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A Machine Learning Approach to Part Scale Microstructure Predictions in LPBF

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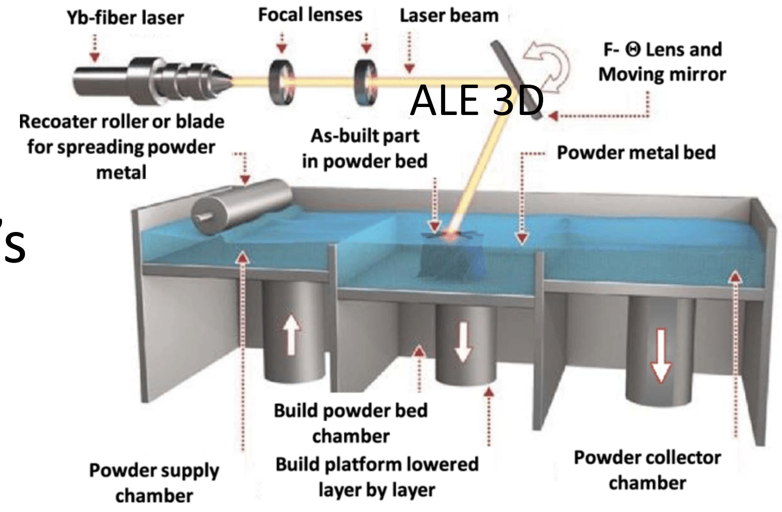
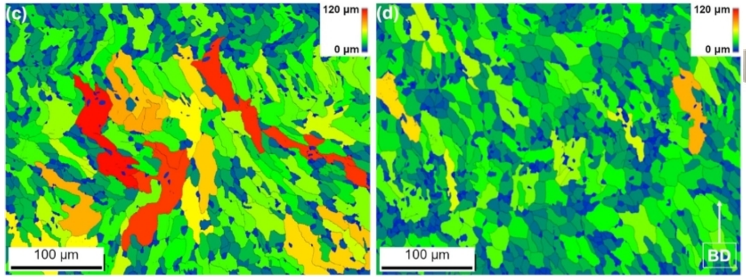
Laser Powder Bed Fusion Process

- Rapid solidification process (>10^5 K/s)
- Discrete control of process parameters at every point (10's of µm)
- Too slow for statistical testing of parts and optimizing process parameters
- Range of models:
  - Complex high-fidelity multi-physics codes
  - Reduced order physics-based models
  - Predictive data-driven models
- Growing literature on reduced-order and data driven LPBF microstructure surrogate models
- Fast models needed to better facilitate process design/optimization



Özel, T., et al., JMSE, 2019



Roehling, T., et al., Acta Materialia, 2018

Siemens

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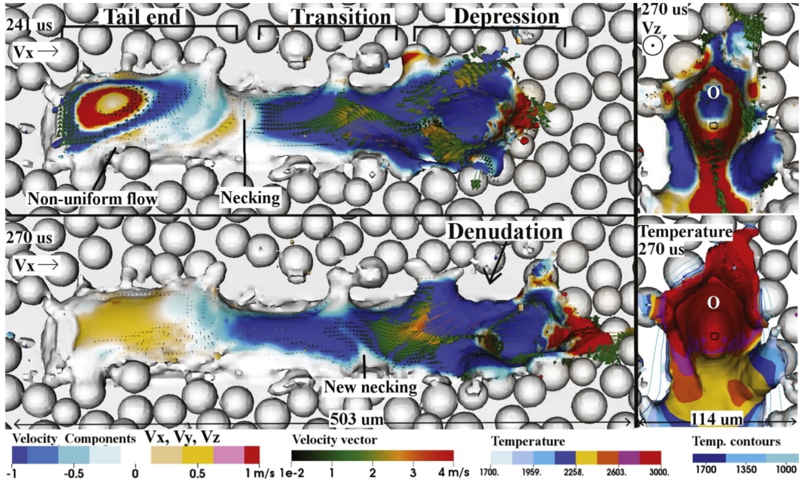
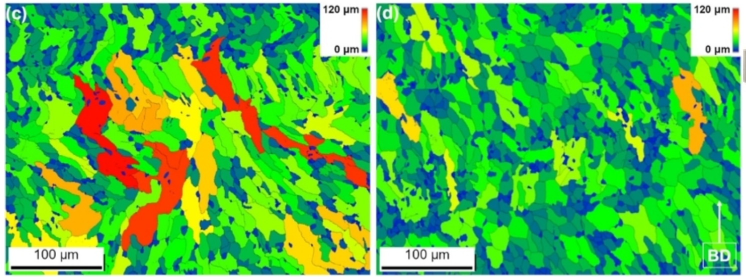


Khairallah, K., et al., Acta Materialia, 2017



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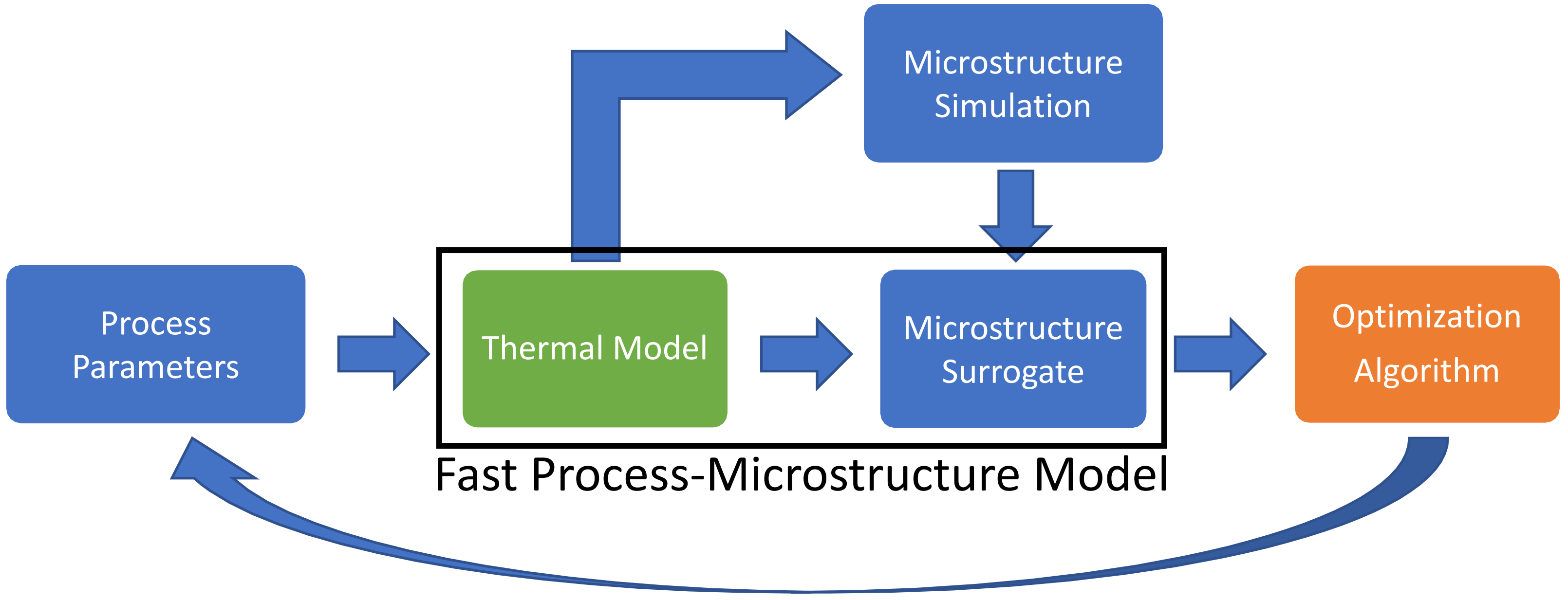
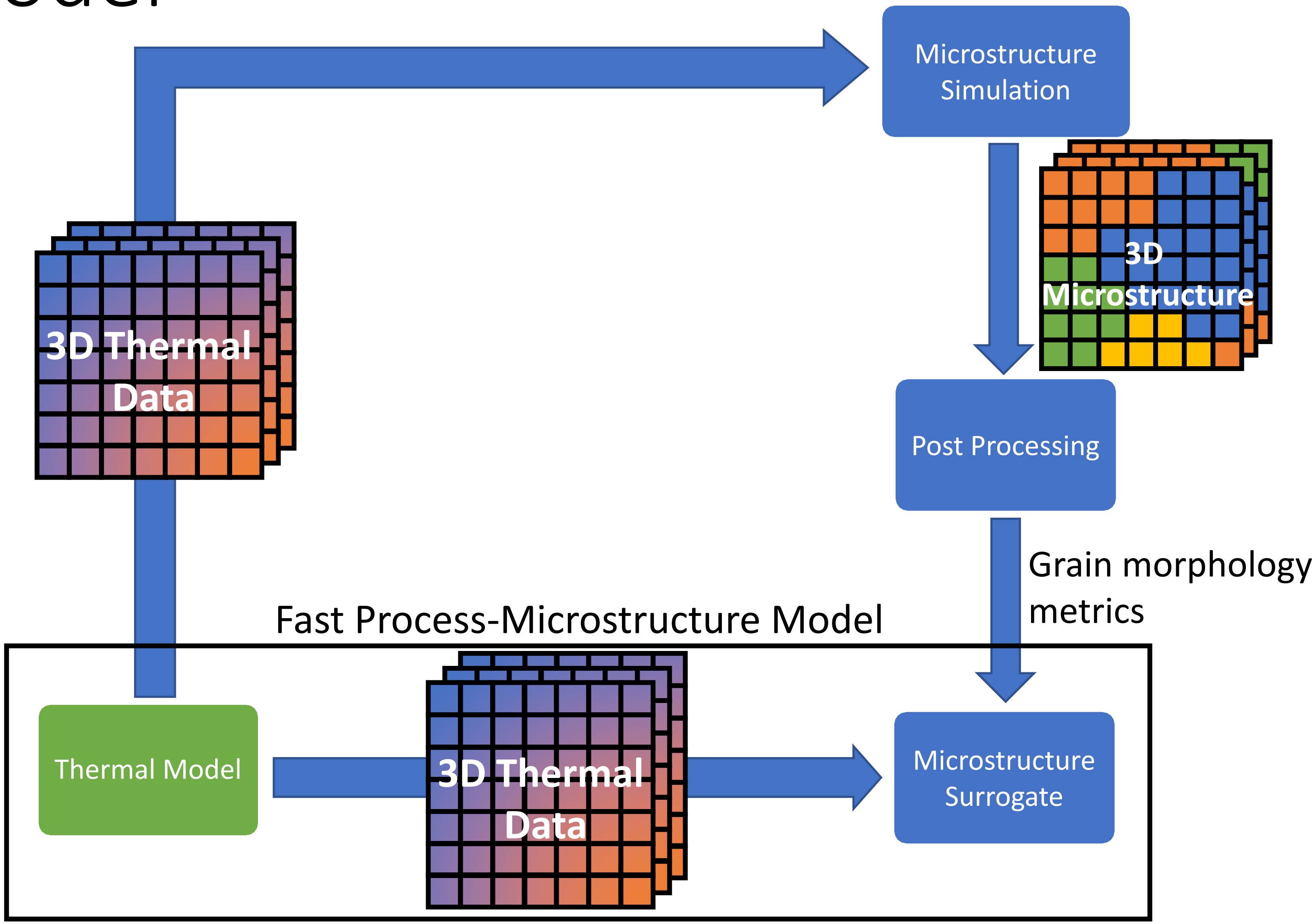
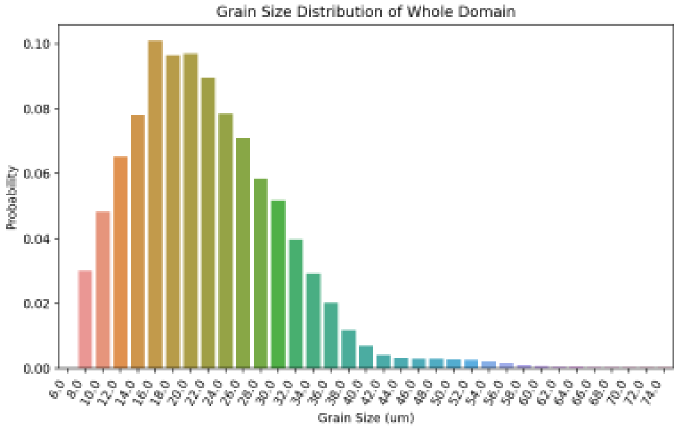
Fast Process-Microstructure Predictions Needed for Process Optimization

- Process optimization and experimentation is expensive
- Goal is to create a model fast enough for process parameter optimization



Framework for Creating a Fast Microstructure Model





Microstructure Simulations With SPPARKS

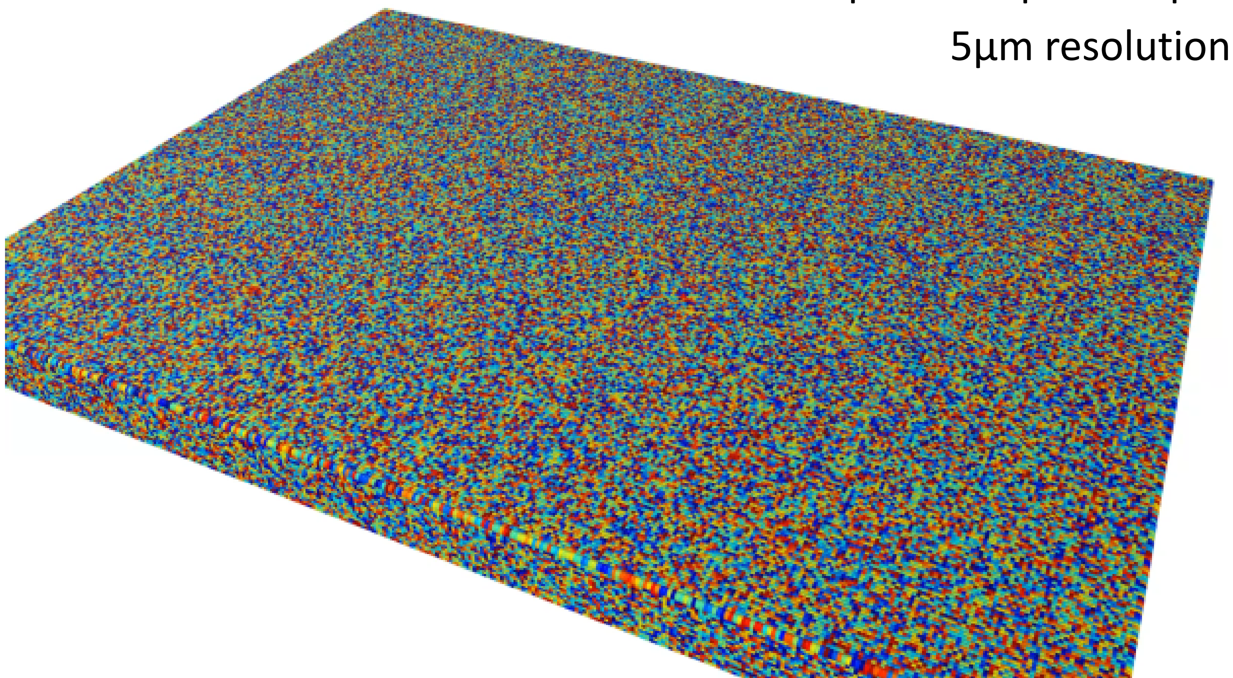
- SPPARKS – Stochastic Parallel PARticle Kinetic Simulator (Plimpton et al 2009)
- Lattice based Monte Carlo microstructure simulation
- Thermal AM module developed by Rodgers et al (2020)
  - Uses finite difference thermal model
  - Models nucleation in mushy zone
  - Uses KMC for solid region
  - 304/316 Stainless Steel
- Full microstructure simulations too slow for optimization
- Use SPPARKS to generate data for surrogate model training

Simulation Process Parameters:

100W, 1m/s, 82µm Gaussian Beam

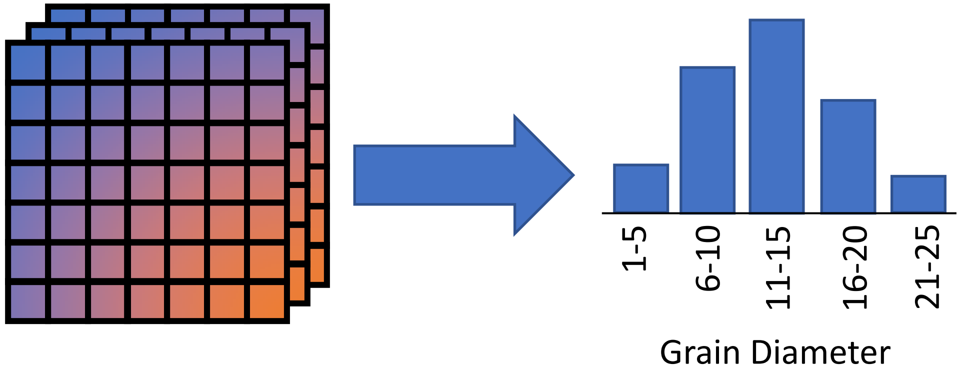
1750µmx1250µmx290µm

5µm resolution



Approach for a Microstructure Surrogate Model

- Want to predict microstructure statistics from thermal model outputs
- Inspired by computer vision models
  - Thermal data is structured like image data
  - Microstructure distributions are probability vectors



https://www.petage.com/kitten-care-101/

Approach for a Microstructure Surrogate Model

- Want to predict microstructure statistics from thermal model outputs
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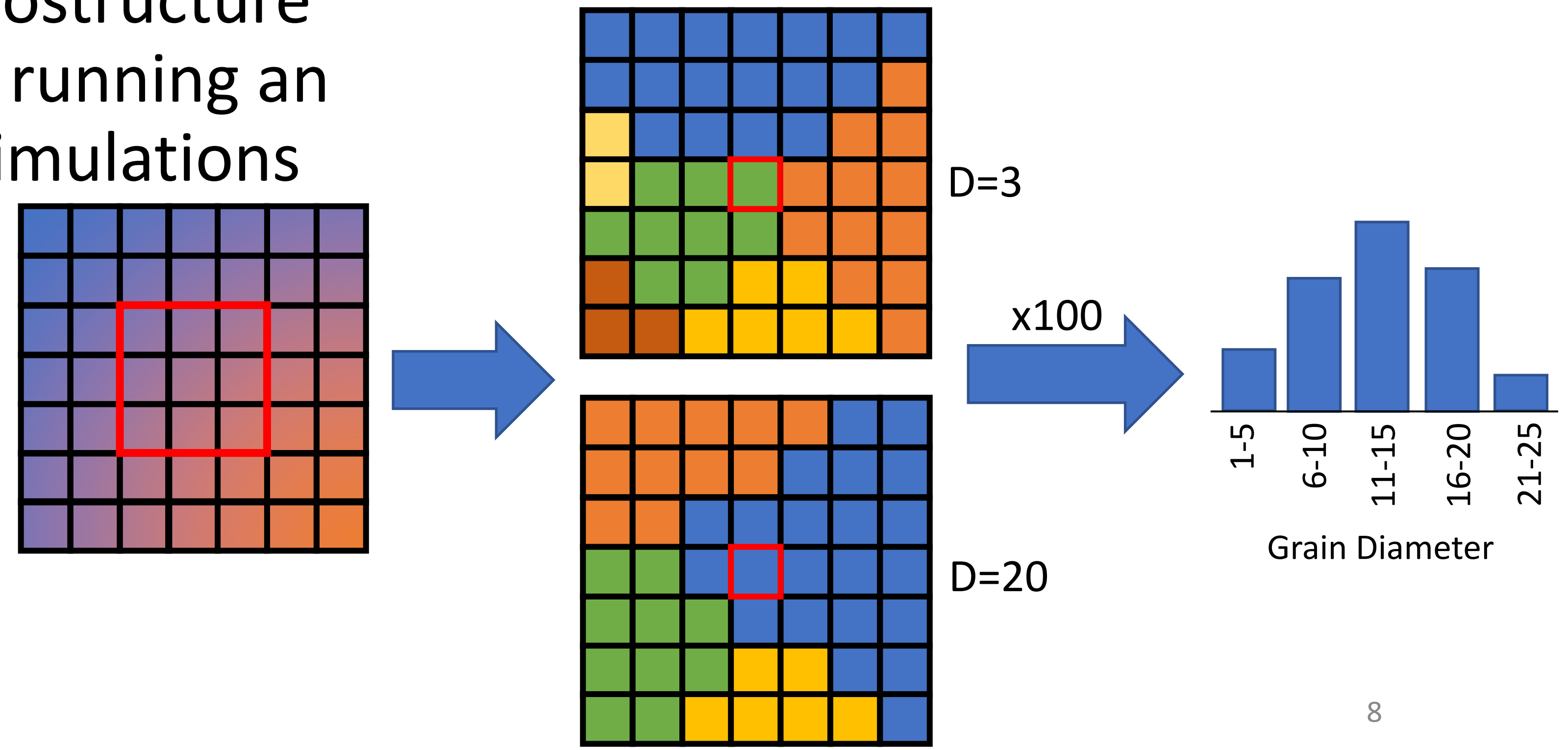
- Produce pointwise microstructure statistics for training by running an ensemble of SPPARKS simulations
- Use moving window on input to make local predictions



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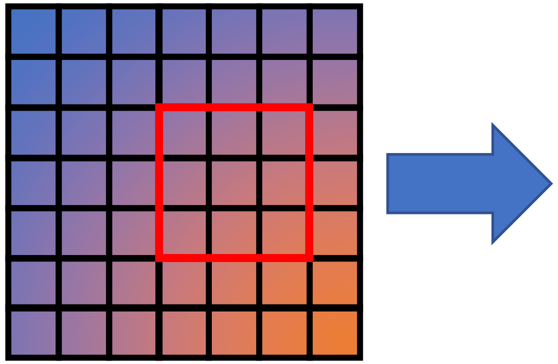
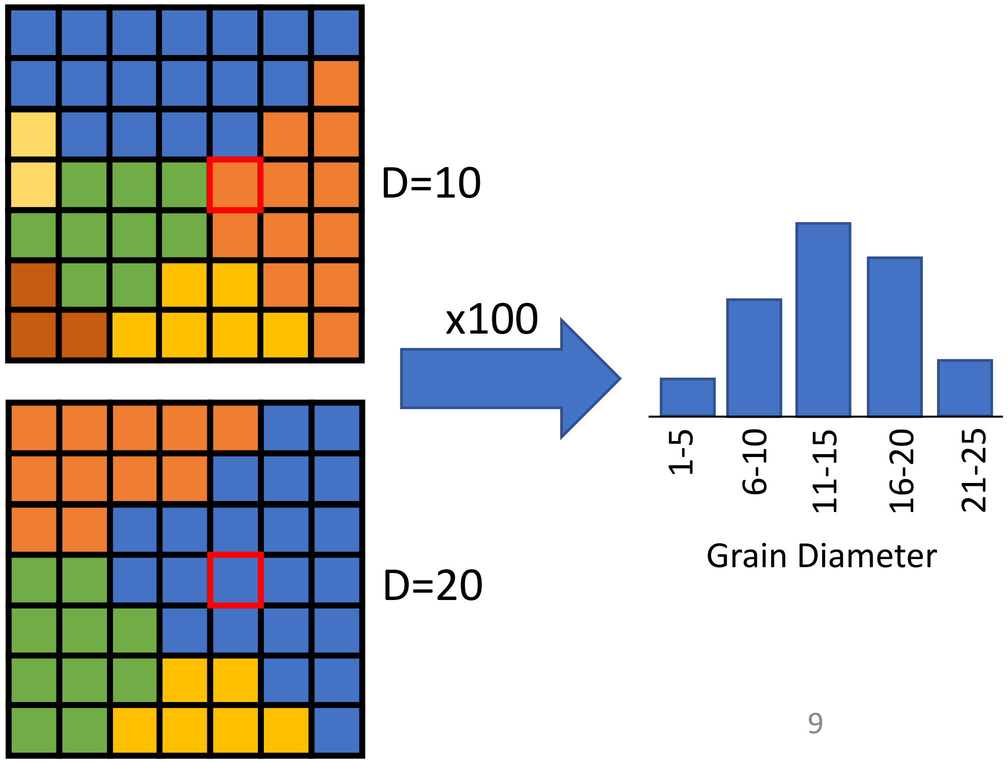
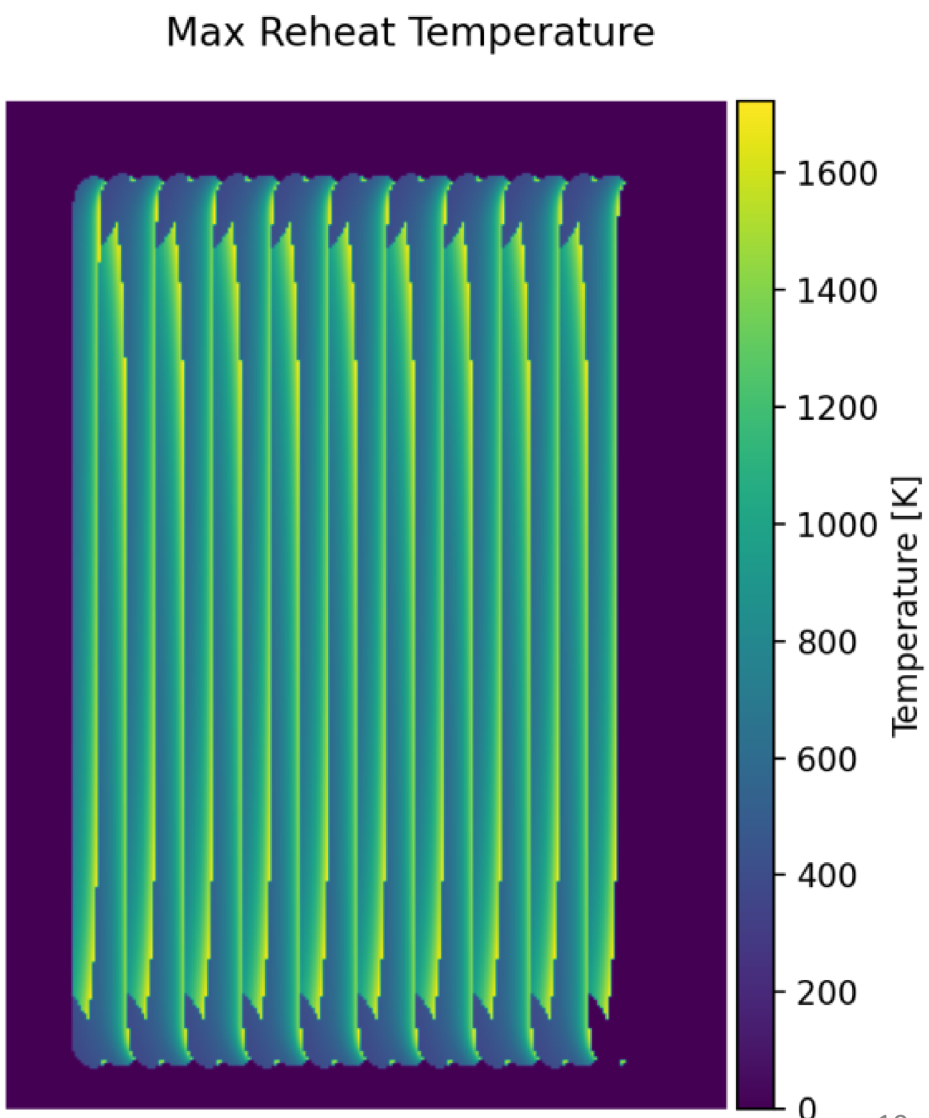
- Use moving window on input to make local predictions
- Multiple thermal characteristic fields analogous to image color channels





9 Thermal Characteristics Selected as Inputs to Microstructure Model

- Max reheat temperature post solidification
- Melt Count
- Cooling rate
- 3 Temperature gradient components
- 3 Cooling times
  - Time above undercooling
  - Time above solidus
  - Time at elevated temperature



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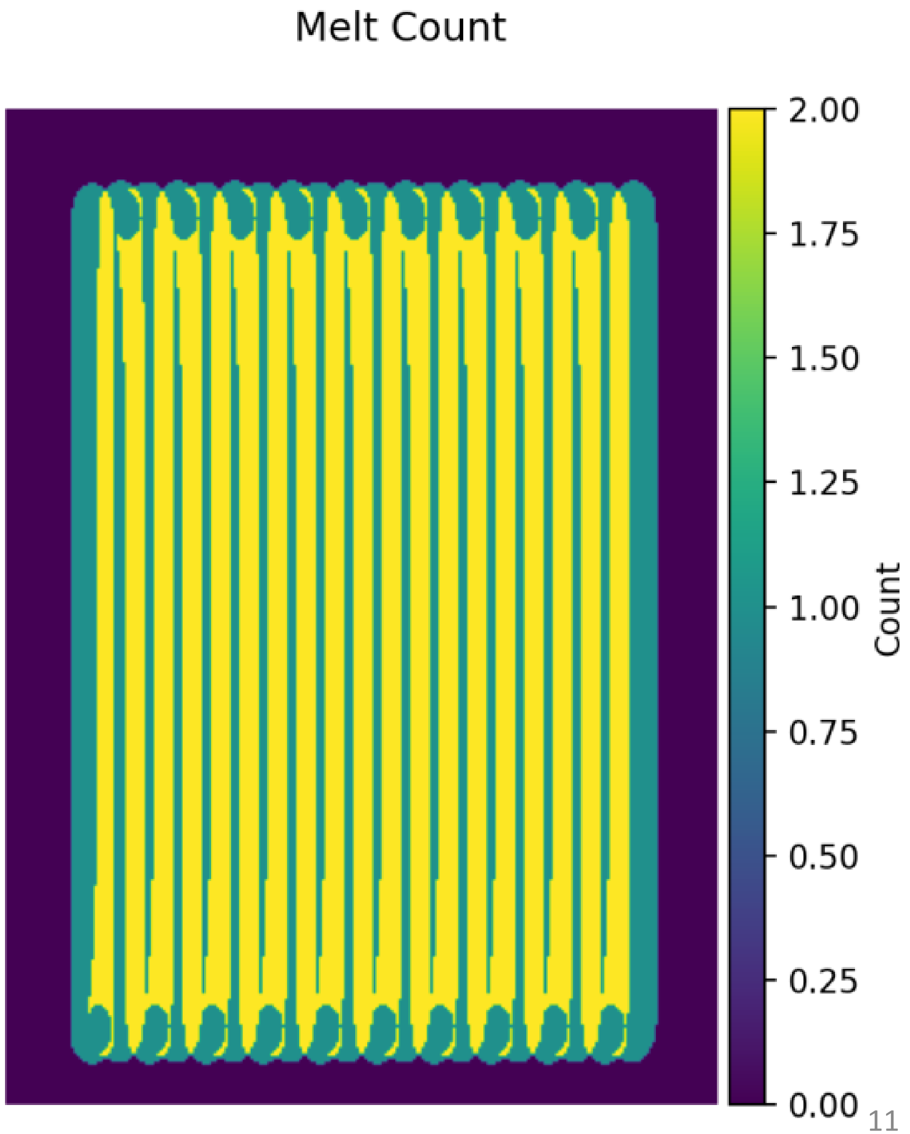

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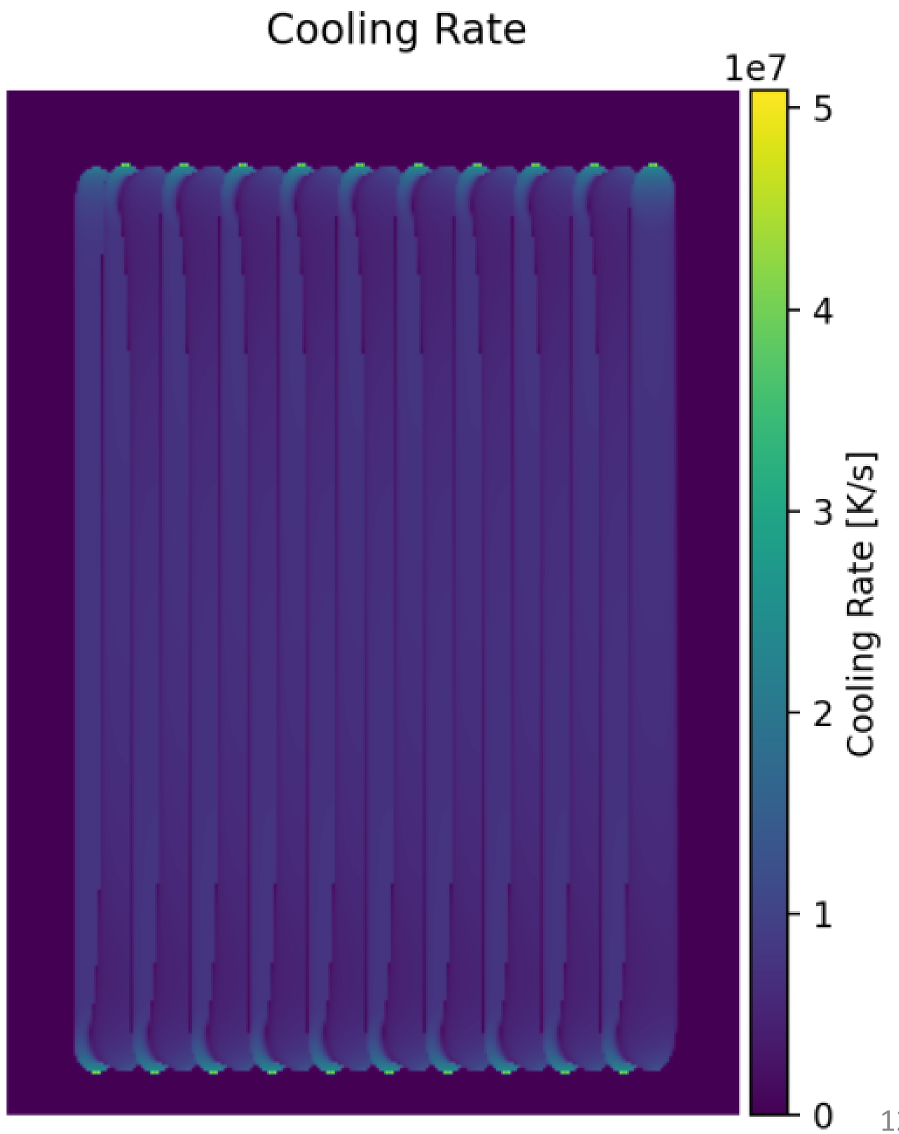

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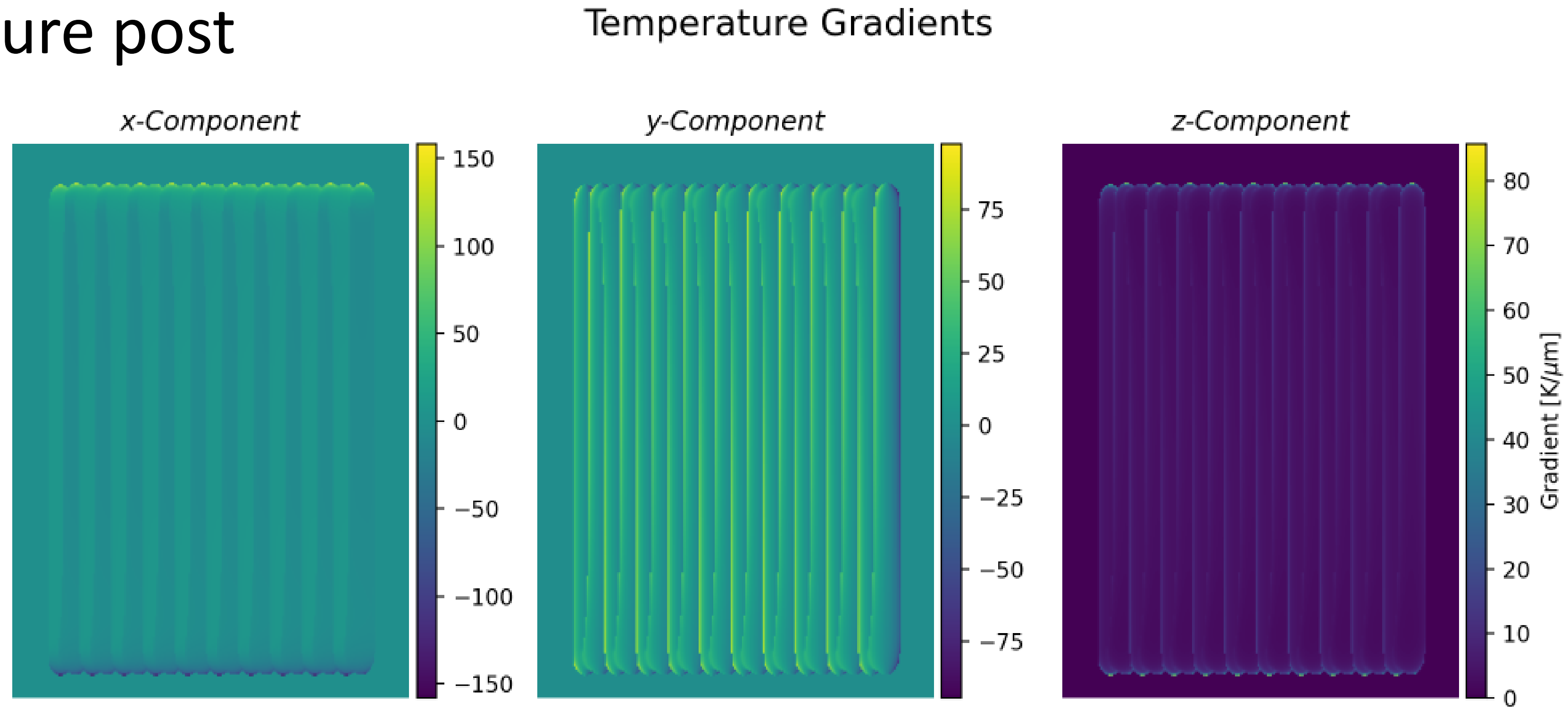

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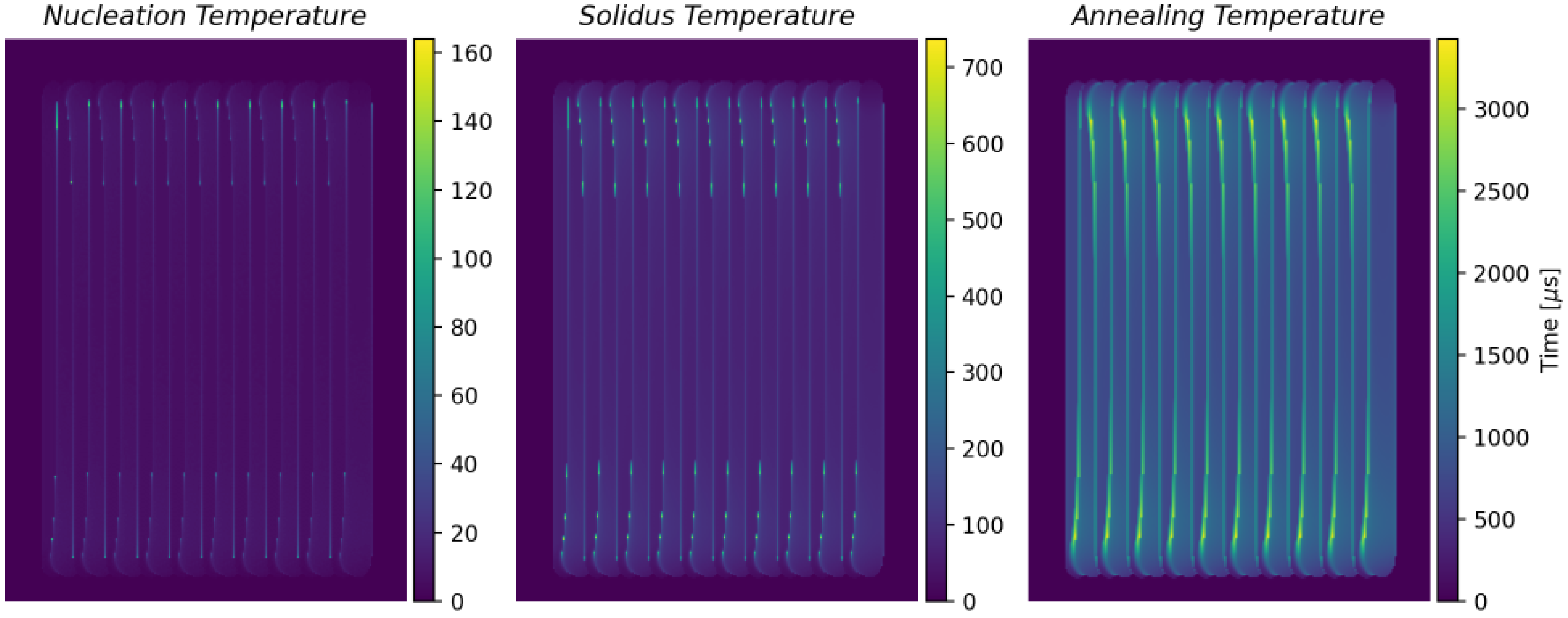
Cooling Times - Time Spent Above:



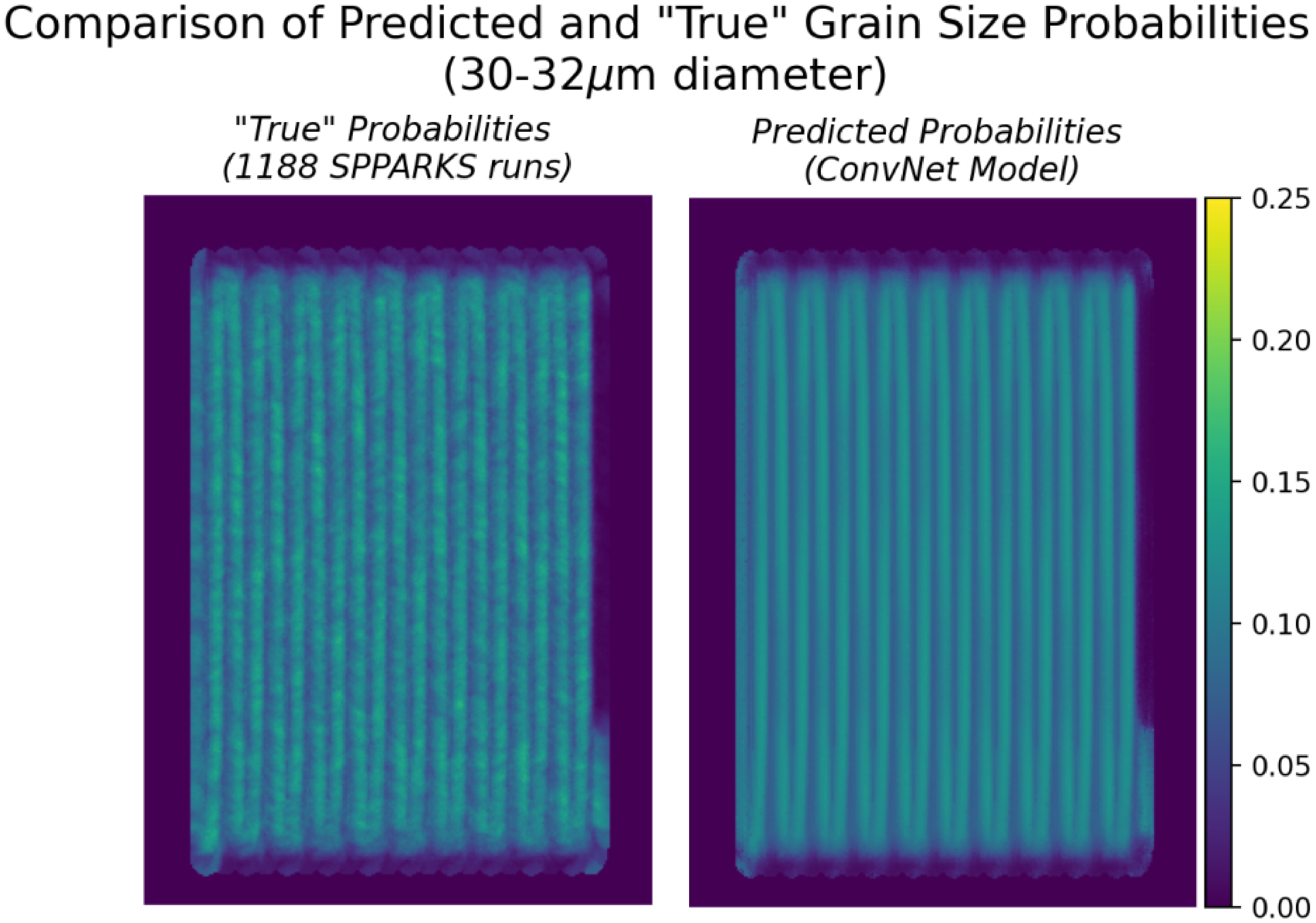
Machine Learning Model Overview

- Inputs are 15x15x15 cube with 9 channels
- ConvNext V1 architecture (Facebook 2022)
  - Convolutional Neural network updated with recent techniques
  - 20% dropout rate
- Modified last layer
  - Softplus activation function to enforce positive values
  - Normalized outputs sum to one
- Mean Squared Error (MSE) as loss function

$$MSE = \frac{1}{N}\sum_{i}(x_i - y_i)^2$$

Resulting Surrogate Model Has Accuracy Equivalent To Running a Much Larger Ensemble

- Model learns to average out the stochastic influence of the training data
- Accuracy of the model is at the limits of what we can measure



Model size was optimized to improve performance

- Initial model had minimal changes from image classification model and had not been optimized for this task
- Performed multi-objective hyperparameter optimization of the model using gaussian process Bayesian optimization
  - Maximize model speed
  - Minimize model error
- Reduced the number of model weights to 5.6M weights from 38.8M weights
- Reduced inference time by 75%

Resulting Surrogate Model is Much Faster Than Running a New Ensemble

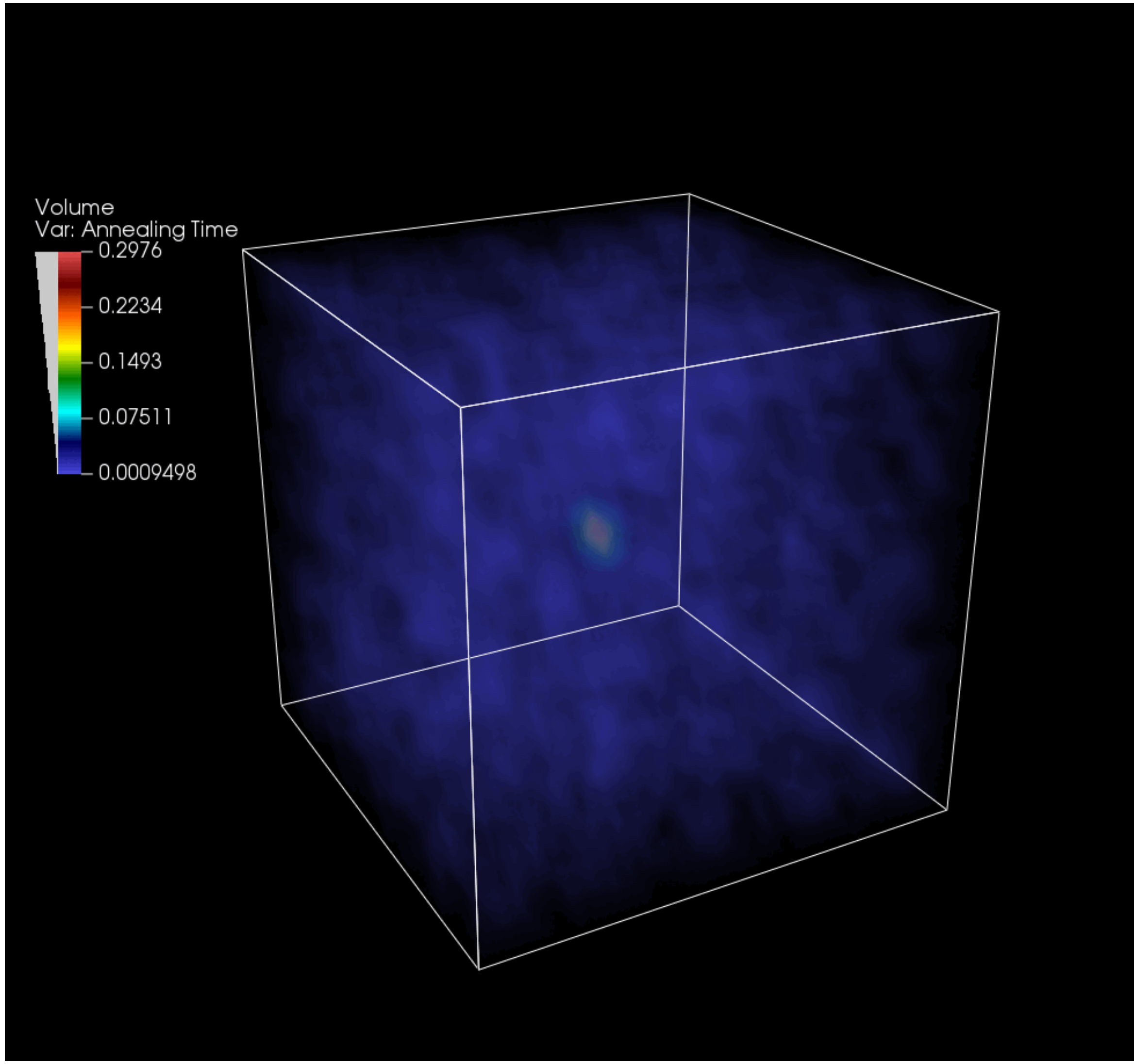
- Inference for 50x40µm layer 0.5mm square takes 9 minutes on an A100
  - Added 3 hours 31 minutes for thermal simulation
- Equivalent SPPARKS run takes 22 hours on 64 Cores (AMD EPYC 7532)
  - Need 100+ run ensemble to get same information as surrogate
  - Surrogate results comparable to 1000+ run ensemble
- Single machine speedup: 600x

Analyzing Importance of Thermal Characteristics

- Thermal characteristics selected were educated guesses, actual impact was unknown
- A significant portion (81%) of the thermal model runtime is spent calculating these characteristics – Reducing the number of characteristics could create significant improvements in process-microstructure model speed
- Taking the Jacobian of the model predictions with respect to the inputs can tell us the influence of each value in the input on the prediction
- Comparing the influence across many predictions tells us if any data is underutilized

Analyzing Importance of Thermal Characteristics

- All characteristics have large regions of low importance
- All characteristics place more importance on center
- No characteristic is obviously less useful
- We will keep them all for now



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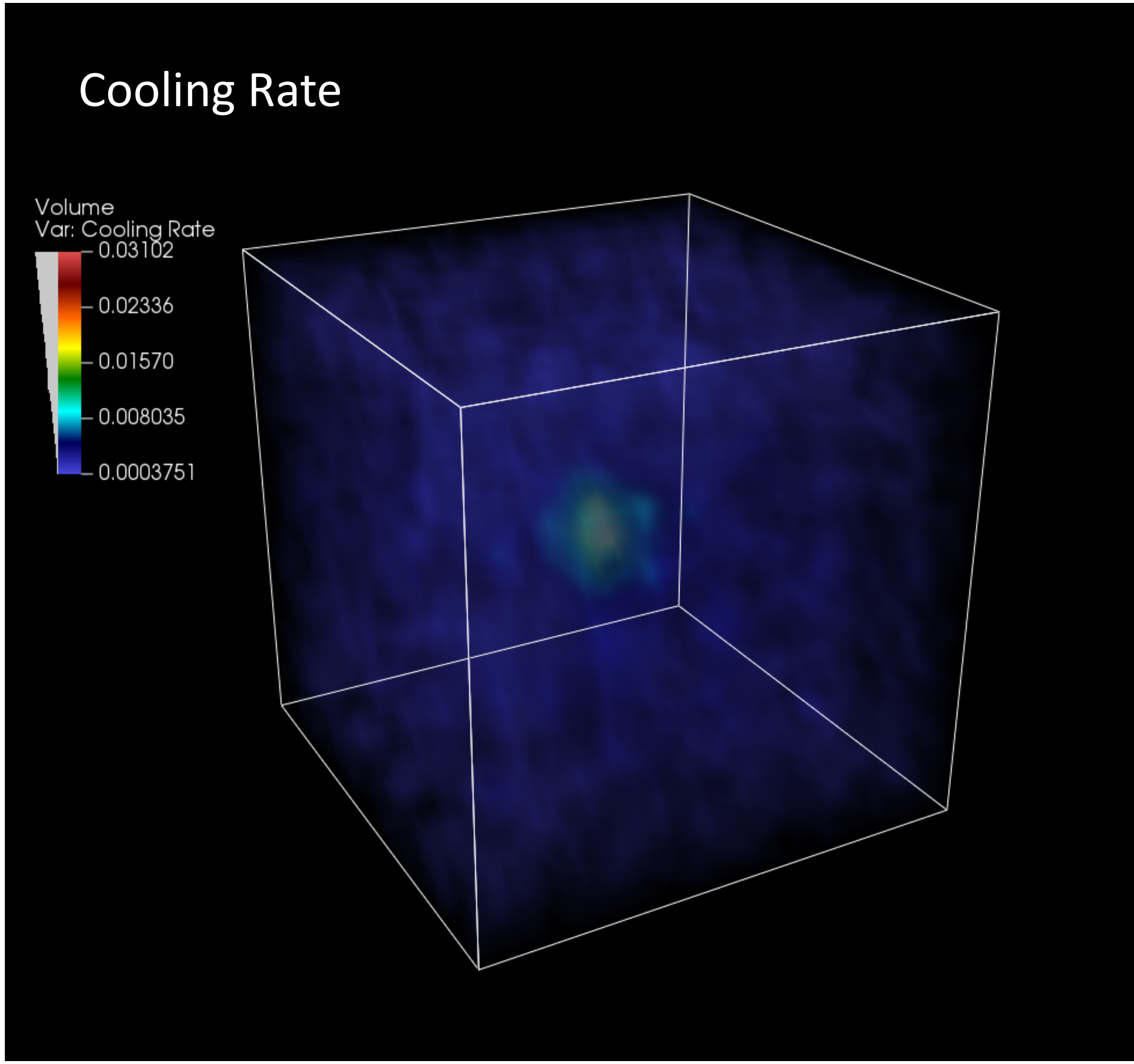

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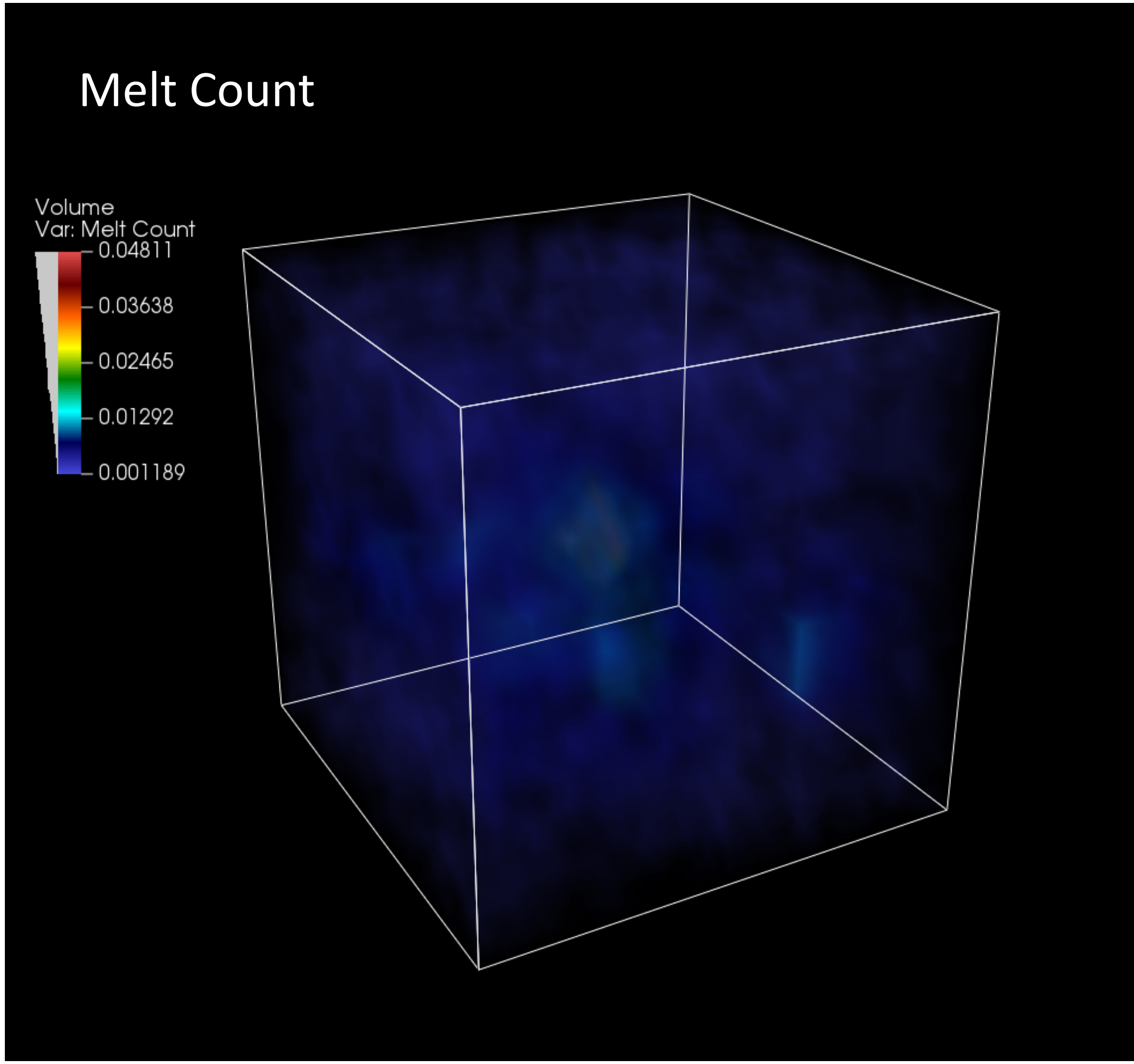

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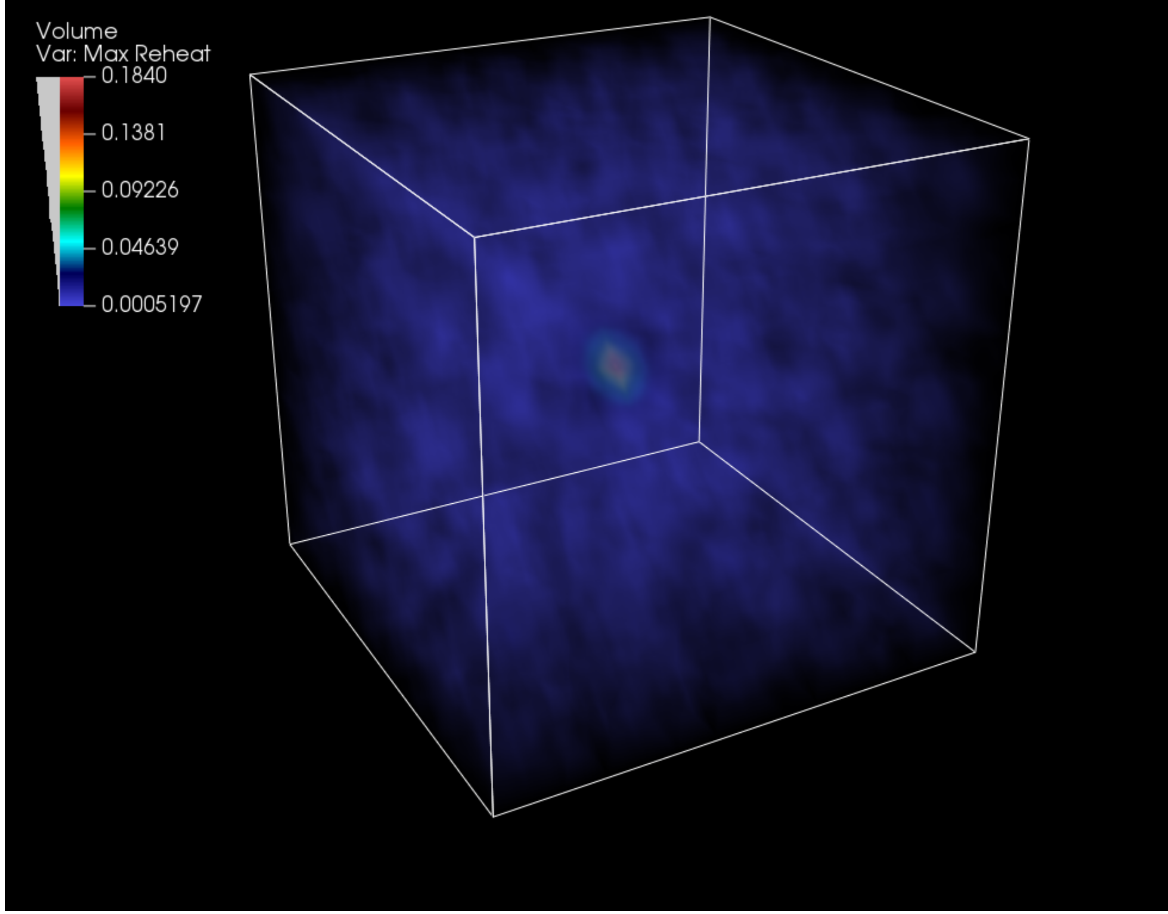
Max Reheat Temperature



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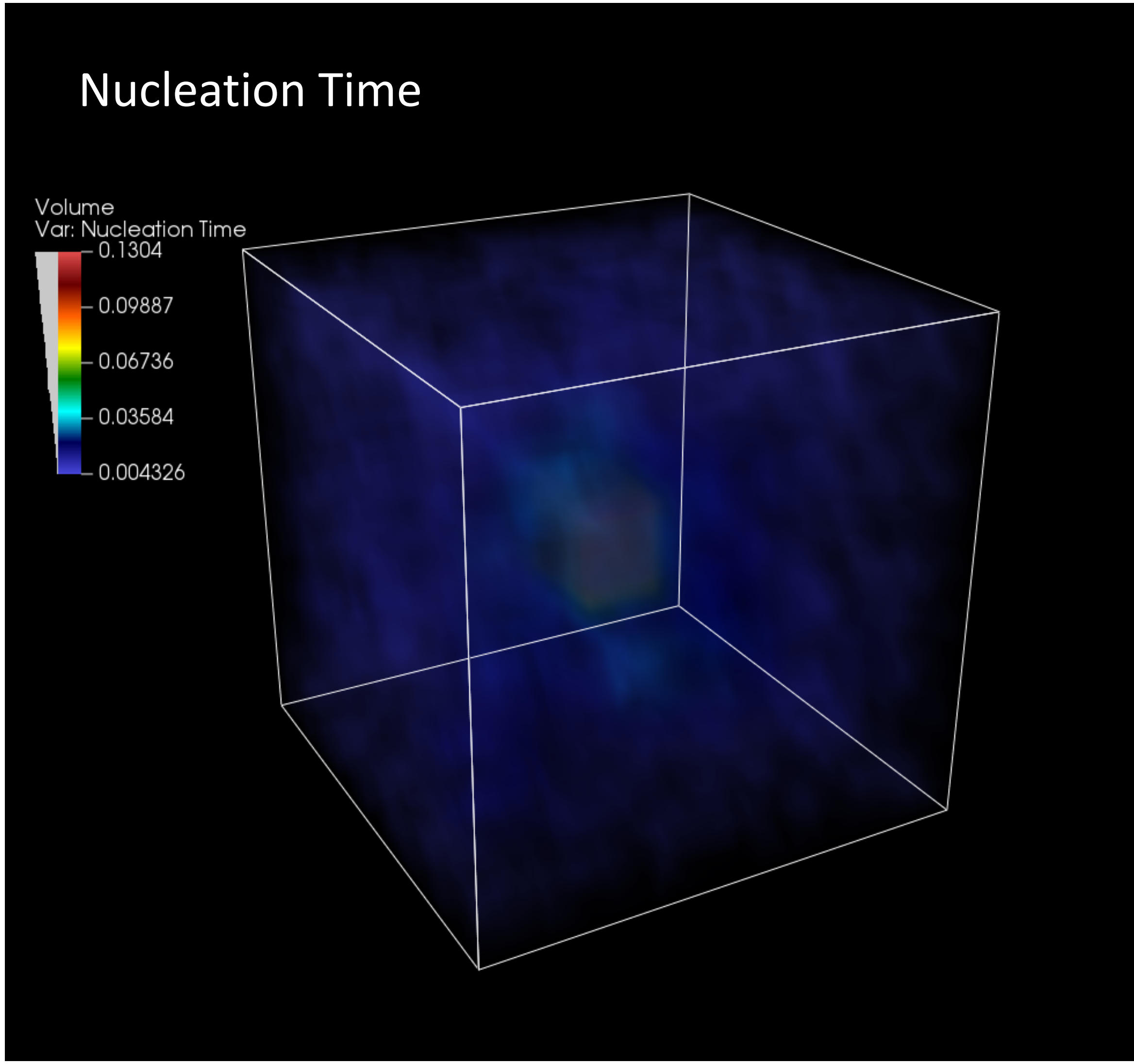

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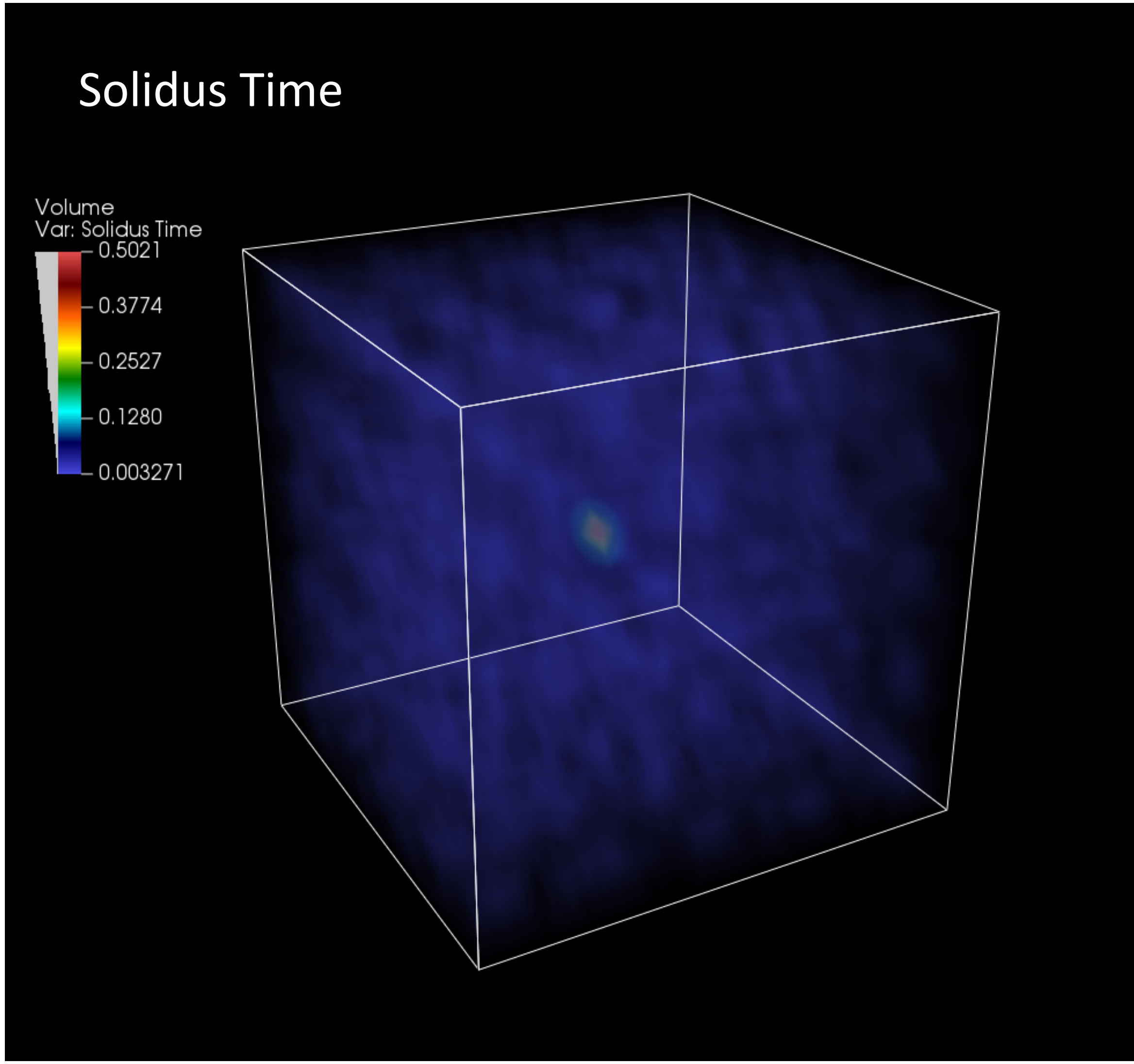

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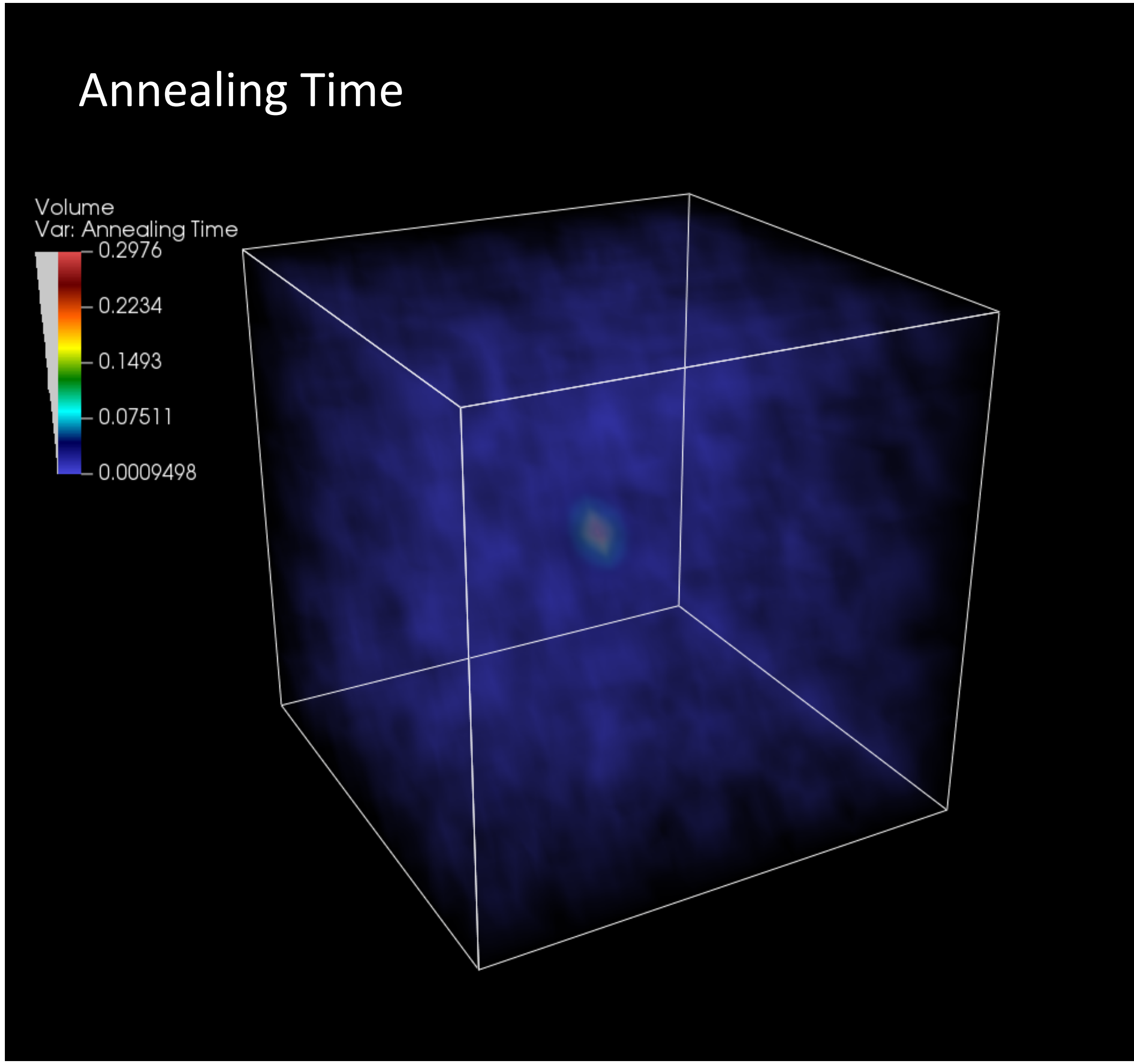

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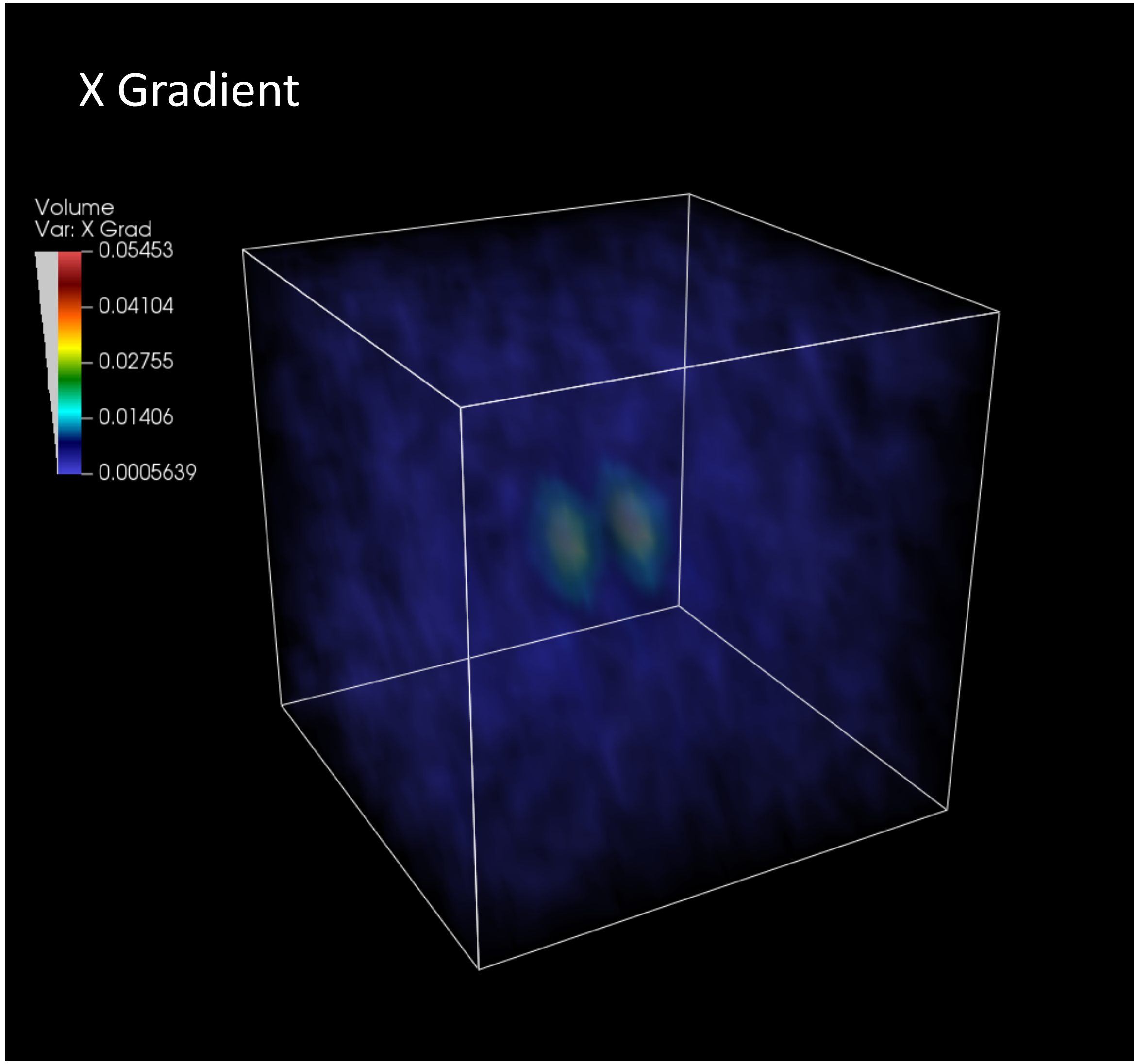

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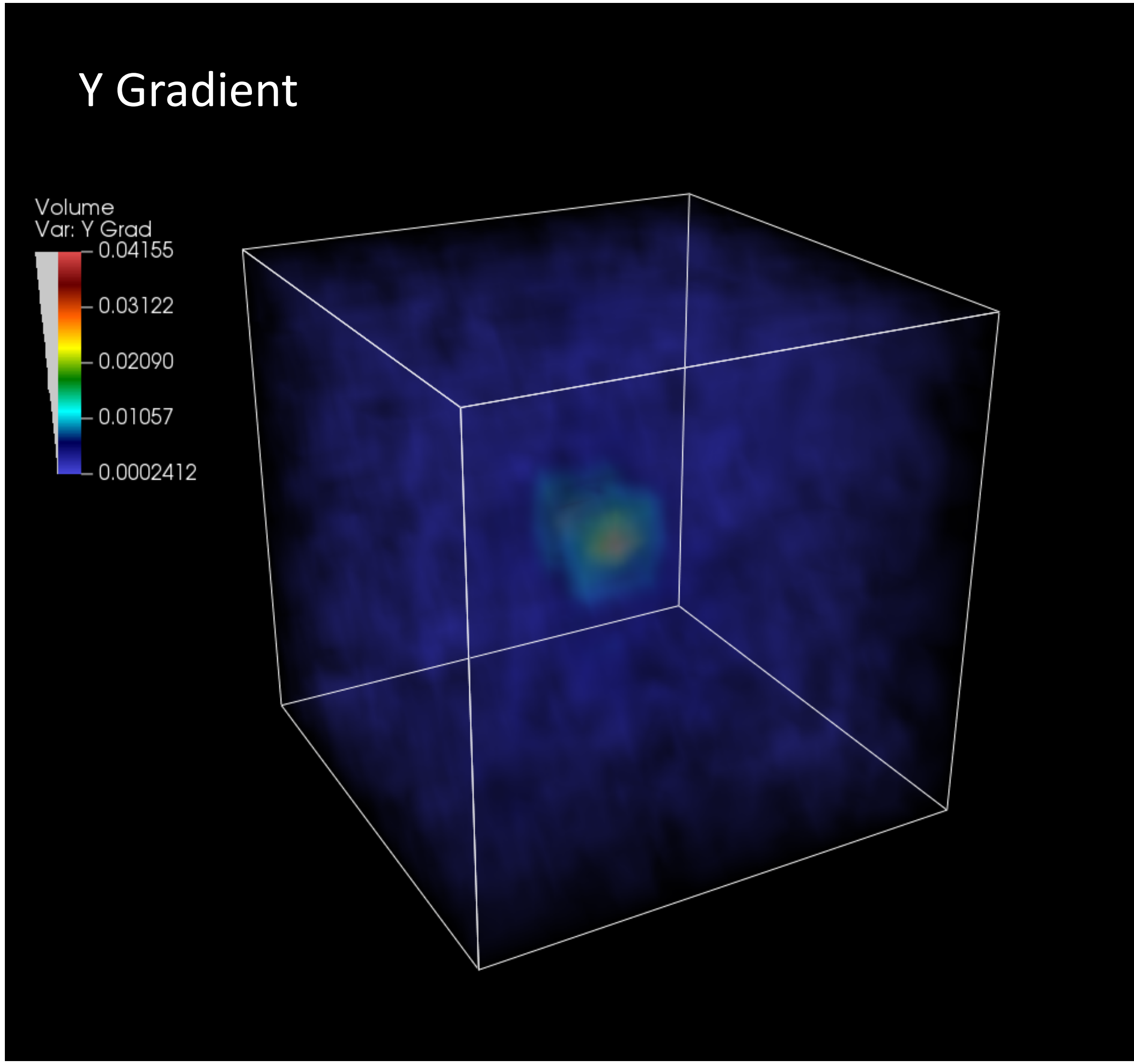

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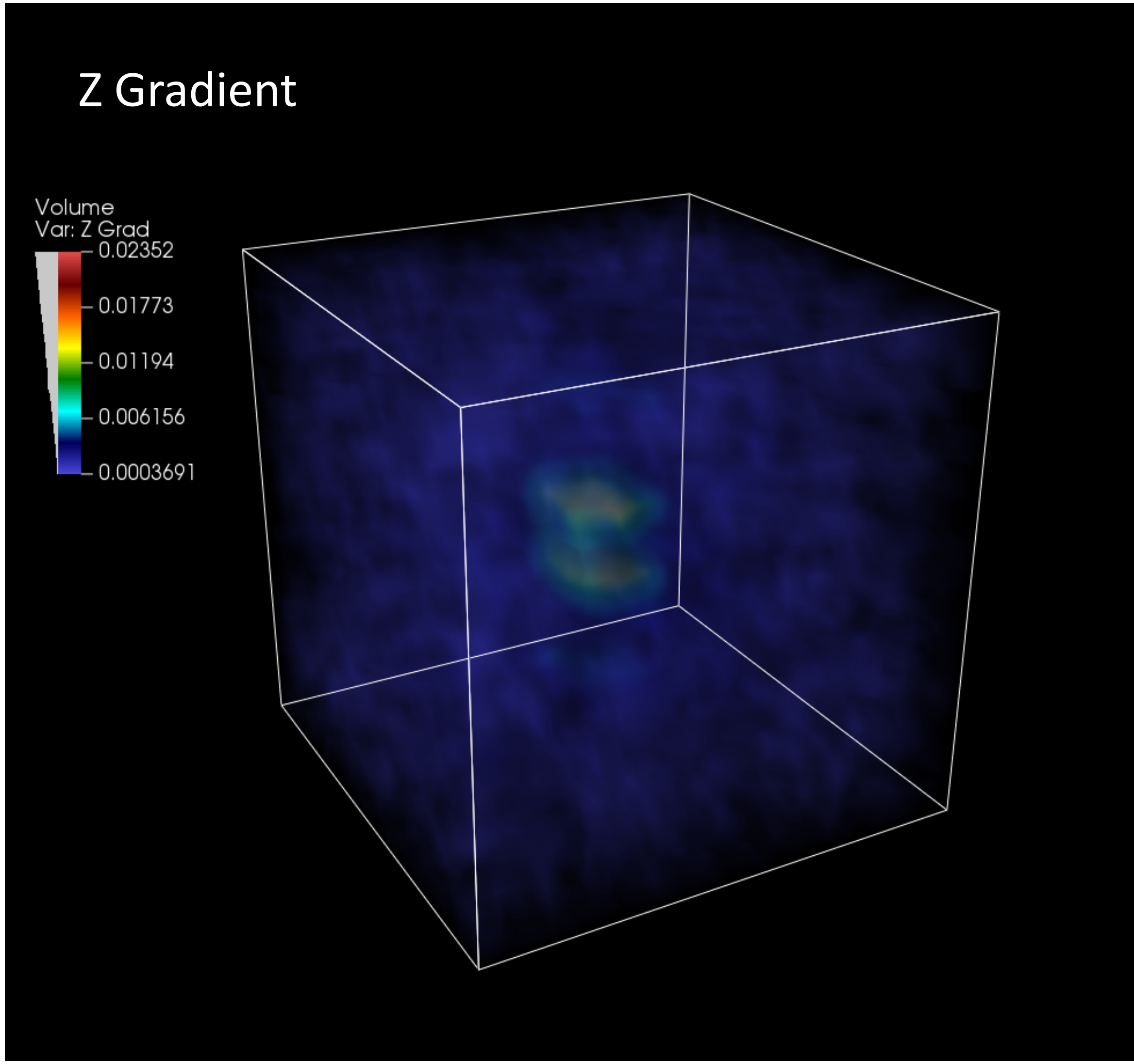


Now that we have a fast model, what is necessary for part scale predictions?

- Problem 1:
  - This model is still not fast enough for centimeter scale parts
  - What is the minimum representative volume element that is statistically meaningful?
- Problem 2:
  - We can’t guarantee accuracy outside of the training data
  - Means we need training data from large complex simulations, but this is expensive

Both require ensembles of expensive simulations to solve

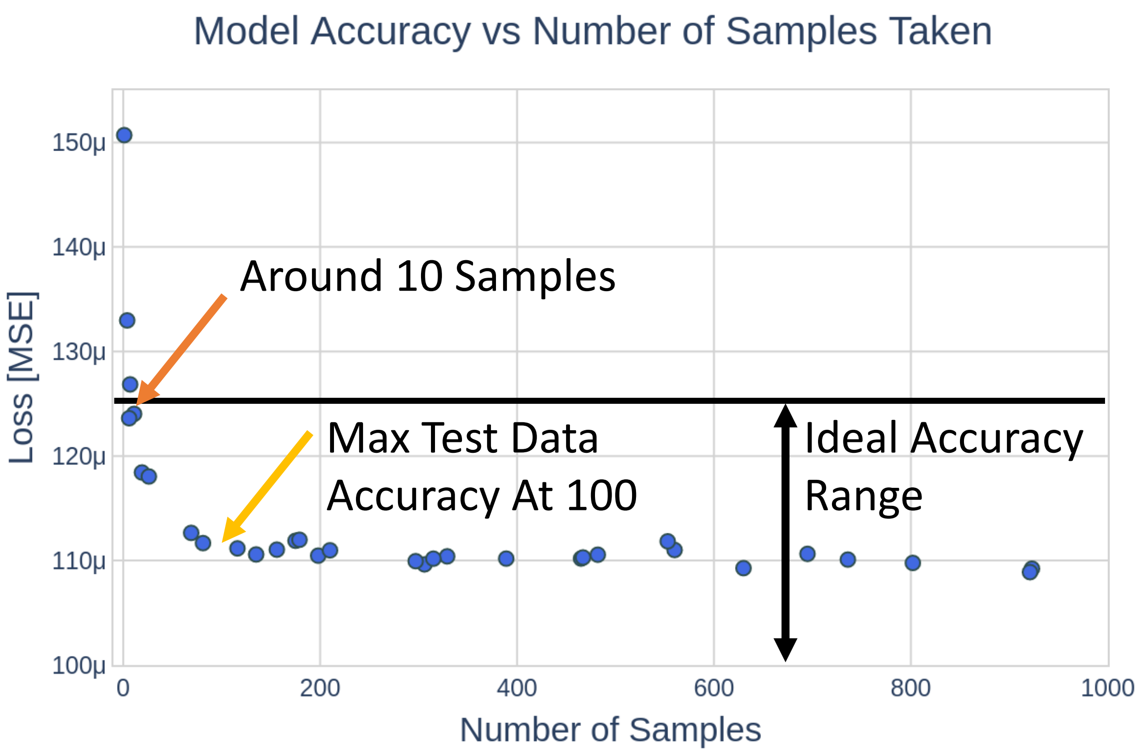
Do We Need Large Ensembles?

- What if we can use a smaller ensemble to train and still make accurate predictions?
- We know that the model can make predictions more accurate than training data
- Significantly faster to tune a model with new training data than to run 100+ SPPARKS sims with large domains
- Use new model to do statistical analysis of RVE

Test this theory by simulating influence of smaller ensembles on training via sampling

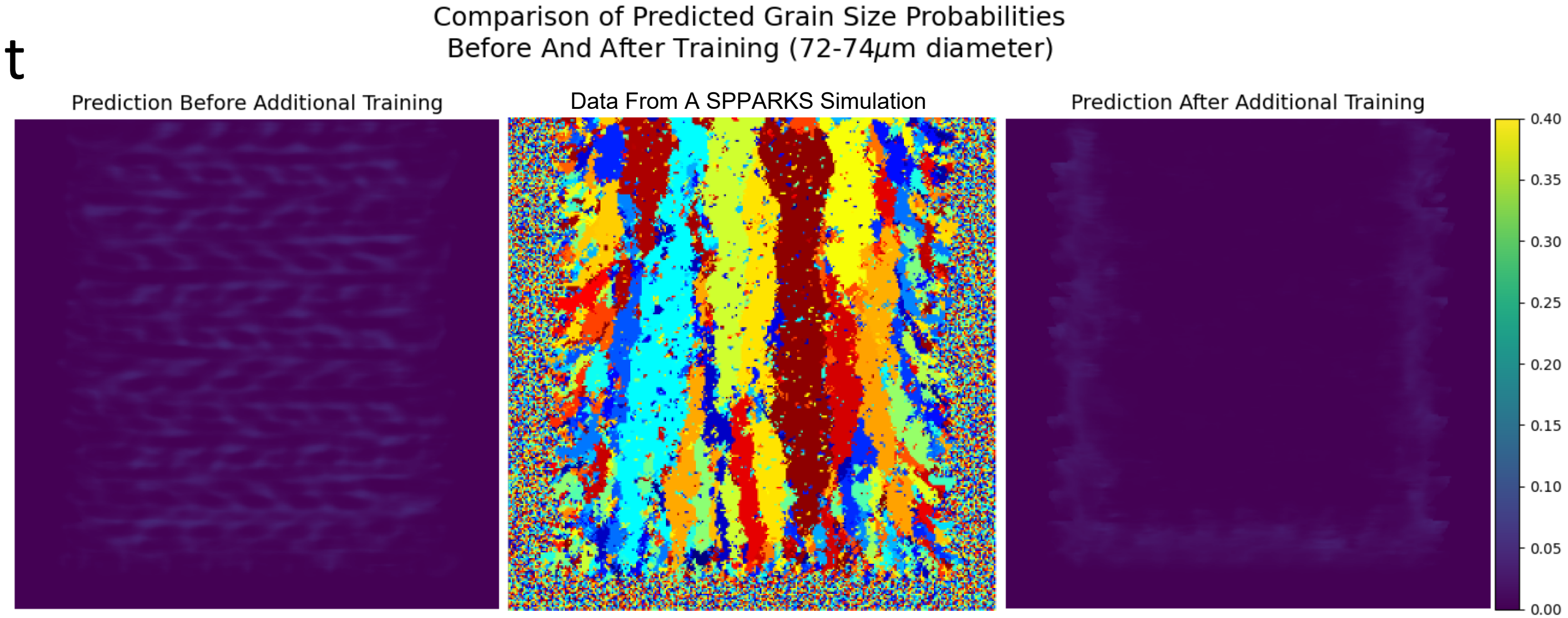
Simulating Varied Ensemble Sizes During Model Training

- Model trains to ideal accuracy with only 10 samples per data point
- Indicates we can get acceptable model accuracy by training with small ensembles
- Caveat: Base data is a large ensemble meaning sampled data will be less correlated than a small ensemble



Applying This Method Make Predictions About Large Simulation Domains

- Significant improvement in predictions when trained on a small ensemble when process parameters far outside other training data
- Still needs validation
- Significant compute savings
  - 400 node-hour sims + 4 hour training
  - 4000 node-hour sims



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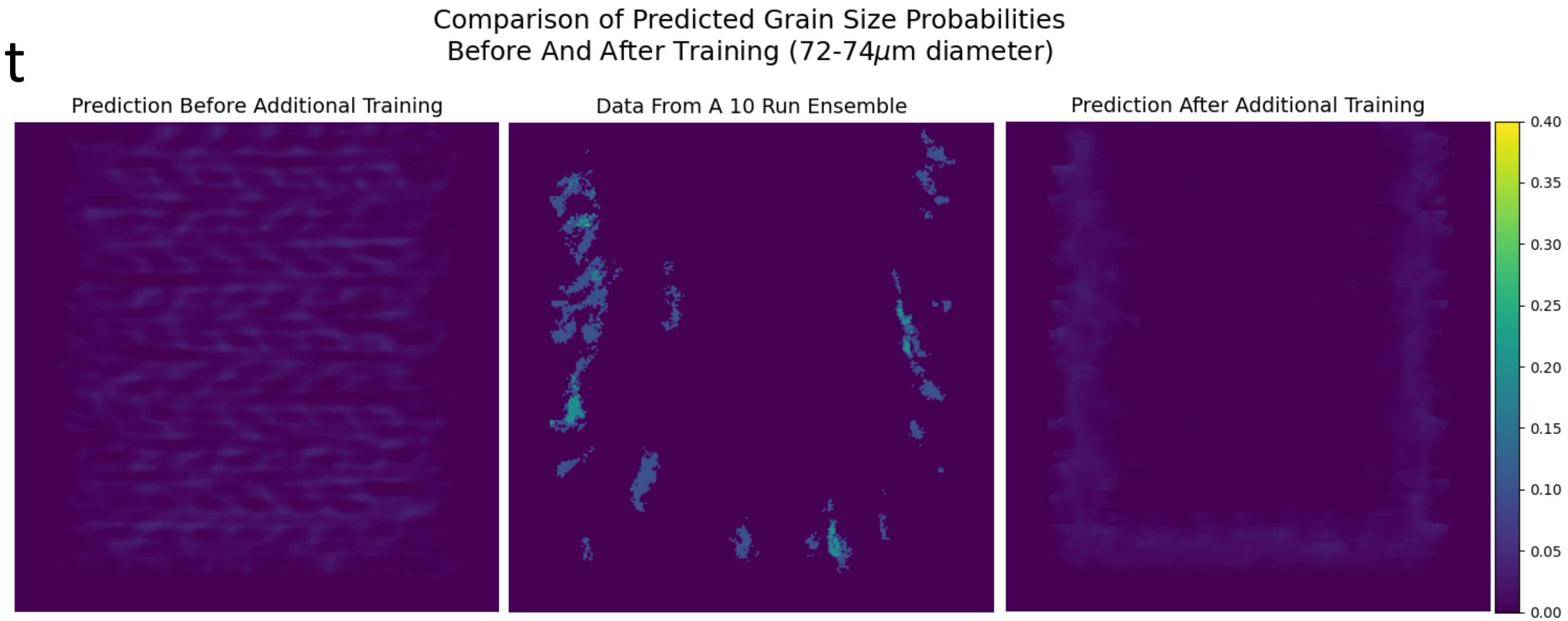

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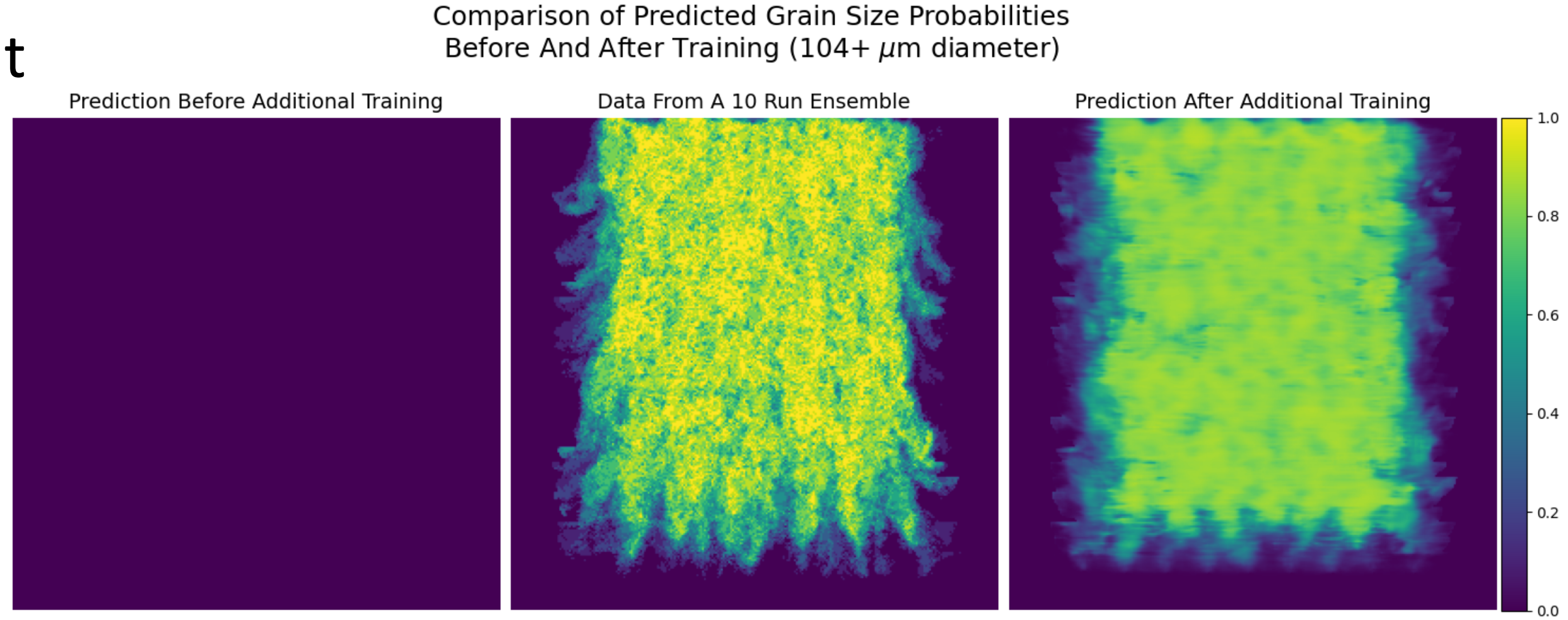


Applying This Method to RVE Analysis

- Work is ongoing
- Next steps are:
  - Validating the small ensemble method with small ensembles
  - Using the model for a statistical analysis of the minimum RVE

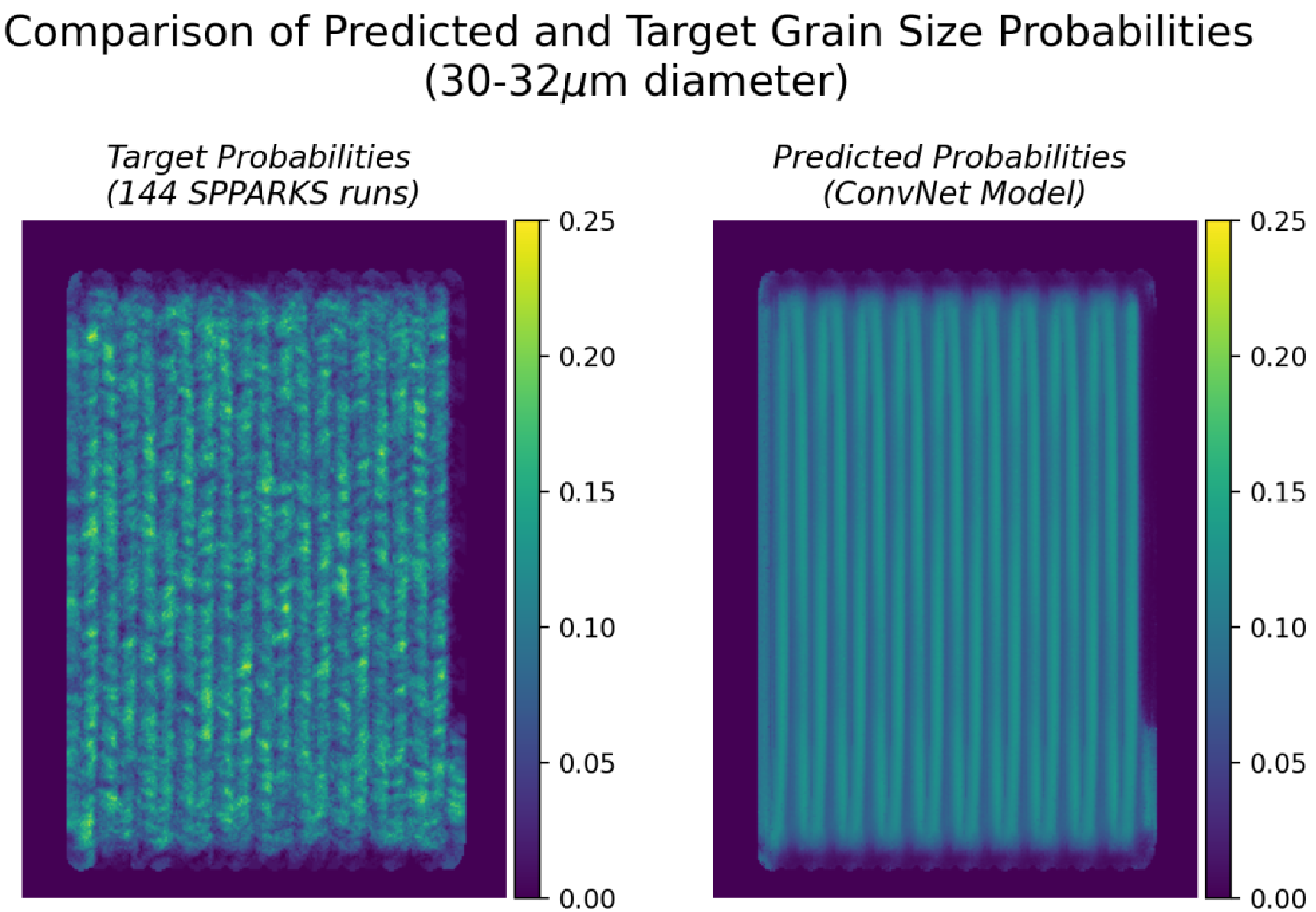
Conclusions

- The LPBF microstructure surrogate model is much faster than running a statistically equivalent SPPARKS ensemble
- Hyperparameter tuning of models is important for maximizing surrogate model speed
- The 9 thermal characteristics chosen as inputs to the surrogate model are reasonable choices
- We can probably use much smaller ensembles for model training
- We can probably use small ensembles for statistical analysis of the minimum RVE by leveraging the surrogate model

Integrate with slide 17

Model Prediction Accuracy

- Model obtains maximum measurable accuracy
- Resulting probability fields resemble those of the training data
- Results shown are from top surface of a 1-layer raster scan path

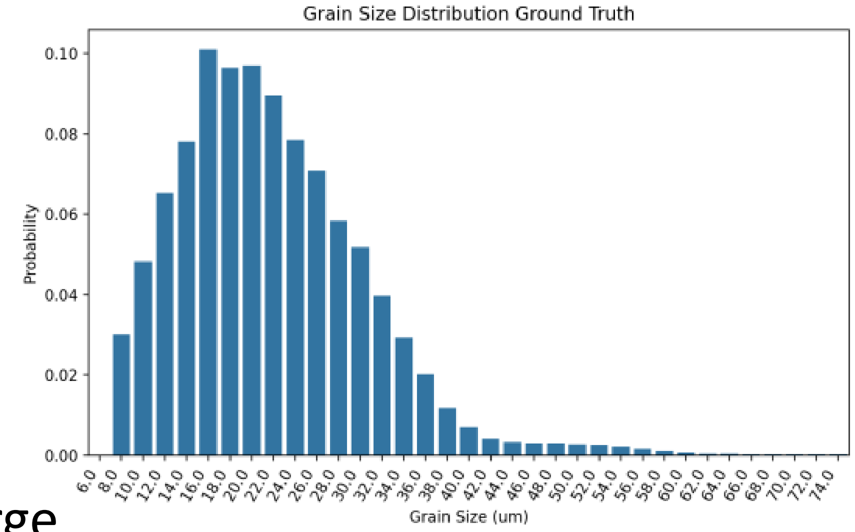


Data Regularization for Surrogate Model Training

- Limits overfitting of model
- Input data is a cube – 48 possible orientations
- Augmentation of target
  - 50% chance that the target microstructure will be re-sampled
  - Add uniform random noise to target
    - Too small to influence non-zero values
    - Keep model from overfitting zero-values

Statistical Experiments to Understand the Loss Magnitude

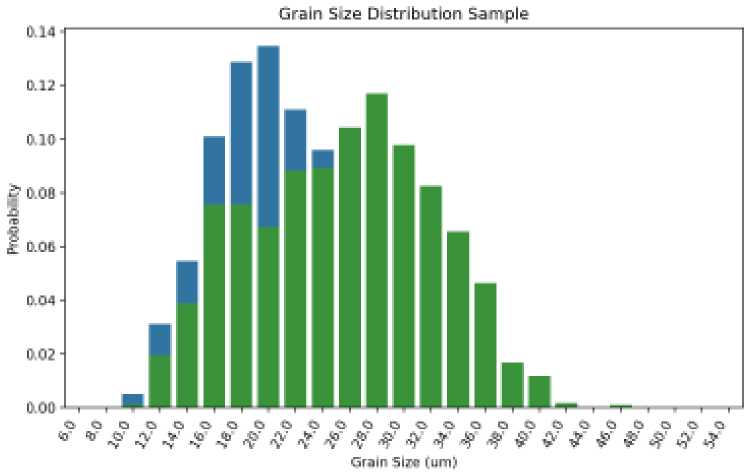
- MSE not an intuitive number
  - How good is “Good Enough”?
- Perform Monte Carlo experiments to gain a better understanding
  - Start with grain size distributions from a large microstructure ensemble (ground truth)
  - Sample the ground truth to get many smaller datasets
  - Calculate the distances between the sampled datasets and:
    - Each other (relative) – model vs training data
    - The ground truth (reference) – model vs “Truth”
- Only tells us what a good loss is



Run 1000+ simulations to obtain ground truth

Take N samples twice to get 2 new distributions

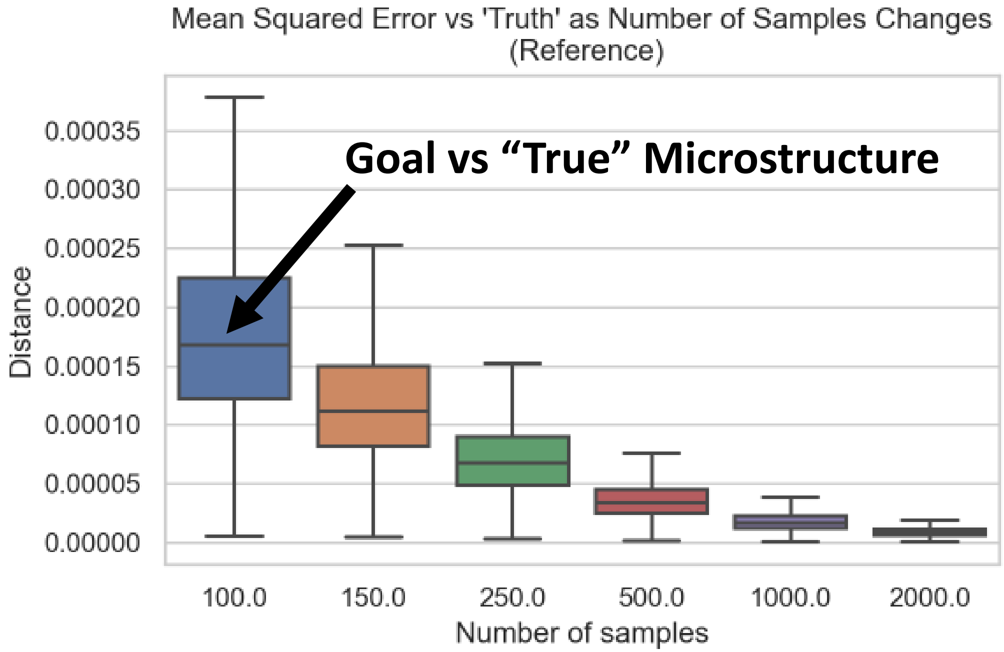
Repeat 4,000,000x

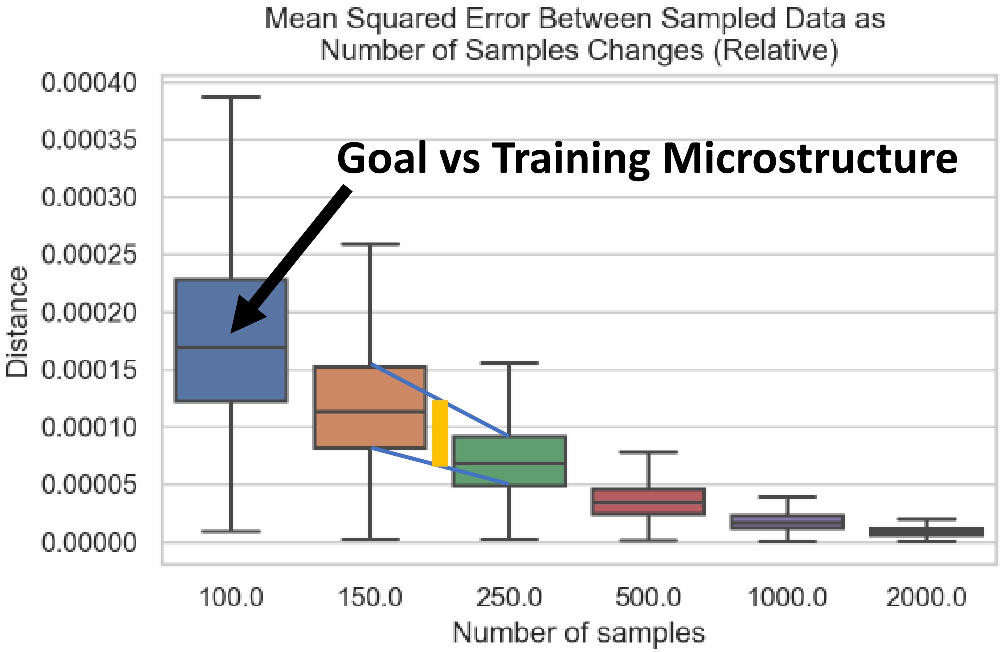


Calculate MSE 3x

Statistical Experiments to Understand the Loss Magnitude

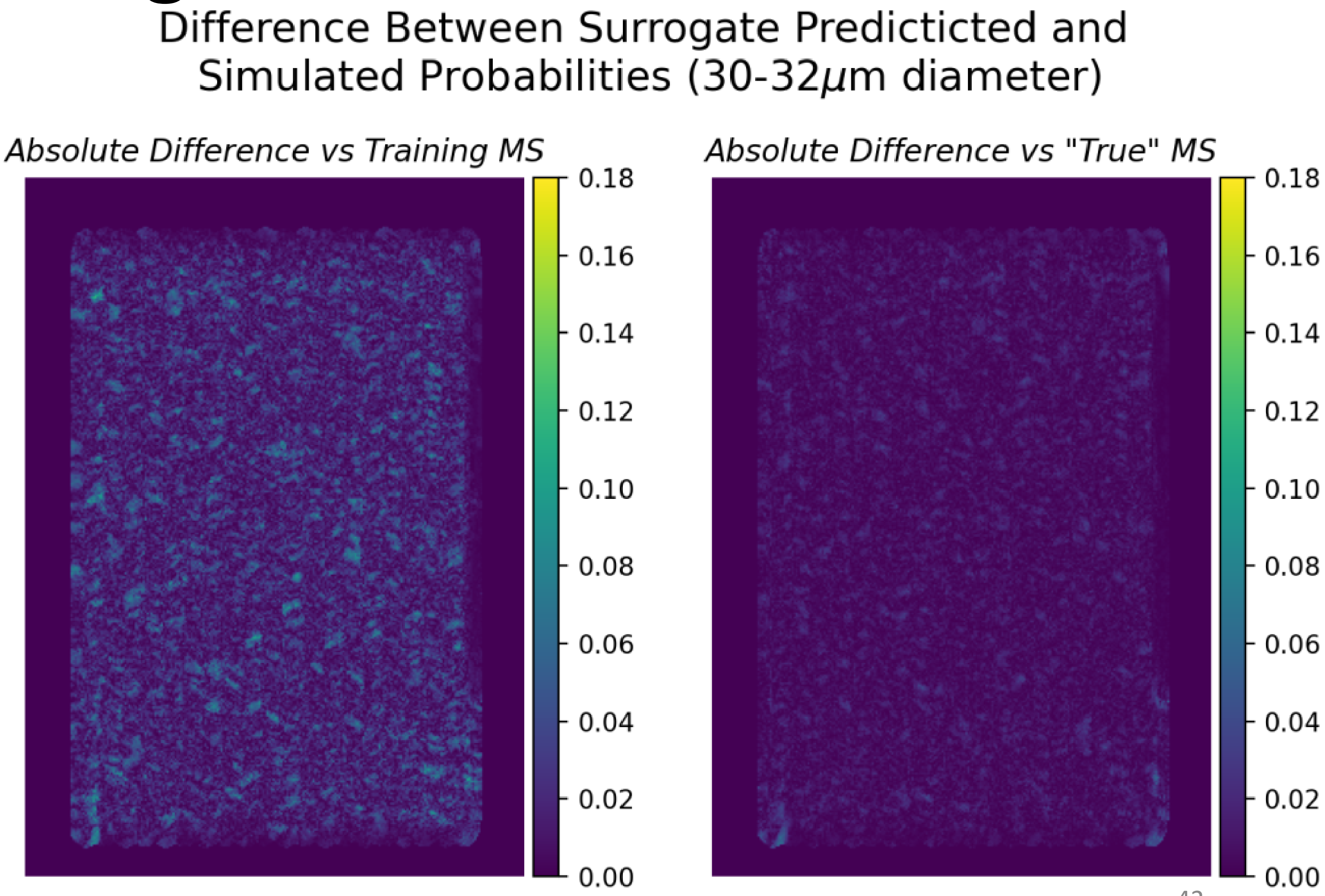
- Reference and relative distances similar
- Want model to be at least as good as 100 samples – Analogous to running a new ensemble of 100
- Smaller distance from "True" microstructure more important





Averaging Effect of the Model is Equivalent to Running a Much Larger Ensemble

- Stochastic effect of ensemble decrease as ensemble size increases
- Model prediction is closer to larger ensembles



Averaging Effect of the Model is Equivalent to Running a Much Larger Ensemble

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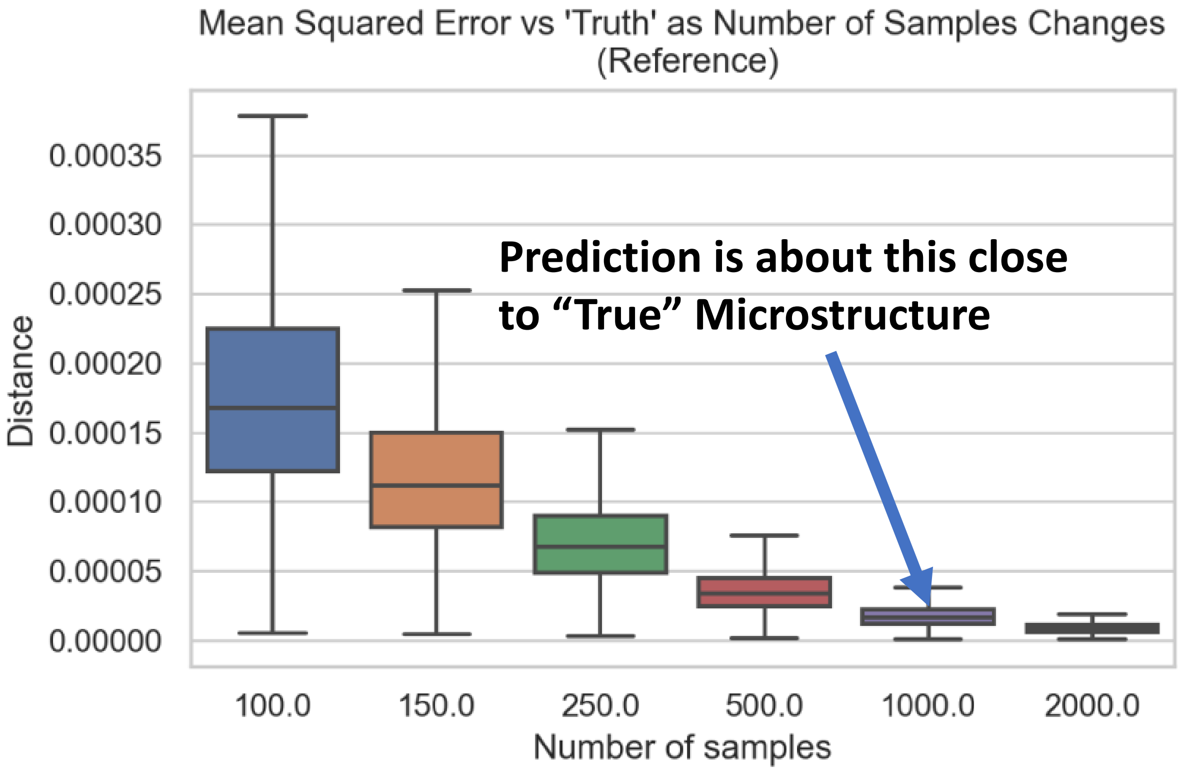
- Model obtains a MSE of 0.00002 on "True" data



“Annealing Temperature”

- Equation for rate of growth has no clear cutoff point (Solidus used in SPPARKS)

$$r^n = K_0 \exp\left(-\frac{Q}{RT}\right)t$$

r = average grain diameter
n, K_0, Q = Growth parameters

- Can approximate “knee” with average slope $\frac{0.315025\, e^{-15432.3/x}}{x^2} = \frac{2.6308 \times 10^{-9}}{1723}$

$x \approx -461877.$

$\boxed{x \approx 1321.26}$

$x \approx 446442.$

- Growth rate at “knee” is 1/10th of maximum

plot	$y = 2.04133 \times 10^{-5} \exp\left(-\frac{128312}{8.3145\, x}\right)$	$x = 0$ to 1723