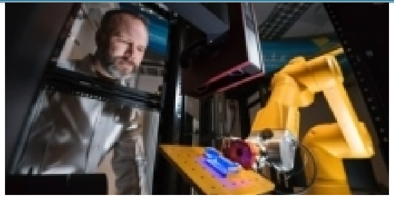
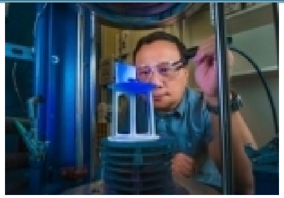
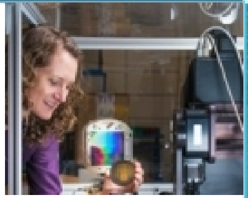
SAND2021-7021PE

Advanced Manufacturing through Machine Learning







David Montes de Oca Zapiain

Senior Member of Technical Staff

Org. 1864 Computational Materials and Data Science

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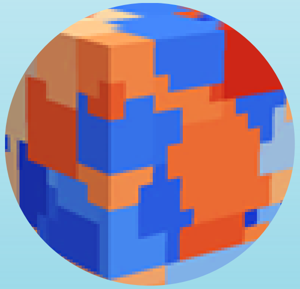
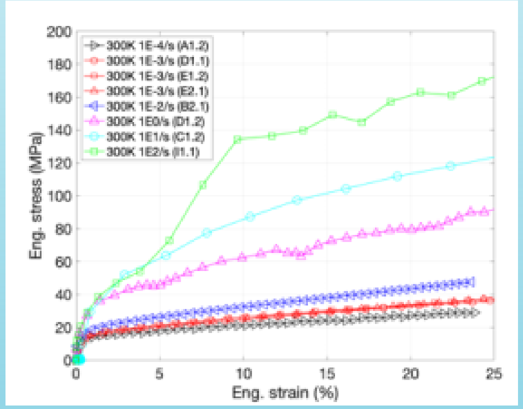
Traditional Manufacturing Process

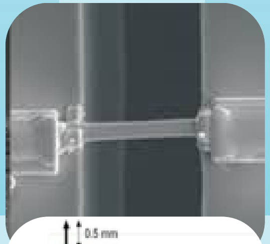
SYNTHESIS PROCESS

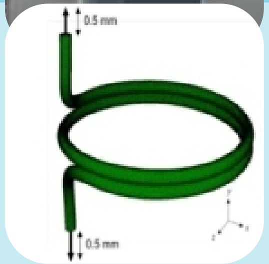
MATERIAL STRUCTURE



PROPERTY





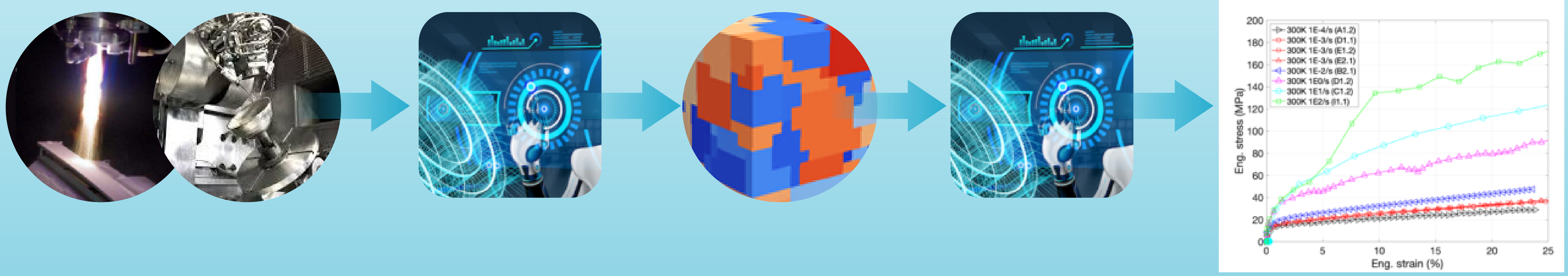


Capital Intensive and Time Consuming

Advance Manufacturing (AdM)

- AdM brings design and testing closer.
- Accelerates the development and deployment of new materials.
- Reduces design cycle for novel components.

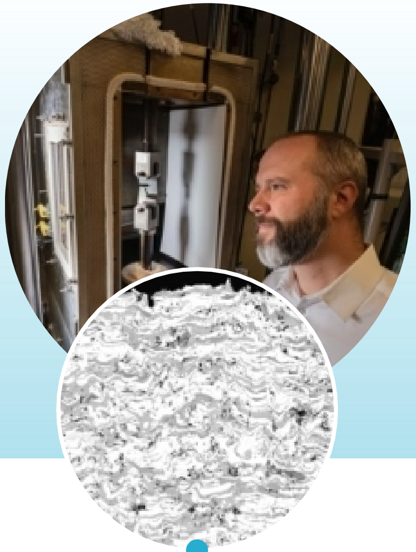
SYNTHESIS PROCESS　　MATERIAL STRUCTURE　　PROPERTY



- Machine Learning (ML) is the perfect tool for enabling AdM because it:
  - Is computationally efficient
  - Enables the usage of previously performed results to predict in new/unseen scenarios.
- ML enables us to link each part of the process with accurate yet computationally efficient surrogate models.

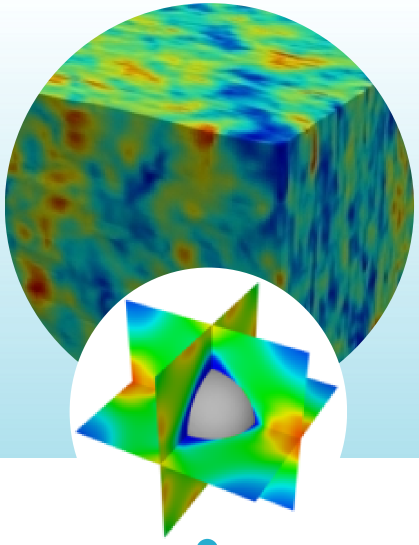
Unique Capability to Establish ML-based Surrogate Models

Material Characterization and Experimentation



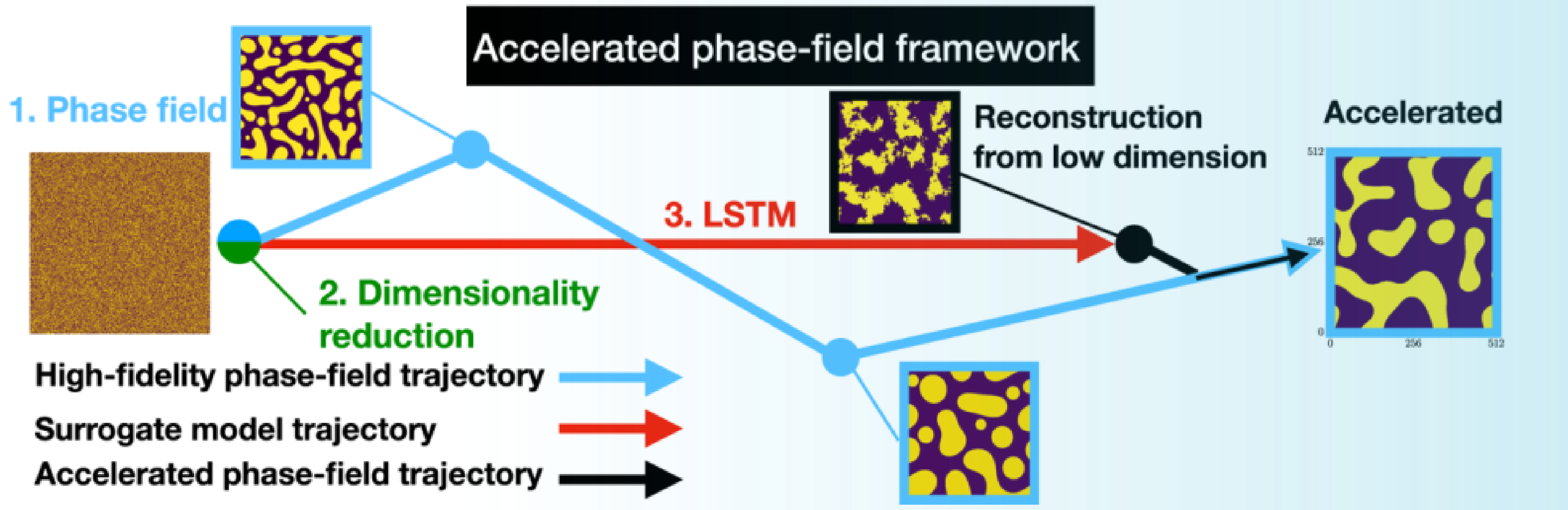
High-Performance Computing

High-Fidelity Multiphysics Codes

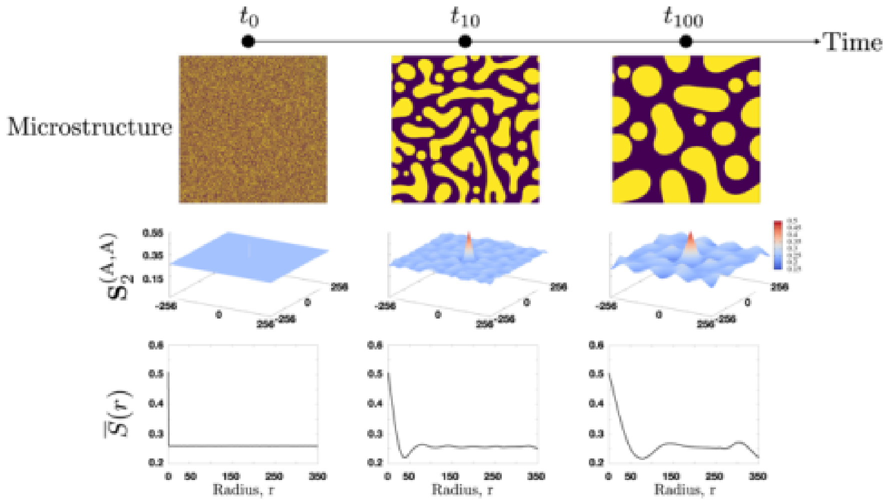


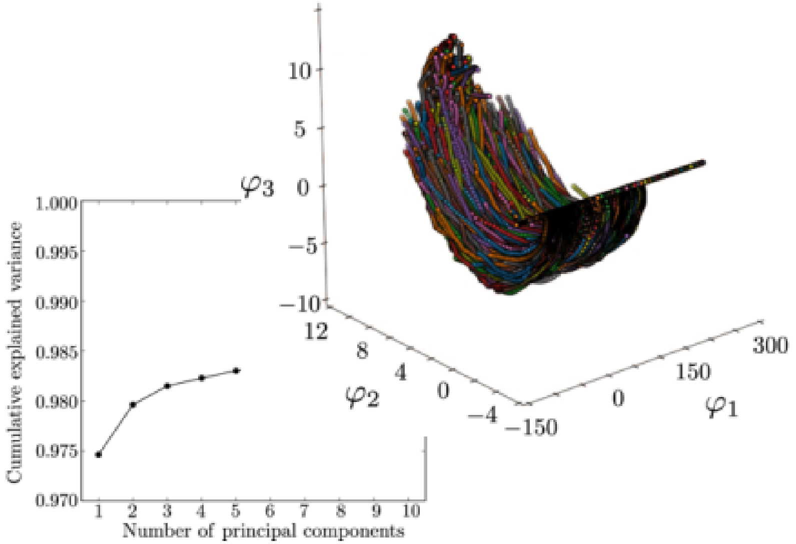
Interdisciplinary Workforce

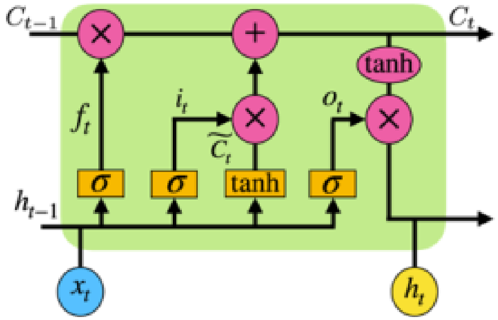
We are National Lab of "Firsts"



First to establish an accelerated phase-field framework capable of predicting microstructure evolution **40,000 times** faster than traditional simulation software with minimal loss in accuracy.





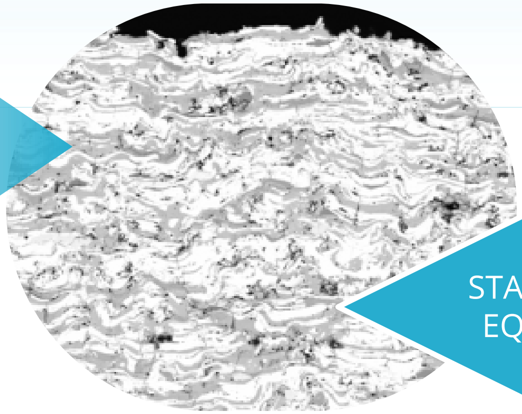


[Montes de Oca et al., npj compu mat, 2021]

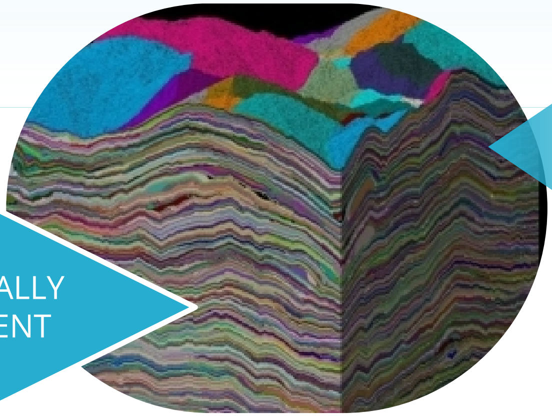
We are National Lab of “Firsts”

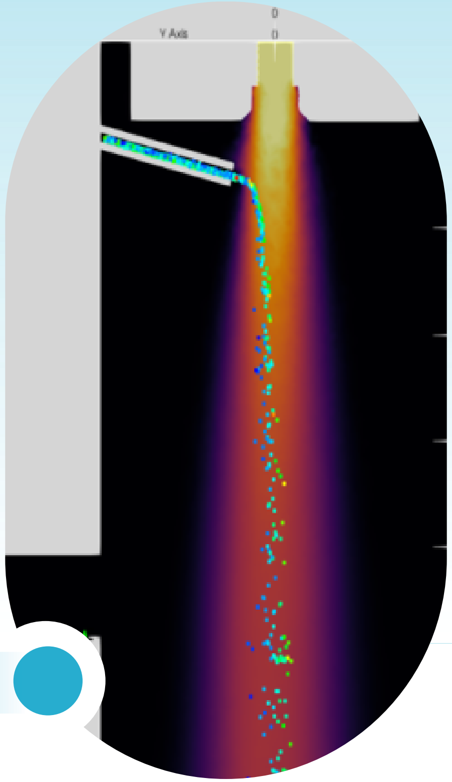
First to establish a computationally efficient protocol to synthetically generate microstructures that are statistically equivalent to experimentally observed microstructures.

ORIGIN OF DATA	PORE VOLUME FRACTION (%)	TIME
Experiment	2.12	
Full-field SPPARKS-DAKOTA optimization	2.25	**6 DAYS** on 3 nodes with 36 processors
ML-based optimization	2.28	**84 SECONDS** on an 8 processor MacBook



STATISTICALLY EQUIVALENT





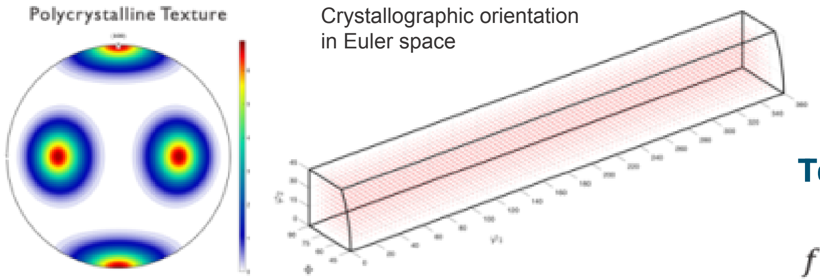
- Experiments performed on thermal spray lab in 1834

- Microstructures were synthetically generated using SPPARKS (1864 Dr. Theron Rodgers)

[Montes de Oca et al., MRS 2021 Spring Meeting]

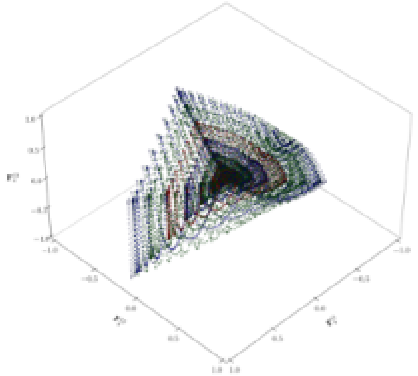
- First to establish a computationally efficient model that links the crystallographic texture of metals to their corresponding anisotropy constants.

Crystallographic textures



54,880 textures represented by generalized spherical harmonics (GSH)

Texture quantification



$$f(g) = \sum_{\mu,n,l} F_l^{\mu n}\, T_l^{\mu n}(g)$$

$$T_l^{mn}(g) = T_l^{mn}(\varphi_1, \Phi, \varphi_2) = e^{im\varphi_1} P_l^{mn}(\Phi) e^{im\varphi_2}$$

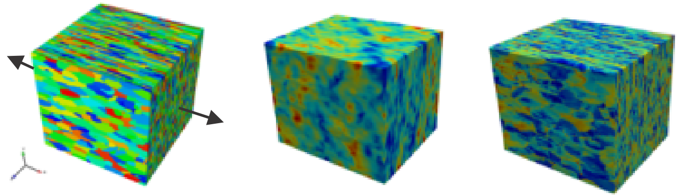
Anisotropy Constants

Crystal plasticity simulations

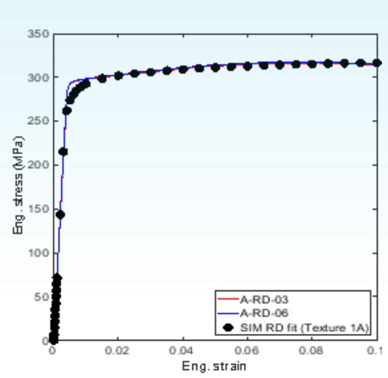
54,880 crystal plasticity simulations performed by Dr. Hojun Lim in 1864 to investigate anisotropic yield behavior and to fit Hill's anisotropic yield model

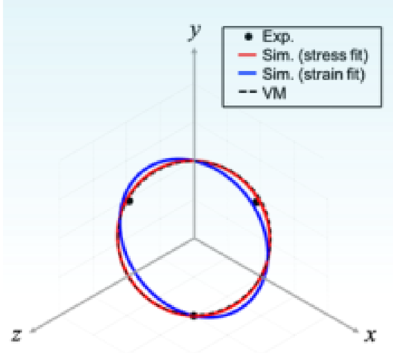
$$f = F(\sigma_{yy} - \sigma_{zz})^2 + G(\sigma_{zz} - \sigma_{xx})^2 + H(\sigma_{xx} - \sigma_{yy})^2 + 2(L\sigma_{yz}^2 + M\sigma_{zx}^2 + N\sigma_{xy}^2)$$

Initial mesh   Deformed mesh (10%)

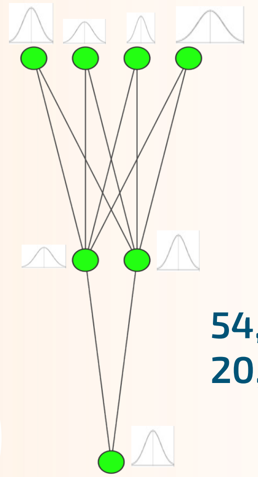


Equivalent plastic strain   VM stress



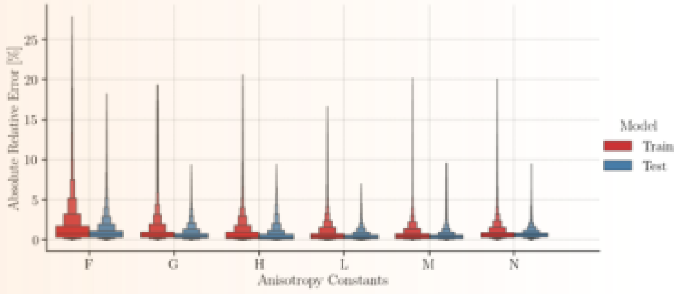


Variational Bayesian Inference Neural Network Model



54,880 training data
20,000 validation data

Distribution of absolute relative error on the training and testing set



The mean error = 0.63%

Lifting as we climb

ENERGY I-CORPS
U.S. Department Of Energy

NNSA
National Nuclear Security Administration

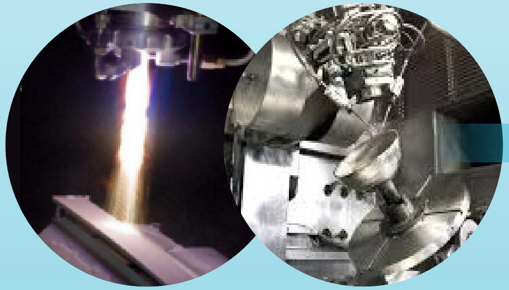
- DOE funded program to foster and develop viable market pathways for national laboratory-developed technologies.
- Intensive two-month training where the researchers define technology value propositions, conduct customer discovery interviews, and develop viable market pathways for their technologies.
- Identify via 75+ customer discovery interviews the most viable path to commercialize our computationally efficient model that links the crystallographic texture of metals to their corresponding anisotropy constants.

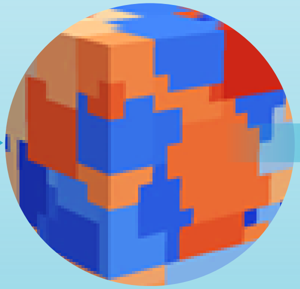
Conclusion

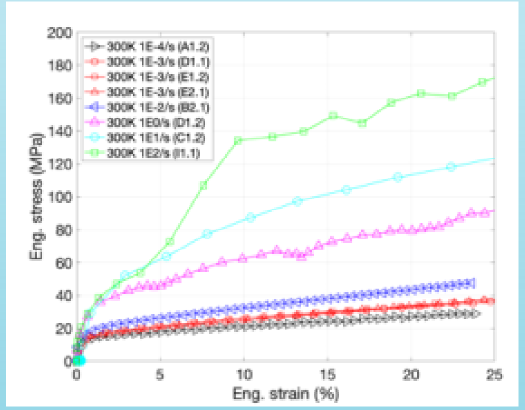
SYNTHESIS PROCESS

MATERIAL STRUCTURE

PROPERTY







Contributors/Collaborators

Dr. Hojun Lim

Dr. Theron Rodgers

Dr. James Stewart

Dr. Remi Dingreville

Sandia National Laboratories

Dr. Mark Chavez

LENS™

U.S. DEPARTMENT OF ENERGY

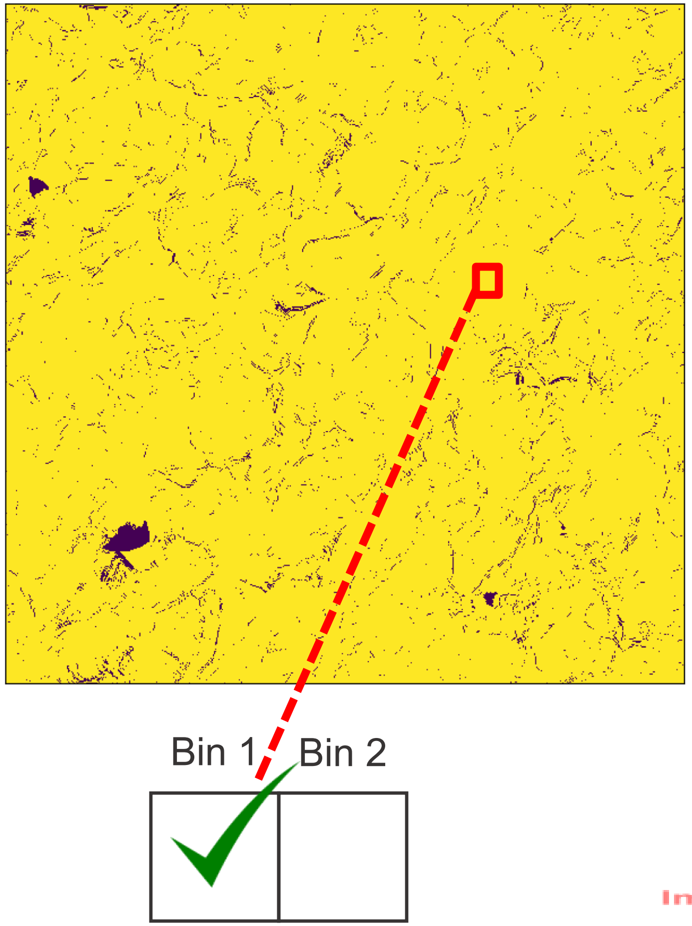
National Nuclear Security Administration

ENERGY I-CORPS U.S. Department Of Energy

Questions?

Obtaining a Robust Descriptor of the Microstructure

Digital Representation



$$m(\boldsymbol{x},n) \approx \sum_{h=1}^{H}\sum_{s=1}^{S} m_s^h \chi_h(n)\chi_s(\boldsymbol{x})$$

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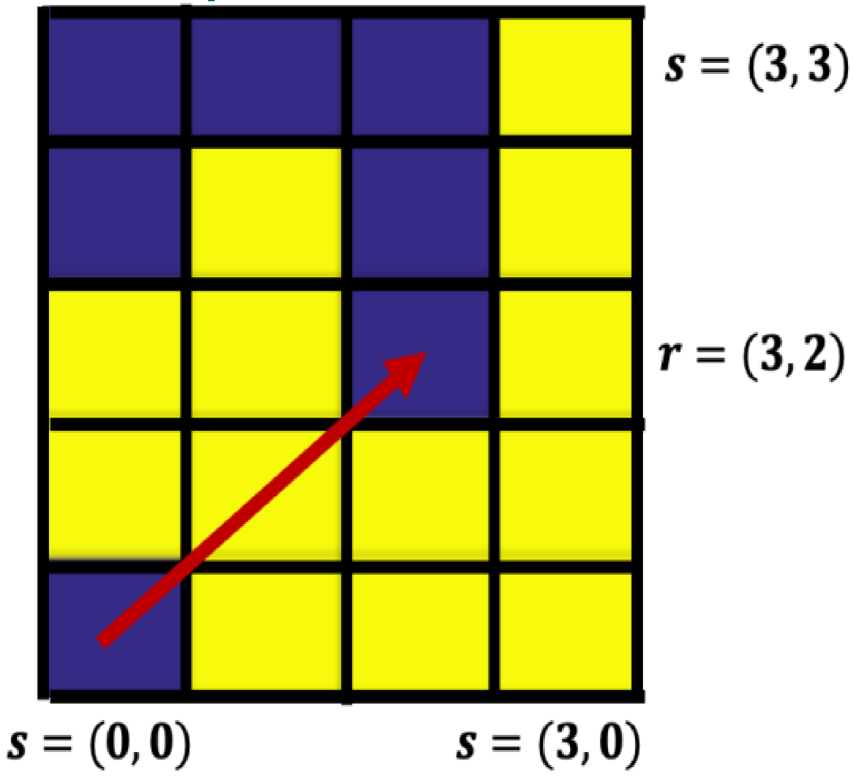
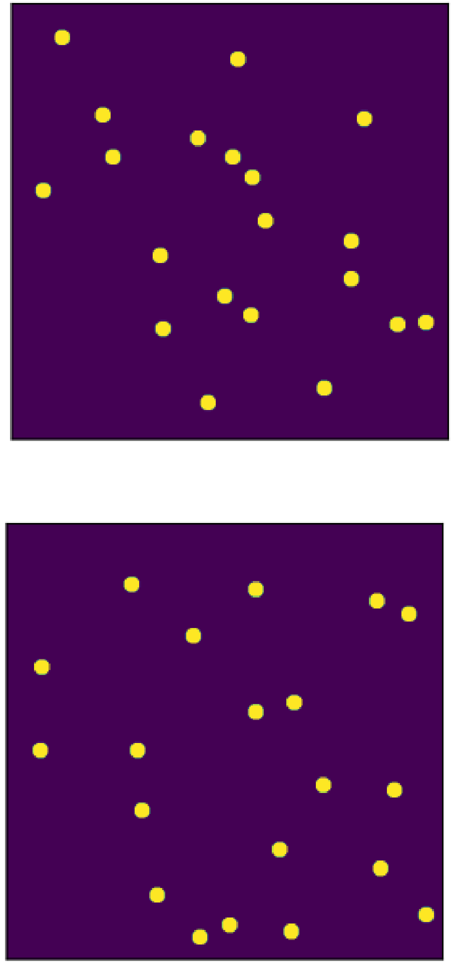
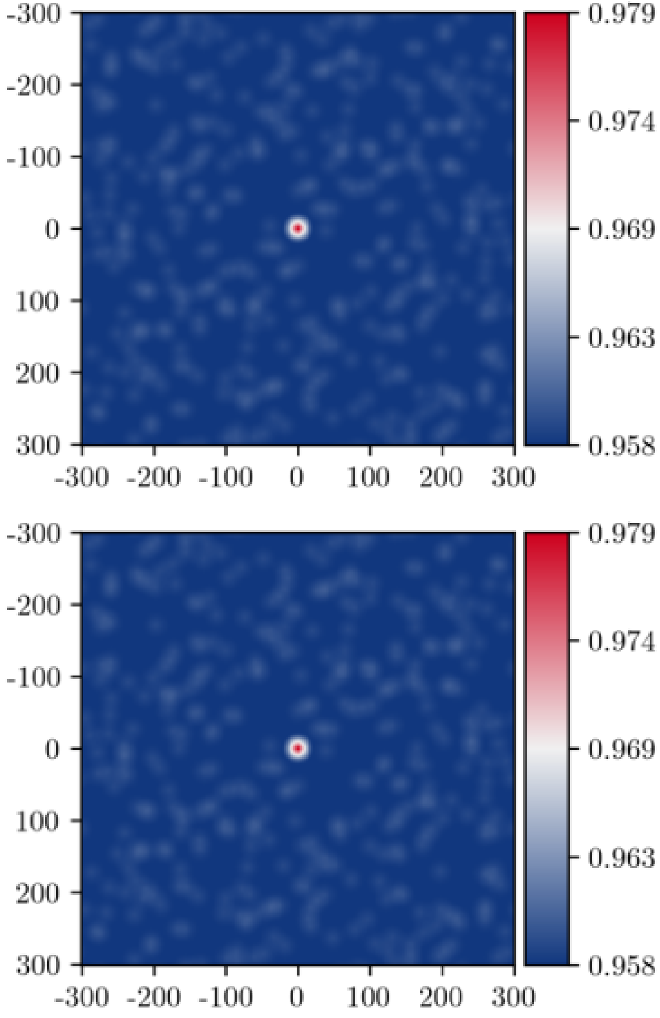
2-point statistics

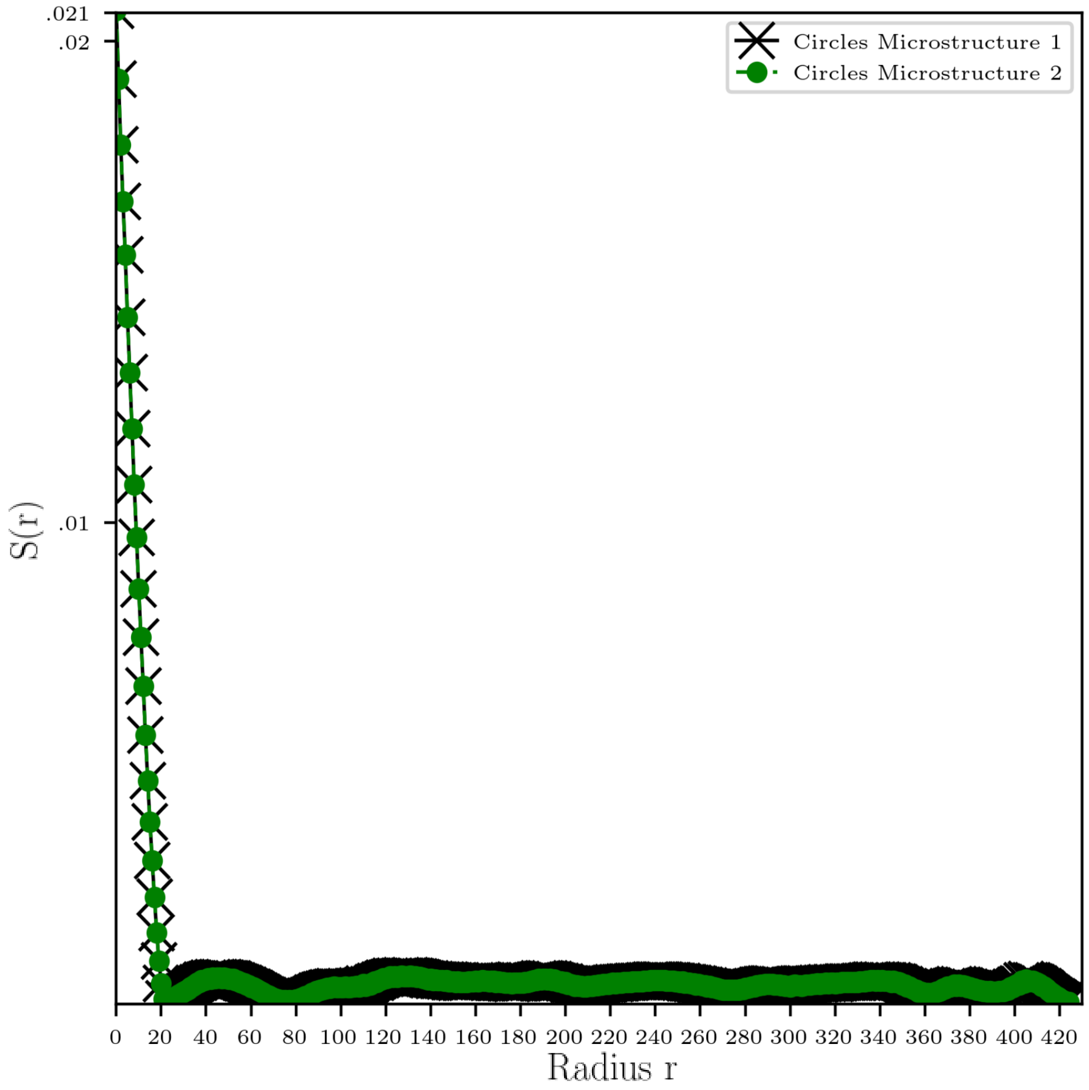


$$f_r^{hh'} = \frac{1}{S}\sum_{s=1}^{S} m_s^h m_{s+r}^{h'}$$

Why 2-point Statistics ?





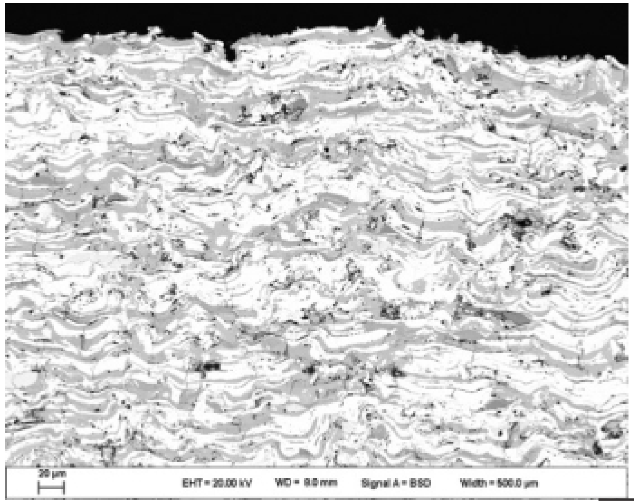


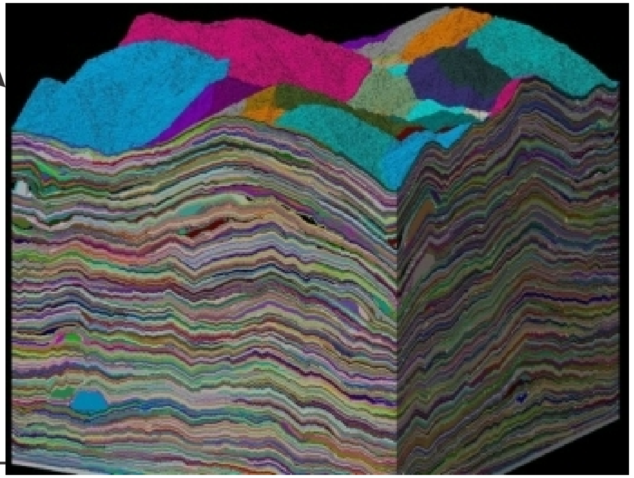
Current Optimization Process for Obtaining a Statistically Equivalent Microstructure

SPPARKS

Each evaluation requires 90 minutes and 3 nodes with 36 processors.

Update Parameters





No

Statistically Equivalent?

Yes

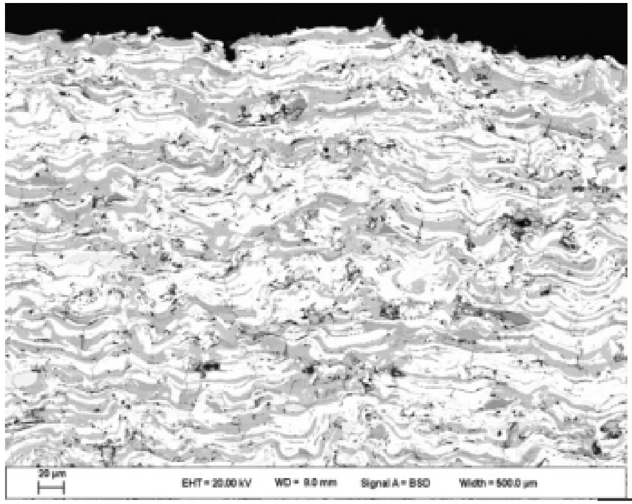
This optimization process takes various days

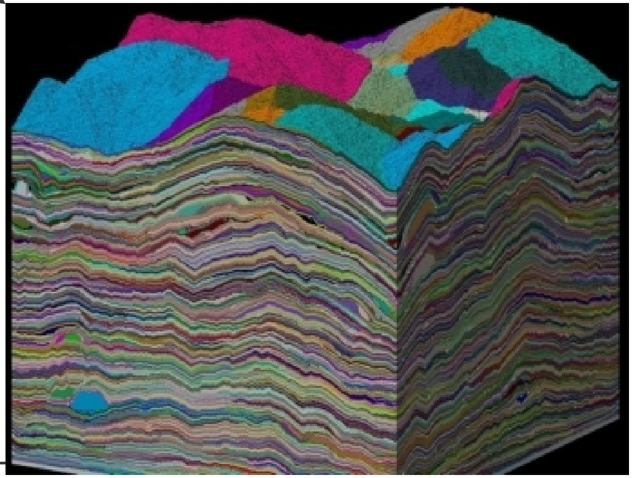
Finish Optimization

ML-based Optimization Process for Obtaining a Statistically Equivalent Microstructure

Each evaluation takes seconds and minimal computational resources

Update Parameters





No

Statistically Equivalent ?

Yes

This optimization process takes minutes

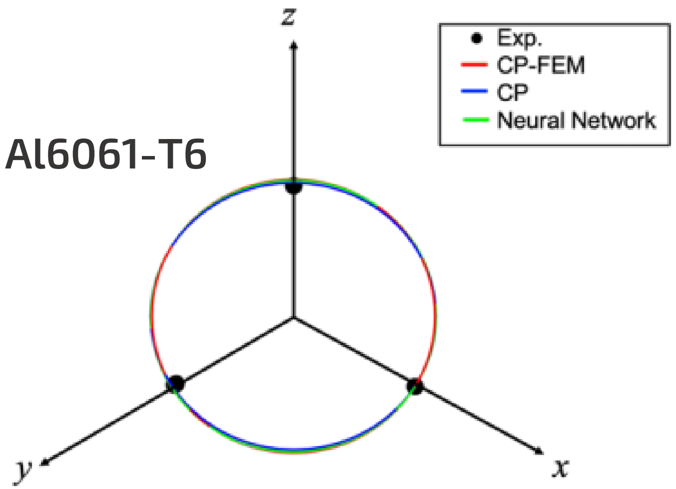
Finish Optimization

Materials Science Research Foundation

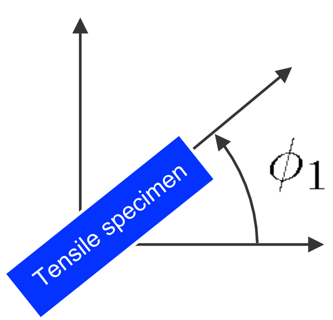
Comparisons with Experiments & High fidelity simulations

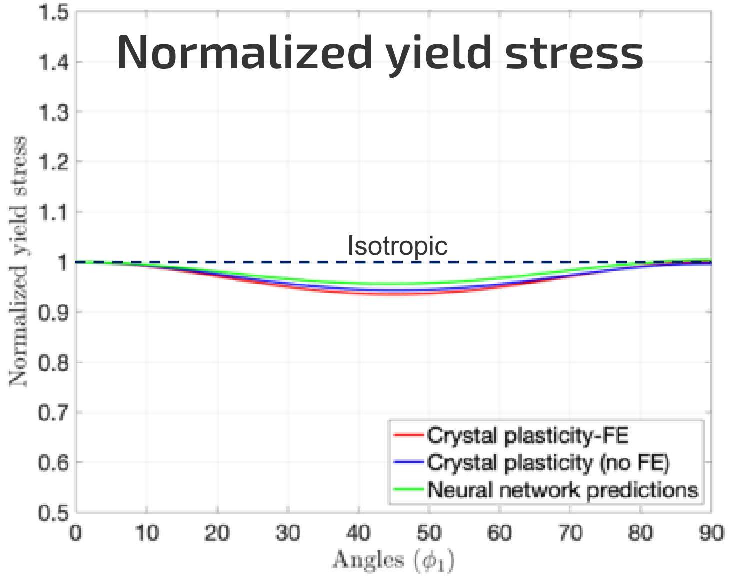
Parameterizing Hill's quadratic anisotropic yield model: $f = F(\sigma_{yy} - \sigma_{zz})^2 + G(\sigma_{zz} - \sigma_{xx})^2 + H(\sigma_{xx} - \sigma_{yy})^2 + 2(L\sigma_{yz}^2 + M\sigma_{zx}^2 + N\sigma_{xy}^2)$

Al6061-T6	*F*	*G*	*H*	*L*	*M*	*N*	*TIME*
Experiments	0.6097	0.5495	0.4061	-	-	-	3-6 months
Crystal plasticity-FE	0.5268	0.5261	0.4739	1.5258	1.4788	1.7604	~10 h in HPC
Neural Network predictions	0.5298 ±0.0013	0.5369 ±0.0010	0.4631 ±0.0010	1.5735 ±0.0017	1.5296 ±0.0013	1.6548 ±0.0015	<1 sec.



π-plane yield surfaces of Al6061





Variation Bayesian Inference Neural Network (VBI-NN) model of Hill's anisotropy model saves computational cost by more than 4 orders of magnitude compared to crystal plasticity finite element simulations.