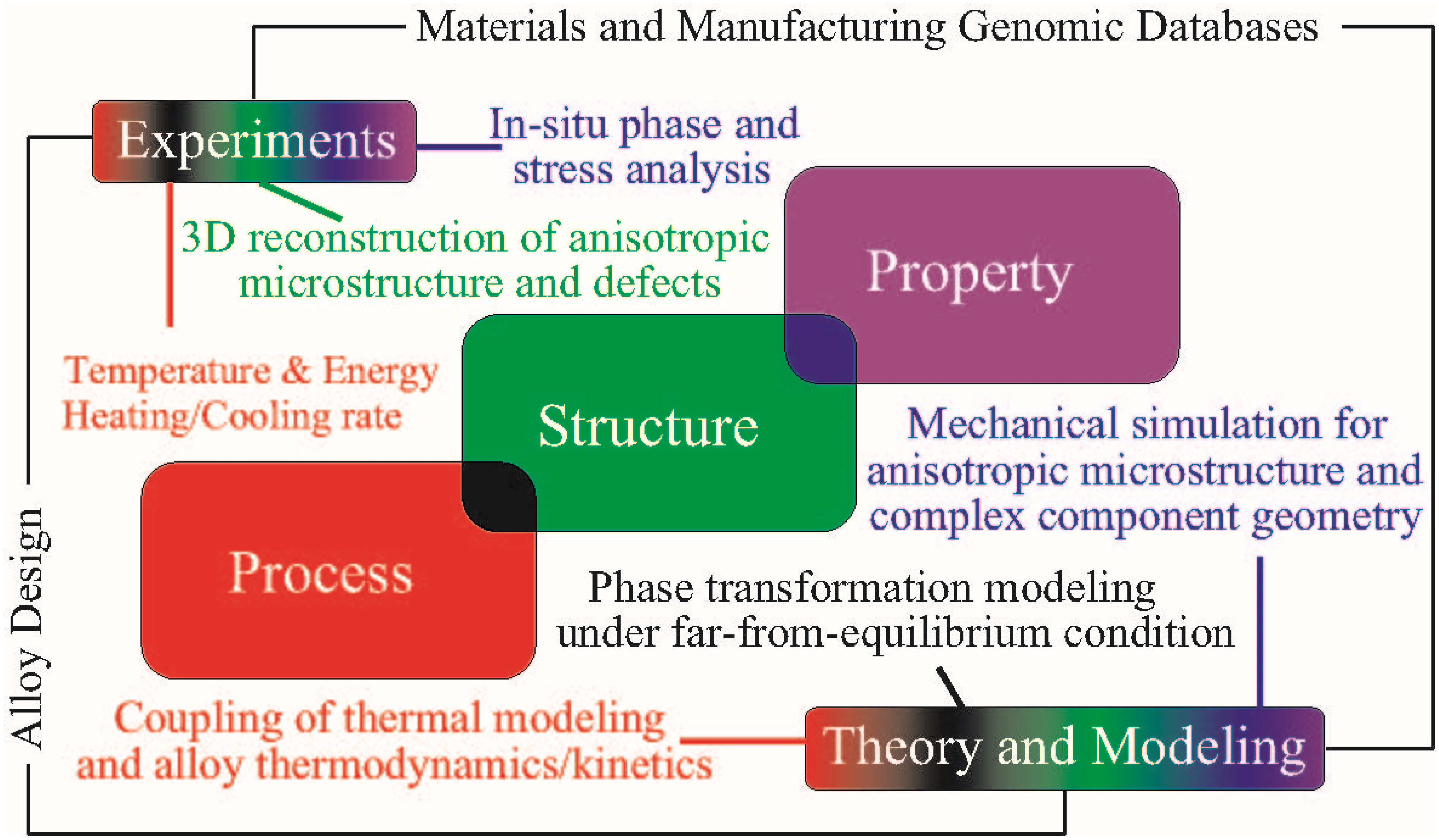
Data Compression

- Principal Component Analysis
- Proper Orthogonal Decomposition

Uncertainty Quantification

- Can the Solution Be Trusted?

Predictive modeling supported by experiments



Materials and Manufacturing Genomic Databases

Experiments

In-situ phase and stress analysis

3D reconstruction of anisotropic microstructure and defects

Property

Temperature & Energy
Heating/Cooling rate

Structure

Mechanical simulation for anisotropic microstructure and complex component geometry

Process

Phase transformation modeling under far-from-equilibrium condition

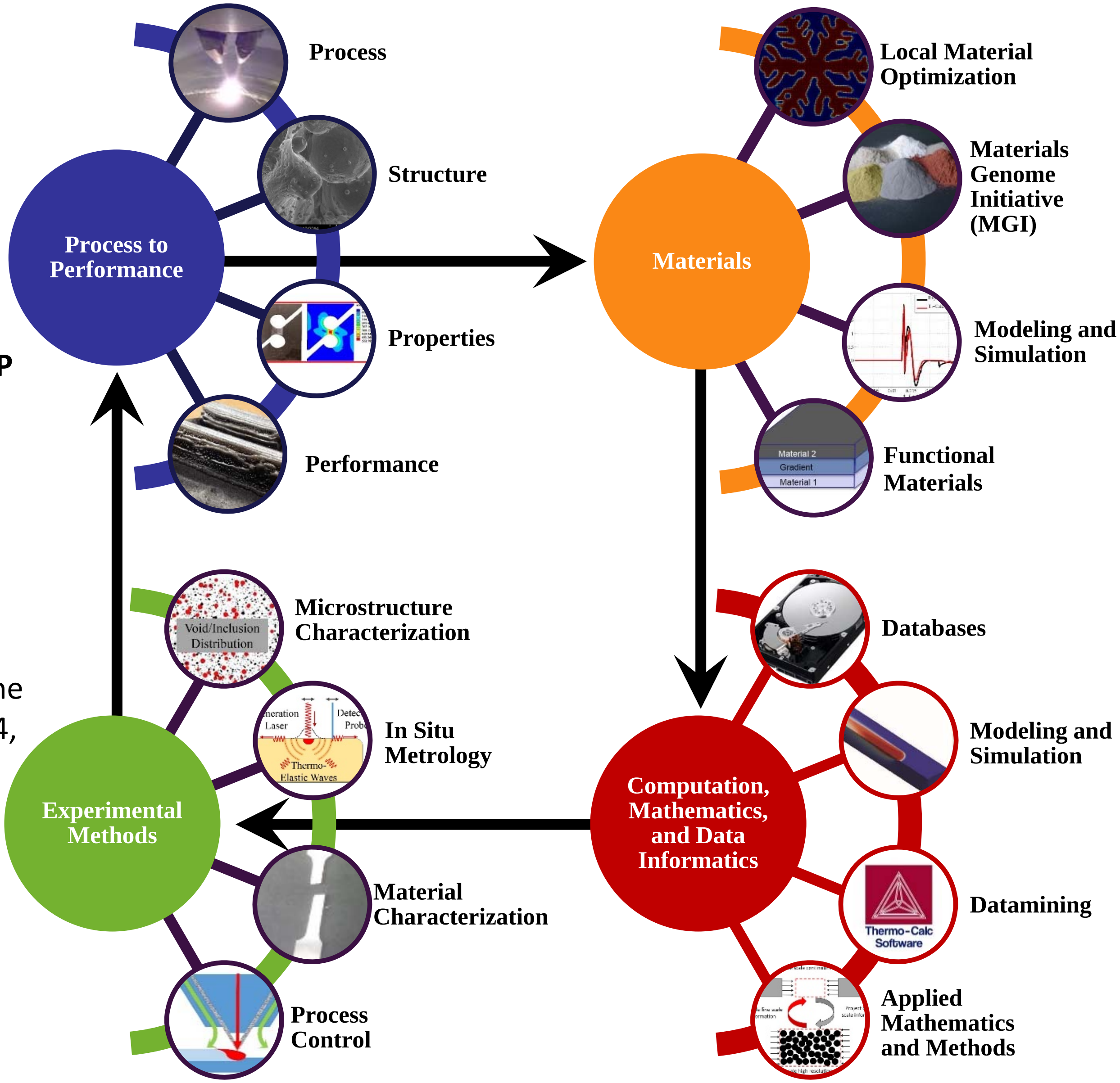
Coupling of thermal modeling and alloy thermodynamics/kinetics

Theory and Modeling

Alloy Design

Impact areas for the future of AM processing

J Smith, W Xiong, W Yan, S Lin, P Cheng, OL. Kafka, GJ. Wagner, J Cao, WK.Liu, “Linking Process, Structure, Property, and Performance for Metal-based Additive Manufacturing: Computational Approaches with Experimental Support,” *Computational Mechanics*, Online DOI 10.1007/s00466-015-1240-4, 2016.



Process to Performance

Process

Structure

Properties

Performance

Materials

Local Material Optimization

Materials Genome Initiative (MGI)

Modeling and Simulation

Functional Materials

Computation, Mathematics, and Data Informatics

Databases

Modeling and Simulation

Datamining

Applied Mathematics and Methods

Experimental Methods

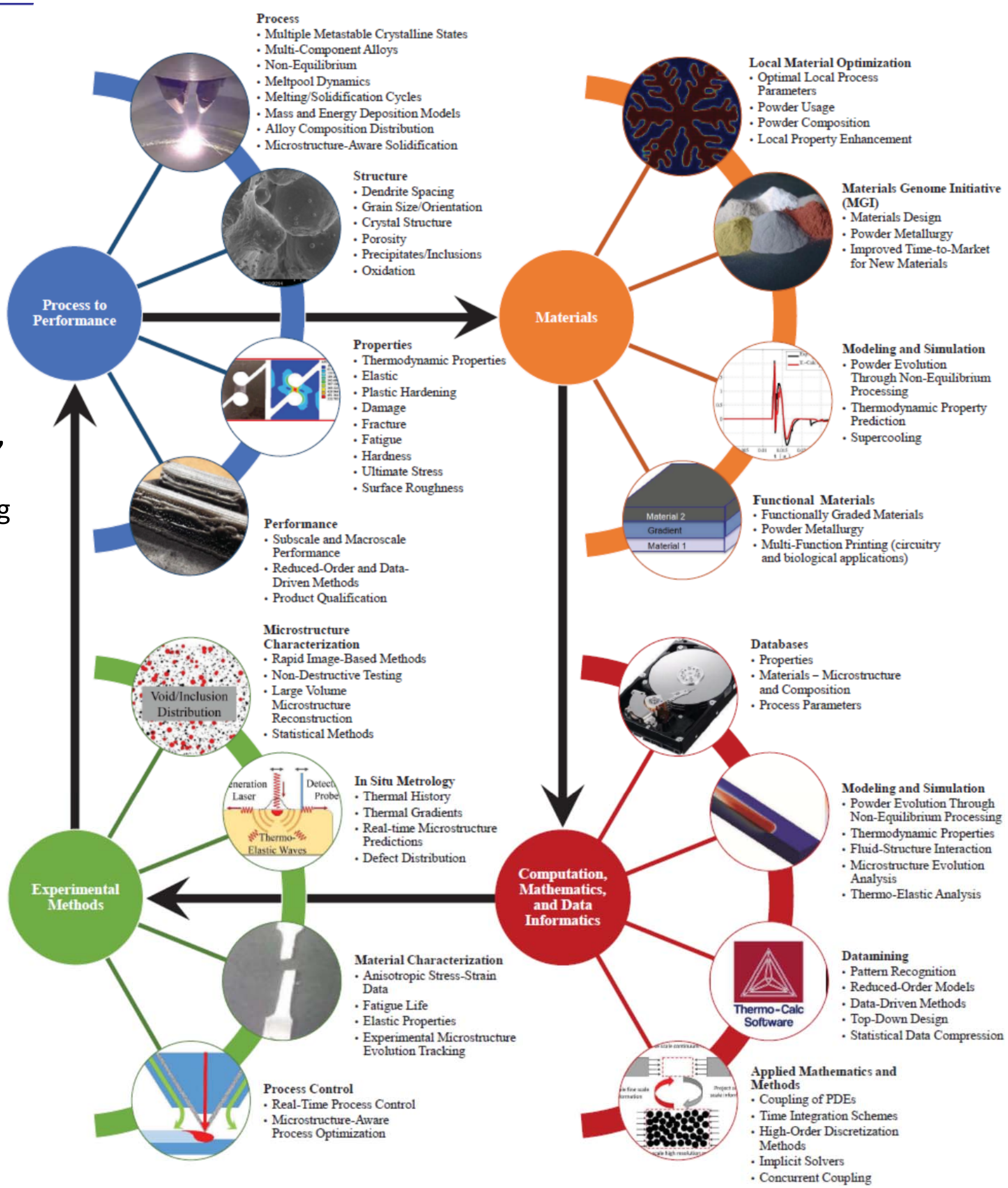
Microstructure Characterization

In Situ Metrology

Material Characterization

Process Control

J Smith, W Xiong, W Yan, S Lin, P Cheng, OL. Kafka, GJ. Wagner, J Cao, WK.Liu, “Linking Process, Structure, Property, and Performance for Metal-based Additive Manufacturing: Computational Approaches with Experimental Support,” *Computational Mechanics*, Online DOI 10.1007/s00466-015-1240-4, 2016.



Process to Performance

Process
- Multiple Metastable Crystalline States
- Multi-Component Alloys
- Non-Equilibrium
- Meltpool Dynamics
- Melting/Solidification Cycles
- Mass and Energy Deposition Models
- Alloy Composition Distribution
- Microstructure-Aware Solidification

Structure
- Dendrite Spacing
- Grain Size/Orientation
- Crystal Structure
- Porosity
- Precipitates/Inclusions
- Oxidation

Properties
- Thermodynamic Properties
- Elastic
- Plastic Hardening
- Damage
- Fracture
- Fatigue
- Hardness
- Ultimate Stress
- Surface Roughness

Performance
- Subscale and Macroscale Performance
- Reduced-Order and Data-Driven Methods
- Product Qualification

Materials

Local Material Optimization
- Optimal Local Process Parameters
- Powder Usage
- Powder Composition
- Local Property Enhancement

Materials Genome Initiative (MGI)
- Materials Design
- Powder Metallurgy
- Improved Time-to-Market for New Materials

Modeling and Simulation
- Powder Evolution Through Non-Equilibrium Processing
- Thermodynamic Property Prediction
- Supercooling

Functional Materials
- Functionally Graded Materials
- Powder Metallurgy
- Multi-Function Printing (circuitry and biological applications)

Computation, Mathematics, and Data Informatics

Databases
- Properties
- Materials – Microstructure and Composition
- Process Parameters

Modeling and Simulation
- Powder Evolution Through Non-Equilibrium Processing
- Thermodynamic Properties
- Fluid-Structure Interaction
- Microstructure Evolution Analysis
- Thermo-Elastic Analysis

Datamining
- Pattern Recognition
- Reduced-Order Models
- Data-Driven Methods
- Top-Down Design
- Statistical Data Compression

Applied Mathematics and Methods
- Coupling of PDEs
- Time Integration Schemes
- High-Order Discretization Methods
- Implicit Solvers
- Concurrent Coupling

Experimental Methods

Microstructure Characterization
- Rapid Image-Based Methods
- Non-Destructive Testing
- Large Volume Microstructure Reconstruction
- Statistical Methods

In Situ Metrology
- Thermal History
- Thermal Gradients
- Real-time Microstructure Predictions
- Defect Distribution

Material Characterization
- Anisotropic Stress-Strain Data
- Fatigue Life
- Elastic Properties
- Experimental Microstructure Evolution Tracking

Process Control
- Real-Time Process Control
- Microstructure-Aware Process Optimization

Materials Genome for Multiscale Modeling and Simulation with Experimental Support for Additive Manufacturing

- **Archetype-Genome exemplar:** the apparent properties of a system depend on the building blocks (archetypes) that comprise it; and apparent system properties create the system genome.
- **Three important entities:** design of archetype properties, conformation of archetypes (as a result of processing), and interactions activated by that conformation. (The combination of these entities into the system genome is called assembly.)
- **Integrated design theory/framework (i.e. assembly)** to bridge the gap between computational methods and scales for a well defined genome for particular application(s)
- **AM has a natural application in this framework: Archetype conformation and interactions are apparent with a cursory inspection of the technology**
  The question is, can we develop detailed *material databases, conformation and interaction (statistical descriptions with uncertainty quantification)* to produce a desired genome with AM techniques?