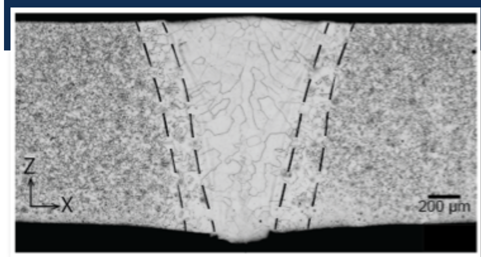
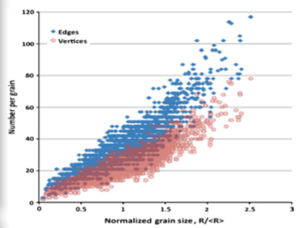
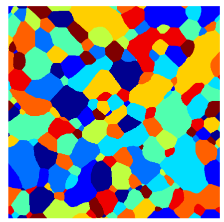
SAND2017-9381C

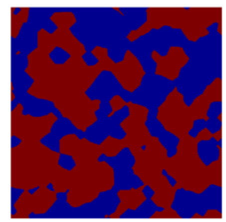
Exceptional service in the national interest

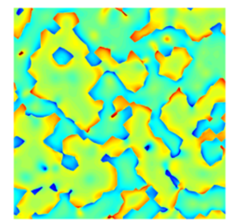
Sandia National Laboratories

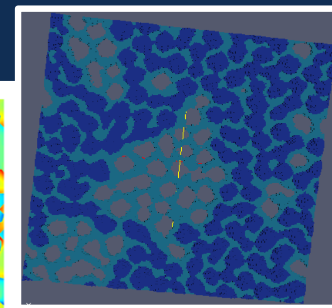


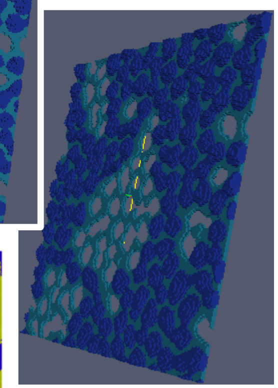


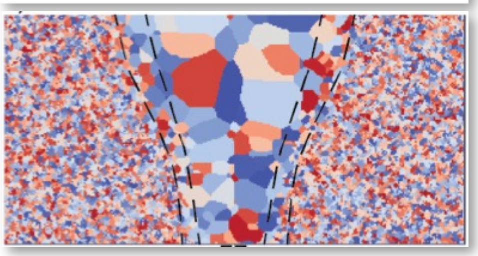


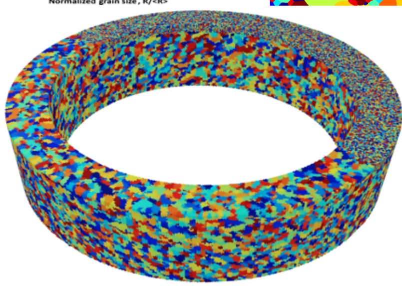


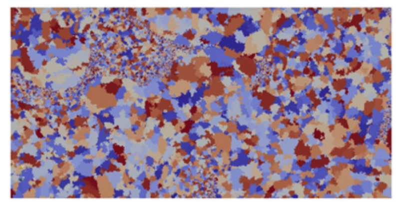


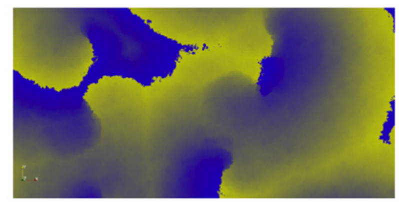












SYNTHETIC MICROSTRUCTURES FOR ADDITIVE MANUFACTURING: GENERATION, QUANTIFICATION & PARTNERING EFFORTS

Jonathan Madison, Theron Rodgers, Kyle Johnson, Joe Bishop, Veena Tikare

[1]*Sandia National Laboratories, Albuquerque, NM*

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND2017-XXXX

Acknowledgements

- ***Steve Plimpton***
- ***Aiden Thompson***
- ***Dave Adams***
- ***Mario Martinez***
- ***Mike Maguire***
- ***Joe Michael***
- ***Ben Reedlunn***
- ***Joe Bishop***
- ***Kyle Johnson***

- ***Todd Palmer et al.**, Pennsylvania State University*
  Center for Innovative Materials Processing through Direct Digital Deposition (CIMP-3D)
- ***Surya Kaladindi et al.**, Georgia Institute of Technology*
- ***Amy Clark et al.**, Colorado School of Mines*
- ***Joe McKeown et al.**, Lawrence Livermore National Laboratories*

Outline

I. **A Database Approach to Additive**

II. **Computational Lengthscales & Tools**

III. **SPPARKS Framework & Approximating Solidification**

IV. **Additive Case Studies**

IV. **Partnering Efforts**

- *Thin Films*
- *Data Science*
- *Thermal History Models*
- *Direct Numerical Simulation for Mechanics*

V. **Concluding Thoughts & Summary**

GRANTA's Approach to Additive

Sandia National Laboratories

Leverage core expertise of MDMC members

- Materials, manufacturing, data management
- Software infrastructure and networks

Focus

- Schema development, software & network integration,
- standards, interfacing with AM initiatives worldwide

MDMC.net

BOEING

Pratt & Whitney
A United Technologies Company

UTC Aerospace Systems

LOCKHEED MARTIN

NORTHROP GRUMMAN

Honeywell

U.S. ARMY

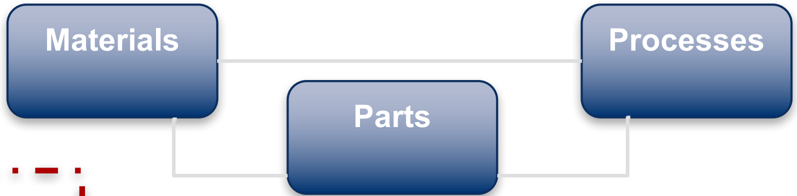
ARL

OAK RIDGE National Laboratory

NASA

and more….

AM Schema Requirements



Feed materials

- Bulk properties
- Simulation input data
- Microstructure

Polymers
Low density alloys
High temp alloys
Medical alloys
Innovative alloys…

Processes (Machines and simulations)

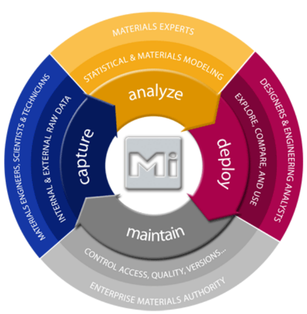
- Type and capabilities details
- Processing parameters stores
- Project-specific data

Direct laser deposition
Laser sintering
Electron beam deposition
Electro-mechanical…

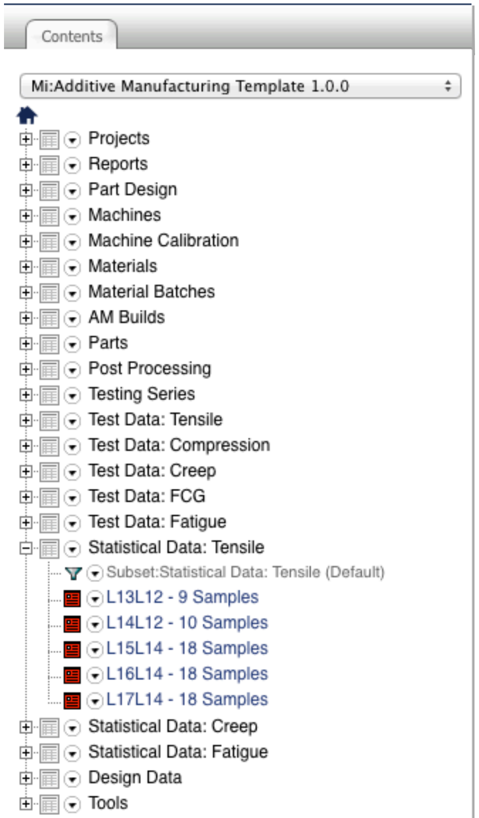
Fabricated parts

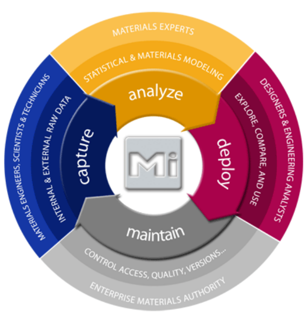
- Characterization, measurements, properties

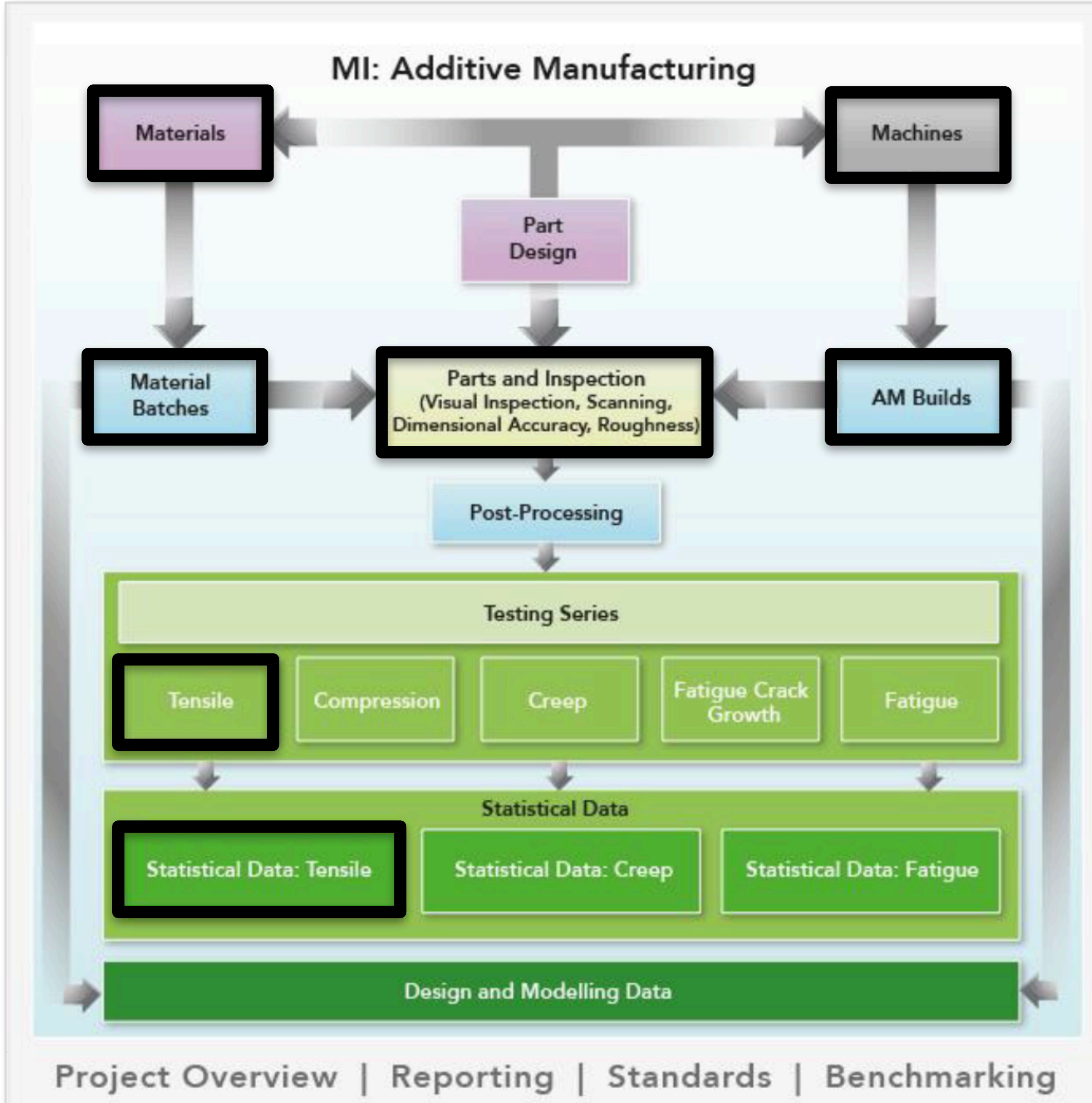
Mechanical testing
Ultrasonic inspection
Computed Tomography
Metallography
Microscopy…



AM Schema Visualized





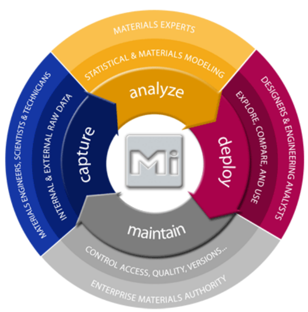


MDMC.net

AM Schema Attributes Count

Granta MI, AM Schema Layout Headings

Layout Headings - Granta AM Schema v1.01					
Machines	Materials	Part Design	Material Batches	Builds	Parts
General Information	General Information	General Information	Project Information	Project Information	Project Information
Calibration	General Properties	Original Design	General Batch Information	General Information	Part Information
Machine Specifications	Composition overview	Re-Design	Manufacturing	Build Information	Part Specifications
Material	Bulk Mechanical Properties	Dimensions	Material Quality	General Build Parameters	Samples
Machine Properties	Bulk Thermal Properties	General Material Properties	Particle Properties and Size Distribution	Build Atmosphere	Visual Inspection
Build Environment	Bulk Electrical Properties	Processing	Interstitial contamination	Material Used	Accuracy Testing
Laser Properties	Biological	Static Tensile Properties	Flowability	Support	NDT Testing
Electron Beam Properties	Chemical	High-cycle fatigue properties	Wire Properties	Filament Information	Post Processing
	Eco	Fracture Toughness	Chemical Analysis and Composition	Substrate	Heat Treatment
	Cost	Fatigue Crack Growth		Quality of Welding Consumables	HIP
	Safety and Handling	Surface Roughness Requested		Build Alarms	Machining
	General Information	Other Requested Properties		Themes Used	Laser Polishing
	Requirements	Final Part Details		Powder Build Parameters	Other Post Processing
	Composition	Quality Assurance		Wire Build Parameters	
	Physical Properties	Key Benefits		Laser Properties	
	Further Information			Electron Beam Properties	
				Arc Properties	
				In-Process Rolling	
				In-Process Analysis	

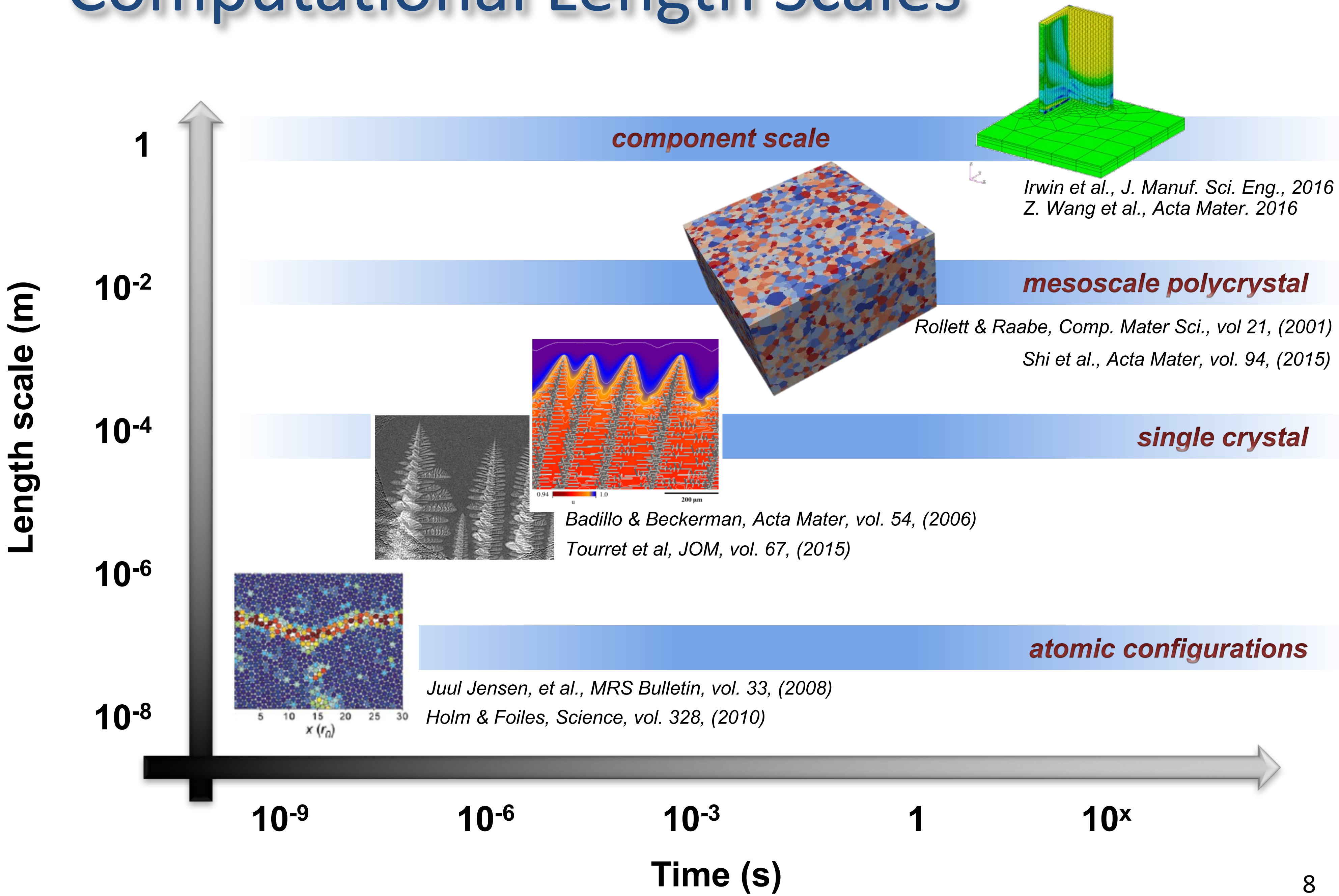


MDMC.net

Currently Includes **800+** individual attributes

Traditional brute force design of experiment approaches are no longer tenable. Efficient & flexible modeling approaches in additive are needed now more than ever.

Computational Length Scales



Computational Tools

Length scale (m)

- **DEFORM** – forming heat-treatment & machining
- **DANTE**
- **ProCast** – solidification
- **Micress**
- **JMatPro** – composition dependent properties (thermo, chemical, mechanical, etc.)
- **PrecipiCalc** – multiparticle diffusive precipitation kinetics
- **PanDat**
- **ThermoCalc** – thermodynamic calculations/predictions
- **MedeA** – combinatorial property predictions by lower length scale simulation(s)
- ***LAMMPS**
- **VaSP**

continuum

mesoscale polycrystals

single crystal

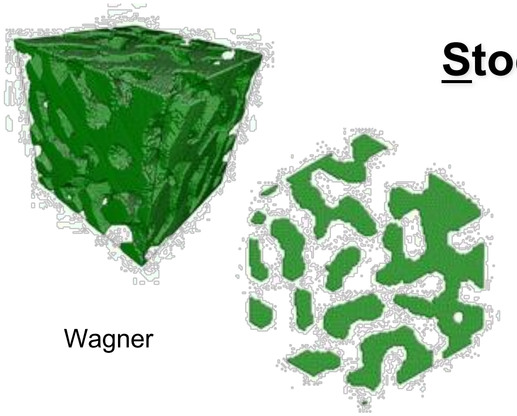
atomic configurations

Sim Framework

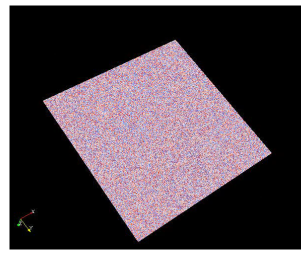
SPPARKS

Stochastic Parallel PARticle Kinetic Simulator

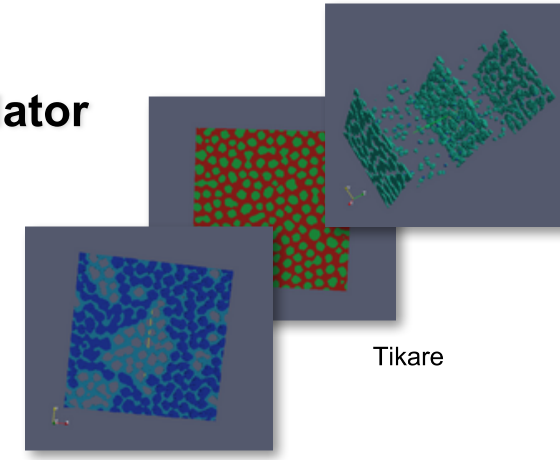
http://spparks.sandia.gov



Wagner

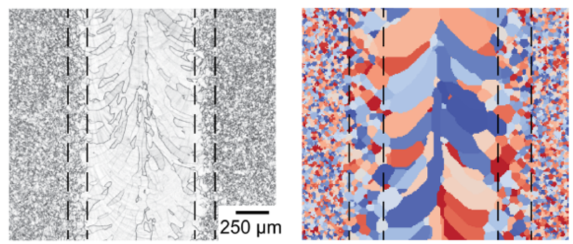


Holm & Battaile, ***JOM*** (2001) vol. 53, pp. 20-23

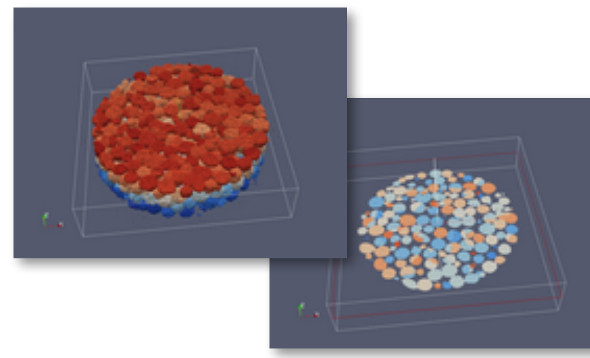


Tikare

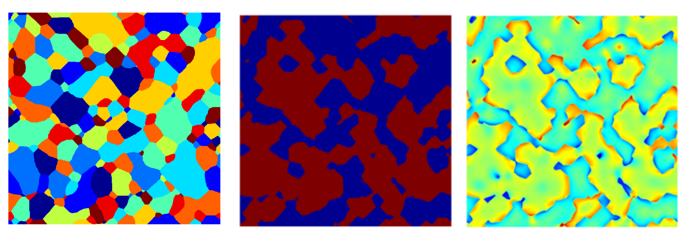
- Open source kinetic Monte Carlo platform with user-editable “apps” for specific applications
- Used to study several mesoscale phenomena including sintering, recrystallization, vacancy diffusion, grain growth and welding
- Problems are easily parallelized and a range of Monte Carlo solvers are available



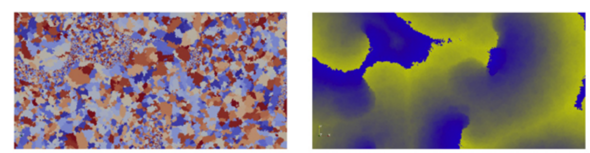
Rodgers, Madison, Tikare & Maguire, ***JOM*** (2016) vol. 68, pp. 1419-1426



Cardona et al. ***J. Am. Ceram. Soc.*** (2012) pp. 1-12



Homer, Tikare & Holm, ***Comp. Mat. Sci.*** (2013) vol. 69 pp. 414-423



Madison, Tikare & Holm, ***J. Nuc. Mat.*** (2012) vol. 425 pp. 173-180

Potts kinetic Monte Carlo

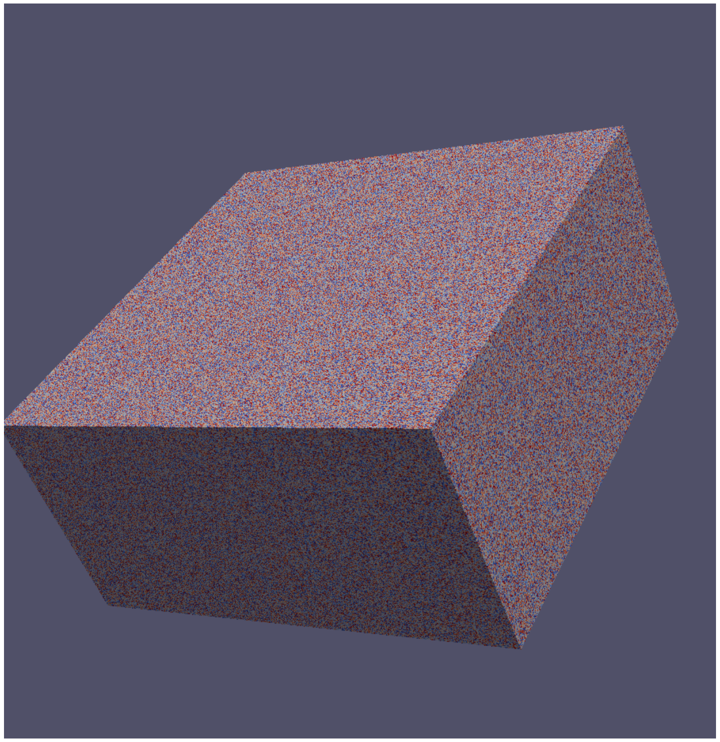
- The Potts model is widely used to simulate curvature-driven grain growth
- The simulation domain is divided into a discrete lattice and each site is assigned a grain ID or "spin".
- Grain boundary motion occurs by changing a site's grain ID to that of a neighboring lattice site and determining the resulting change in system energy.

- The change is accepted/rejected via the
  - Metropolis function:

$$P = \begin{cases} \exp\left(\frac{-\Delta E}{k_B T_S}\right) & if\ \Delta E > 0 \\ 1 & if\ \Delta E \leq 0 \end{cases}$$

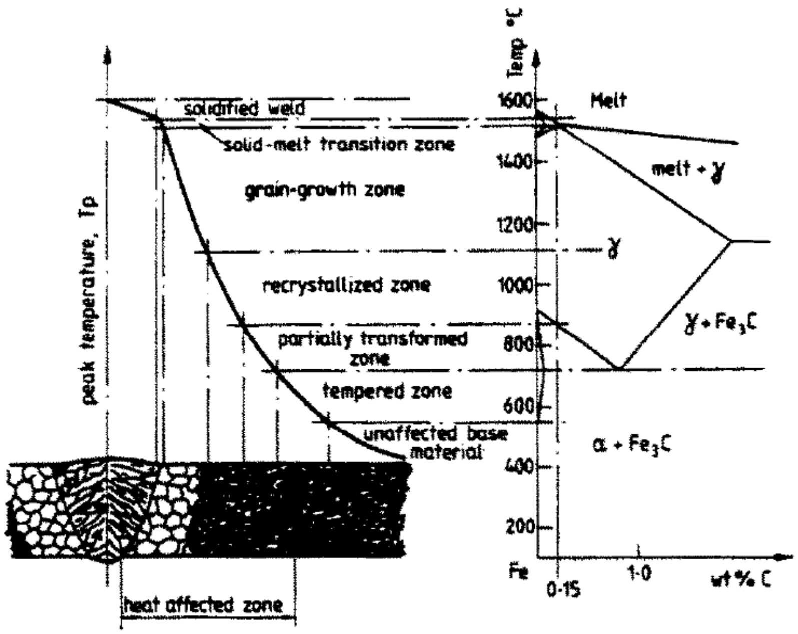
  - where system energy, E, is determined by:

$$E = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{26}\left(1-\delta\left(q_i, q_j\right)\right)$$

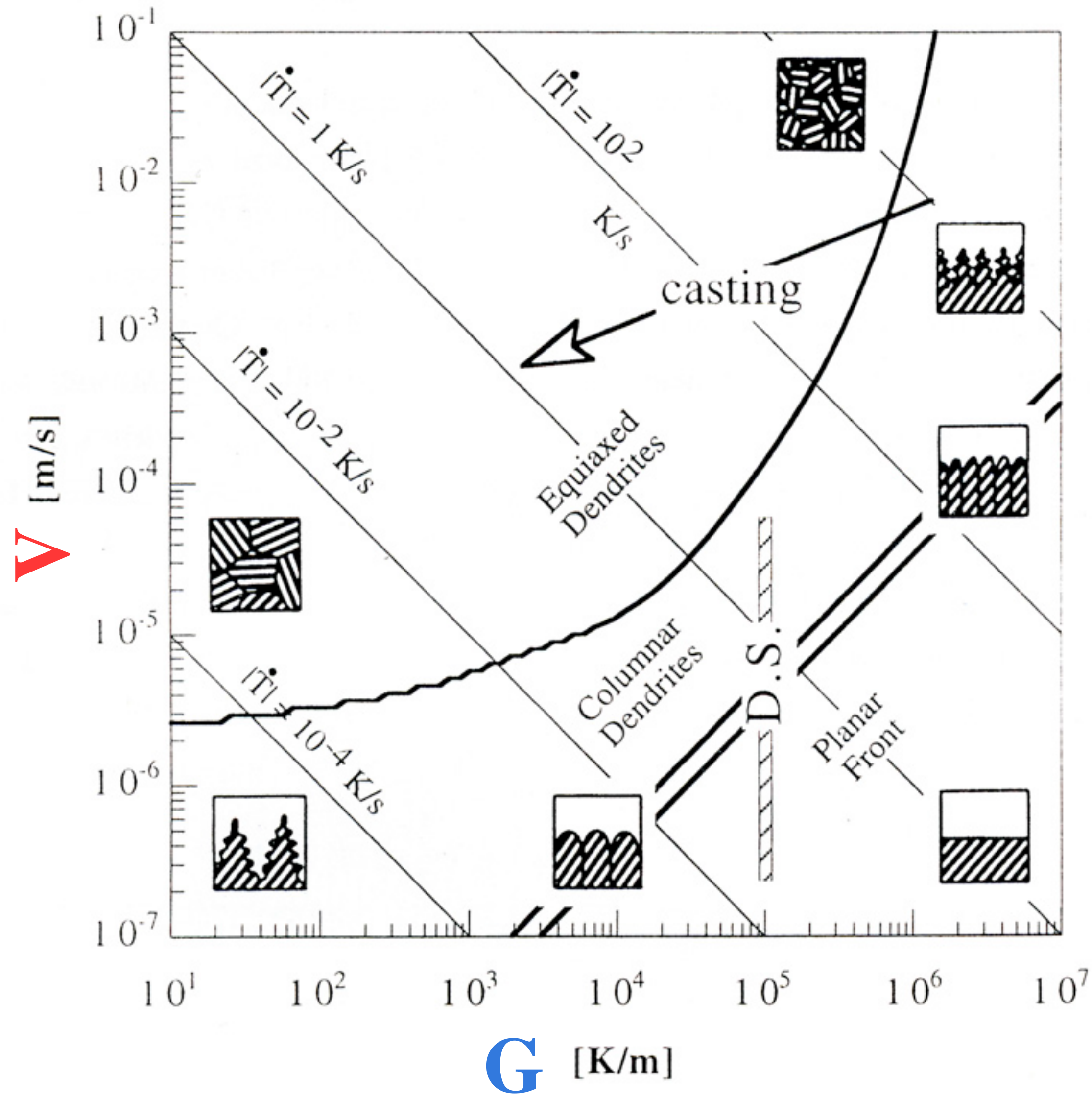


Solidification

- In directional solidification, it has been widely understood that select combinations of ***thermal gradient (G)*** and ***solidification front velocity (V)*** produce specific grain morphologies in single phase metallic systems



M.F. Ashby, K.E. Easterling, ***Acta Metall.***, (1982) vol. 30, pp. 1969-1978

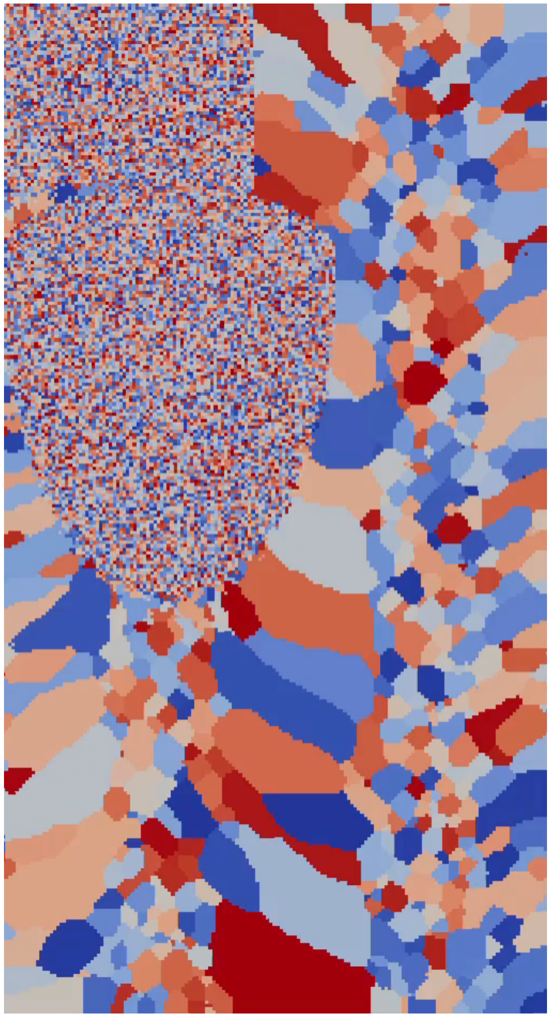


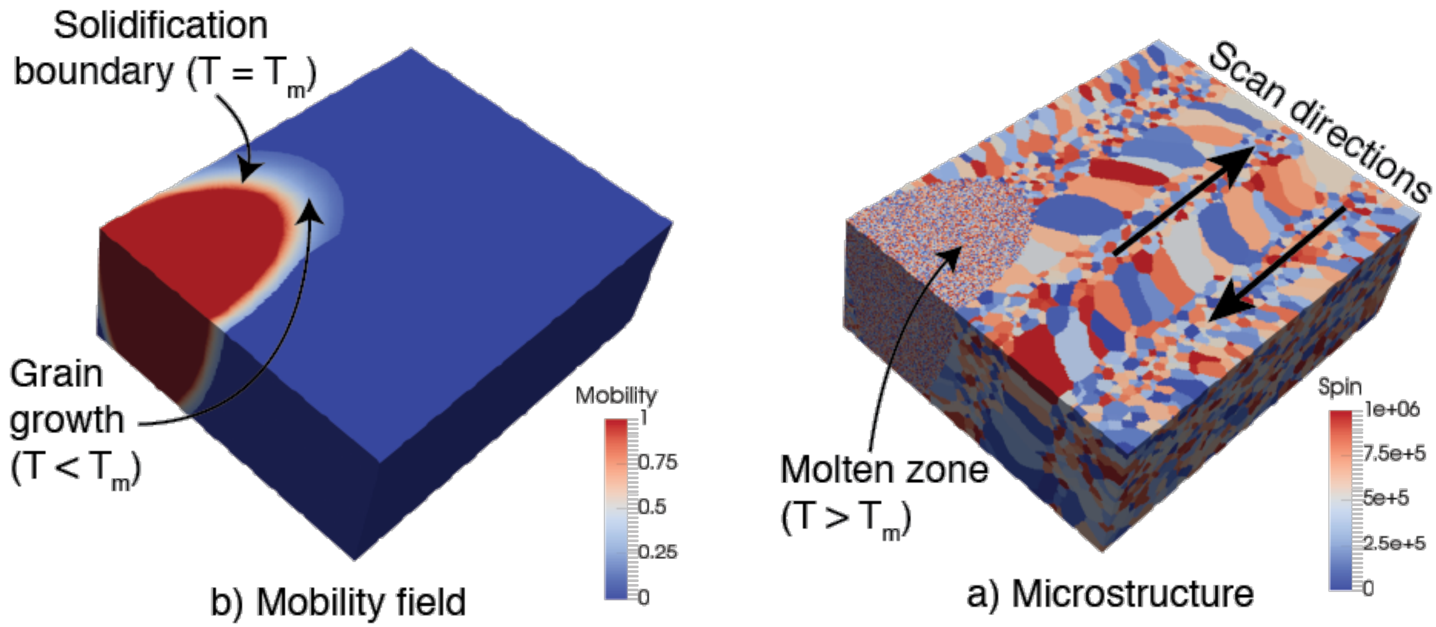
W. Kurz, & D.J. Fisher, Fundamentals of Solidification, Chapter 4: Solidification Microstructure, Trans Tech Publications (Enfield, NH, 1998)

kMC & Solidification

$$M(T) = M_o \exp\left(\frac{-Q}{RT}\right)$$

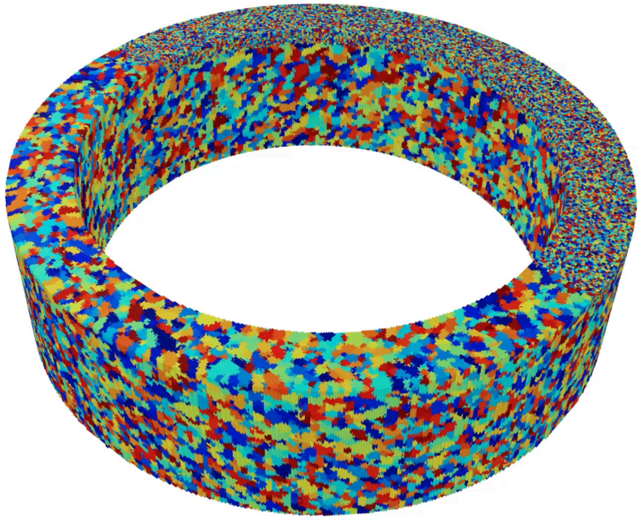
$$P = \begin{cases} M(T)\exp\left(\frac{-\Delta E}{k_B T_s}\right), & if\ \Delta E > 0 \\ M(T), & if\ \Delta E \le 0 \end{cases}$$

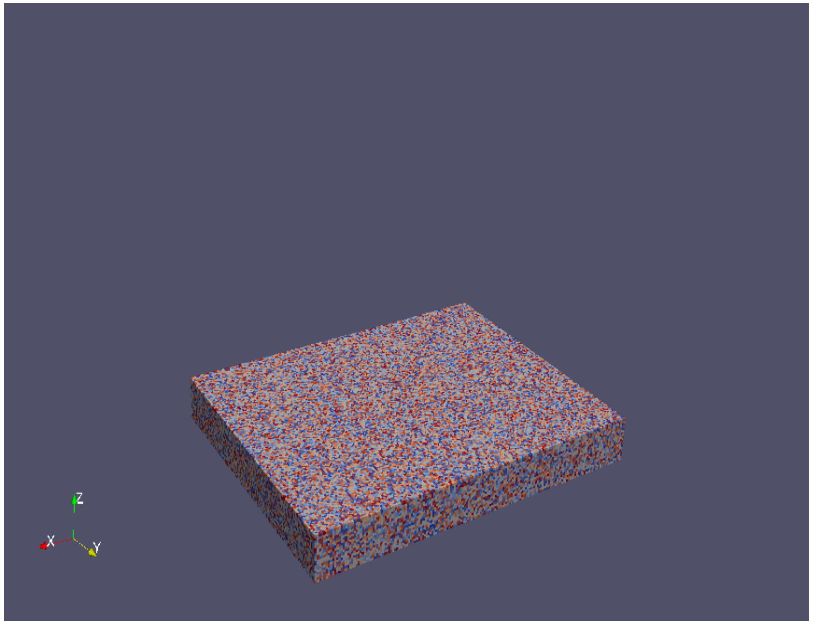




- The molten zone randomizes grain identities when it enters a region.
- Along the trailing surface, voxels either join existing columnar grains or form new grains.
- The temperature gradient creates a corresponding gradient of grain boundary mobilities via an Arrhenius relationship.

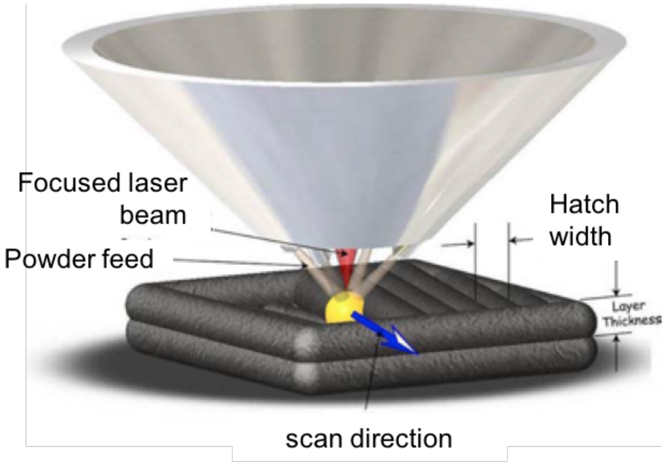
Additive Processes



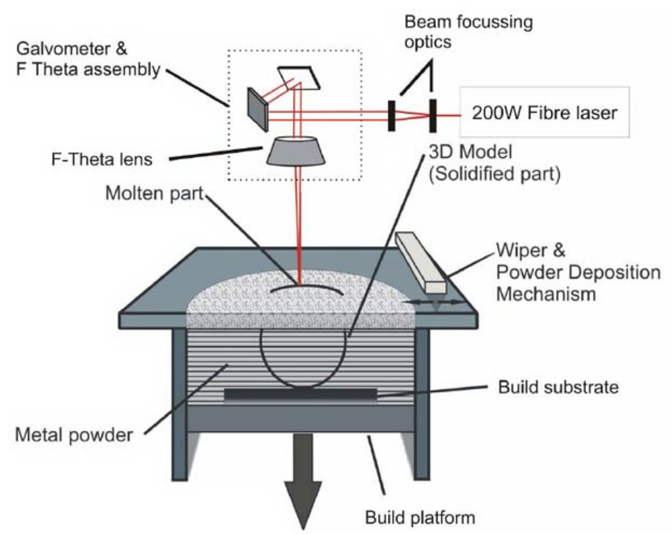


modified Kinetic Monte Carlo (MkMC) via SPPARKS

LASER ENGINEERED NET SHAPING



POWDER BED FUSION



http://www.fusionimplants.com

Additive Case Studies

- Thin-wall builds of Inconel 718 by DED

  Parimi et al., ***Mater. Charact.*** (2014), vol. 89, pp. 102-111

- Two-pass build of Ti-6V-4Al by SEBM

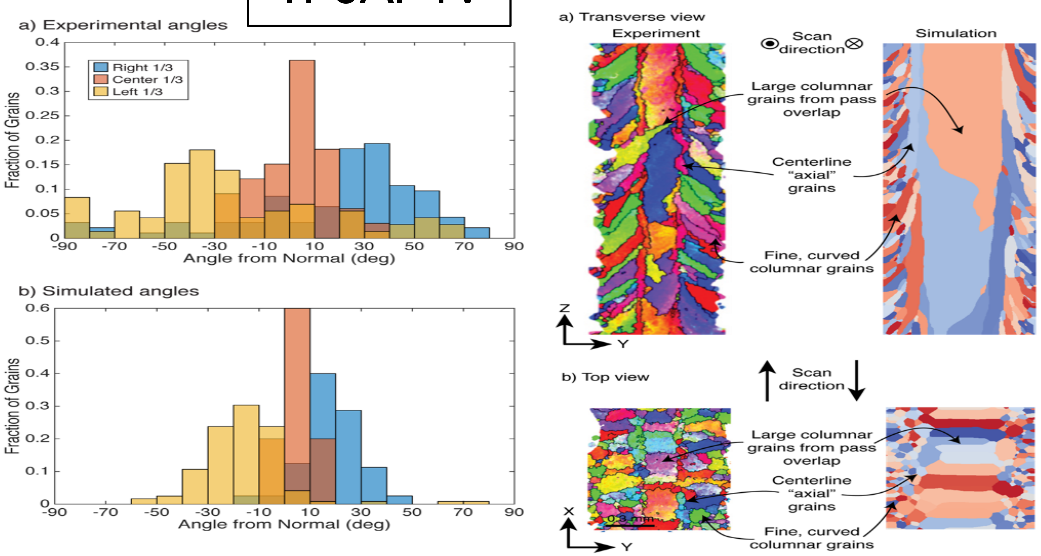
  A. Antonysamy et al., ***Mater. Charact.*** (2013), vol. 84, pp. 153-168

- High-power LENS build of 304L Stainless Steel

  Nishida et al., **Proc. of DYMAT 2015**

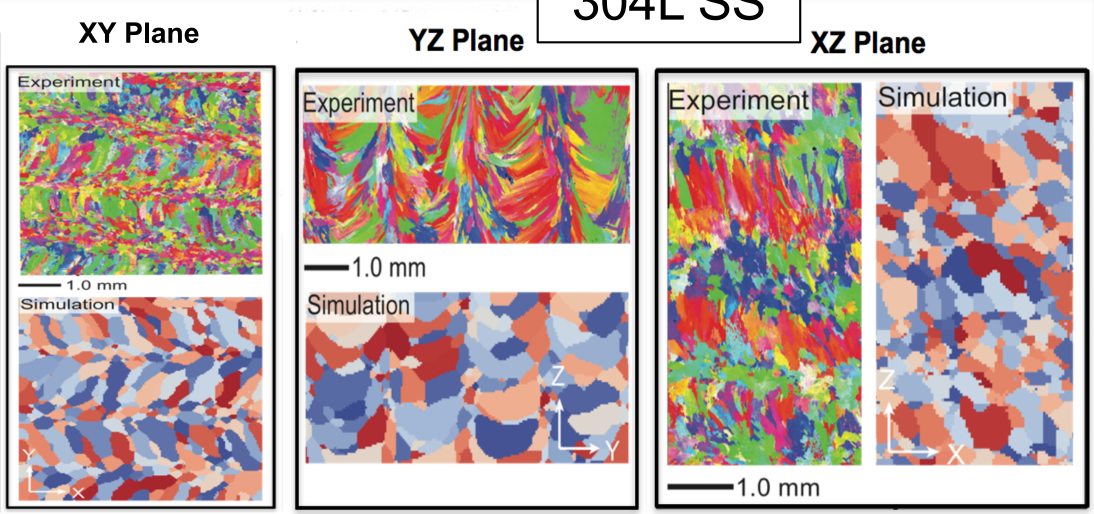
Additive Case Studies

Ti-6Al-4V



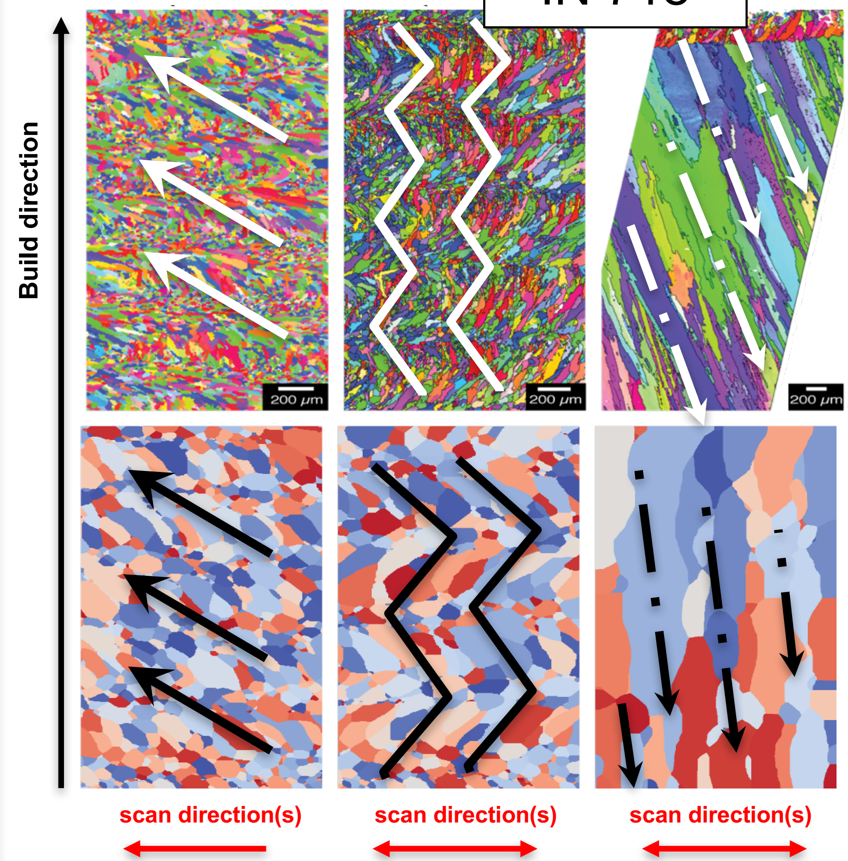
A. Antonysamy et al., ***Mater. Charact.*** (2013), vol. 84, pp. 153-168

304L SS

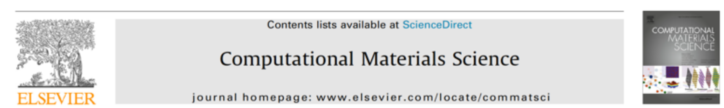


Nishida et al., **Proc. of DYMAT 2015**

IN 718



Parimi et al., ***Mater. Charact.*** (2014), vol. 89, pp. 102-111



Computational Materials Science 135 (2017) 78–89

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Simulation of metal additive manufacturing microstructures using kinetic Monte Carlo

Theron M. Rodgers[a,*], Jonathan D. Madison[b], Veena Tikare[c]

[a] Computational Materials & Data Science, Sandia National Laboratories, PO Box 5800 MS-1411, Albuquerque, NM 87185, USA
[b] Materials Mechanics, Sandia National Laboratories, PO Box 5800 MS-0889, Albuquerque, NM 87185, USA
[c] Multiscale Science, Sandia National Laboratories, PO Box 5800 MS-1321, Albuquerque, NM 87185, USA

Application to Thin Film Grain Growth

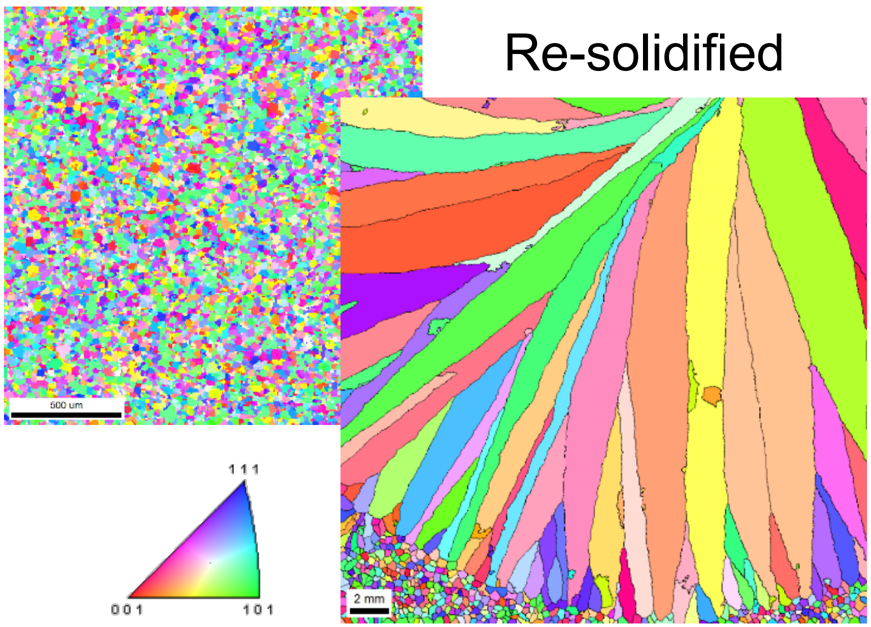
Grain Growth in Thin Films

- Thin Films of Al-Si binary alloys melted to undergo rapid solidification while being observed in a time-resolved dynamic TEM (DTEM).
- Solidification interface profiles are extracted and used as inputs for a 2D kMC model.
- Simulations are now being modified to allow incorporation of crystallographic texture

Experimental ASTAR

Initial

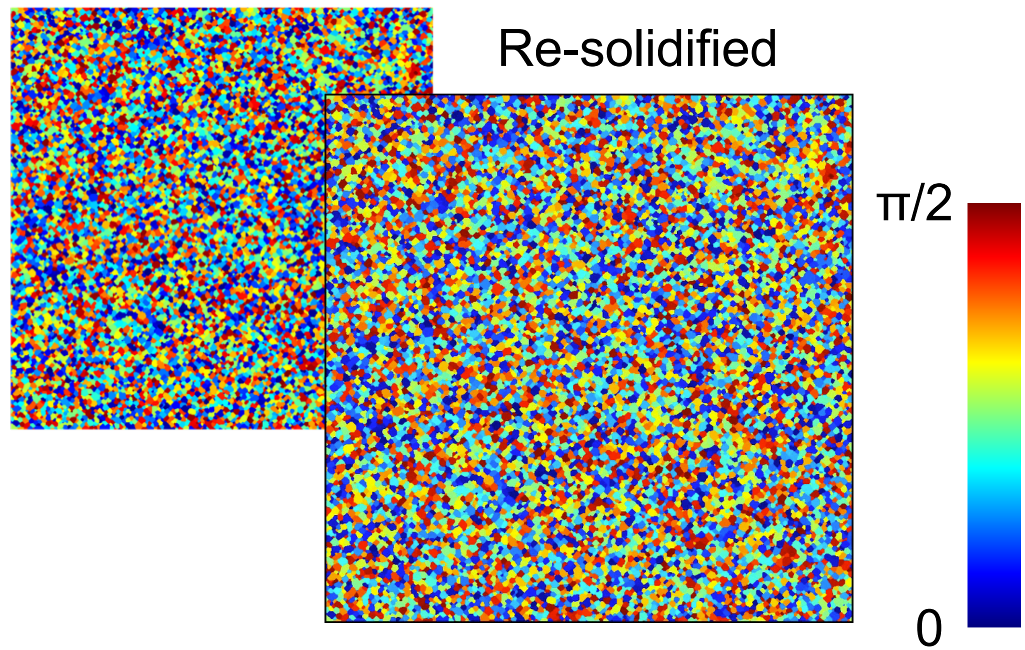
Re-solidified



Simulation

Initial

Re-solidified



Lawrence Livermore National Laboratory

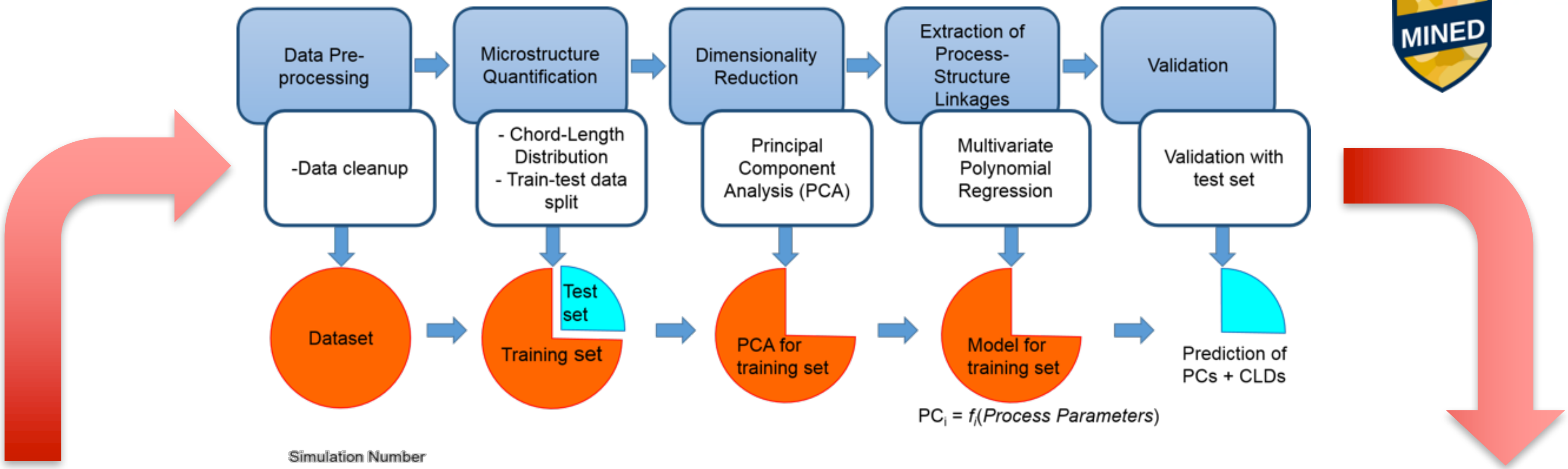
COLORADO SCHOOL OF MINES
EARTH • ENERGY • ENVIRONMENT

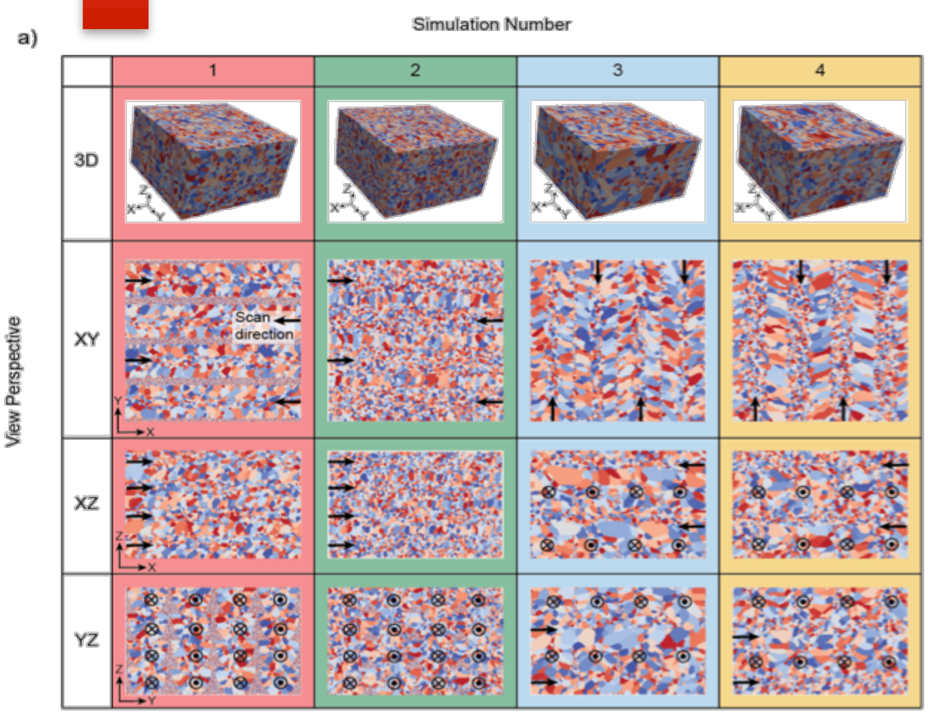
J. McKeown (LLNL), A. Clarke (CSM), J. Gibbs (LANL), T. Rodgers, J. Madison (SNL)

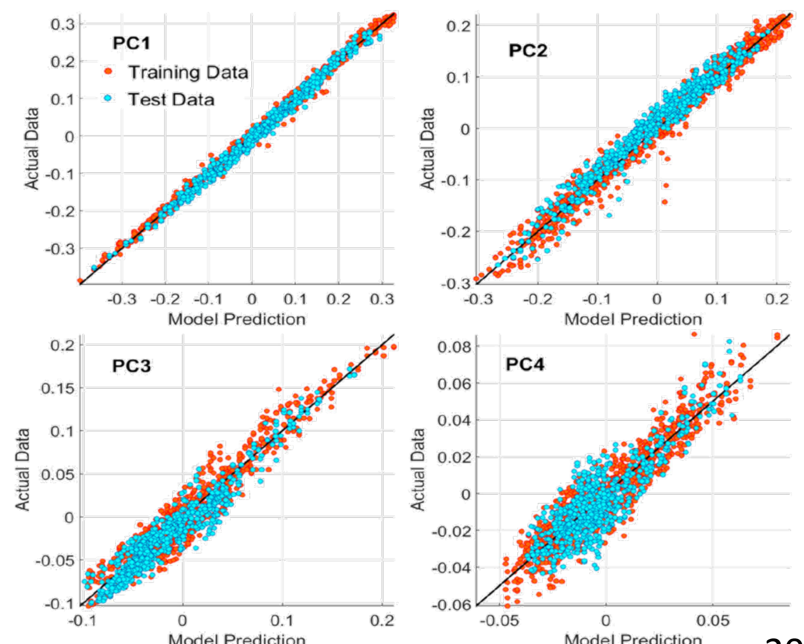
Application to Data Science

Exploring AM via Data Science I

- Developed a reduced-order model for microstructure prediction using chord length distributions (CLDs).



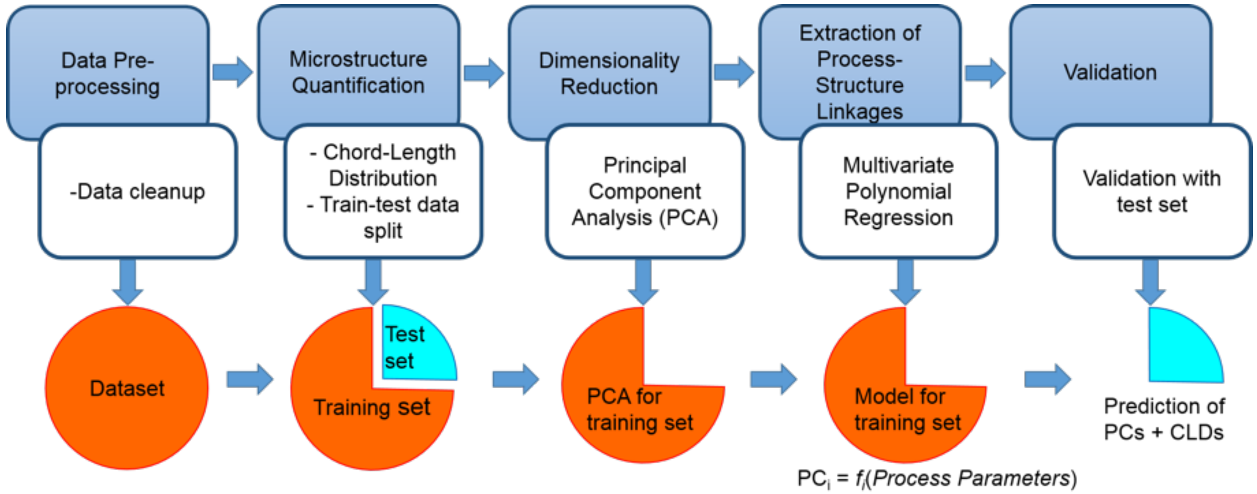


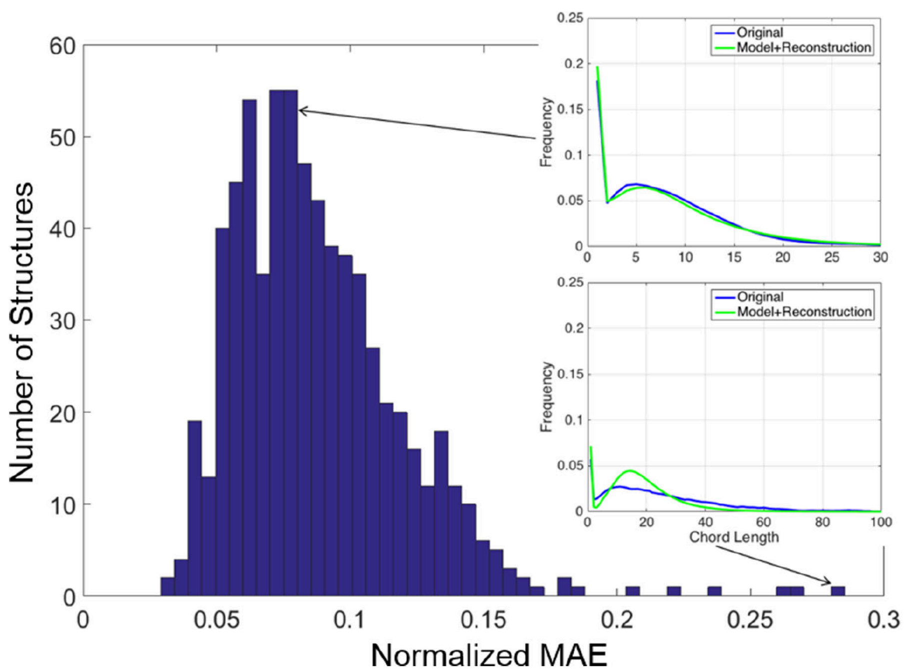


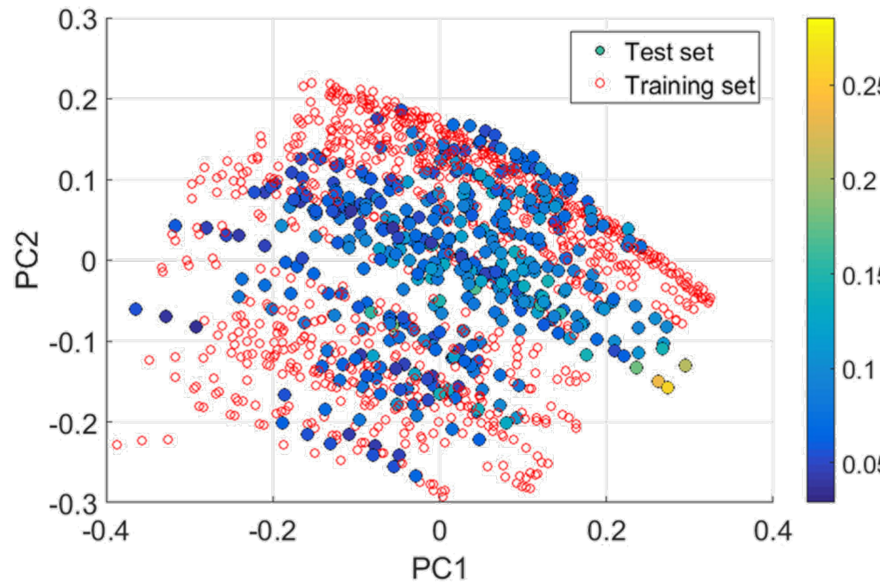
E. Popova, S. Kaladindi, T. Rodgers, J. Madison, et. al., ***IMMI,*** *(2017) vol. 6, pp. 54-68*

Exploring AM via Data Science II

- Developed a reduced-order model for microstructure prediction using chord length distributions (CLDs).





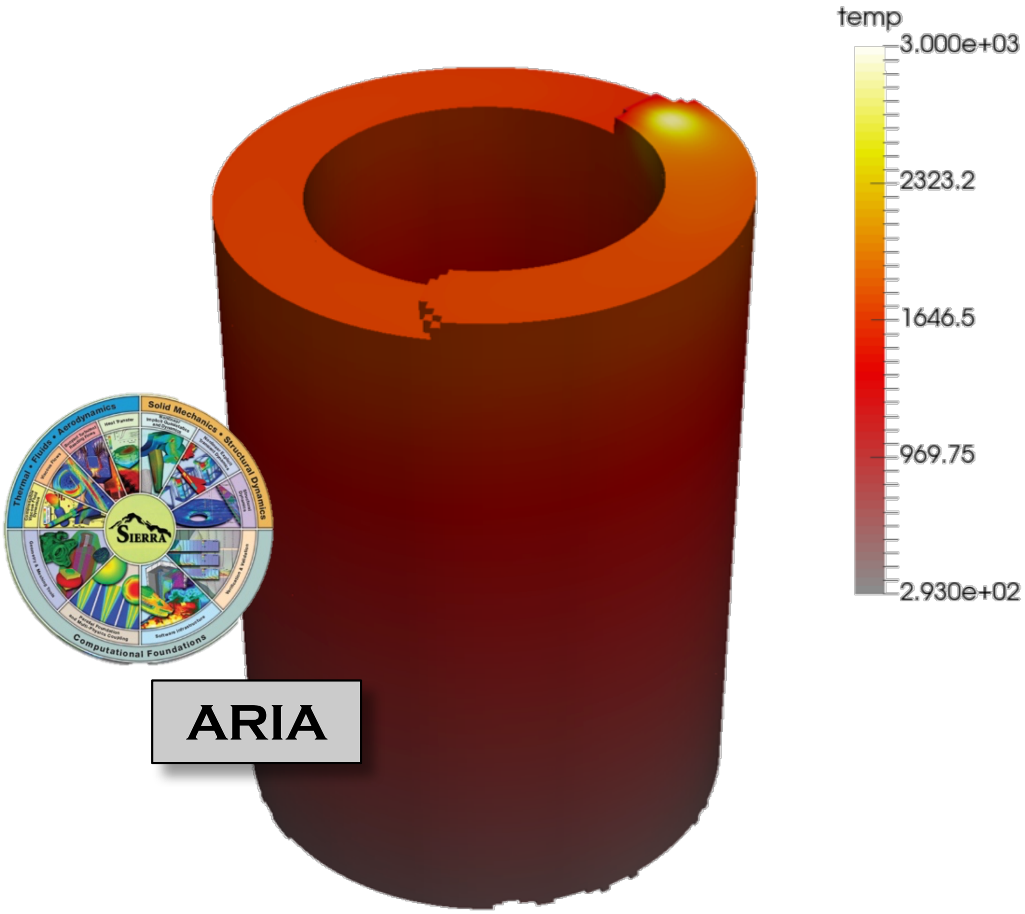


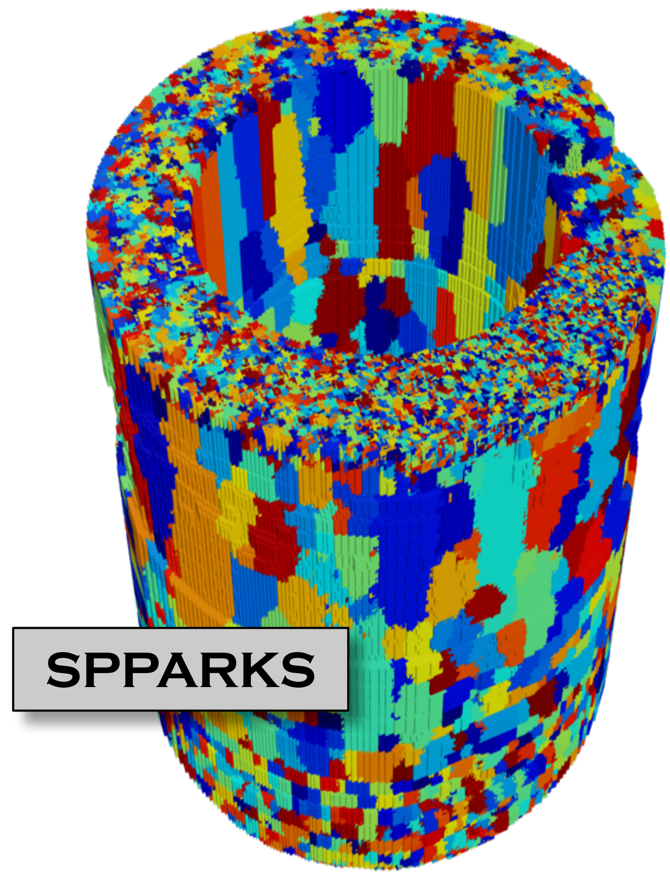
E. Popova, S. Kaladindi, T. Rodgers, J. Madison, et. al., ***IMMI,*** (2017) vol. 6, pp. 54-68

Application to Thermal History Models

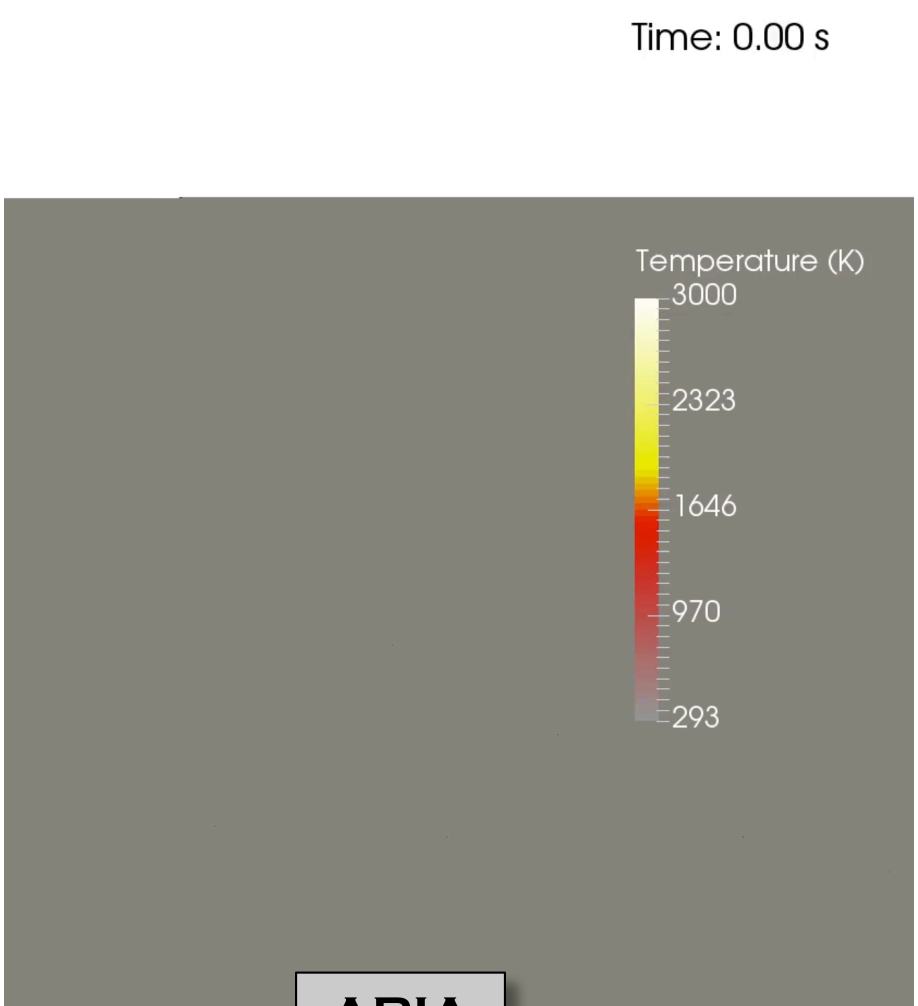
Linking to Thermal Models I

- Using thermal histories simulated within SNL's production code, ARIA as an input, the modified Monte Carlo Potts model within SPPARKS is coupled to predict grain morphologies within an additive manufacturing build. This demonstrates an ability to predict grain morphology from a rigorous multi-physics model as opposed to a simplified and idealized approximation of the molten zone.

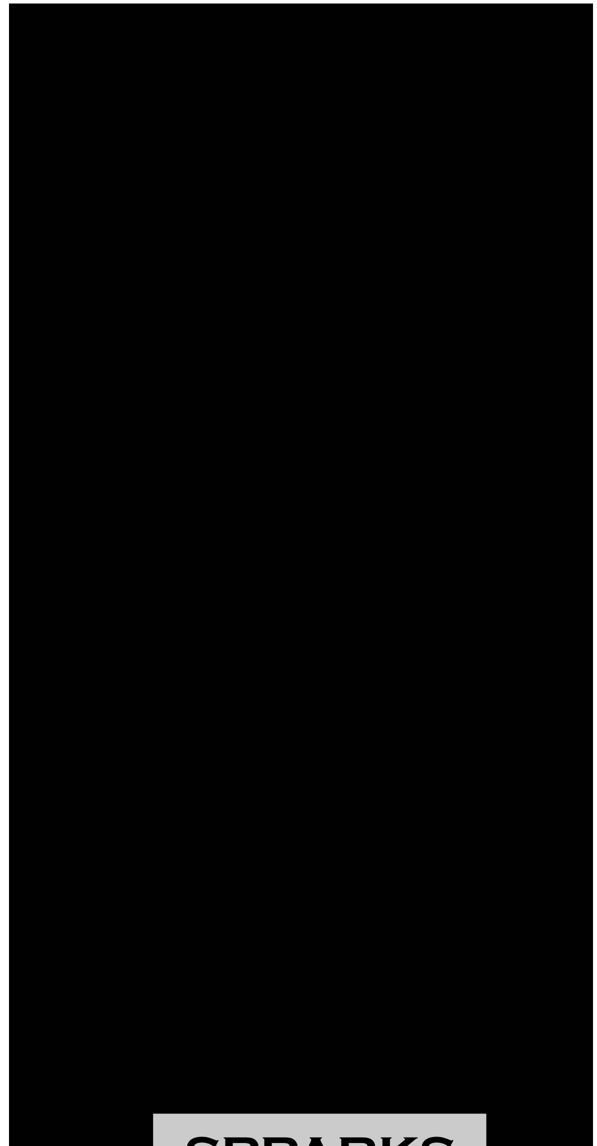




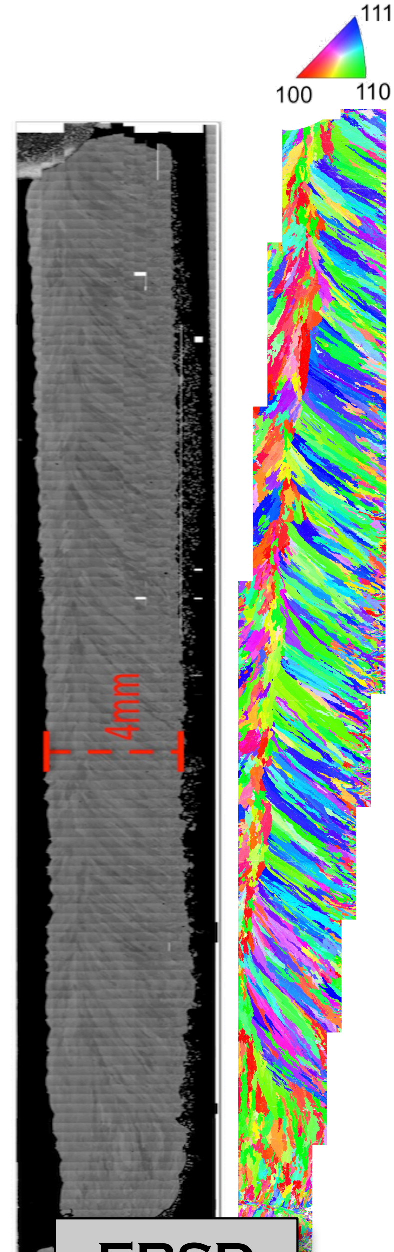
Linking to Thermal Models II



ARIA



SPPARKS



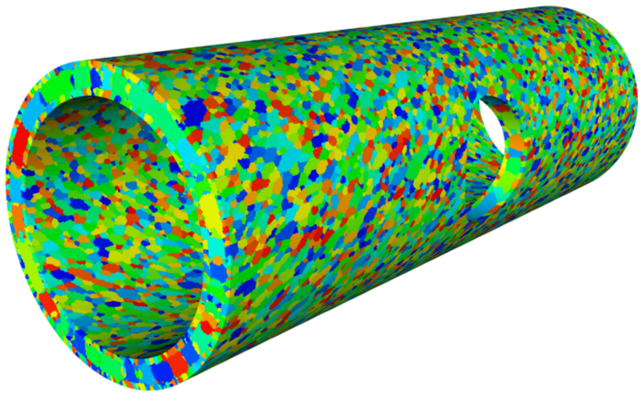
EBSD

K. Johnson, T. Rodgers, O. Underwood (Sandia National Labs)

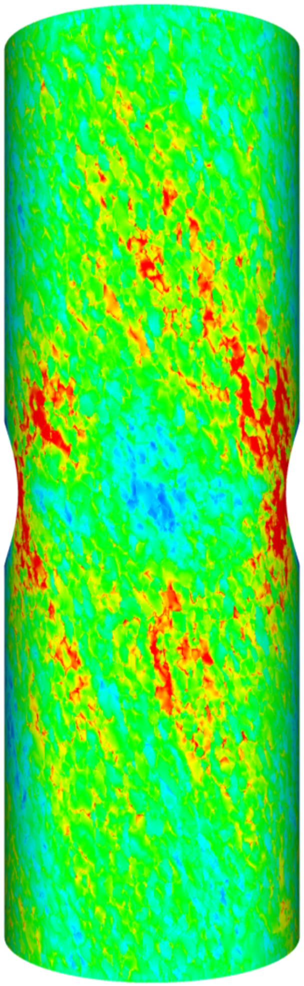
Application to Mechanics

DNS Inputs for Mechanics

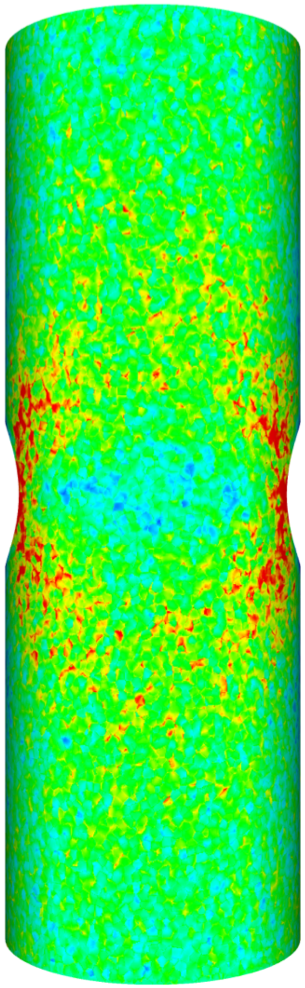
- AM simulations have been performed on cylindrical domains and the resulting microstructures used in solid mechanics simulations.



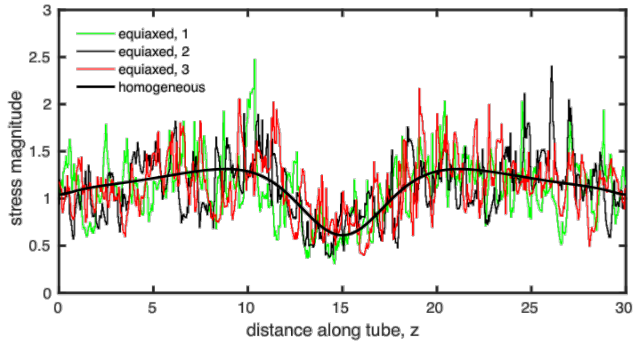
AM-micro stresses

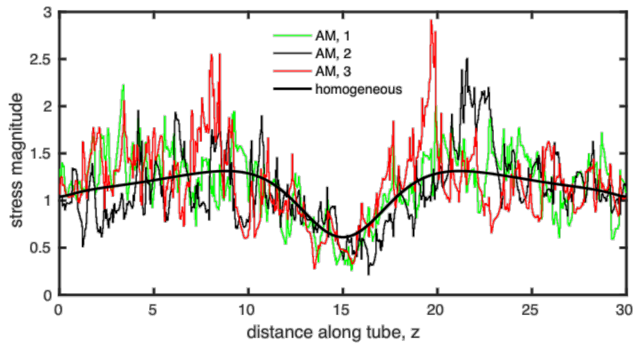


Equiaxed stresses



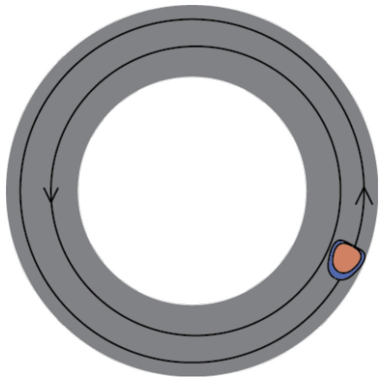
- Stress fields along tube for several equiaxed (top) and AM (bottom) microstructures.





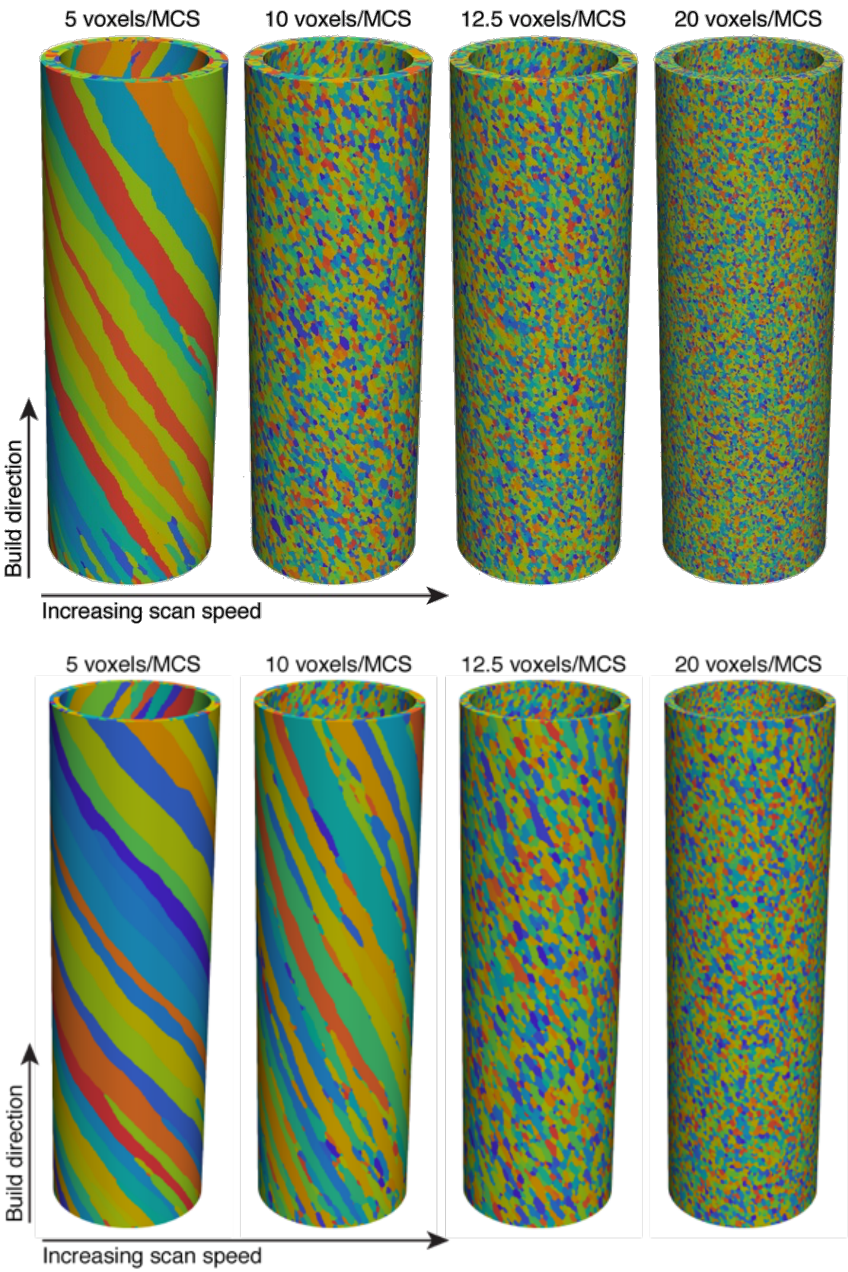
J. Bishop, T. Rodgers, J. Madison, (Sandia National Labs)

DNS Inputs for Mechanics



Synthetic AM builds

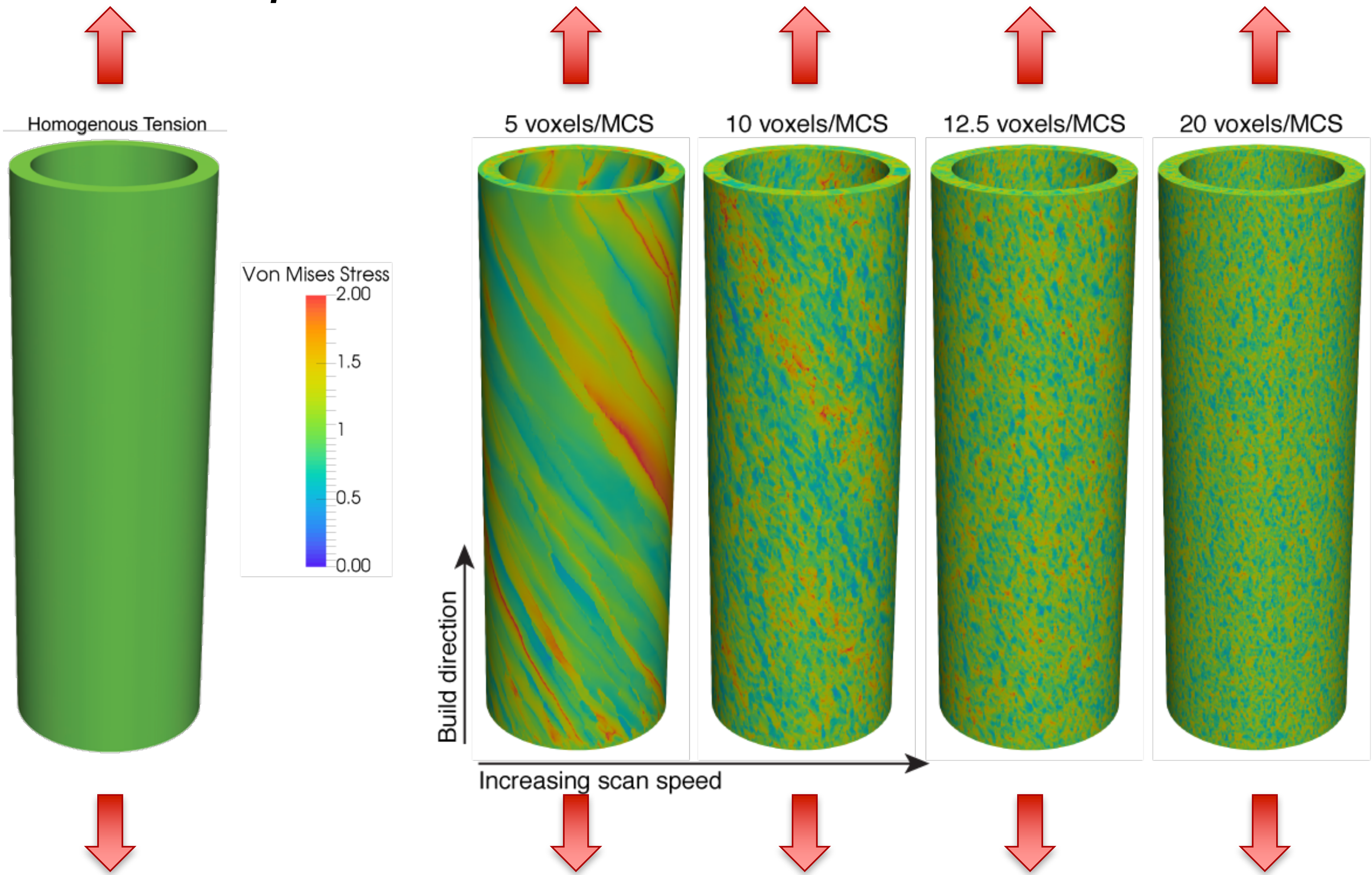
- 4 scan velocities.
- 2 concentric circular scan paths per layer.
- Idealized molten pool
- Significant microstructure variation w.r.t. scan velocities and w.r.t. wall thickness.



J. Bishop, T. Rodgers, J. Madison, (Sandia National Labs)

Direct Numerical Simulation

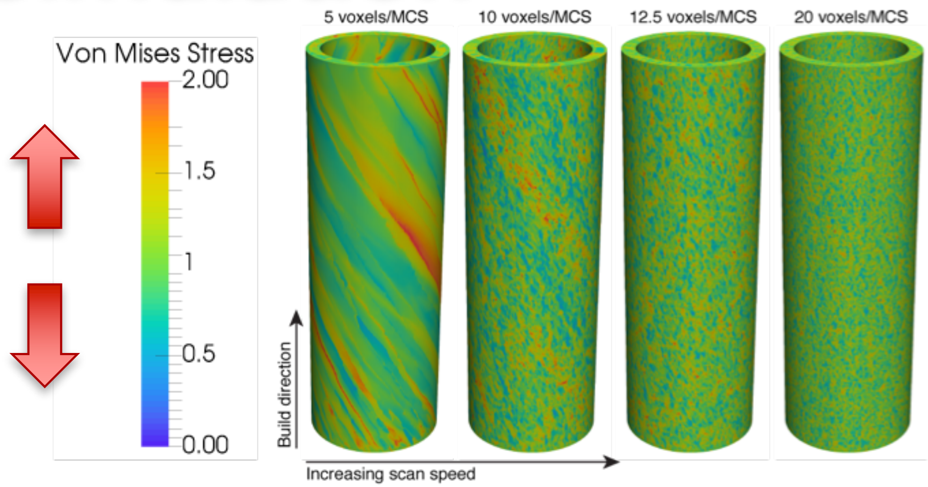
Stress response in tension

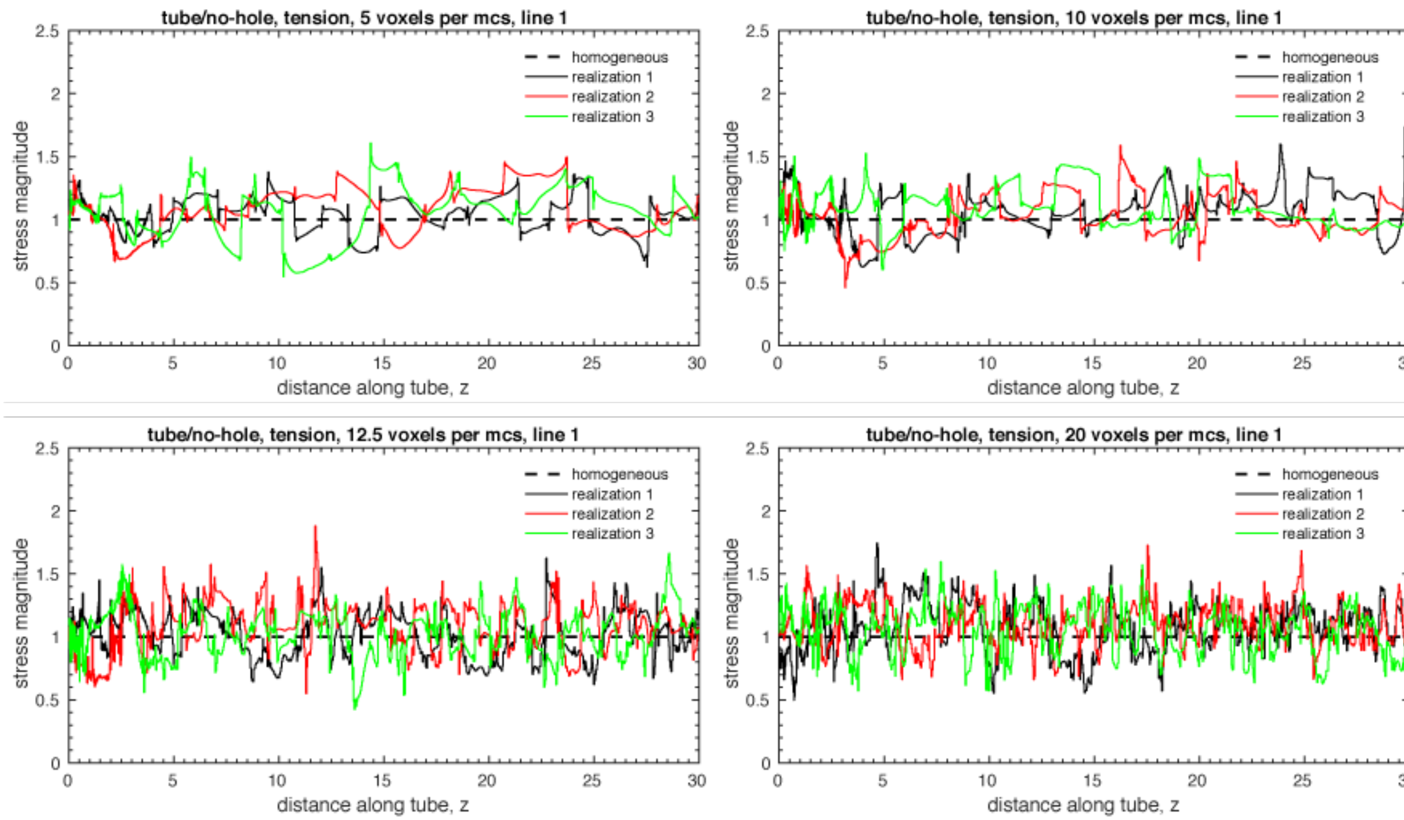


J. Bishop, T. Rodgers, J. Madison, (Sandia National Labs)

Direct Numerical Simulation

Stress response in tension

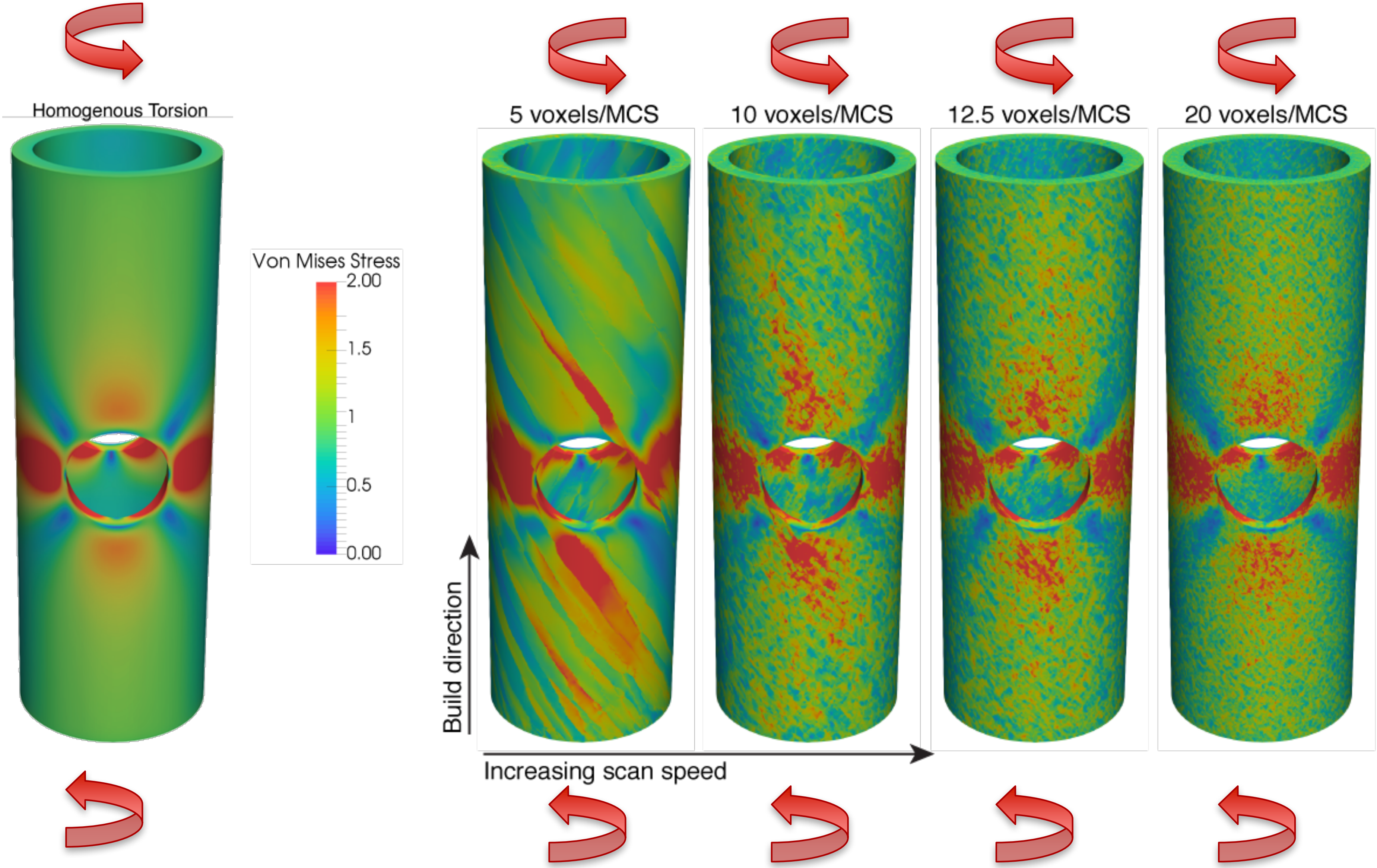




J. Bishop, T. Rodgers, J. Madison, (Sandia National Labs)

Direct Numerical Simulation

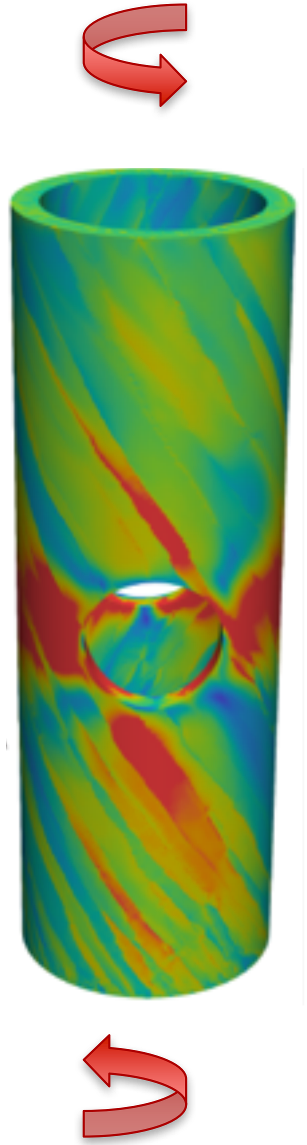
Stress response in torsion (w/stress concentrator)

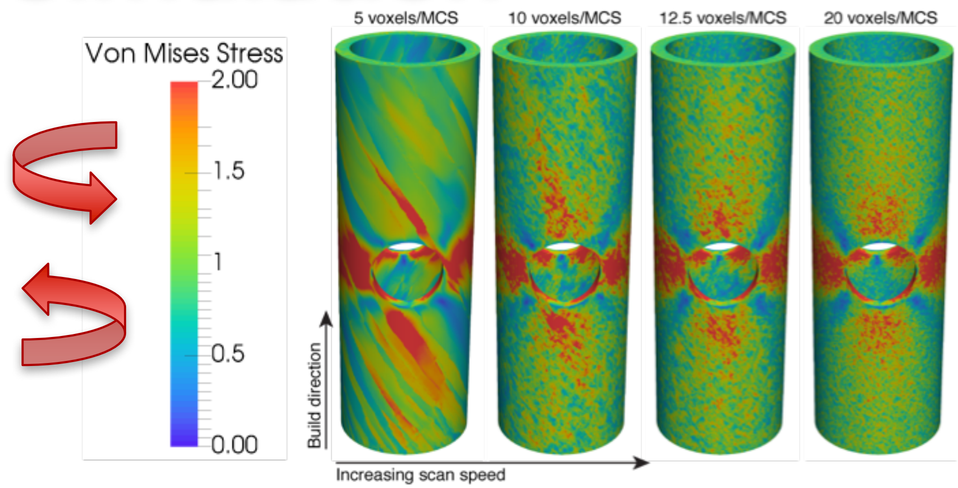


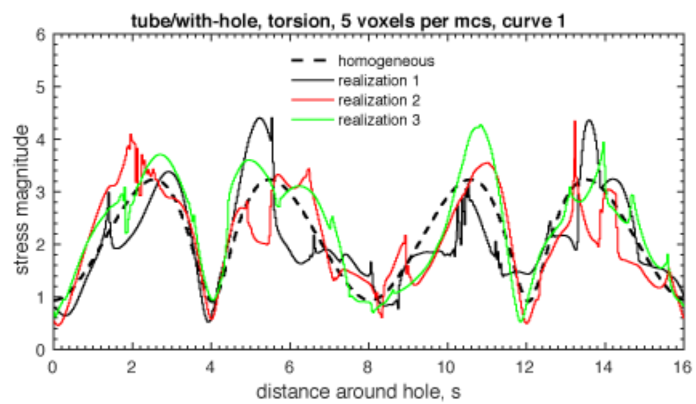
J. Bishop, T. Rodgers, J. Madison, (Sandia National Labs)

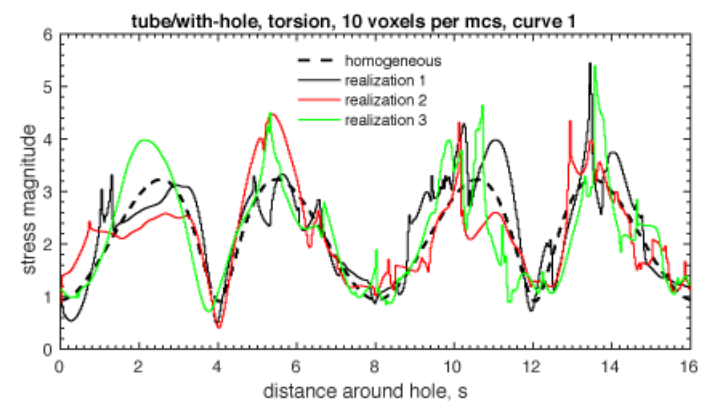
Direct Numerical Simulation

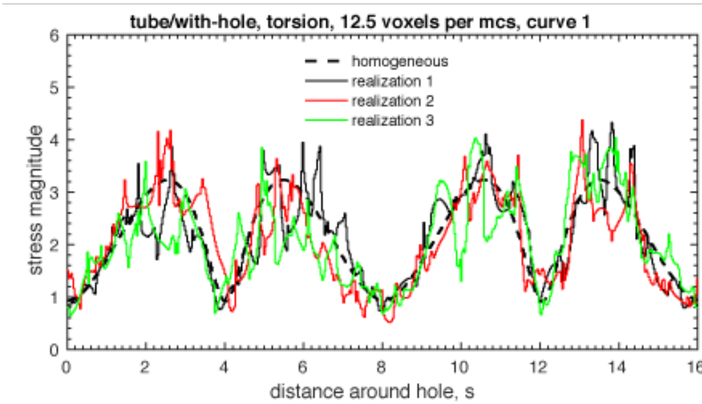
Stress response in torsion

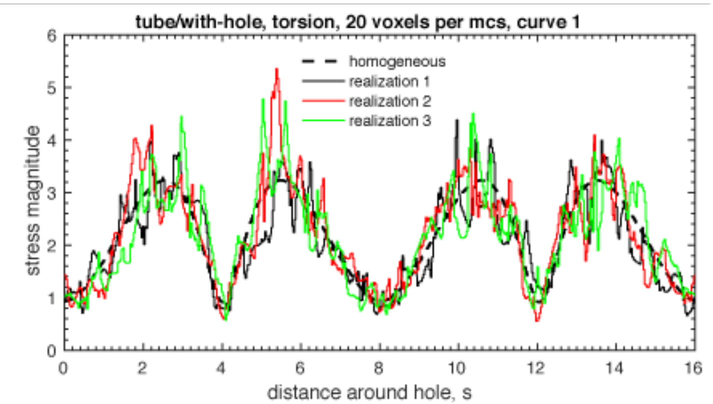












J. Bishop, T. Rodgers, J. Madison, (Sandia National Labs)

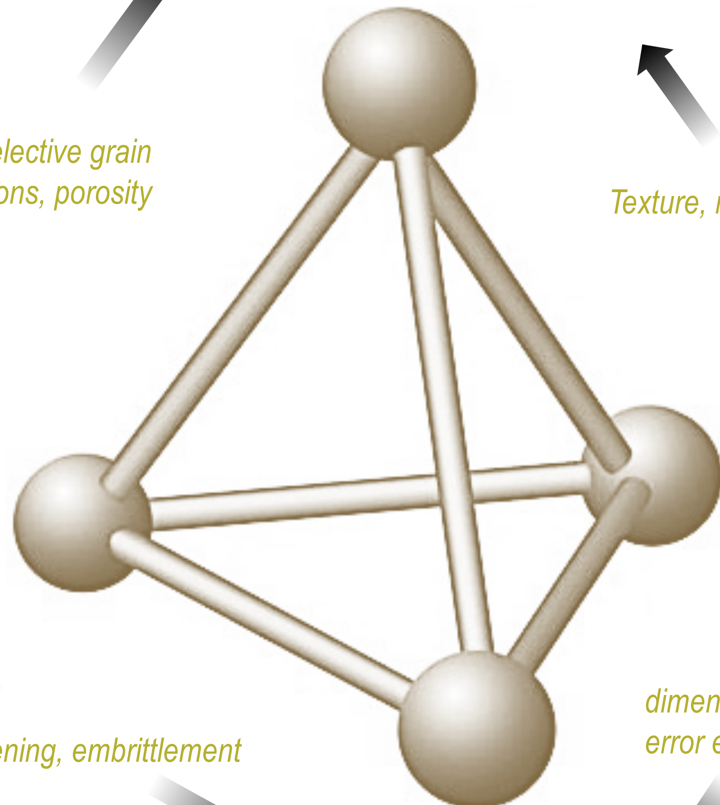
P-S-P-P Linkages by Simulation

Synthetic <u>MICROSTRUCTURE</u> Prediction

- *(kMC) Kinetic Monte Carlo*
- *(PF) Phase Field*

compositional change, selective grain orientations, porosity

Texture, residual stress, dislocation density



Extraction of Relevant Physics for Additive Manufacturing <u>PROCESSING</u>

- *Thermal-fluid Simulation*
- *Heat & Mass Transfer*

Constitutive Models; Material <u>PROPERTY</u> Definitions

- *Crystal Plasticity*
- *Viscoplasticity*

crystallographic texture, hardening, embrittlement

dimensional form, homogenized response, SROM error estimation, UQ

Modeling Mechanical <u>PERFORMANCE</u>

- *(DNS) Direct Numerical simulation*
- *(FE) Traditional FEA*

Summary

- Process-Parameter space in additive manufacturing is so large and so rapidly evolving, traditional design of experiment approaches are inadequate to reliably ascertain conclusive and exhaustive understanding of AM product

- Versatile modeling tools are needed to help scope, inform and aid our understanding of AM product

- SPPARKS is a versatile, open source, on-lattice Monte Carlo simulation suite containing a variety of microstructural evolution apps and has been adapted to simulate first order approximations of AM microstucture in 2- and 3-dimensions

- Synthetic SPPARKS microstructures are now being utilized to:
  - Rapidly explore process-parameter space via data science methods
  - Link with more rigorous thermal-fluid models
  - Serve as inputs for mechanics simulations

Questions

1. T. Rodgers, J. Madison, V. Tikare, *"Simulation of Metal Additive Manufacturing Microstructures Using Kinetic Monte Carlo"* **COMPUTATIONAL MATERIALS SCIENCE,** vol. 135, (2017) pp. 78-89

2. E. Popova, T. Rodgers, X. Gong, A. Cecen, J. Madison, S. Kalidindi, *"Process-Structure Linkages Using a Data Science Approach: Application to Simulated Additive Manufacturing Data"* **INTEGRATING MATERIALS AND MANUFACTURING INNOVATION,** vol. 6, (2017) pp. 54-68

3. T. Rodgers, J. Madison, V. Tikare, *"Predicting Mesoscale Microstructural Evolution in Electron Beam Welding"* **JOM,** vol. 68, no. 5, (2016) pp. 1419 – 1426

4. M. Francois, A. Sun, W.E. King, et al., *"Modeling of Additive Manufacturing Processes for Metals: Challenges and Opportunities"* **CURRENT OPINION IN SOLID STATE AND MATERIALS SCIENCE,** (2017) *in press*

5. J. Madison, *"Integrated Computational Materials Engineering: Tools, Simulations and New Applications"* **JOM**, vol. 68, no. 5, (2016) pp. 1376-1377

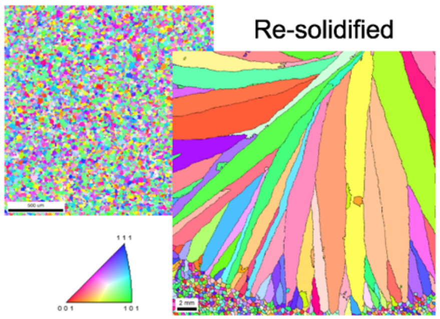
6. **http://spparks.sandia.gov**

Backup Slides

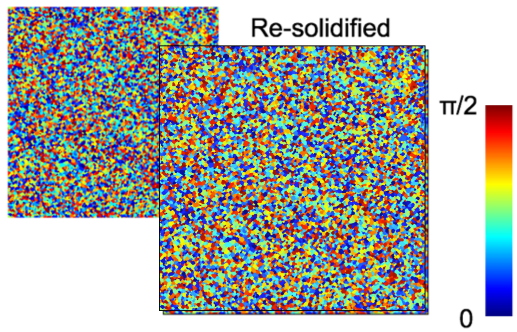
Grain Growth in Thin Films

- Thin Films of Al-Si binary alloys melted to undergo rapid solidification while being observed in a time-resolved dynamic TEM (DTEM).
- Solidification interface profiles are extracted and used as inputs for a 2D kMC model.
- Simulations are now being modified to allow incorporation of crystallographic texture

Experimental ASTAR



Simulation



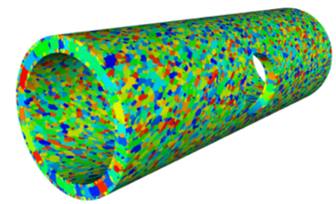
Lawrence Livermore National Laboratory

COLORADO SCHOOL OF MINES
EARTH • ENERGY • ENVIRONMENT

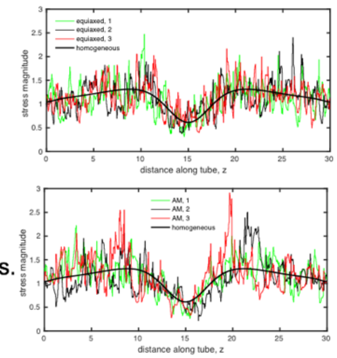
J. McKeown (LLNL), A. Clarke (CSM), J. Gibbs (LANL), T. Rodgers, J. Madison (SNL)

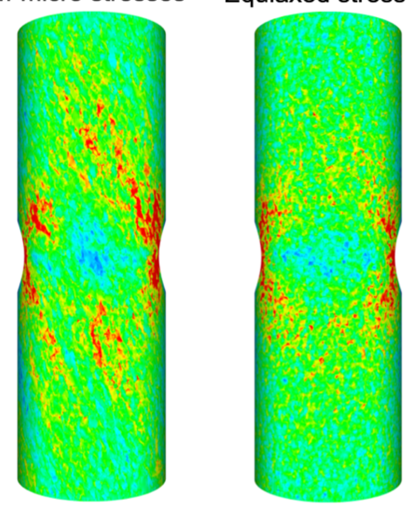
Inputs for DNS for Mechanics

- AM simulations have been performed on cylindrical domains and the resulting microstructures used in solid mechanics simulations.



- Stress fields along tube for several equiaxed (top) and AM (bottom) microstructures.

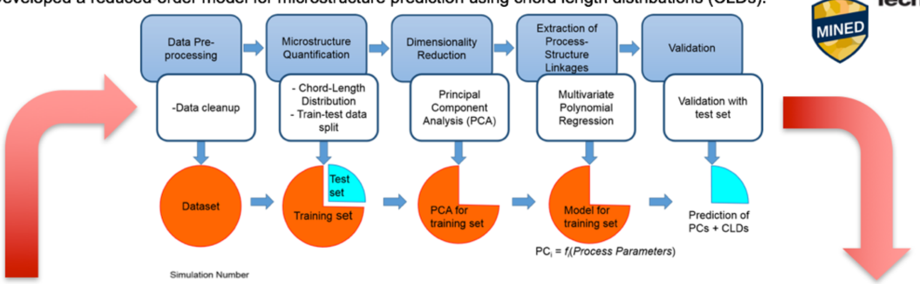




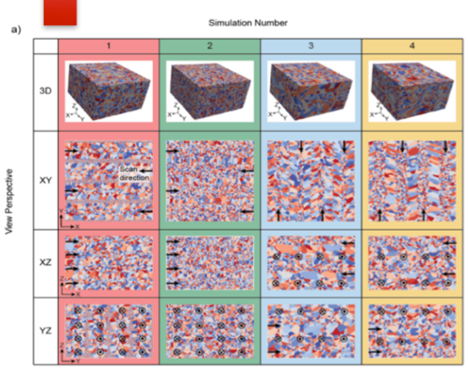
J. Bishop, T. Rodgers, J. Madison, (Sandia National Labs)

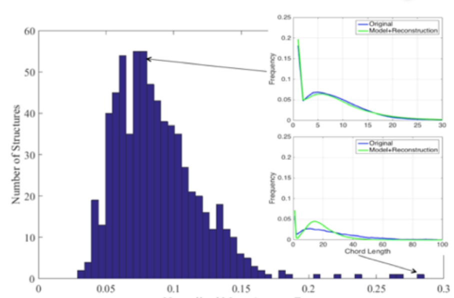
Exploring AM via Data Science

- Developed a reduced-order model for microstructure prediction using chord length distributions (CLDs).



Georgia Tech
MINED

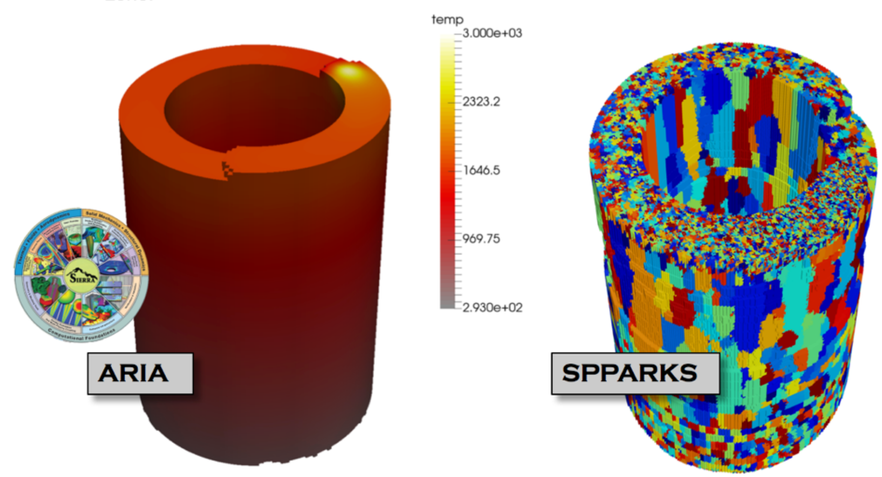




E. Popova, S. Kaladindi, T. Rodgers, J. Madison, et. al., ***IMMI***, (2017) vol. 6, pp. 54-68

Linking to Thermal Models

- Using thermal histories simulated within SNL's production code, ARIA as an input, the modified Monte Carlo Potts model within SPPARKS is coupled to predict grain morphologies within an additive manufacturing build. This demonstrates an ability to predict grain morphology from a rigorous multi-physics model as opposed to a simplified and idealized approximation of the molten zone.



K. Johnson, T. Rodgers, (Sandia National Labs)