SAND2021-5615C

Mechanics of Materials Utilizing Machine Learning: Examples at Sandia National Laboratories

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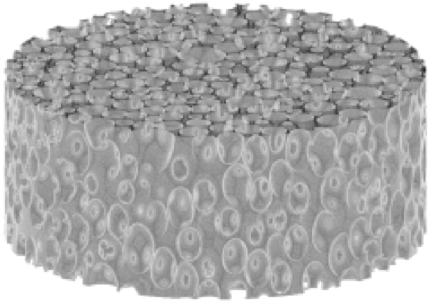
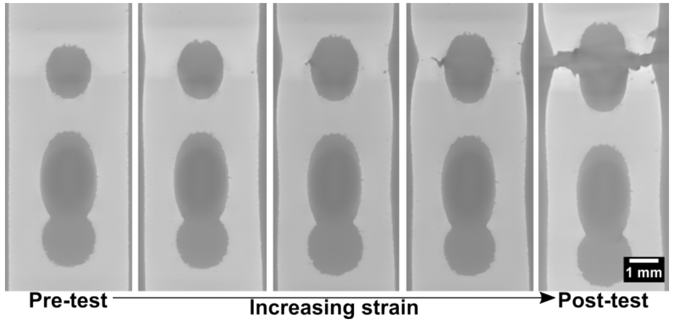
SAND2021-XXXXX

Demystifying Machine Learning

Classification



Pore or Solid Phase?

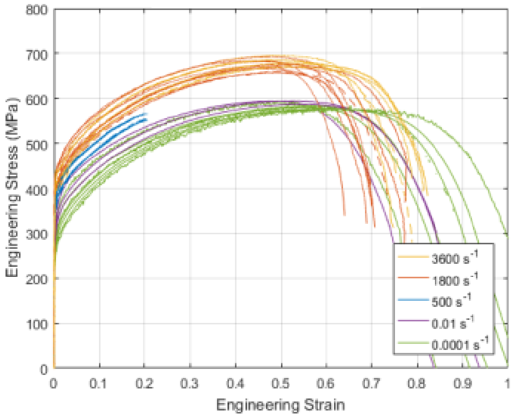


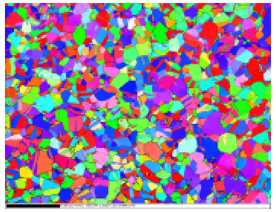
Crack Evolution Identification

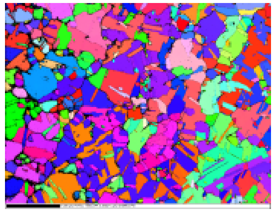
ML Automated Classification → Faster Identification

Regression

304L-VAR Rate-Dependent Tensile Behavior







Simple Regression → Ignoring Some Variables

ML Regression → Incorporates More Variables

ML models can perform automated classification ("a cat or not a cat") and regression in high dimensionality ("fancy curve fitting").

Mechanical Properties Mapping to AM Build Plate Location

PI: Laura Swiler

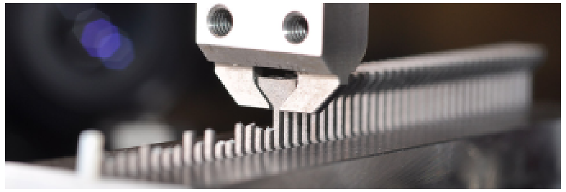
Goal: Characterize mechanical performance of AM materials and relate that to variability in the AM build process

ML Task

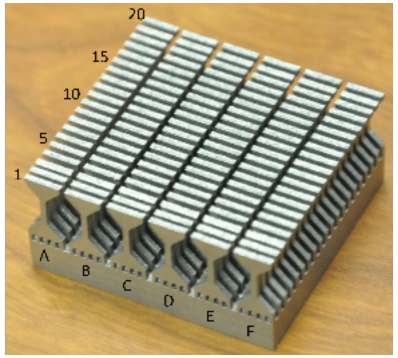
Correlate mechanical properties of 120 specimens together with build plate location

Data

High-throughput tensile testing producing 15 mechanical properties and AM build location of each specimen

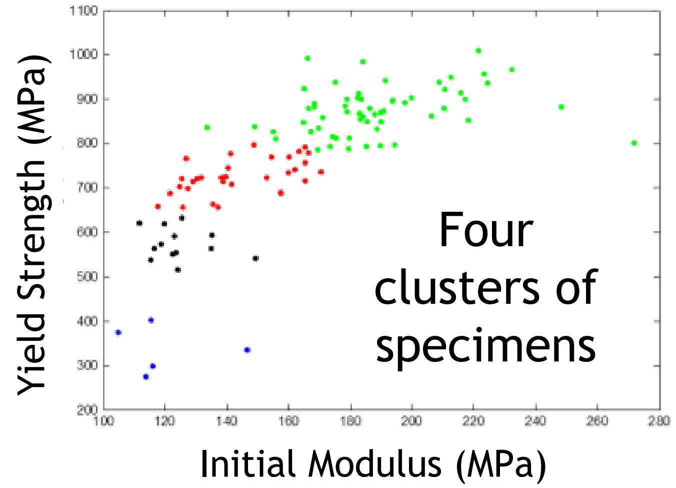


Salzbrenner BC, et al (2017) High-throughput stochastic tensile performance of additively manufactured stainless steel. J Mater Process Technol 241:1-12



Outcome

Unsupervised learning algorithm, K-means clustering, grouped specimens with similar properties into four coherent subsets called clusters. The four clusters were mapped to build location showing some correlation.



	A	B	C	D	E	F
1	3	3	3	3	3	3
2	3	3	3	3	3	2
3	3	3	3	3	3	3
4	3	3	3	3	3	3
5	3	3	3	3	3	3
6	3	3	4	3	3	3
7	3	3	3	3	3	1
8	3	3	3	3	3	1
9	3	1	1	1	4	3
10	3	1	4	3	4	1
11	3	1	1	1	1	3
12	1	1	2	1	2	3
13	3	1	4	1	1	3
14	1	3	4	4	4	3
15	1	1	1	1	1	
16	3	1	4	2	1	
17	3	1	2	4	1	
18	3	3	4	1	1	
19	1	4	1	4	1	

Cluster Number Mapping to Build Plate

Laura P. Swiler, *et. al.* “Data Analysis for the Born Qualified LDRD Project.” Sandia Report, SAND2018-11244, Sept. 2018.

P-S-P-P relationships are the key to unlocking emerging materials, and ML methods can correlate many specimens across several properties to discover those relationships.

Classification

Predicting Behavior of AM Parts Using Deep Learning

PI: Kyle Johnson

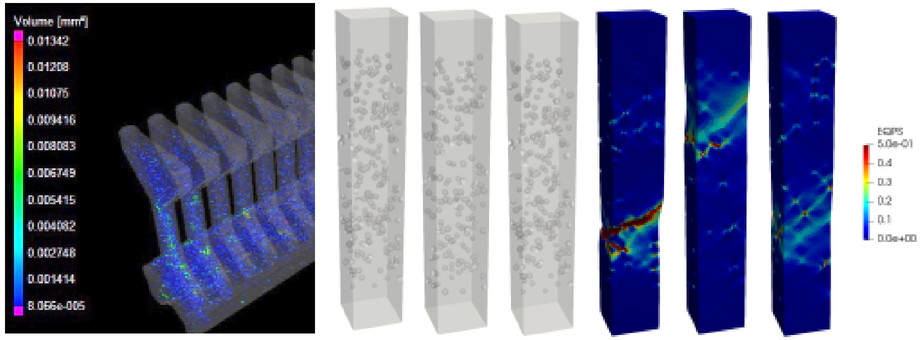
Goal: Rapidly predict mechanical part performance based on AM pore networks

ML Task

Predict AM part failure based on material behavior and pore network

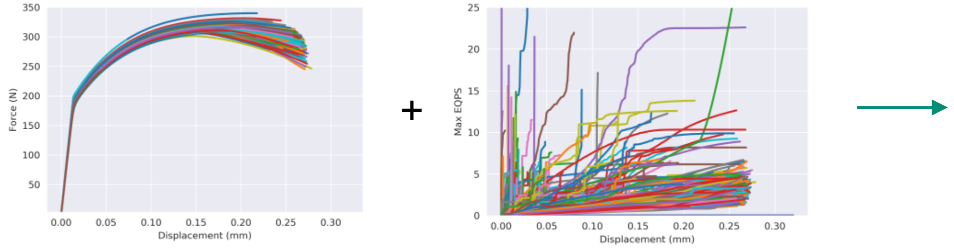
Data

Experimental pore distributions from CT were used to generate synthetic pore networks in tension samples, providing synthetic stress-strain and pore network data

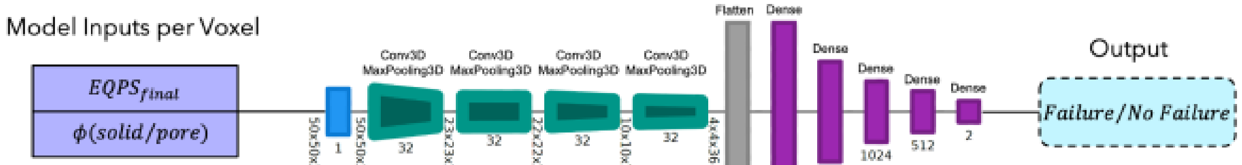


Outcome

Deep Learning was used to classify part performance based on failure metrics. The 3D convolutional neural network used pore network data to predict failure five orders of magnitude faster than traditional FEA.



Fail / No Fail Prediction



3D CNN Formulation

Johnson, KL, et al. SAND2020-10285
Johnson, KL, et al. “Predicting Mechanical Performance of Additively Manufactured Parts Using Deep Learning”, *Additive Manufacturing*. (Submitted)

ML can predict failure based on local variability faster than traditional methods.

Classification

Credible Automated Meshing of Images (CAMI)

PI: Scott Roberts

Goal: Build a 3D computational mesh directly from 3D images

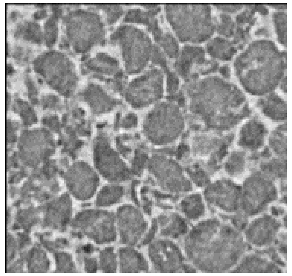
ML Task

Identify boundaries and different phases of materials, as applicable, from a 3D images

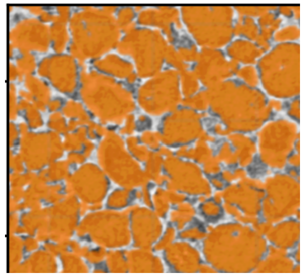
Data

Training: Human-labeled 3D images
New Data for Meshing: 3D Images similar to training images

Slice from CT image of graphite electrode



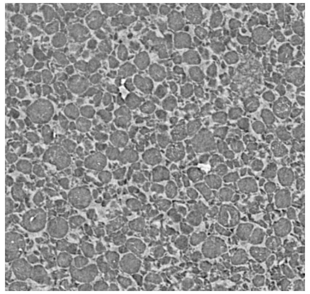
Human label (orange) overlaid on CT scan of battery



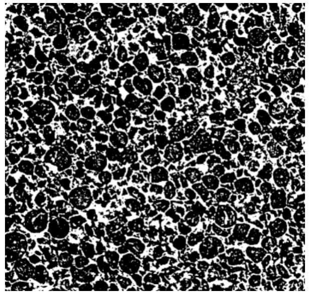
Outcome

Automated meshing techniques from ML output of a Bayesian CNN, propagating UQ to physics predictions. Exemplars: Battery materials, woven composites, laser welds, and polymer foams.

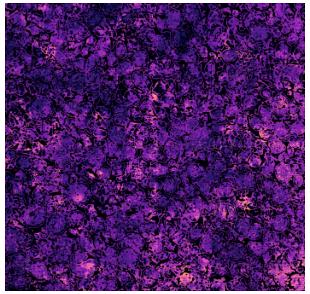
CT scan slice

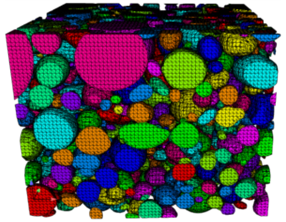


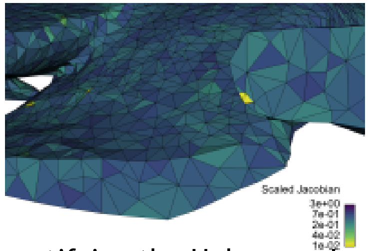
ML segmentation



Uncertainty Map







Michael C. Krygier *et.al.* “Quantifying the Unknown: Impact of Segmentation Uncertainty on Image-Based Simulations.” arXiv:2012.09913

ML is capable of flexible and accurate image segmentation, enabling representative meshes.

ML Models of Plasticity for Metals with Microstructure

PI: Reese Jones

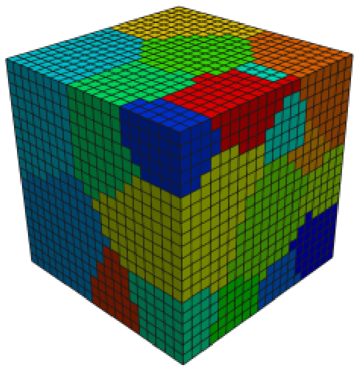
Goal: Accurate modeling of metal plastic deformation based on microstructure

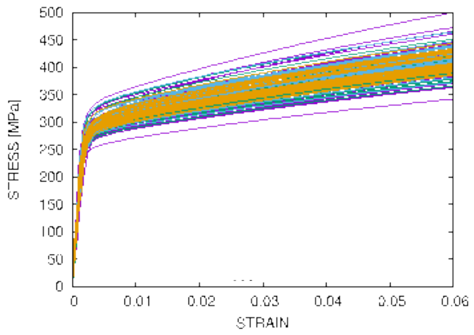
ML Task

Utilize crystal microstructure to predict deformation

Data

Computational simulations of four different representative crystal microstructure with local and global stresses and strains

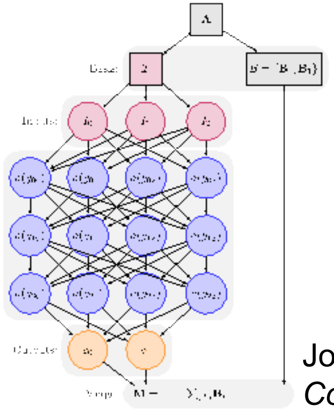




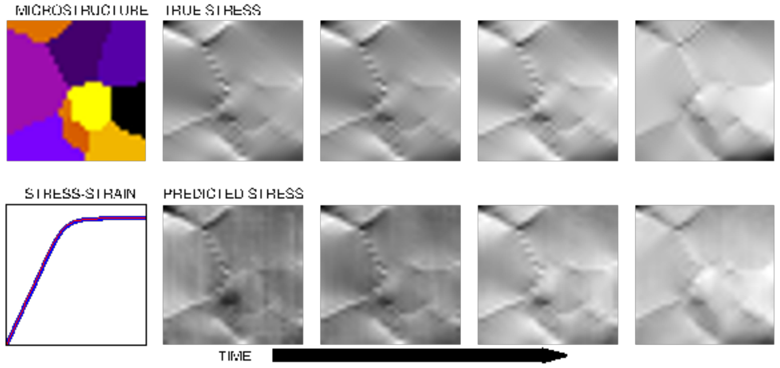
Outcome

A tensor-basis neural network that preserves physical constraints was developed. A second novel convolutional neural network approach discovered the microstructural features needed for a good prediction. These methods predicted local and homogenized stress responses for an unfamiliar microstructure.

A tensor-basis neural network



Stress field predictions of a novel CNN



Jones, RE et al. *Comp.Mod,Eng.Sci.*, 2019; Frankel, A et al. *Comp.Mat.Sci.*, 2019; Frankel, A et al. *arXiv,* 2019

ML can link lower length-scale information to continuum response, enriching material modeling.

Physics-Informed Machine Learning (PIML) for Material Modeling

Regression

PI: Sharlotte Kramer

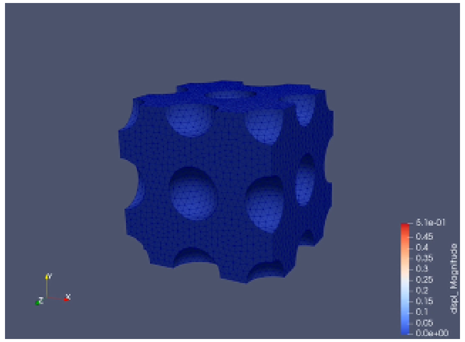
Goal: Accurately predict large-deformation behavior of materials with porosity

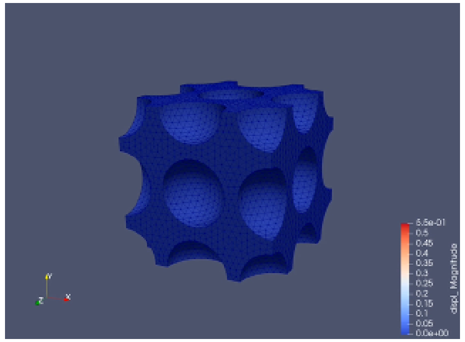
ML Task

Predict mechanical response of materials with porosity

Data

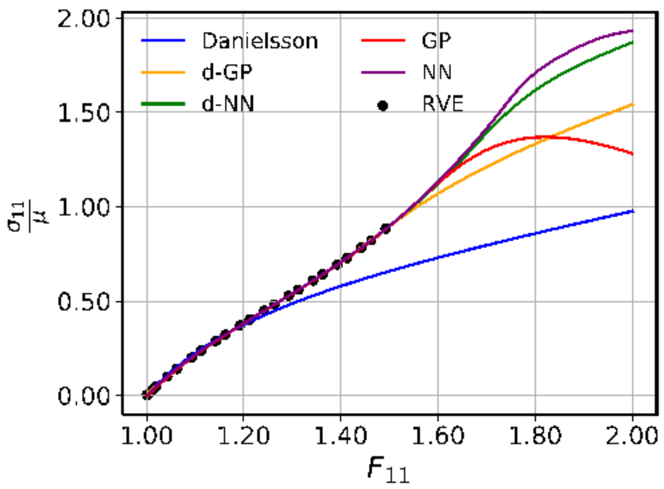
Synthetic stress-strain trajectories from Representative Volume Element (RVE) simulations of idealized foam structures with different porosities



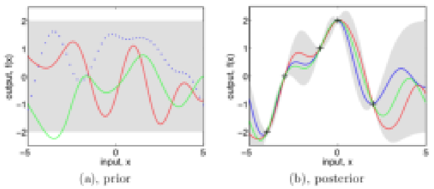


Outcome

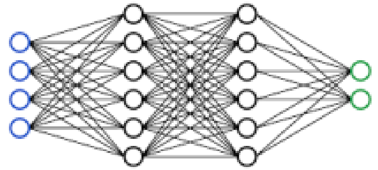
A hybrid model that includes a traditional foam model with an ML-discrepancy model predicts stresses better than the traditional model and pure ML models with strain and porosity inputs.



Gaussian Process (GP) Regression



Neural Network



A.Frankel, C. Hamel, D. Bolintineanu, K. Long, C. Kramer, "Machine Learning Constitutive Models of Elastomeric Foams" (submitted to CMAME)

ML boosts traditional constitutive models to give more accurate and robust results.

Opportunities and Challenges for ML for Mechanics of Materials

Opportunities

- Discovery of P-S-P-P relationships
- Connections between disparate data
- Reducing human-in-the-loop requirements for large data sets
- More efficient models, once trained
- New paradigm of constitutive models

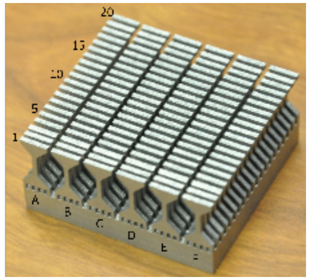
Challenges

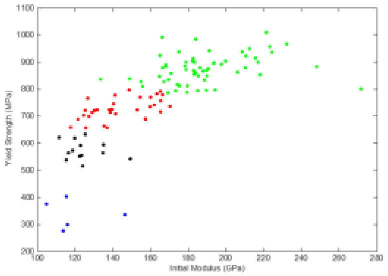
- Discovery of physical intuition from ML models
- Explainability or Interpretability of ML models
- Extrapolation beyond training data for purely data-driven models
- Education of ML methods for the mechanics community

ML can be a disruptive capability in mechanics if used with care.

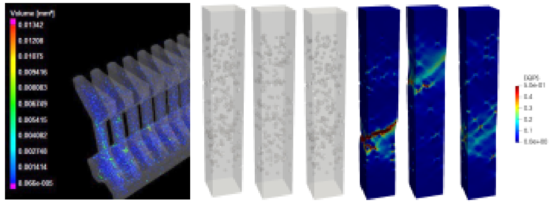
Summary: ML for Mechanics at Sandia

Classification ML



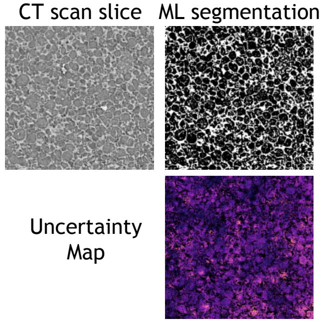


Mechanical Properties Mapping to AM Build Plate Location (K-means Clustering)



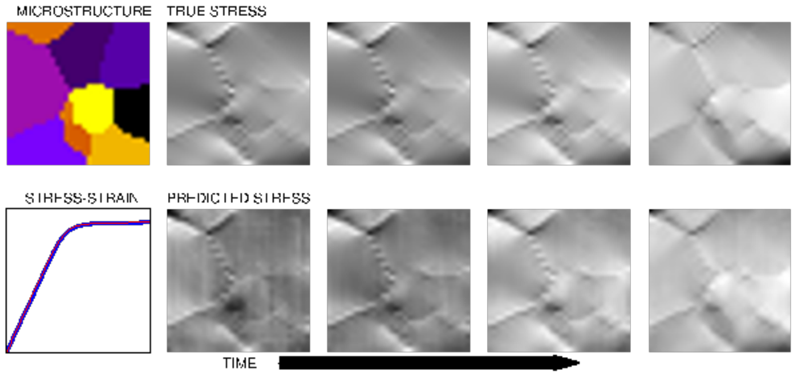
Pore and Mechanical Data for Failure Prediction in AM Metal (3D Convolutional Neural Network)

Automatic 3D Computational Mesh Generation Directly from 3D Images (Bayesian Convolutional Neural Network)

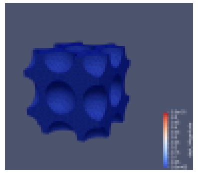


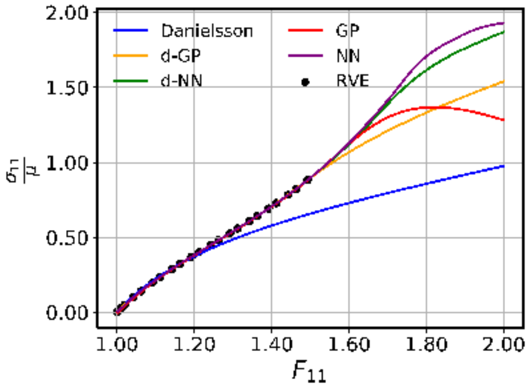
Regression ML

ML Models of Plasticity for Metals with Microstructure (Convolutional Neural Network)



Physics-Informed ML for Material Modeling (Hybrid Traditional + Gaussian Processes and Neural Network)





ML research for mechanics of materials at Sandia looks to discover new mechanics relationships from our large data sets and to appropriately and efficiently model them.