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Recent Advancements in SPPARKS Metal Additive Manufacturing Simulation Capabilities

TMS 2022

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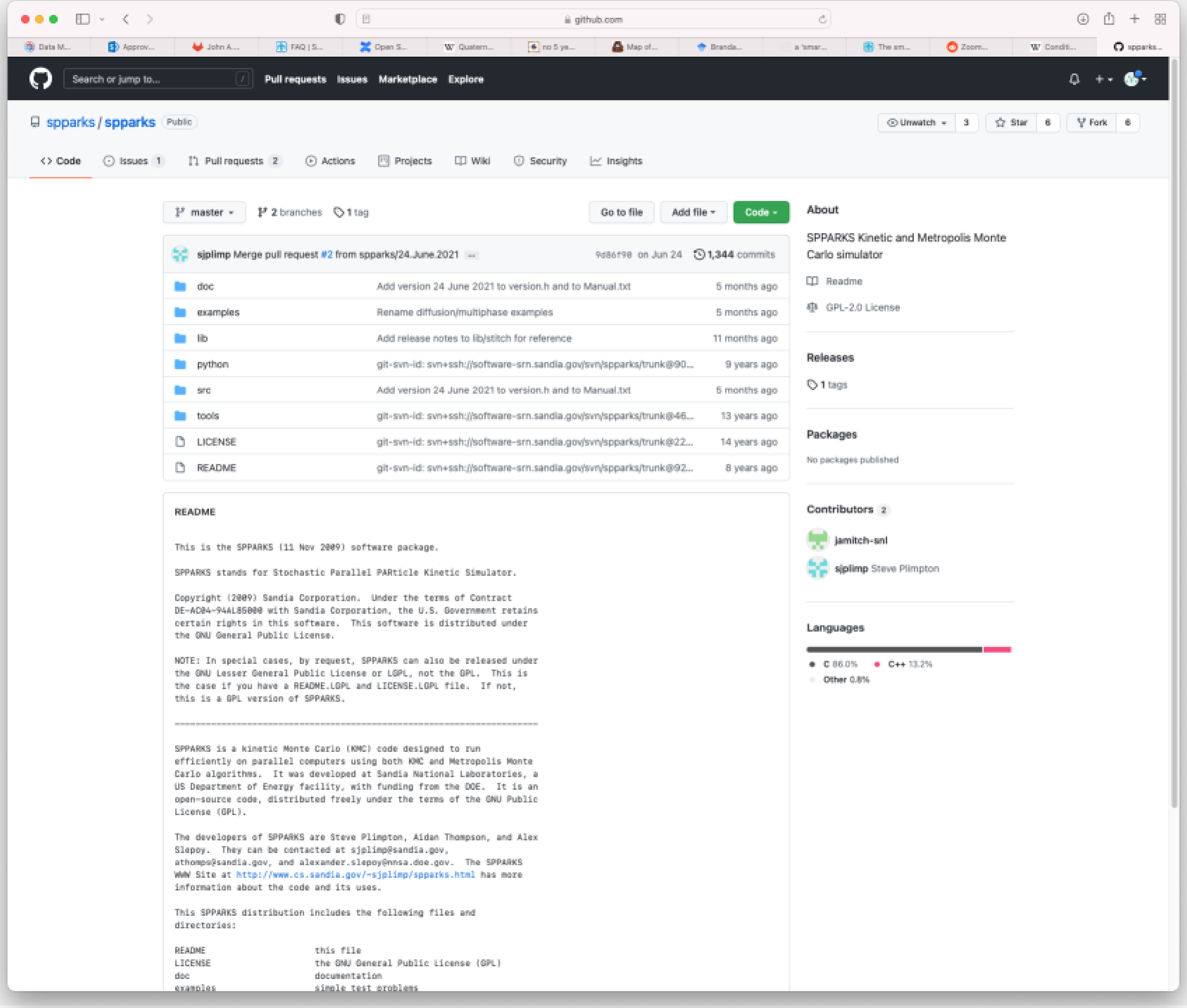
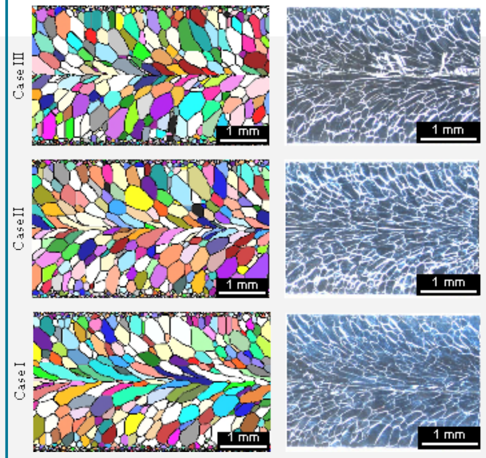
Microstructure simulations performed in SPPARKS



- Open source mesoscale microstructure simulation software
- Focused on Monte Carlo methods but extensible to virtually any on-lattice simulation method
- Massively parallel capability.
- Similar structure to LAMMPS MD code
- Now on Github for easier external collaboration!

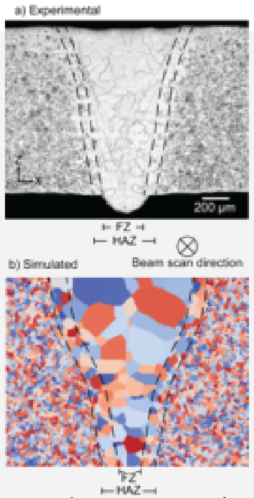
Previous microstructure solidification work

Potts/Weld



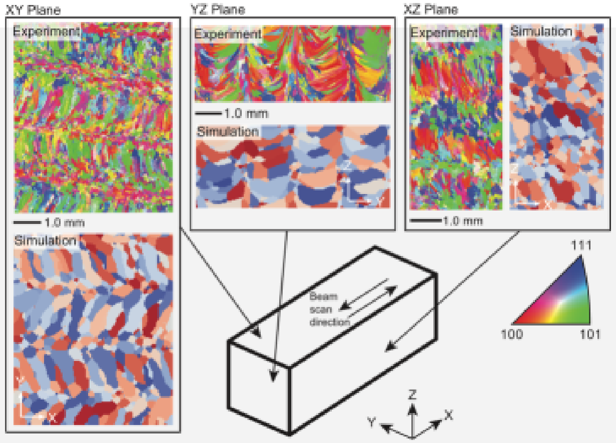
Rodgers et al., MSMSE 2017

Potts/Weld/JOM

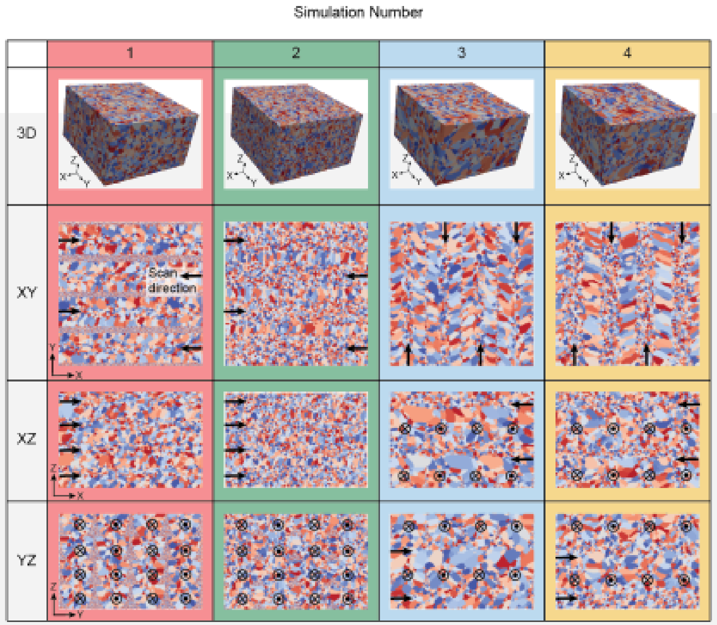


Rodgers et al., JOM 2016

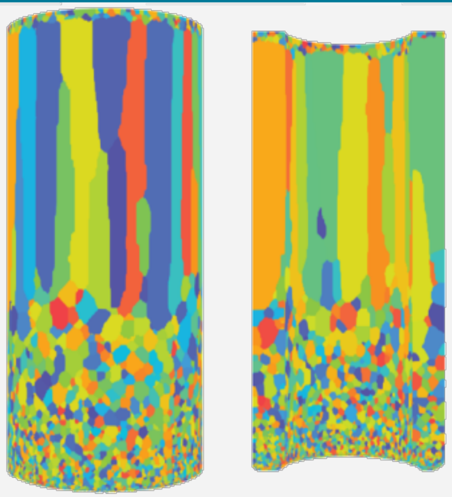
Potts/Additive



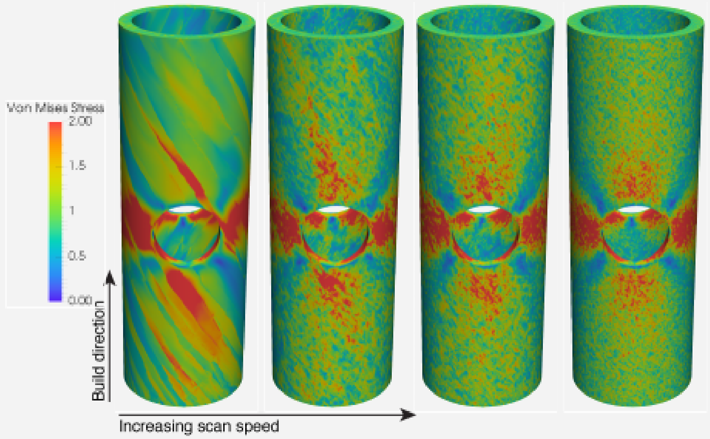
Rodgers et al., Comp Mater Sci 2017



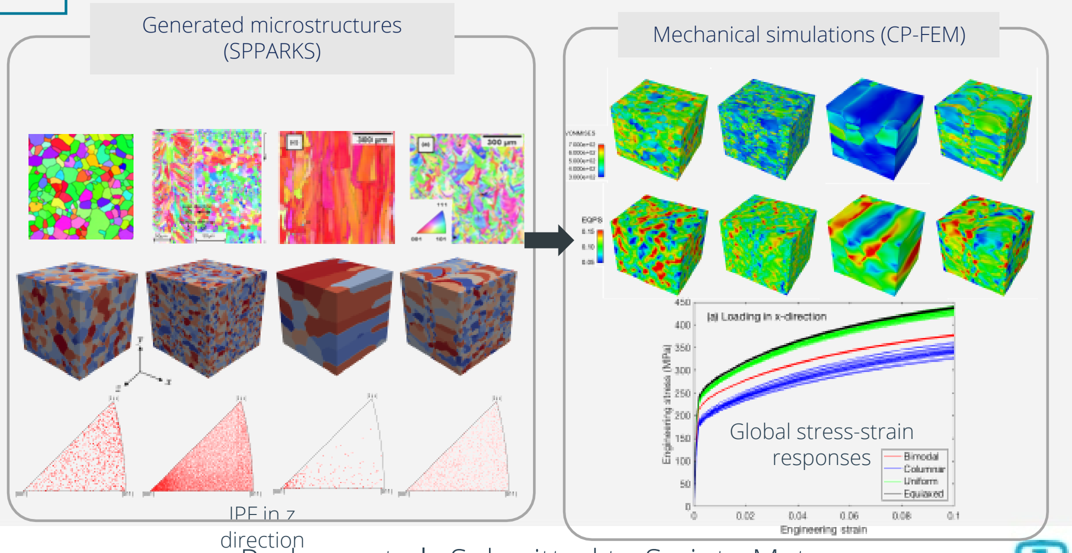
Popova et al. IMMI 2017



Johnson et al., Computational Mechanics 2018



Rodgers et al., MSMSE 2018



Rodgers et al., Submitted to Scripta Mat.

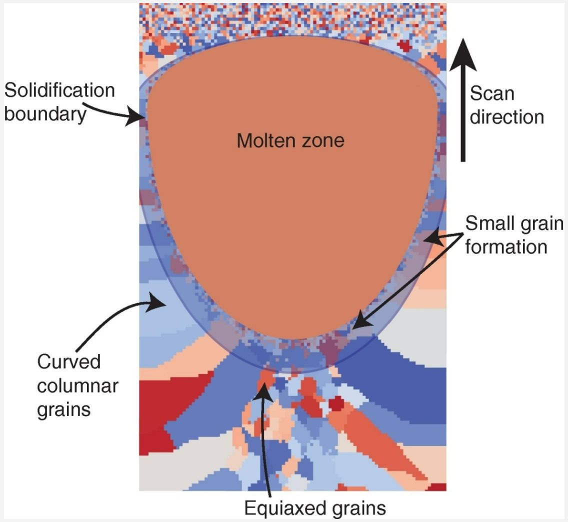
Incorporating material-specific solidification properties

Rodgers et al, *Additive Manufacturing* 2021

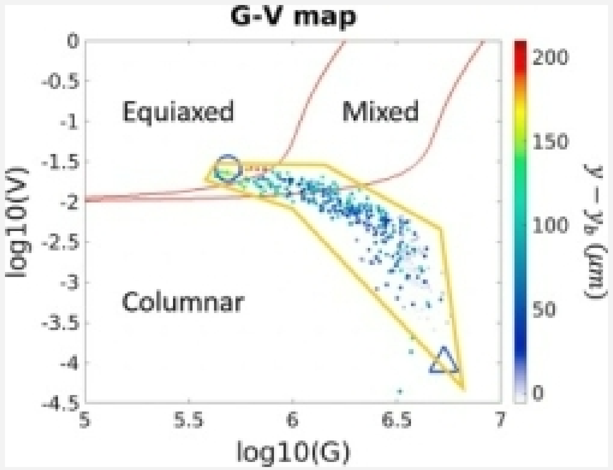
Metal Additive Manufacturing - Microstructure

Types of Microstructures seen in MAM:

- Columnar – Long, highly textured unidirectional grains
- Equiaxed – More isotropic, randomly oriented grains



Various microstructures forming during a laser pass.



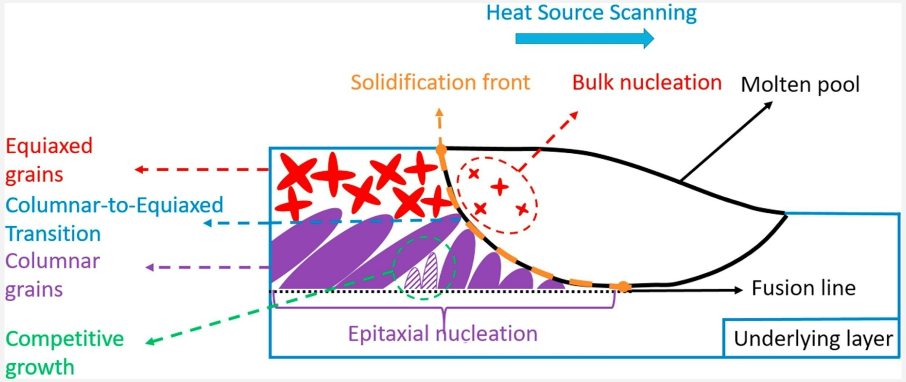
Hunt's Columnar to Equiaxed Transition as a function of G vs V.

Variables Leading to Transitions Between Different Microstructures:

- Temperature Gradients (G)
- Solidification Rate (R or V)
- Nuclei Density (N_0)

Reason for Inconsistent Microstructure Generation:

- Non-uniform solidification behavior
- Changing temperature gradients and directions
- Remelting & resolidification

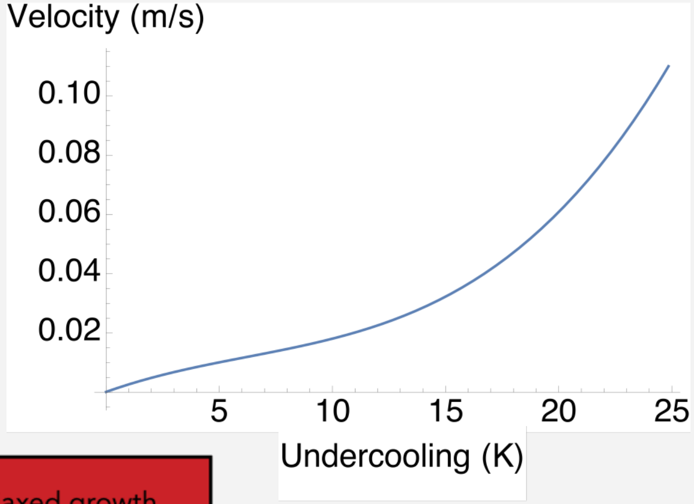


View of the CET criteria during a laser pass.

Incorporating material-dependent parameters

Nucleation site density, N_0, is the number of possible nucleation sites per m^3 (typically 10^{12}-10^{15} m^{-3}). Implemented by allowing a fraction of grain IDs to survive the liquid->solid transition without changing grain ID.

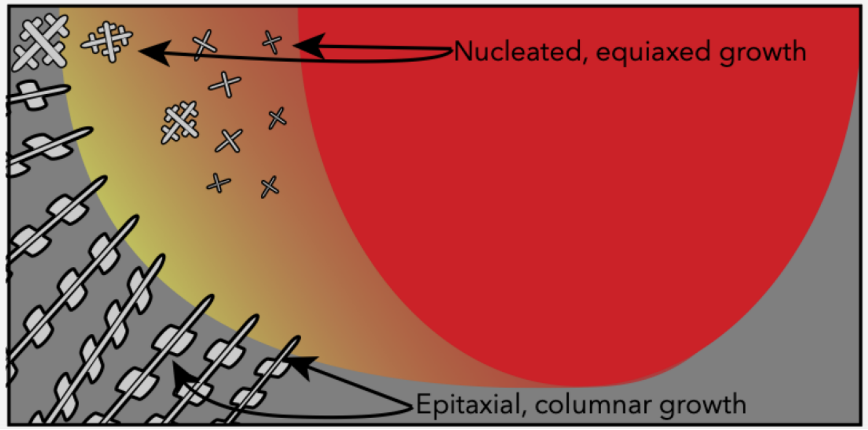
$$N_{frac} = N_0 \Delta x^3$$



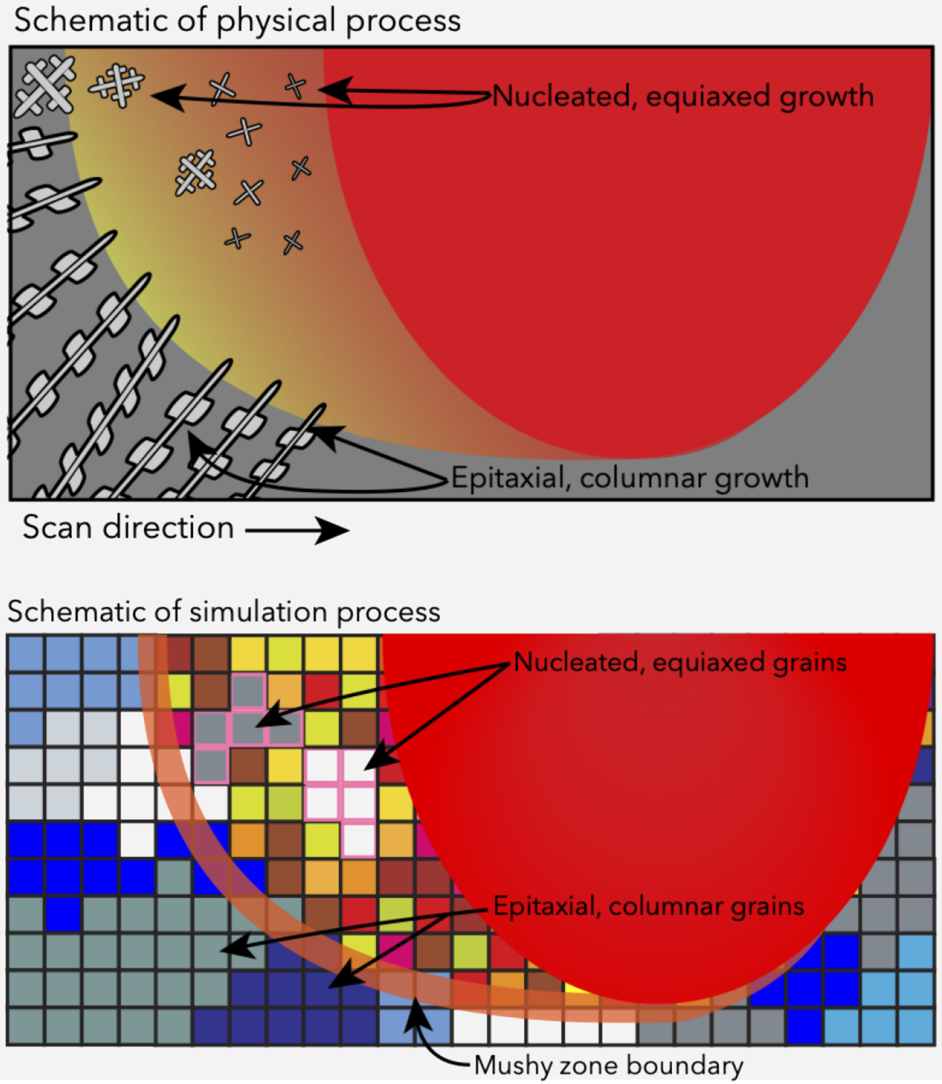
Undercooling ($\Delta T = T_l - T$)-dependent **solidification front velocity,** $\boldsymbol{V}(\Delta \boldsymbol{T})$.

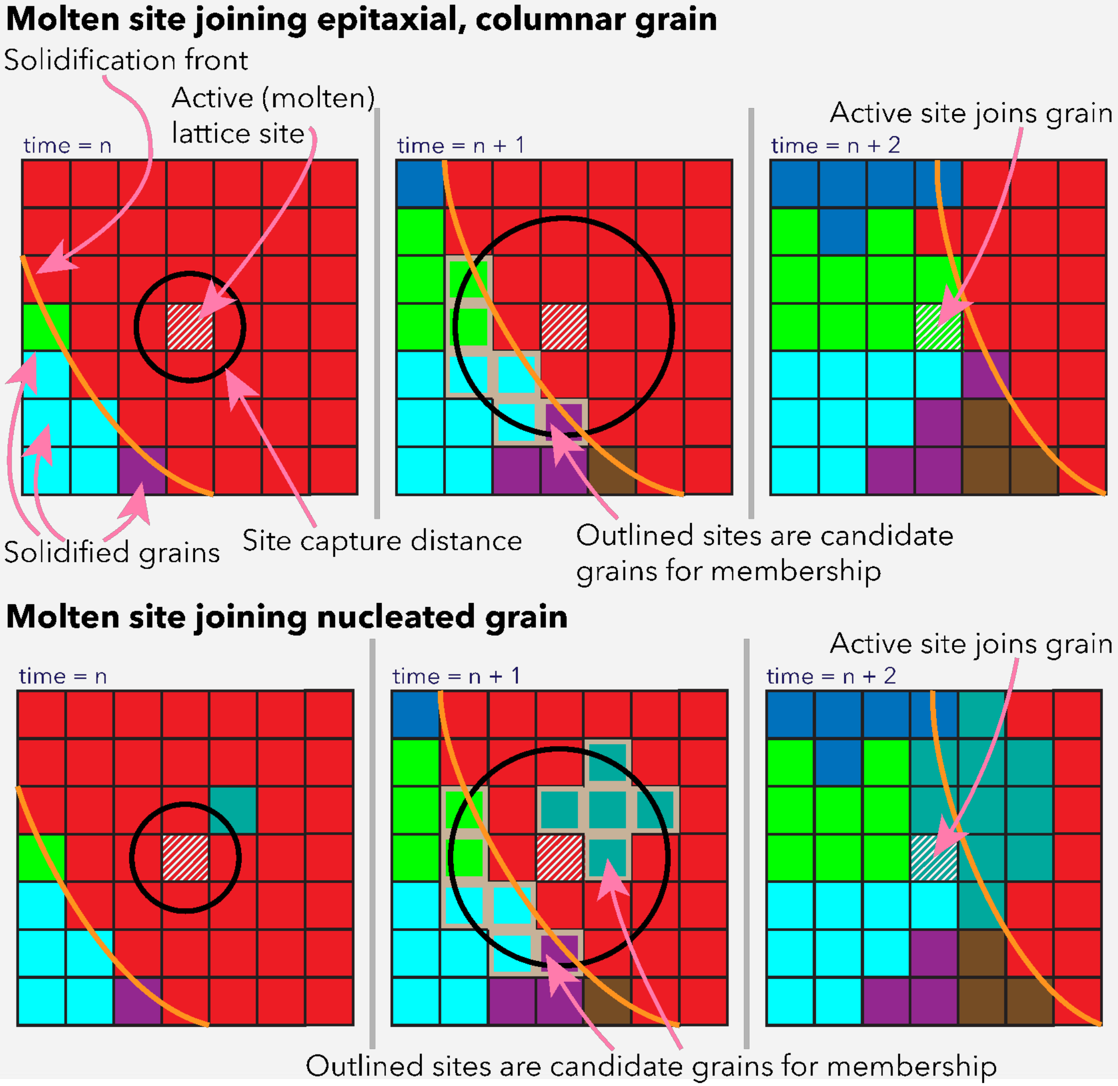
$$V(\Delta T) = a(\Delta T)^3 + b(\Delta T)^2 + c(\Delta T) + d,$$

the coefficients are determined from dendrite-scale solidification simulations or experiments.



New Monte Carlo solidification approach

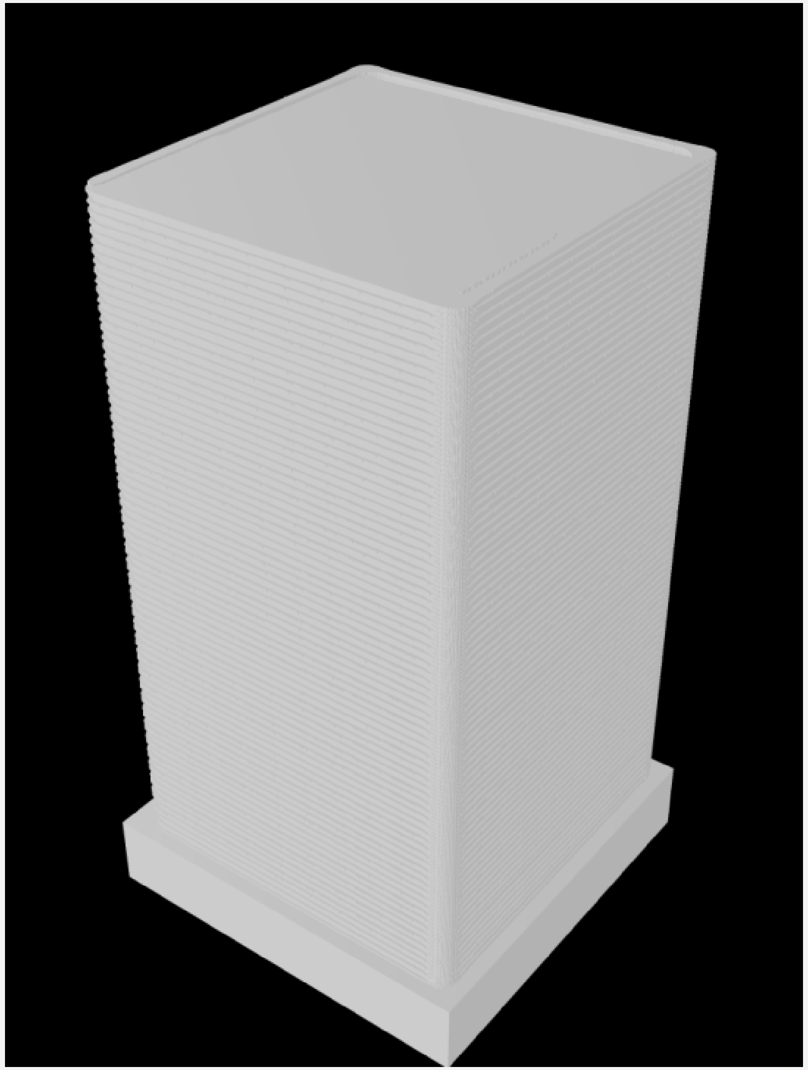




Rodgers et al, *Additive Manufacturing* 2021

Example Simulated Pillar

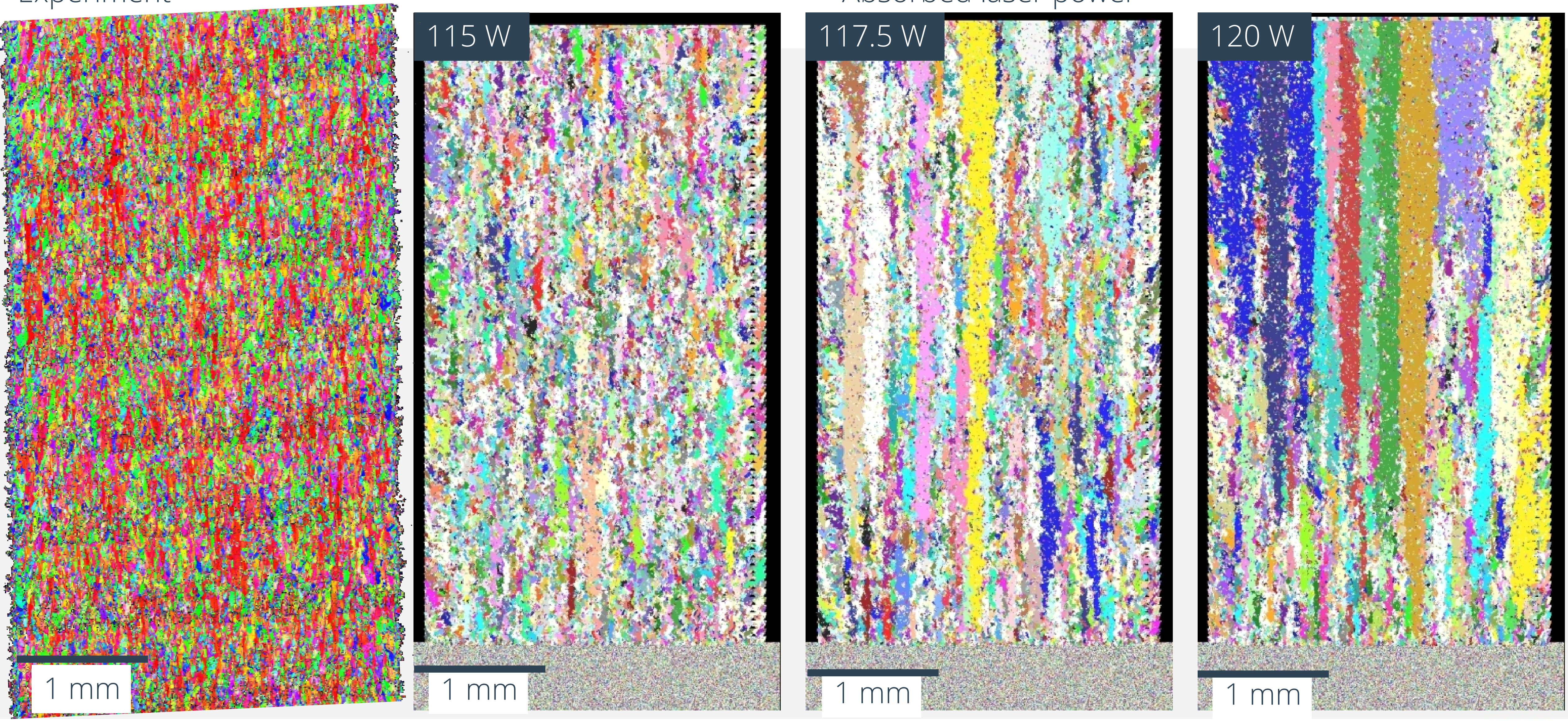
- 2.8 x 2.8 x 5.5 mm domain ~ 340 million lattice sites
  - 2,340 cores for 30 days
- Process parameters calibrated for 3D Systems ProX DMP 200 machine
  - Layer thickness = 30 µm
  - Hatch spacing 50 µm
  - Scan rate = 1400 mm/s
  - Laser power = 129 W
  - Scan strategy = +/-90 alternating
- Includes powder phase with 0.01 of solid conductivity
- Simulation domain boundaries fixed at 300K
- 5 µm grid
- 21.8 m of scan path simulated
- 157 layers
- Critical undercooling 5K



Microstructure evolution is quite sensitive to thermal parameters

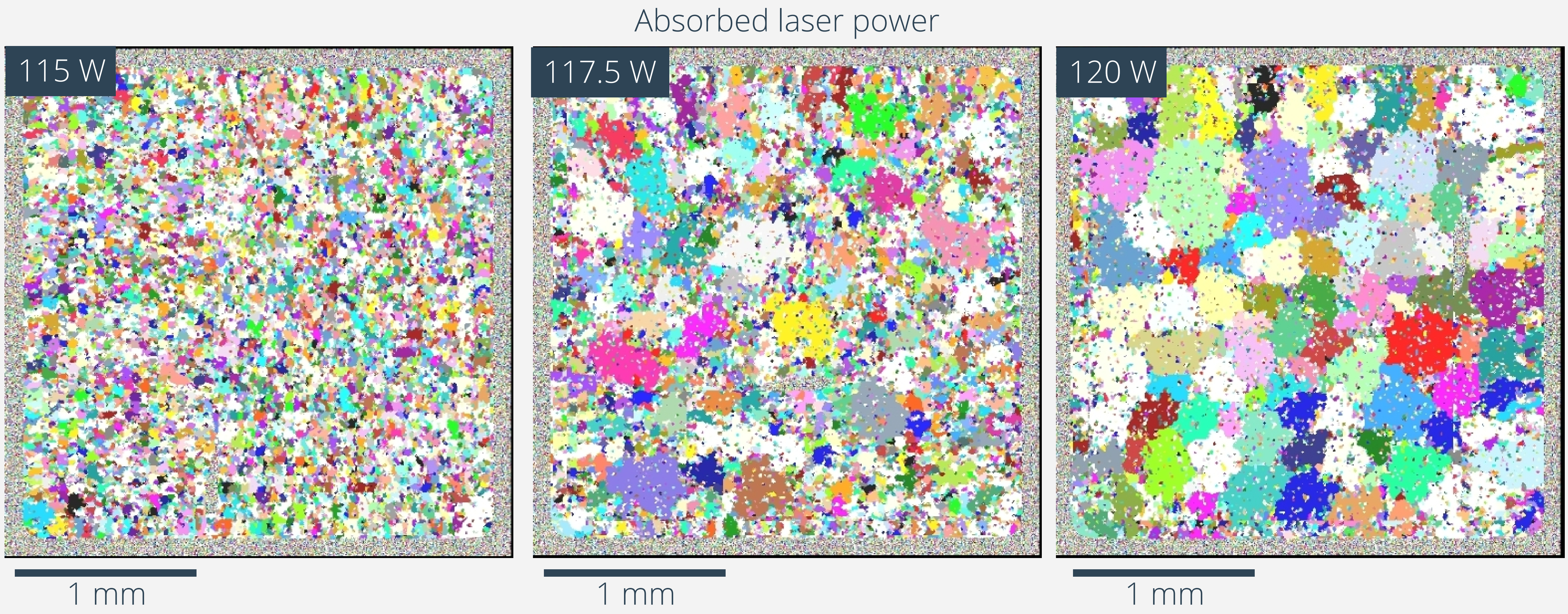
Experiment

Absorbed laser power

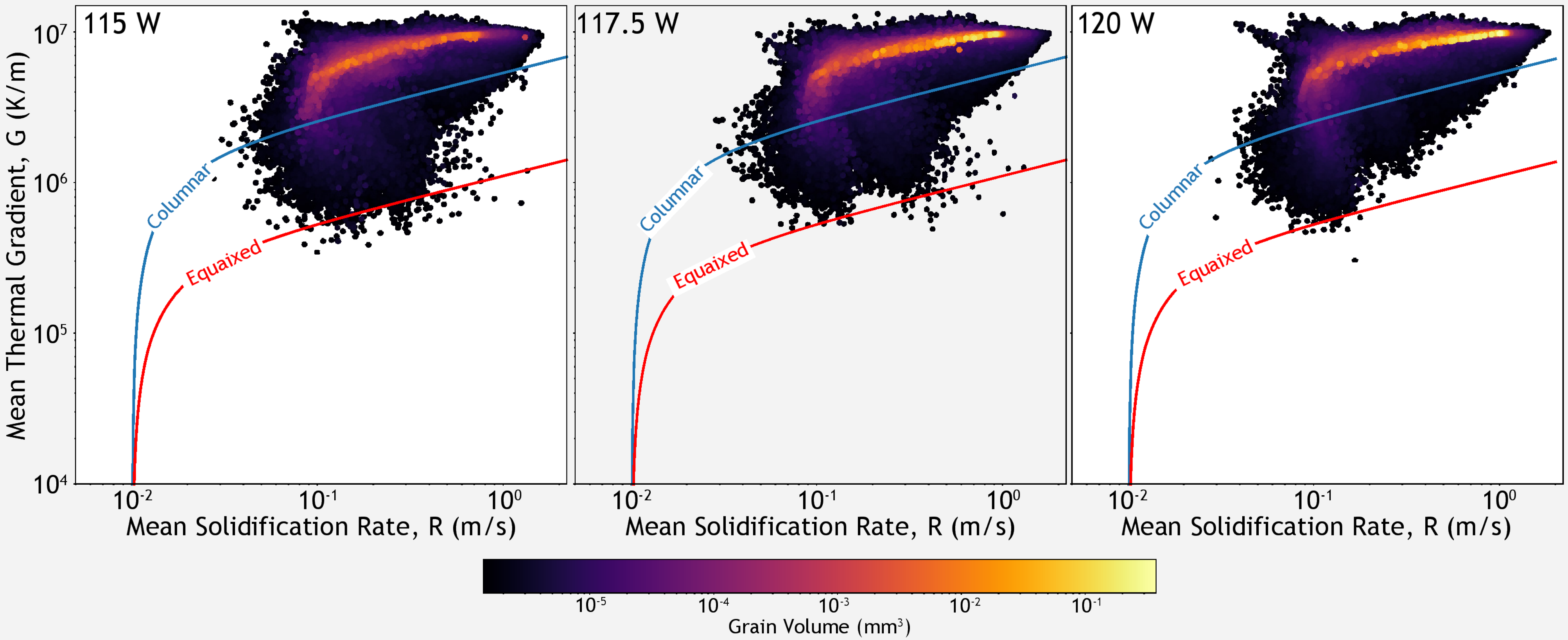


All simulations performed with nucleation densities of 8e13

Top view of build



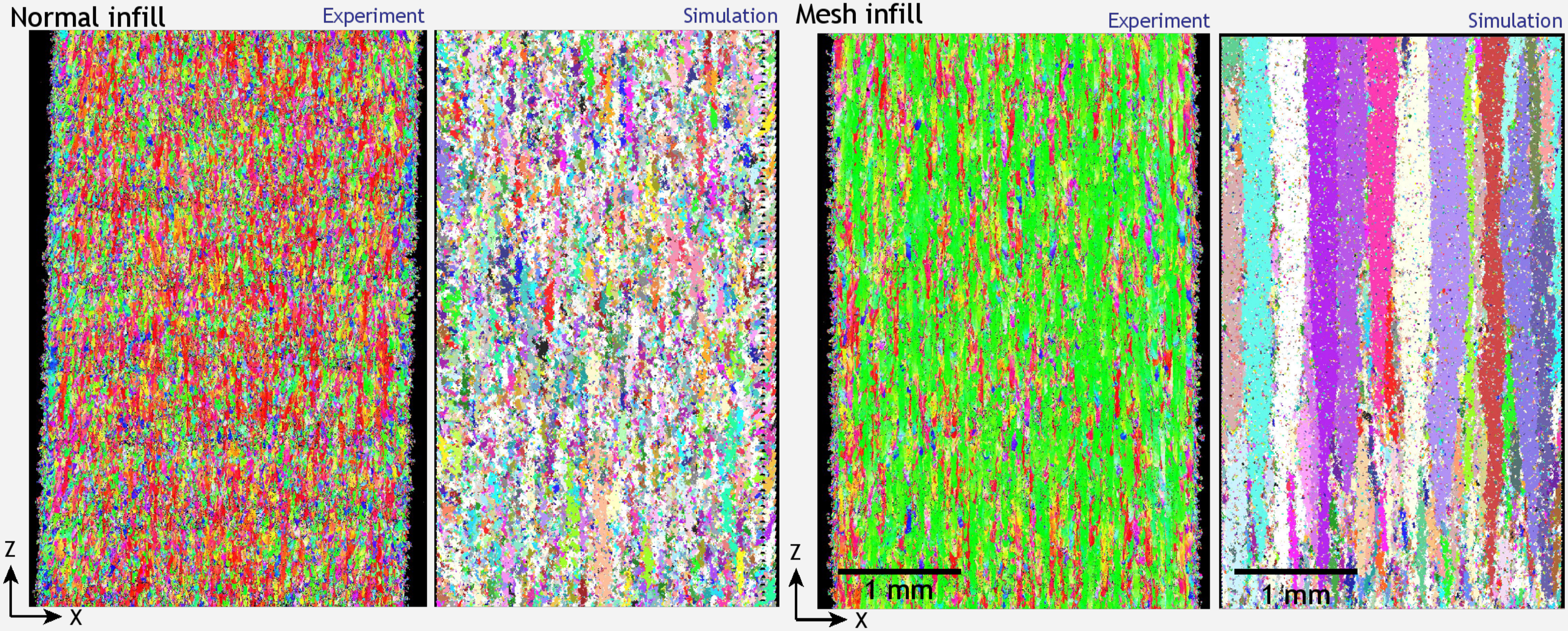
G/R and grain size plots



- Maximum grain size increases significantly with power
- Increasing power results in subtle shift upwards into mixed/columnar regime
- G/R formulation does not account for multiple melting/solidification cycles

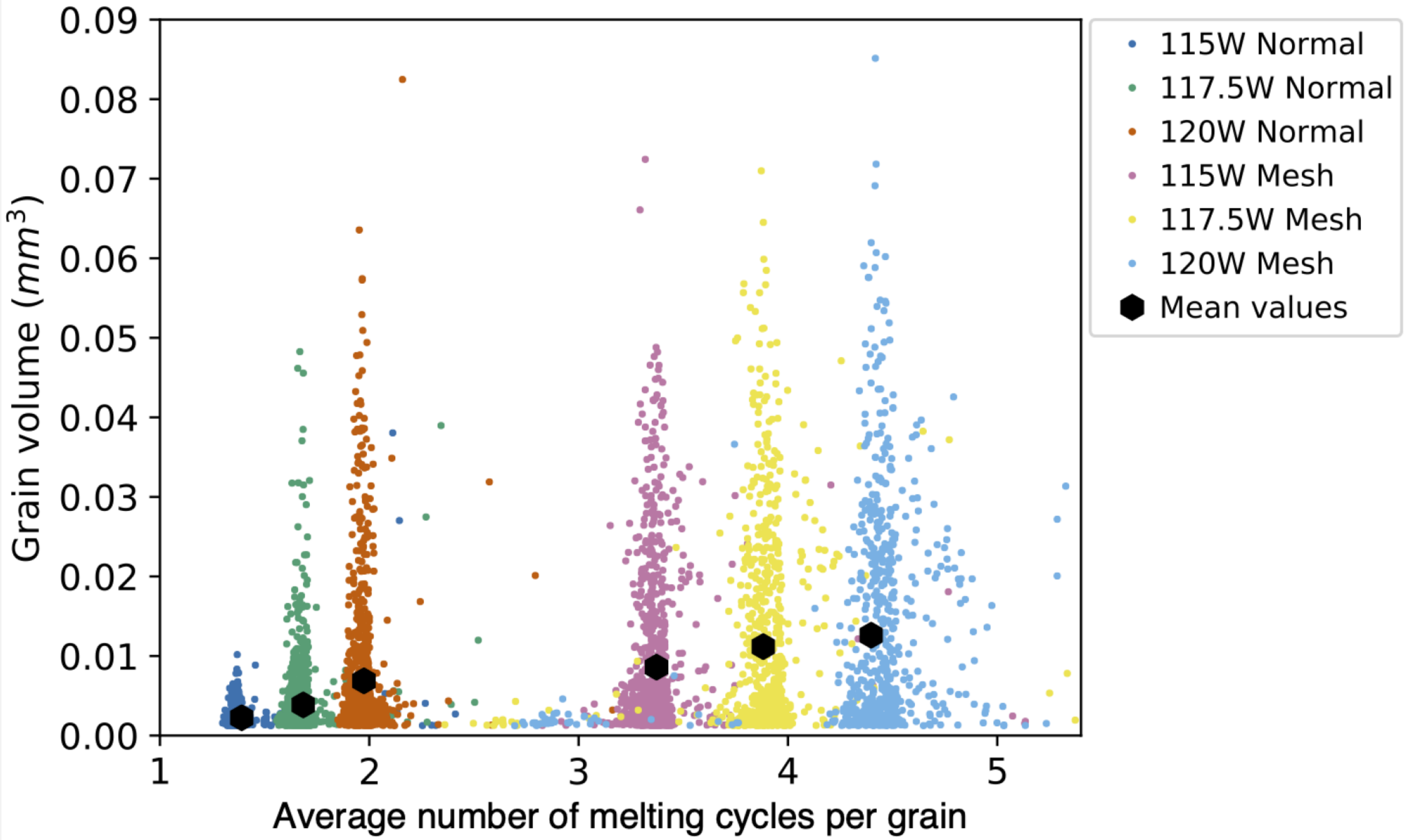
Effect of remelting raster pattern

The addition of a second “remelt” laser raster each layer results in larger, more columnar grains with a strong crystallographic texture.



Grain size dependence on melting/remelting cycles

Dan Bolintineanu

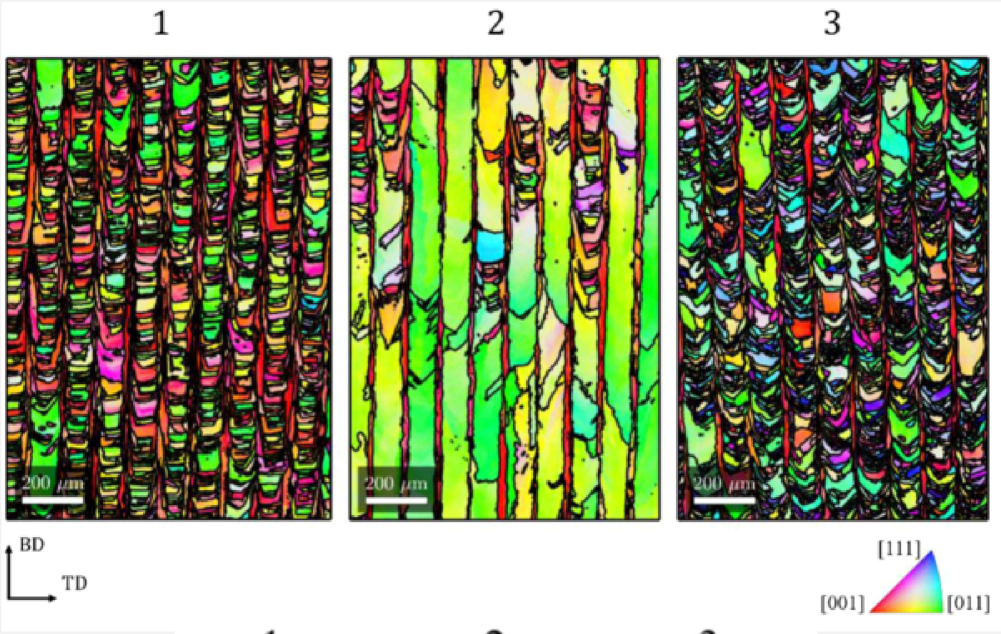


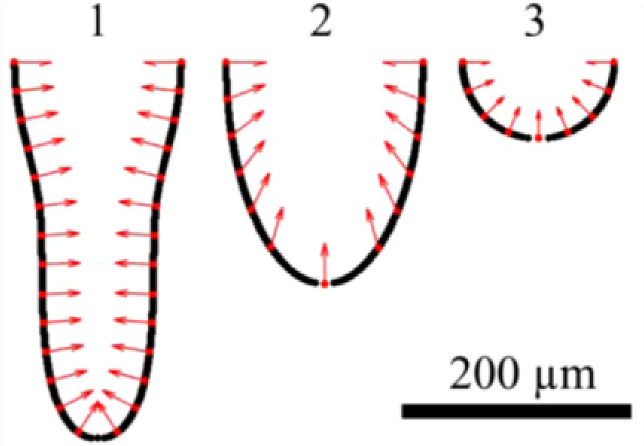
- Laser power & scan pattern combine to control the number of melting cycles experienced by the material.
- The average number of melting cycles increases with both laser power and remelting.
- Maximum and mean grain sizes also increase.
- Nucleation is less influential with additional remelting.

Adding crystallographic texture to MC solidification model

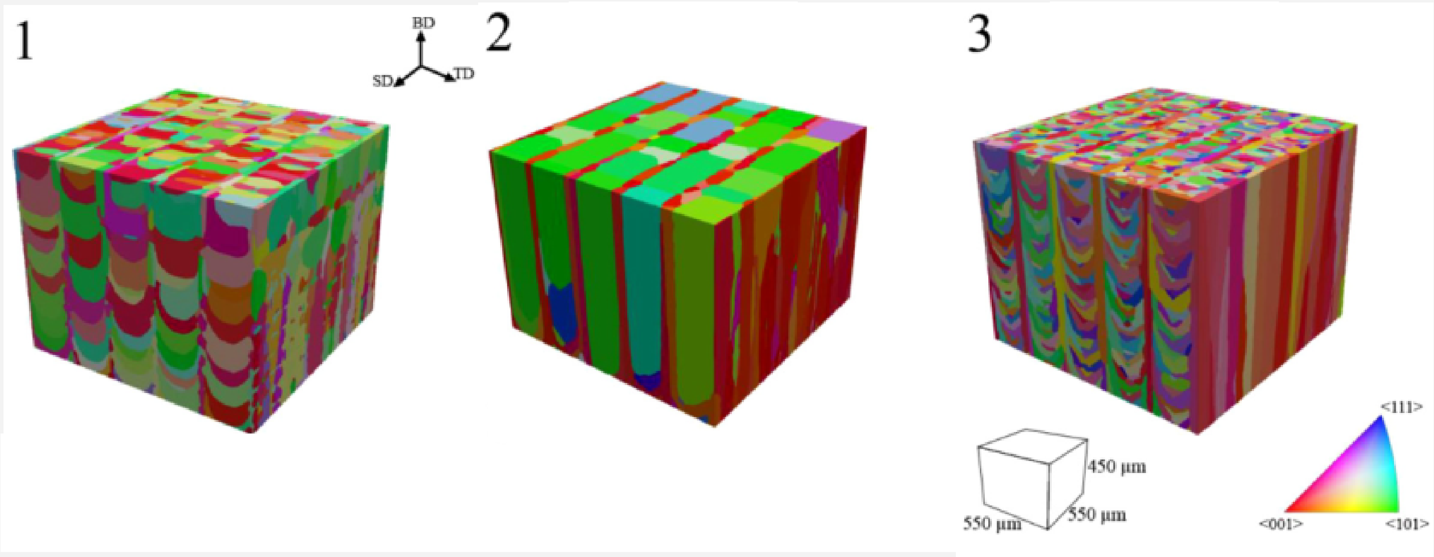
SPPARKS Texture Prediction

Joseph Pauza (CMU)



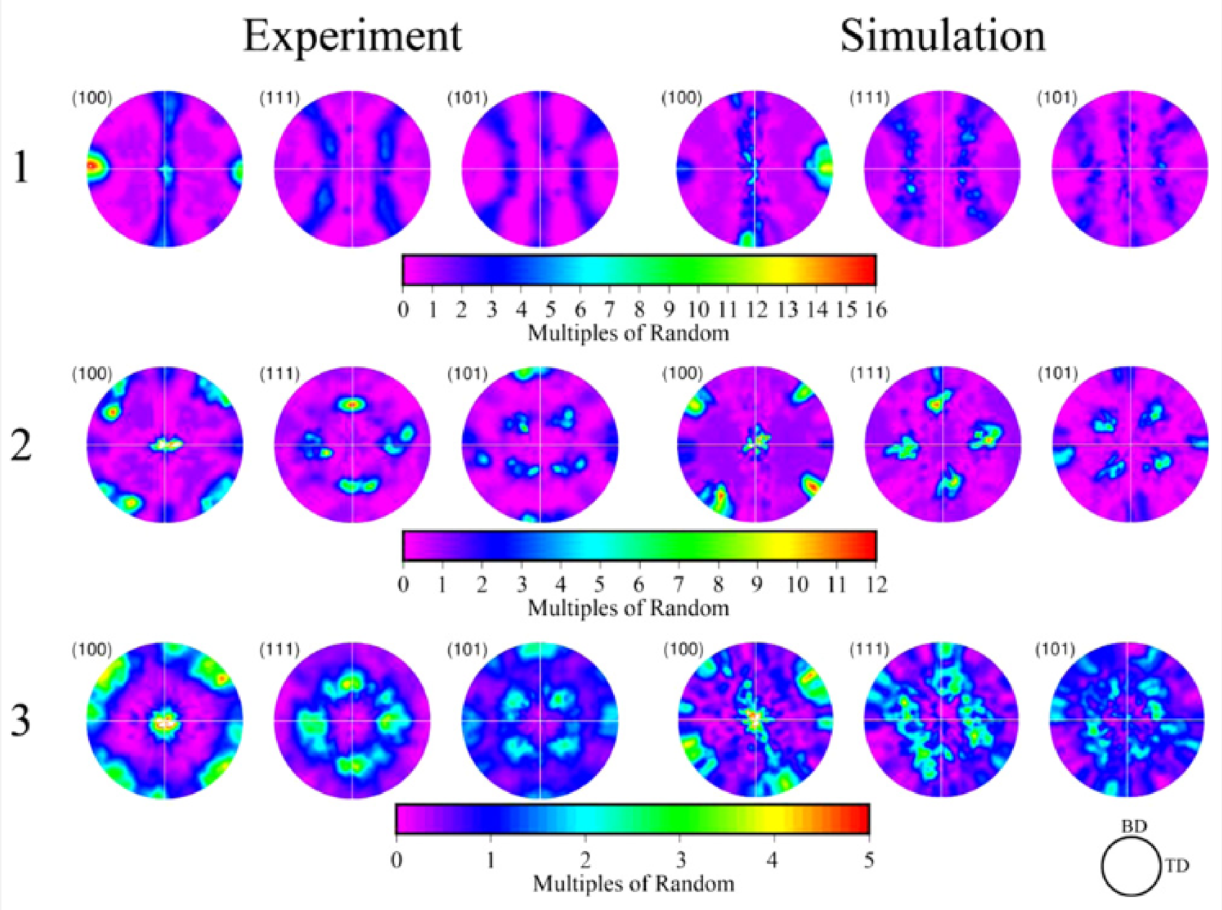


- The Monte Carlo-based grain selection algorithm used in SPPARKS AM app was modified to weight selection based on misorientation between grains and solidification direction.
- Study with In625 successfully replicated texture variation with scan velocity and melt pool shape.

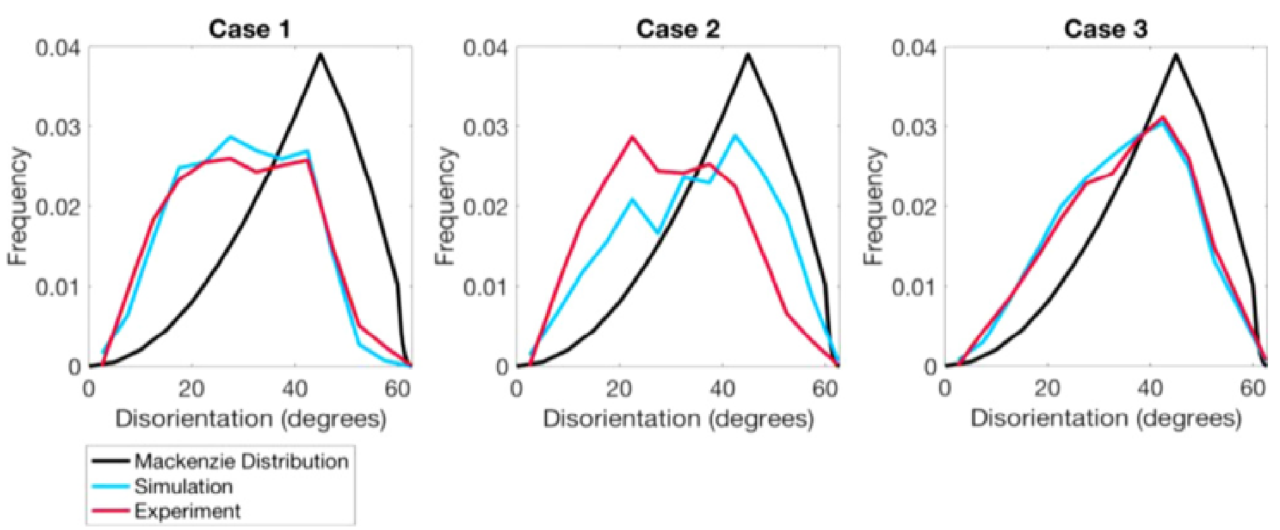


SPPARKS Texture prediction – Orientation distributions

Joseph Pauza (CMU)



Experimental and simulated pole figures show good agreement.



New meltpool models for computational efficiency

Melt pool generation – Rosenthal and the Adaptive Solution

Robert D Moore

Analytical steady-state solution to the heat diffusion equation:

Point Source[4]: $T - T_0 = \frac{\lambda Q}{2\pi R k} exp\left(\frac{-V[\xi+R]}{2\alpha}\right)$

Extended Solution[4]: $T - T_0 = \frac{\lambda_p Q}{2\pi R k} exp\left(\frac{-V[\xi+R]}{2\alpha}\right) + \int_d^{-d} \frac{\lambda_l Q}{2\pi R' k} exp\left(\frac{-V[\xi+R']}{2\alpha}\right) dD$

Advantages of the Rosenthal Solution

No requirement for specific time step (Steady State Solution)

4-6x speedup compared to the Finite Difference method.

Disadvantages of the Rosenthal Solution

Transitions between rasters are poorly modeled by this solution

Previous melted regions are forgotten during subsequent raster passes.

Solution to Transition Problem:

- Form a joint or flexi-Rosenthal solution that morphs with the raster path to capture the transition regions.

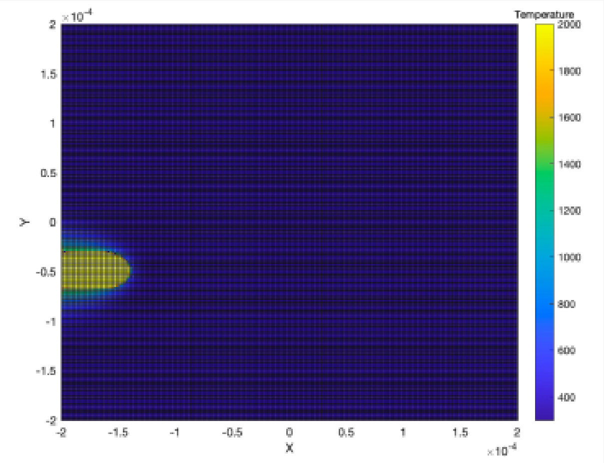


Figure 19: Rosenthal solution implemented in a C++ App.

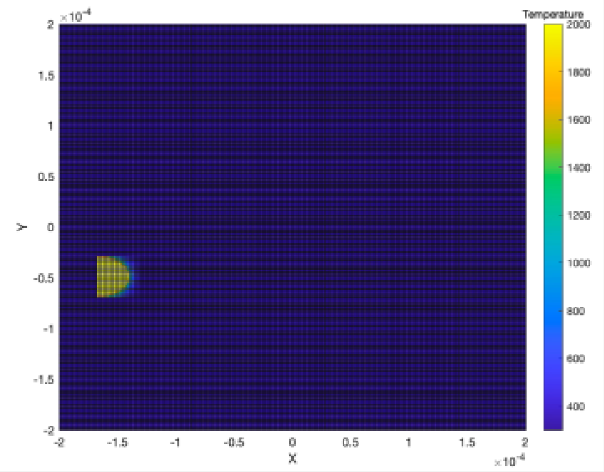
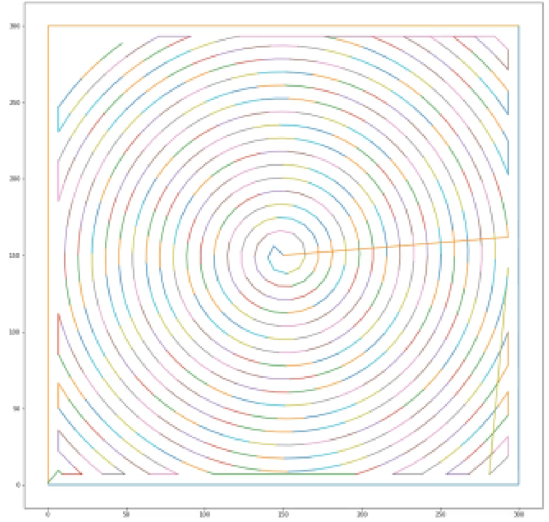


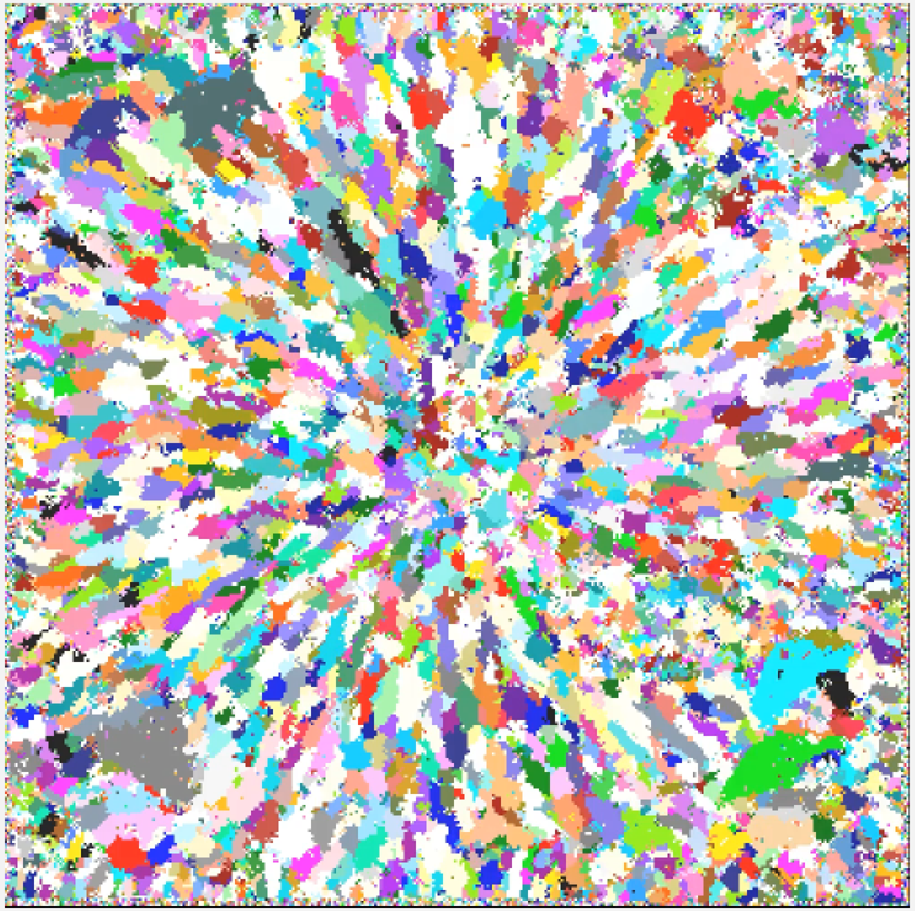
Figure 20: Flexi-Rosenthal solution implemented in a C++ App.

Microstructure Comparison: More Complicated Rasters

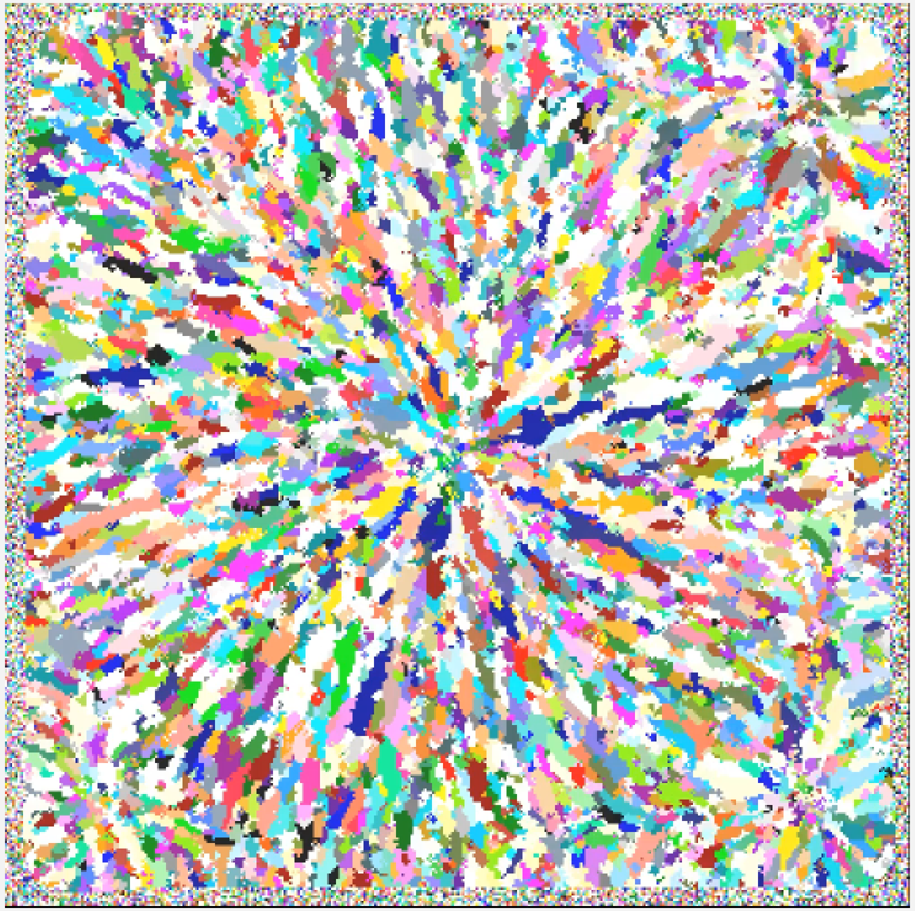
Robert D. Moore



Flexi



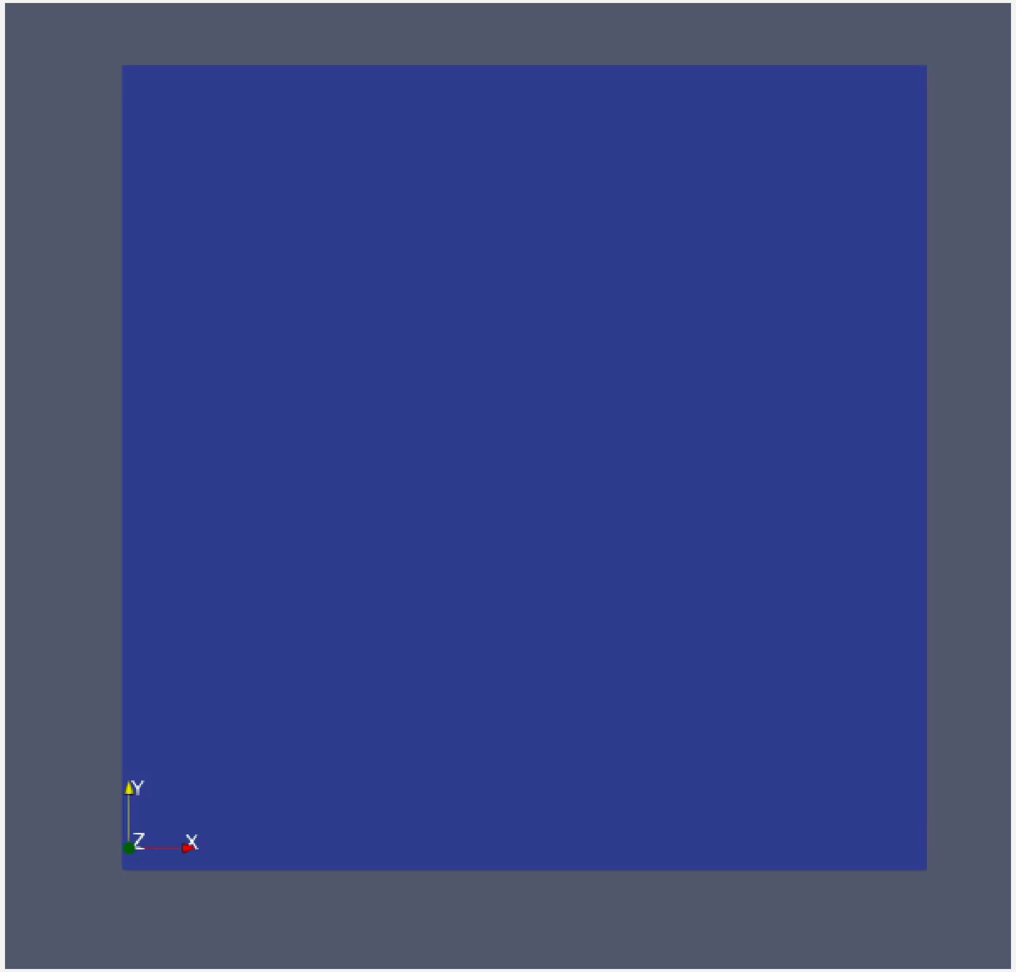
Finite Difference



Part-scale thermal model with parallel Green's function solver

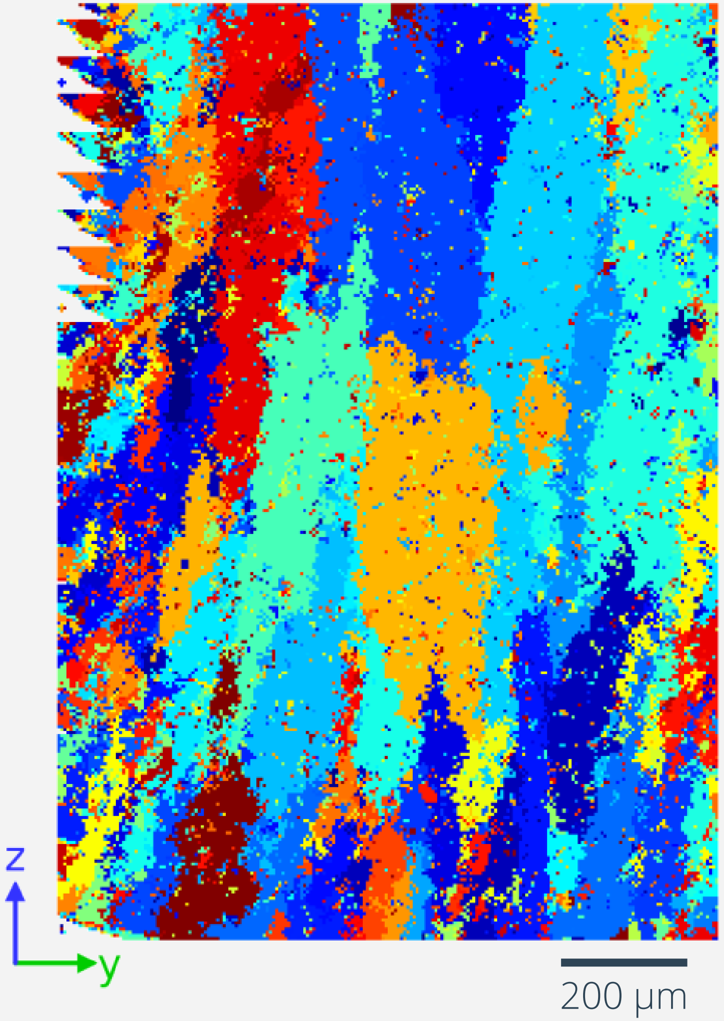
Dan Moser

- Thermal history constructed using massively parallel Green's function solver
  - Previously developed as part of SNL LDRD
- Fully time resolved, linear, time-dependent solution
  - Ellipsoidal Gaussian source
  - Calibrated to mesoscale model melt pool dimensions
  - Adaptive space-time grid solution representation
- Embarrassingly parallel in space and time
- ~3 days run time on 1500 processors
- First full thermal history calculation for part of this size



Full thermal history of first layer

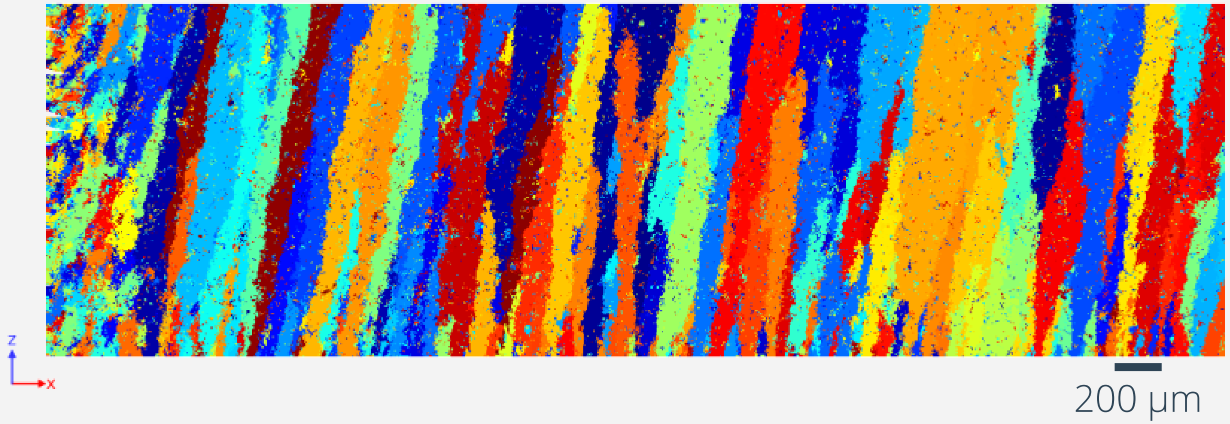
Microstructure prediction using subvolume of thermal model

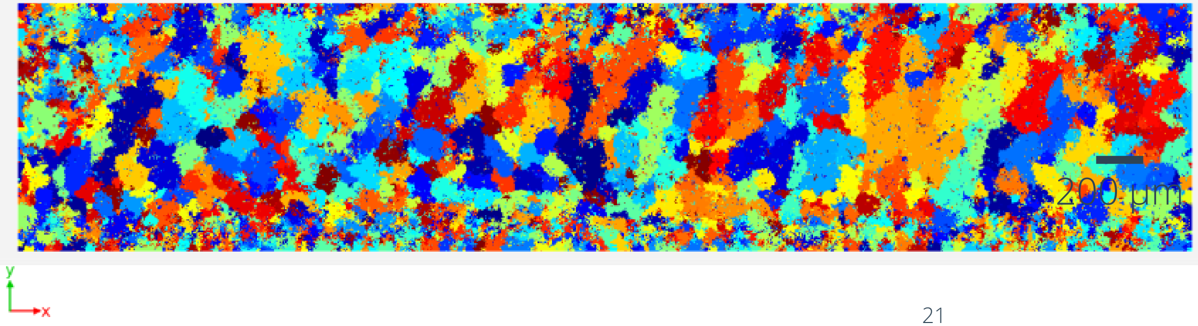


Base nucleation case: N_0 = 5.4e14 #/m^3, ΔT_c = 5K, $\sigma_{\Delta Tc}$ = 3K.

Columnar microstructures with most grains propagated through many build layers.

Future work will use Stitch library to simulate much larger volumes.

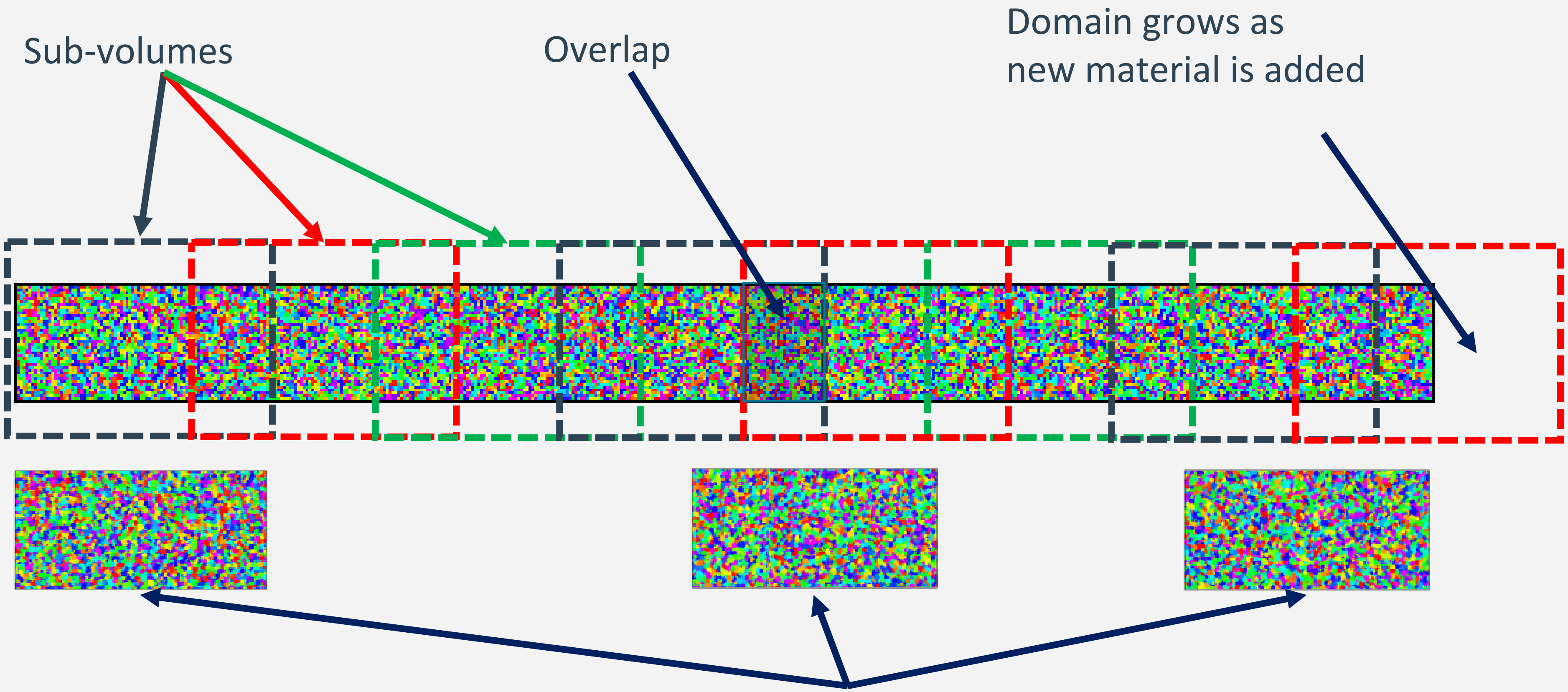




Matching part-length scales with STITCH

John Mitchell

Large domain is simulated using a series of smaller overlapping sub-volumes.



Post-process, visualize and analyze on arbitrary sub-volumes and arbitrary times

Conclusions

- Monte Carlo-based AM microstructure simulation is maturing to include more physics including material-dependent solidification and crystallographic texture.
- The finite difference thermal model source code has been released in the open source SPPARKS Github repository and is available for use/development.
- New, efficient thermal models allow for faster simulations of larger build geometries.

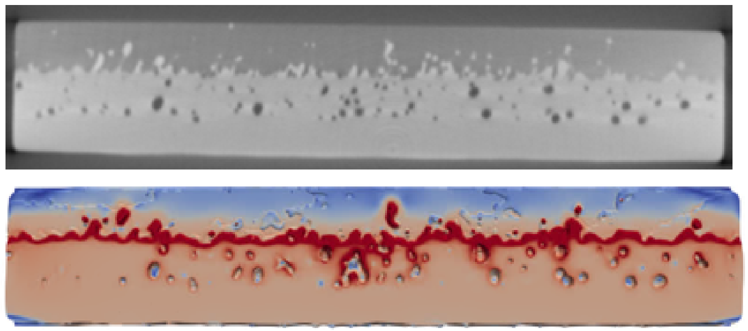
Outline

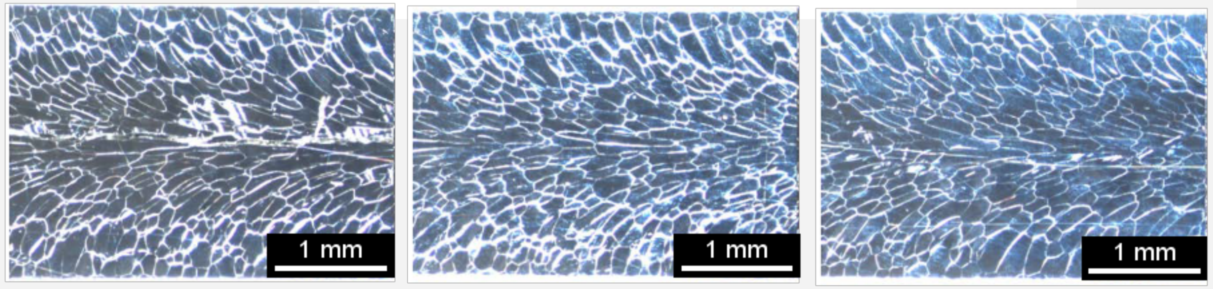
- Introduction to advanced manufacturing microstructure simulation
- Adding material-parameters to SPPARKS AM model
- Predicting crystallographic texture
- Structure->Property linkages for AM materials
- New thermal models for efficient simulation
- Part-scale simulation

Simulation Needs for Advanced Manufacturing

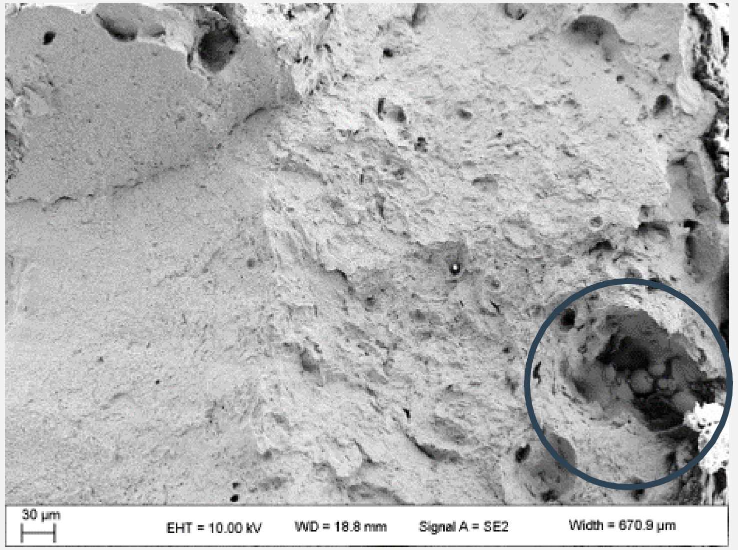
Many processing methods result in materials with non-traditional microstructures, significant defect populations, and residual stresses.

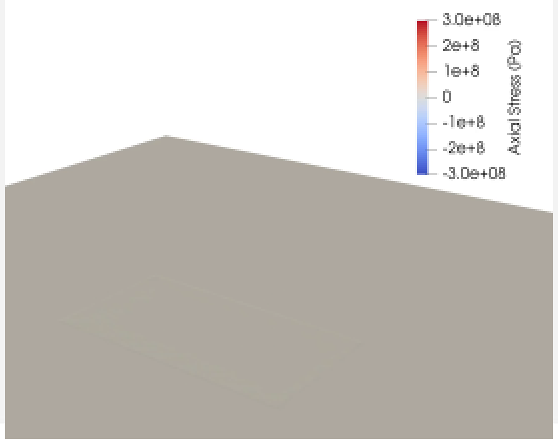
Laser welding

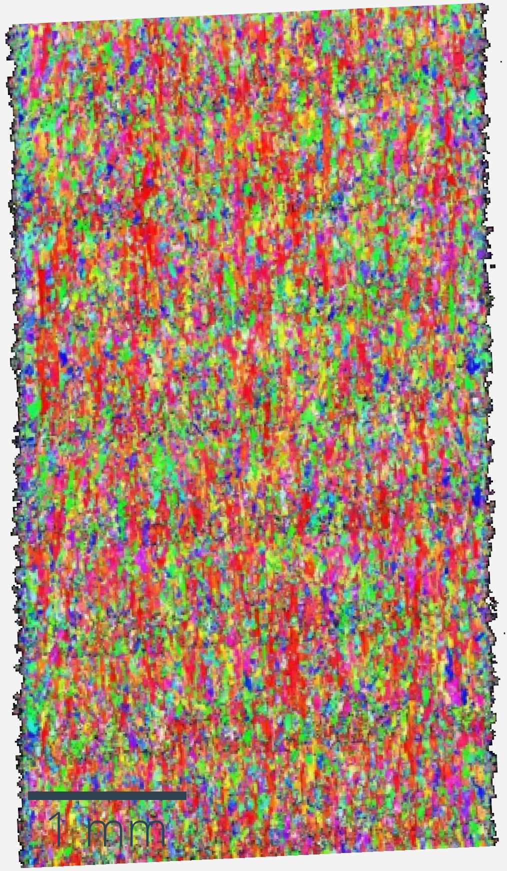




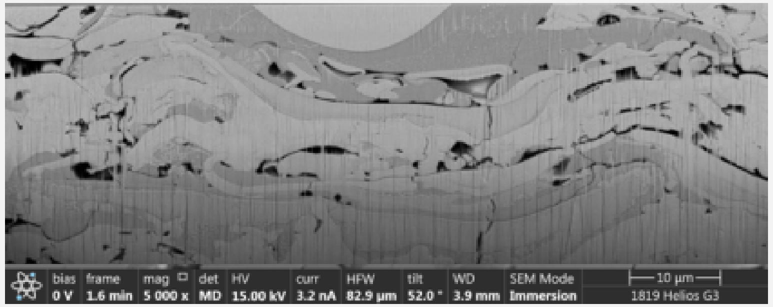
Additive manufacturing

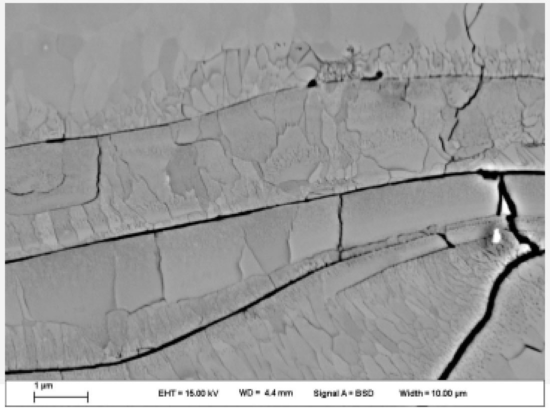






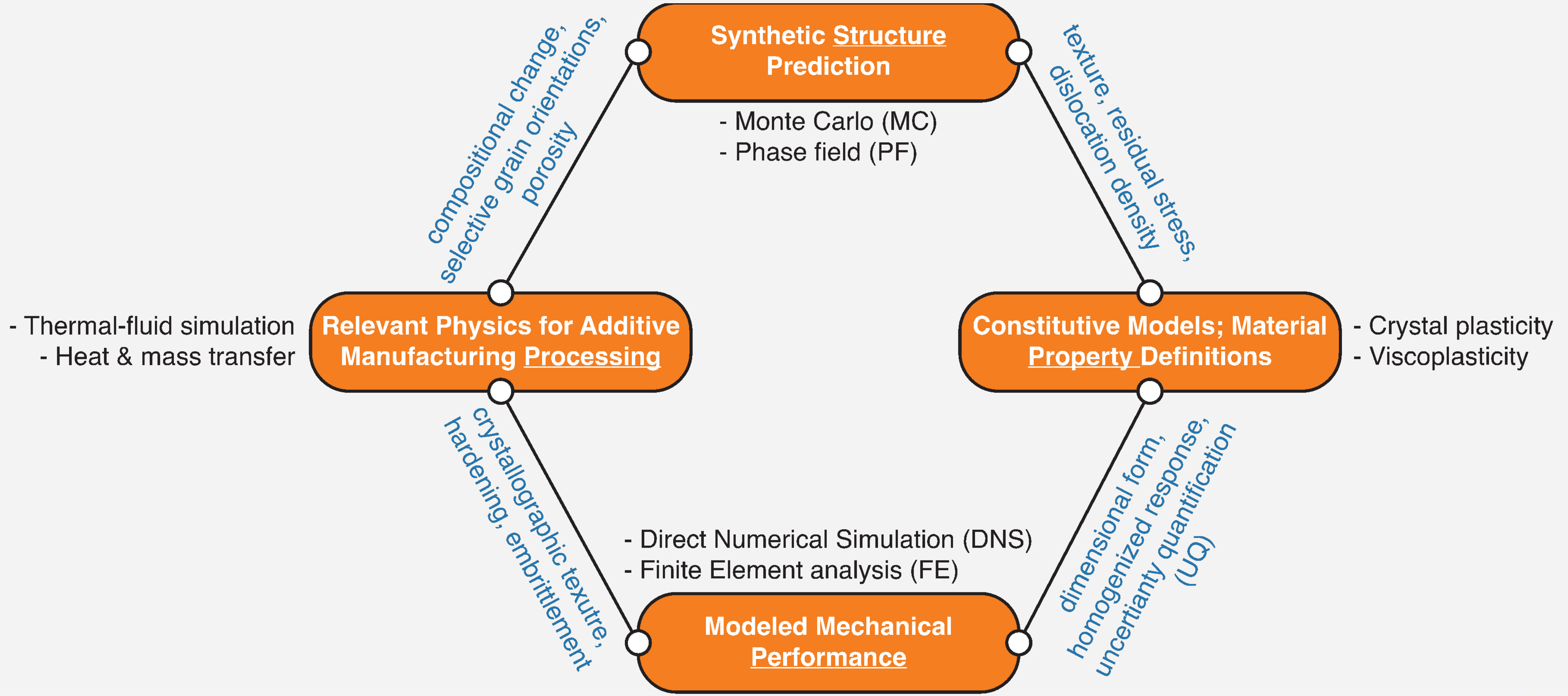
Thermal Spray





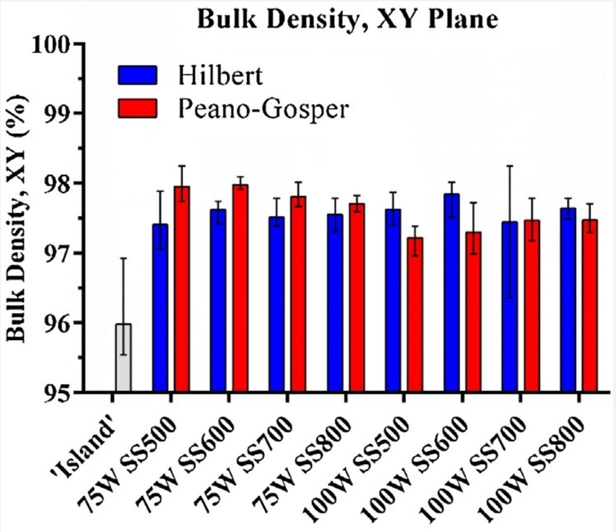
Rodgers et al, *CMS* 2021

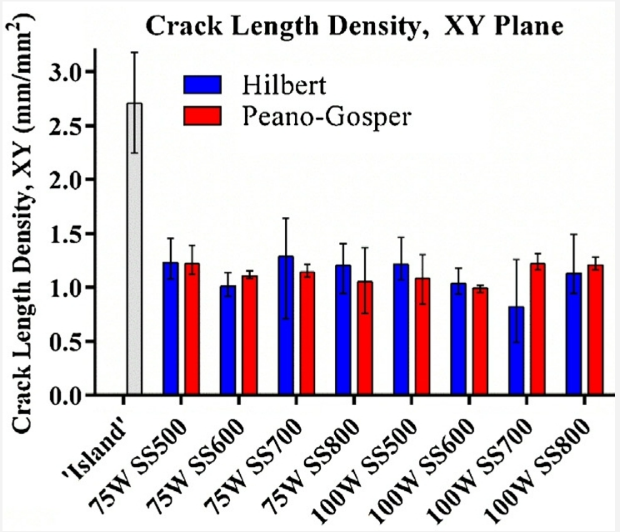
Making PSPP linkages at microscale and above

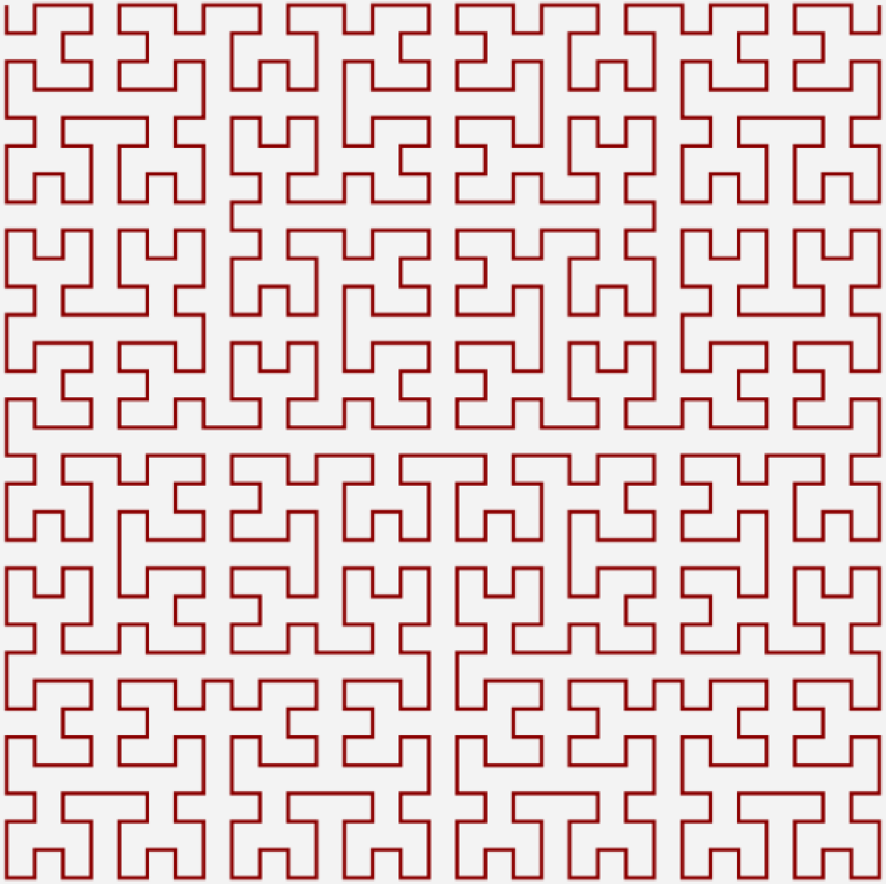


Flexi-Rosenthal challenge problem – Fractal infill patterns

- Fractal curves allow for space-filling, evenly spaced raster patterns.
- Used in some FDM plastic printing and commonly accessible in open source slicer programs.
- Experimental work indicates reduction in crack length and increased density vs typical linear raster “island” scan patterns for difficult to print metals (CM247L Ni-superalloy shown)

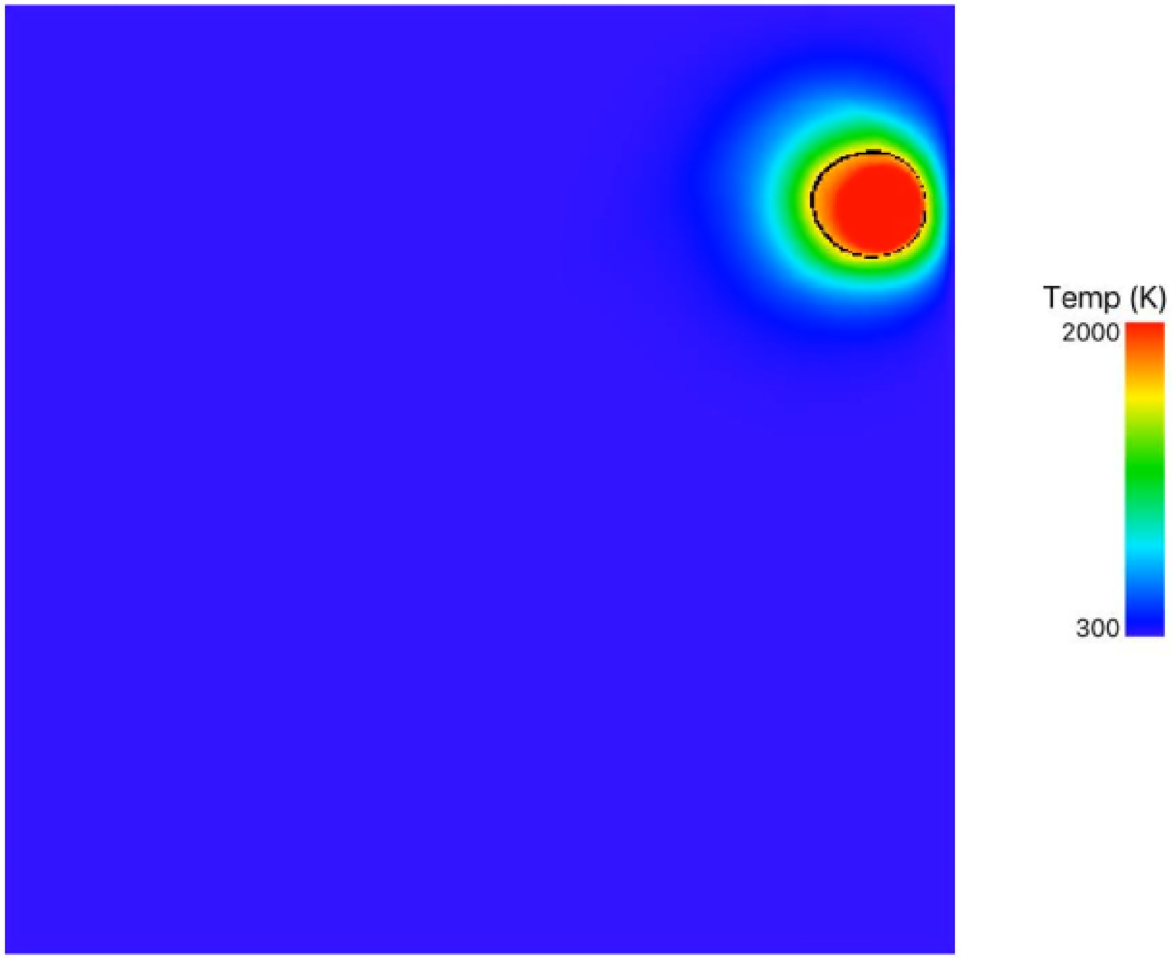


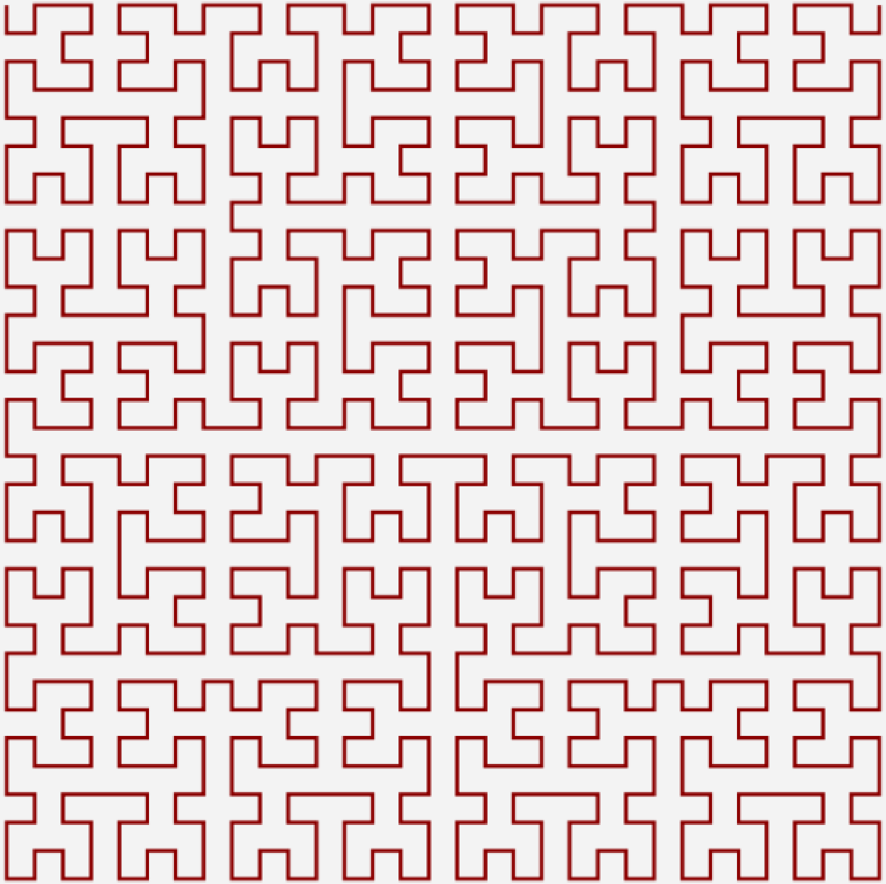




Catchpole-Smith et al, *Additive Manufacturing* 2017

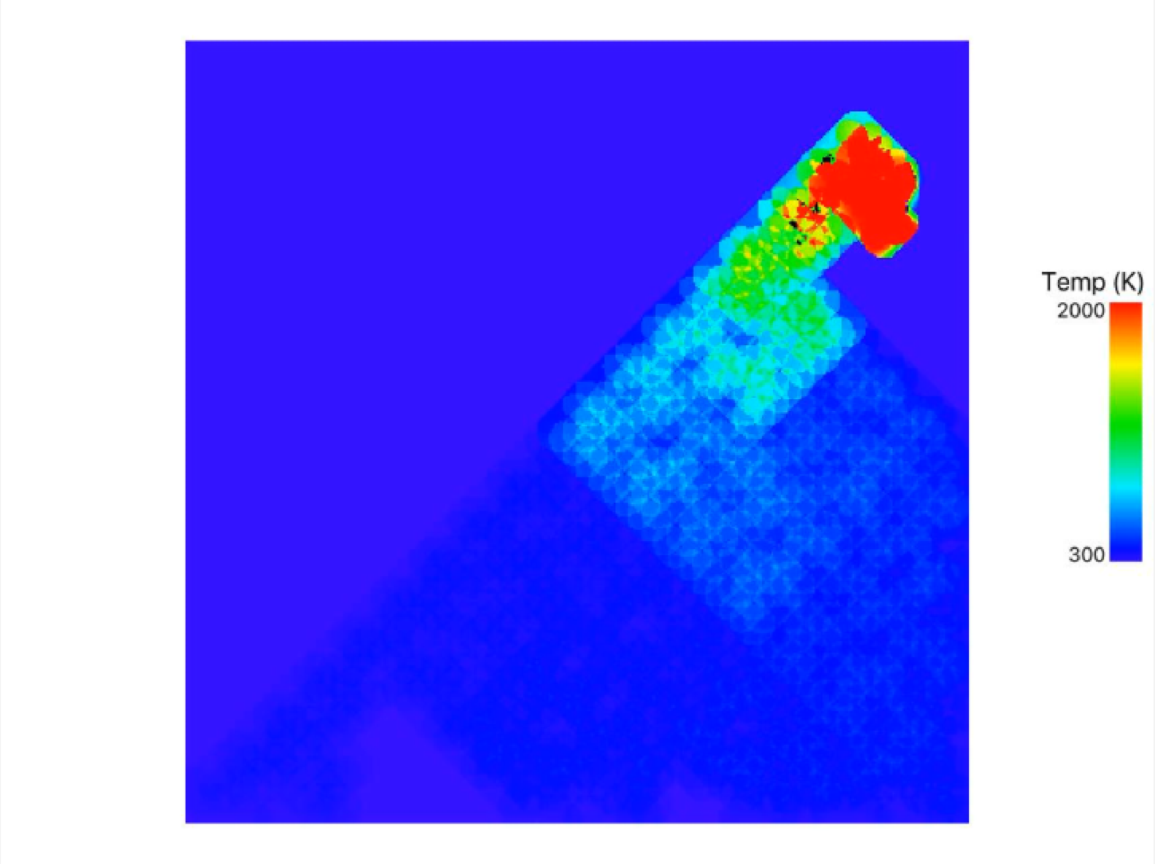
Fractal infill patterns– Finite Difference Results



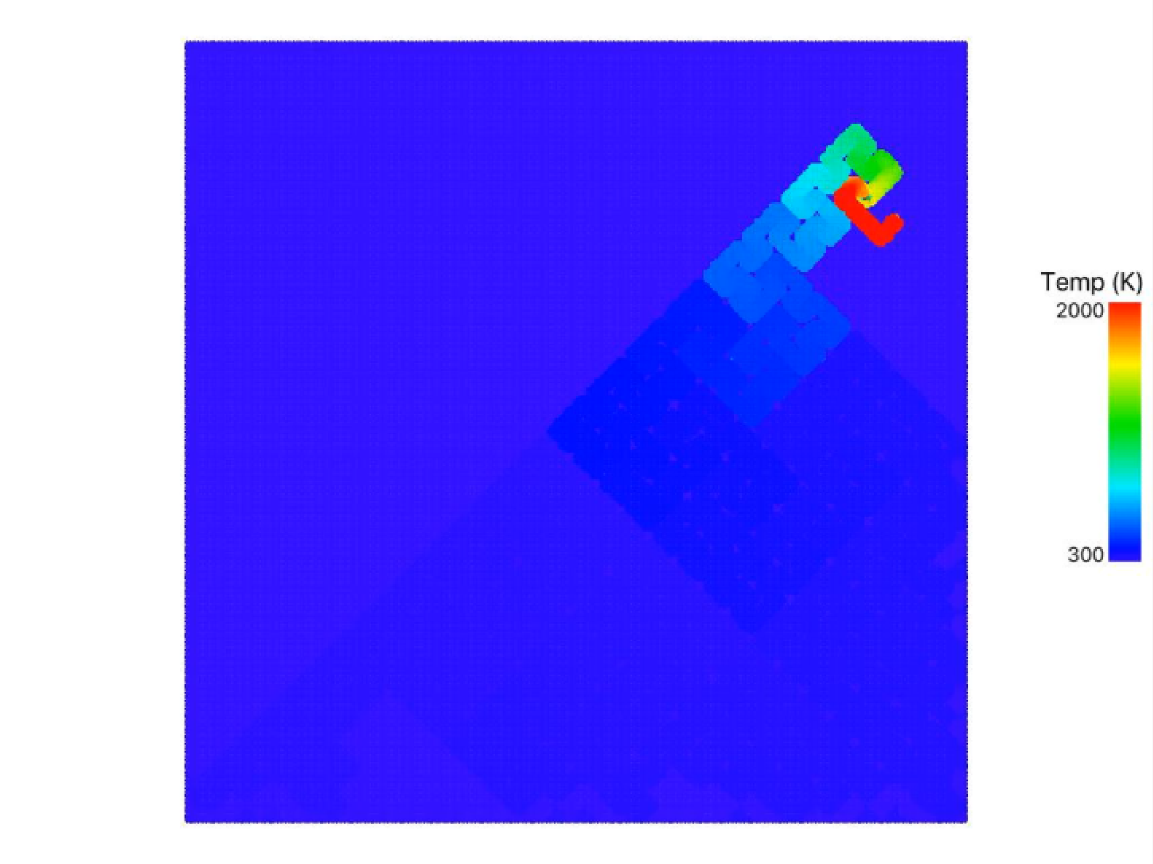


Fractal infill patterns– Flexi-Rosenthal Results

Temperature flux summed over rasters



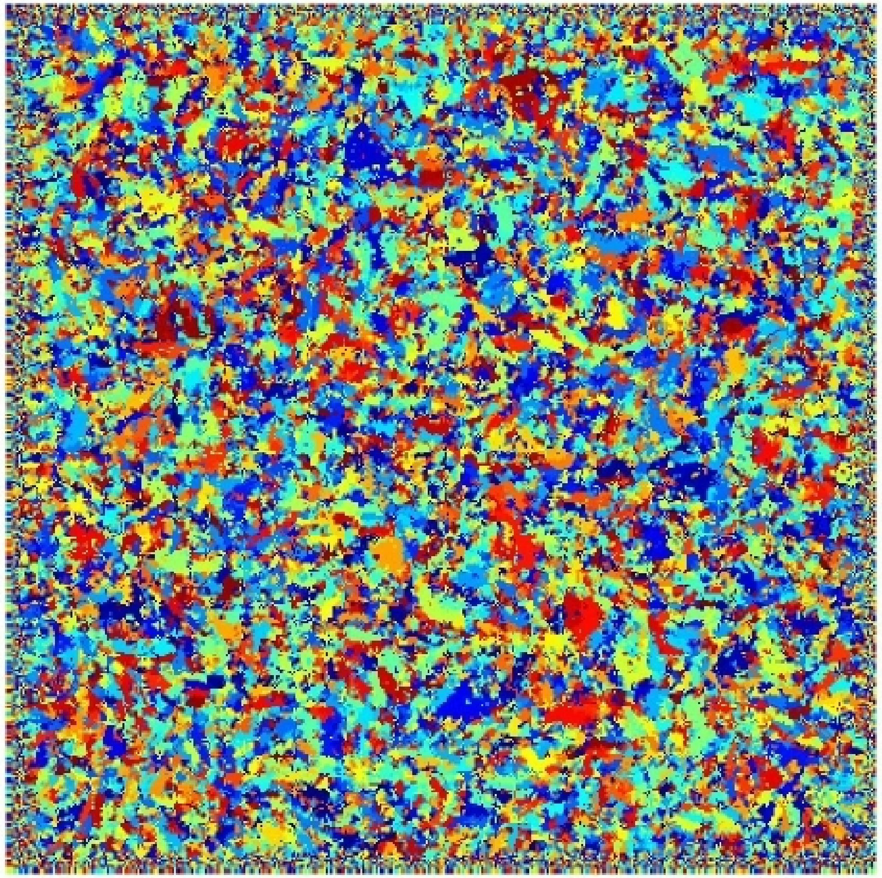
Temperature flux overwritten between rasters



Promising but needs normalization to prevent over-estimating temperature!

Hilbert curve microstructure results

Finite difference method



Flexi-Rosenthal method