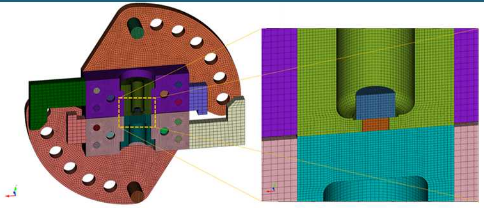
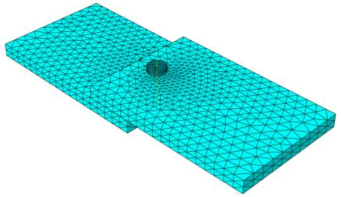
SAND2020-3879PE

Machine learning applications for solid mechanics at Sandia





PRESENTED BY

Michael Tupek, Prof. Julián Rimoli (GA Tech), John Mersch, Tim Shelton, Payton Lindsay, Dan Bolintineanu, Kevin Long, Robert Waymel, Enrico Quintana, Reese Jones, Ari Frankel, Scott Roberts, Justin Newcomer, David Stracuzzi, Laura Swiler, Kyle Johnson, John Emery, Demitri Maestas and Sharlotte Kramer.

September 25th, 2019

GA Tech students: Aarohi Shah, Hernán Logarzo, Germán Capuano

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Fastener surrogate modeling motivation

Part of Sandia’s mission is predicting performance of systems and structures subjected to abnormal environments

Fasteners are an integral connector in many of these system and structures

This is a complicated problem…

Numerous fasteners exist in these systems and can be:
- Different sizes
- Loaded at various rates
- Subjected to diverse loadings

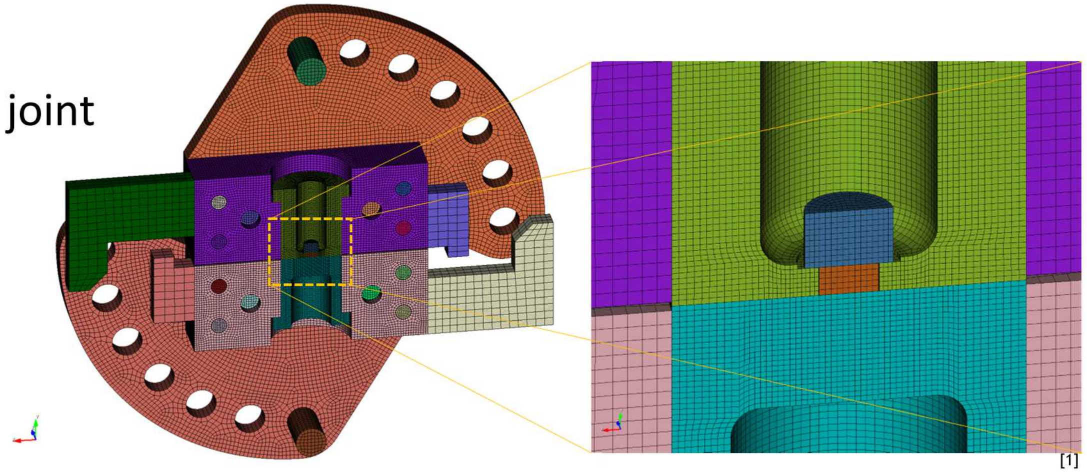
Difficulties:
- It is infeasible to test all fasteners
- Model fidelity requirements of system models are restrictive.
- Modeling fasteners is difficult, time-intensive, and repetitive.

Goal: Develop machine learning surrogate models that are efficient, predictive, robust, and easy to implement.

Fastener challenges

Want to capture the mechanical behavior of the fastener and joint

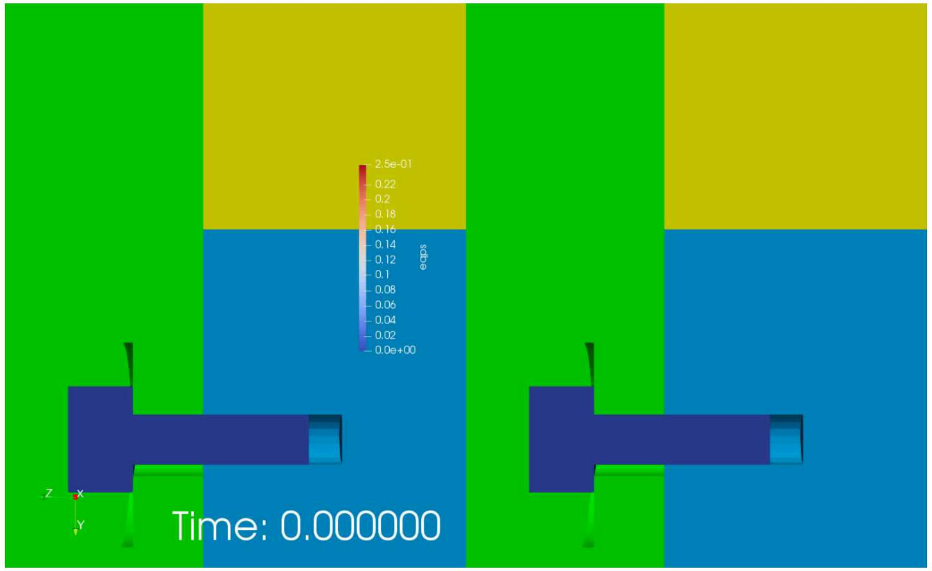
- Load-Displacement Response
- Failure
- Stiffness
- Preload
- Etc.



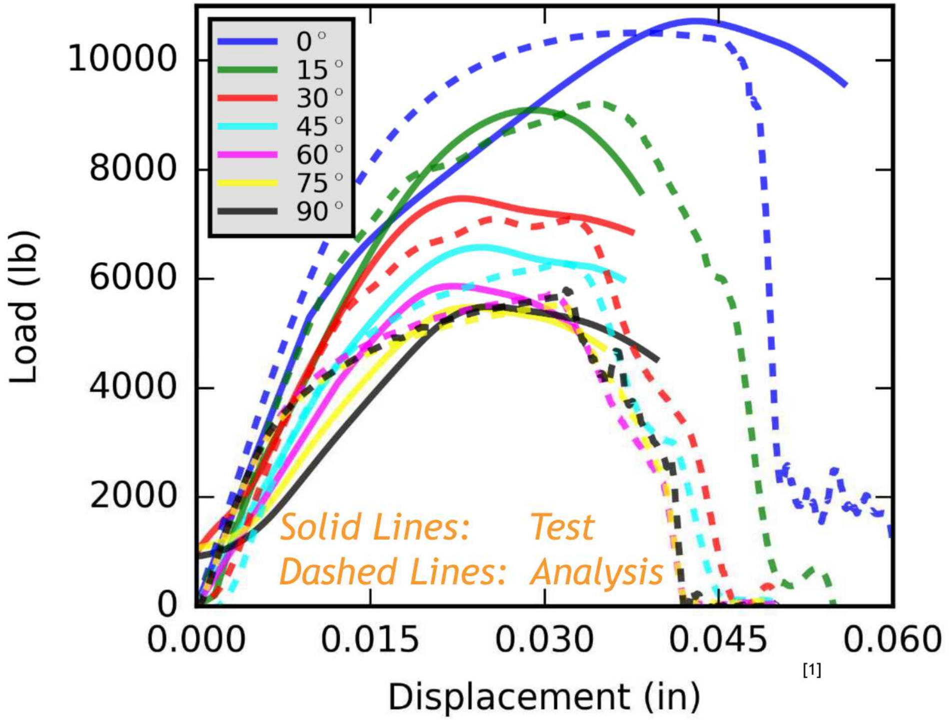
[1]

Perform tests and calibrate a mechanical material model (relate stress to strain)

- Test data does not span all possible loadings or conditions
- Calibration tools are limited



[2]



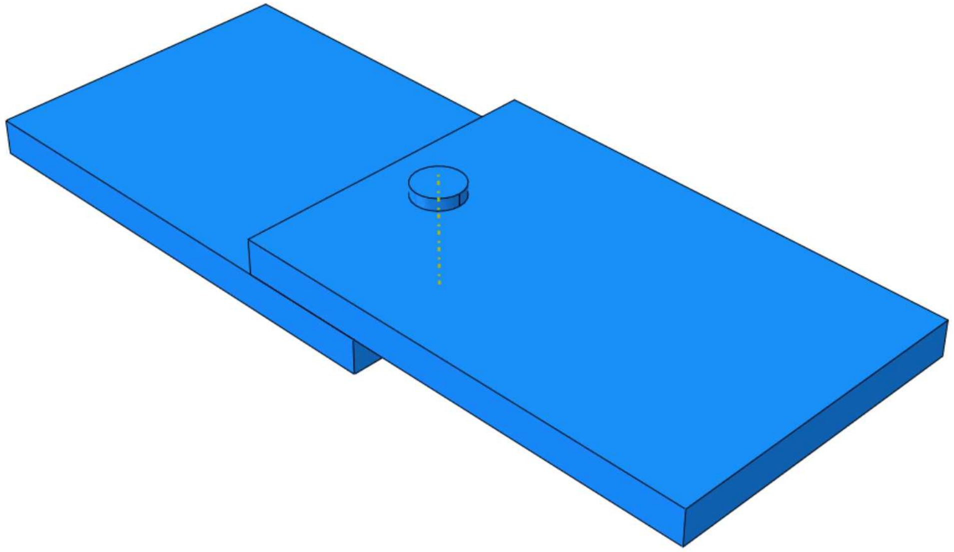
[1]

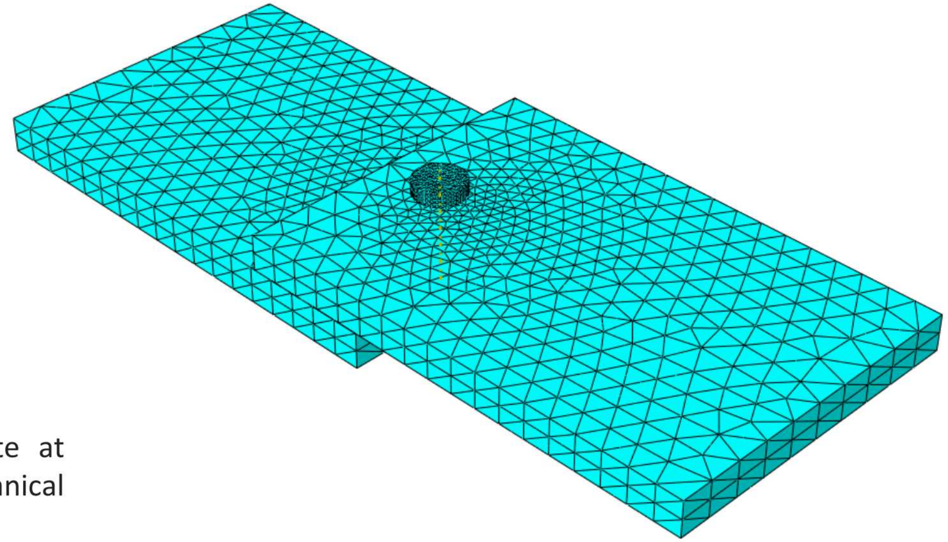
[2] Mersch, J. P., Smith, J. A., Johnson, E. P., Bosiljevac, T., "Evaluating the Performance of Fasteners Subjected to Multiple Loadings and Loading Rates and Identifying Sensitivities of the Modeling Process," *2018 AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference*, AIAA SciTech Forum, AIAA2018- 1896, Kissimmee, FL, 2018.

[1] Mersch, J., Smith, J., Orient, G., Grimmer, P., Gearhart, J., "*Calibration Strategies and Modeling Approaches for Predicting Load-Displacement Behavior and Failure for Multiaxial Loadings in Threaded Fasteners" ASME International Mechanical Engineering Congress and Exposition, IMECE2019-10521, ASME, Salt Lake City, Utah, 2019.*

FEM PROBLEM SCHEMATICS:
model and material

- Bolt and Flange assembly modeled: crucial sub-structure of a bigger structural component
- Model : Rectangular flanges with M8 bolt which forms lap joint
- Material Used: Stainless Steel 304 L (industry grade) Plasticity material data obtained from literature[1]

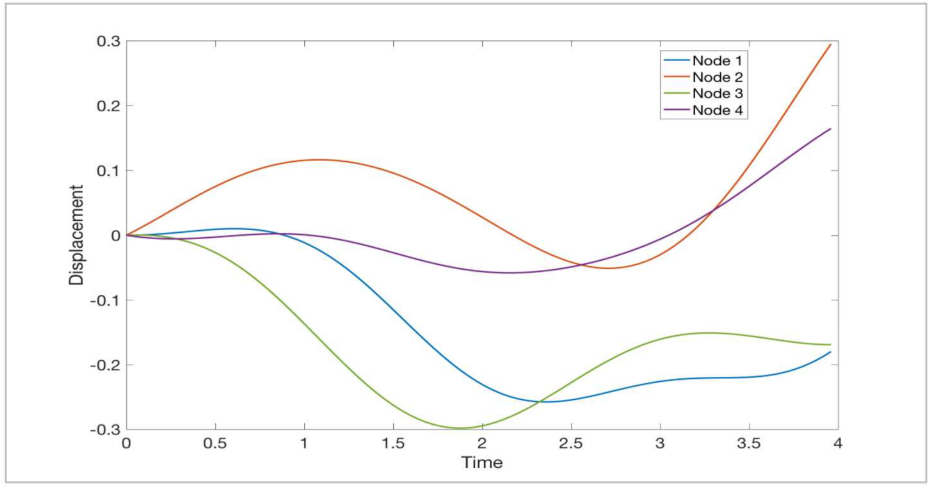




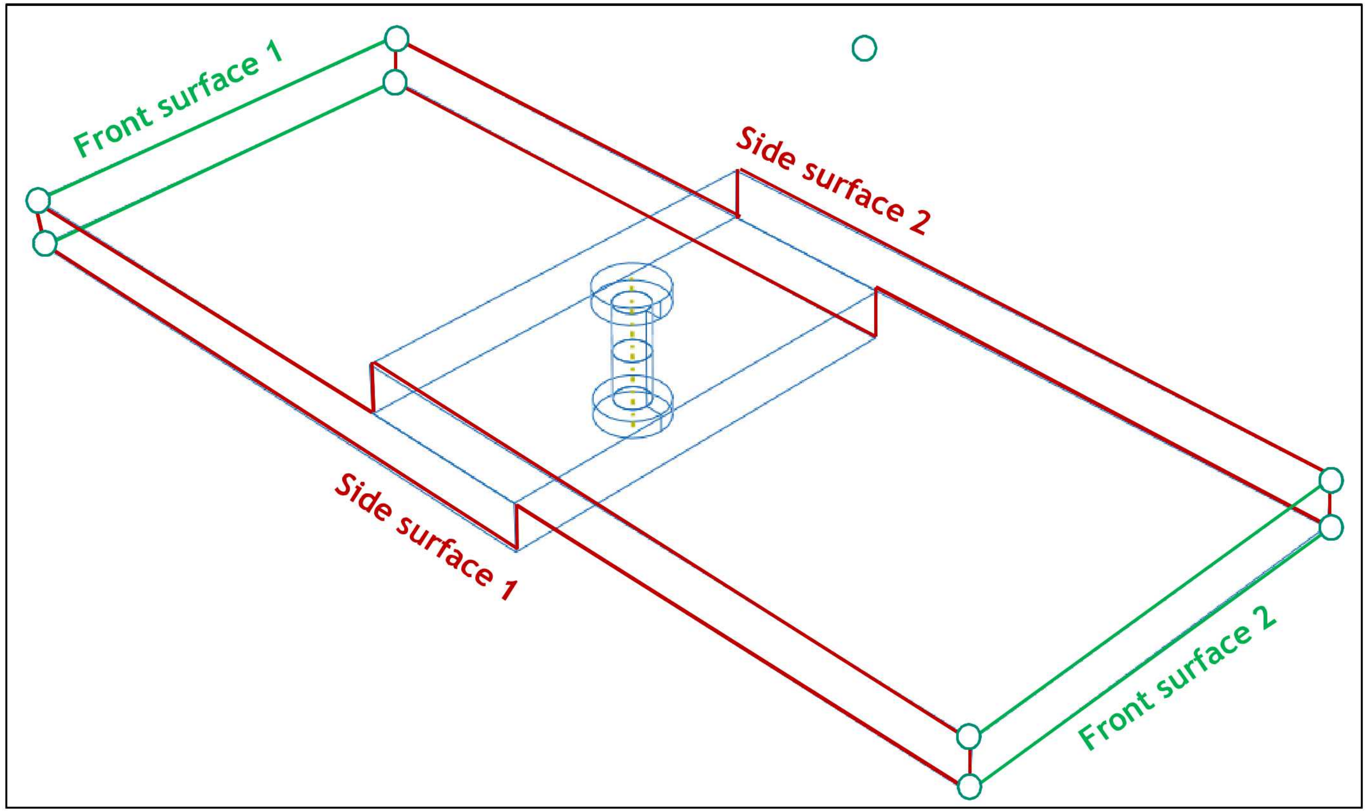
[1]Blandford, R. K., et al. "Tensile stress-strain results for 304L and 316L stainless steel plate at temperature." *ASME 2007 Pressure Vessels and Piping Conference*. American Society of Mechanical Engineers, 2007.

FEM PROBLEM SCHEMATICS:
boundary conditions

- Boundary Conditions applied as displacements on input and side surfaces
- Displacements (3 components) defined at each of the 8 corner nodes using <u>Gaussian processes</u>
- Corner displacements used to determine boundary conditions for nodes on the 4 surfaces using <u>bilinear interpolation</u>



Sample Gaussian processes for 4 nodes



Boundary surface definition

FEM PROBLEM SCHEMATICS: corotational formulation

- Corotational formulation is required to include frame indifference in the component during prediction.
- Compute rigid body motion (translation and rotation) and removing its contribution from the total displacement.

- Equations and Schematic:

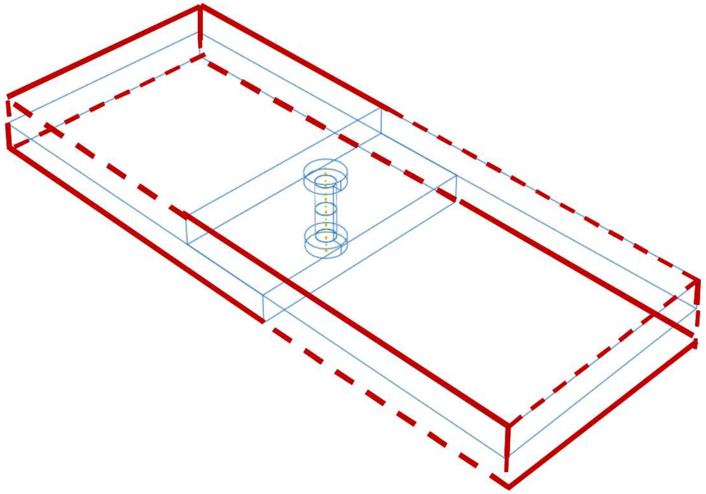
$$U_i = \sum_j u^e_{ij} N_j$$

$$\frac{\partial U_i}{\partial x_k} = \sum_j u^e_{ij} \frac{\partial N_j}{\partial x_k}$$

$$F = \frac{\partial U_i}{\partial x_k} + I \qquad U = \sqrt{F^T F}$$

At center of element

$$F = RU$$



$$X_i = \sum_j X^e_{ij} N_j$$

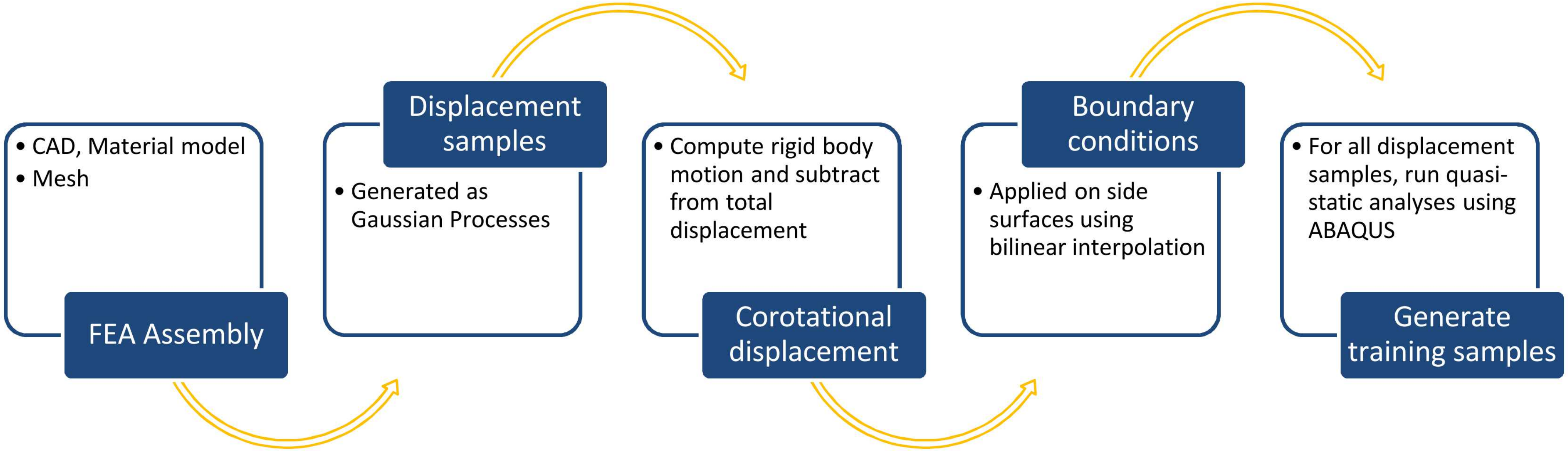
$$u^{et}_i = \frac{1}{8} \sum_j u^e_{ij}$$

$$u^{ed}_i = R(u^e_i - u^{et}_i + X^e_i - X^e_c) - (X^e_i - X^e_c)$$

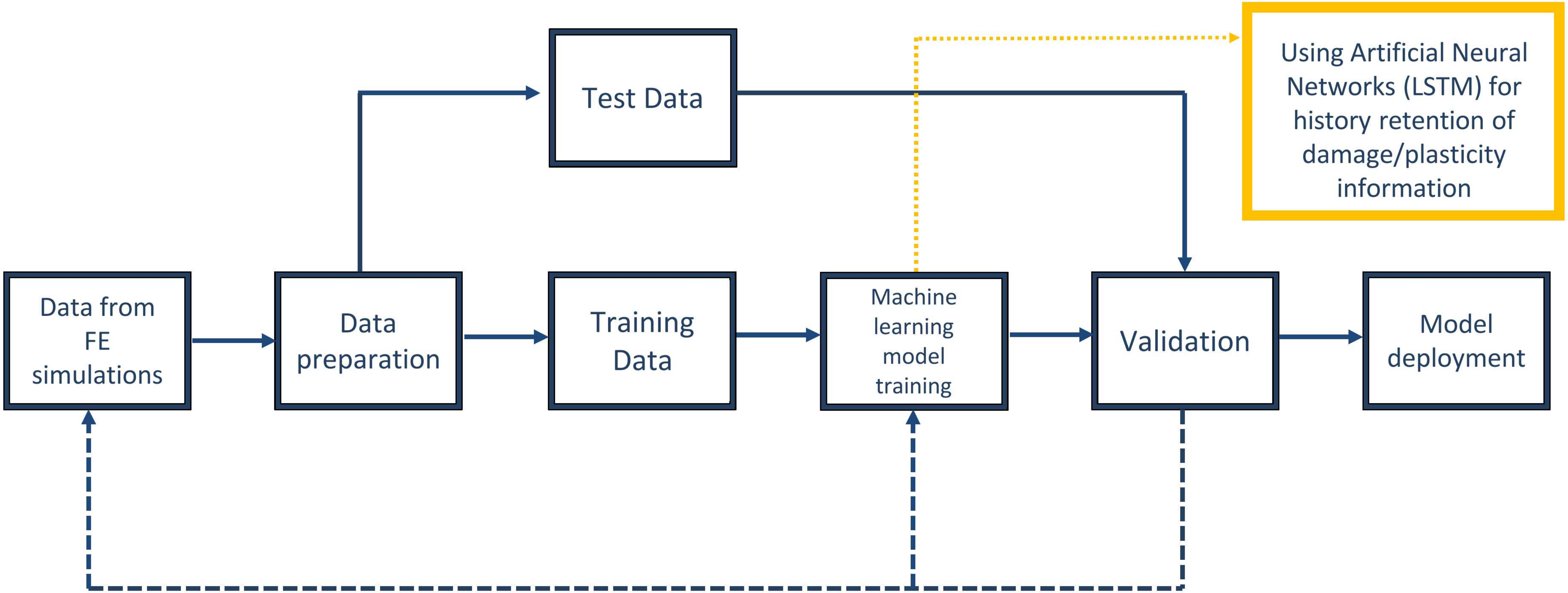
Corotational displacement[1]

[1]Battini, Jean-Marc. "A non-linear corotational 4-node plane element." *Mechanics research communications* 35.6 (2008): 408-413.

FEM PROBLEM formulation: summary



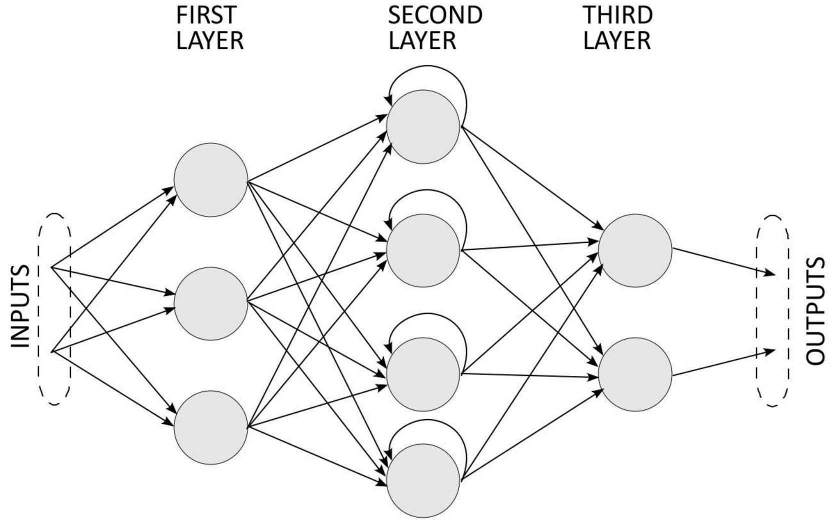
ML APPROACH: overview



ML APPROACH: model architecture

Recurrent Neural Networks (using Keras)

- Similar to Feedforward Neural Networks (FNN) but they allow connections to earlier layers
- They have memory!



Recurrent Neural Network Details

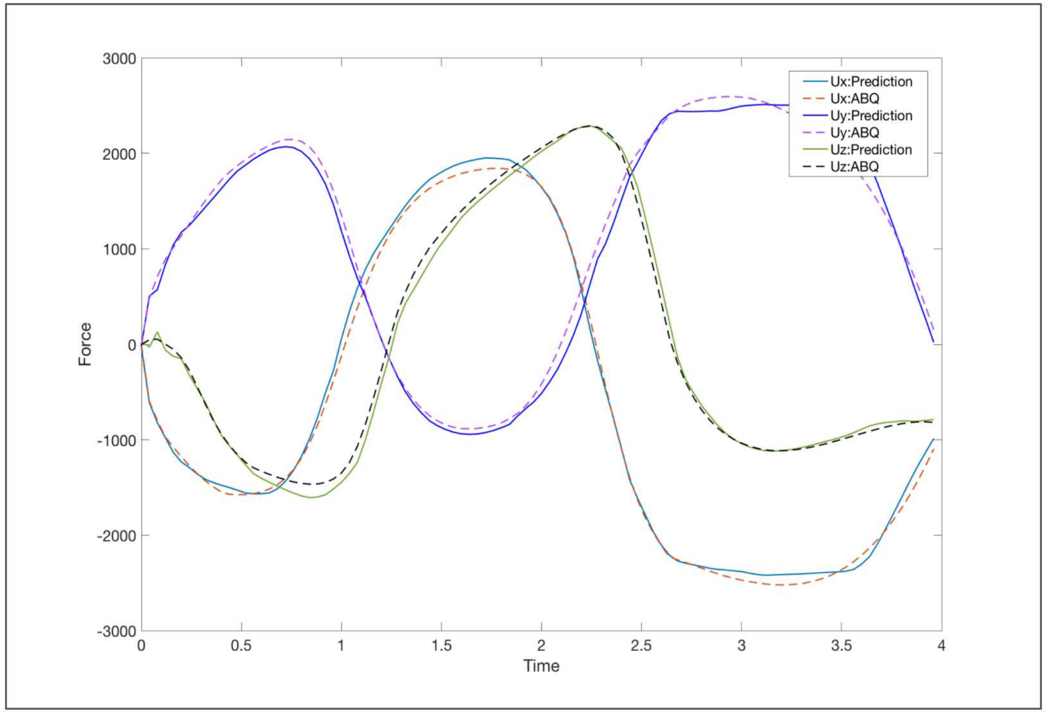
- 2 LSTM layers of size 200 are used with 3 Dense layers of size 200 and final Dense layer of the output size
- Model is trained with 9000 samples with a validation split of 20%
- Adam optimizer and mean squared error is used for loss calculation

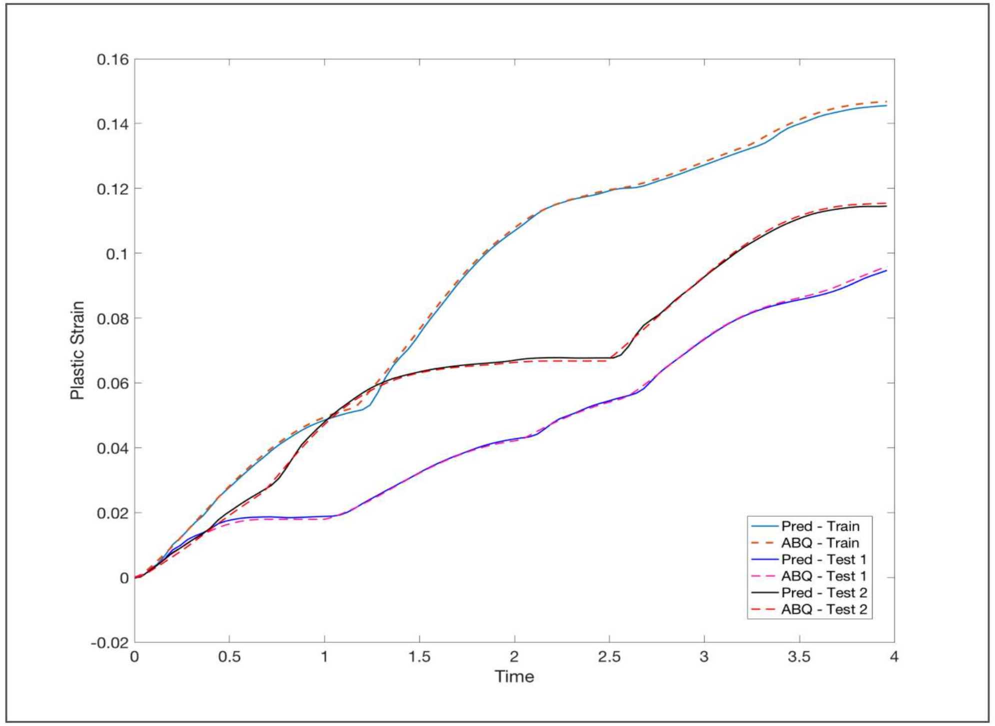
Training Data Details

- Input: - Displacements (3 components) at 8 corner nodes
  - Initial plastic strain
- Output: - Forces (3 components) at 8 corner nodes
  - Max. equivalent plastic strain

RESULTS

- Results indicate good prediction when validated for a test case (unknown to the trained network) and compared with FEA results obtained from commercial software (ABAQUS).
- Left figure: prediction of x, y and z displacement components for a particular node.
- Right figure: maximum equivalent plastic strain history.





Runtime: ~1 hour → ~10 seconds

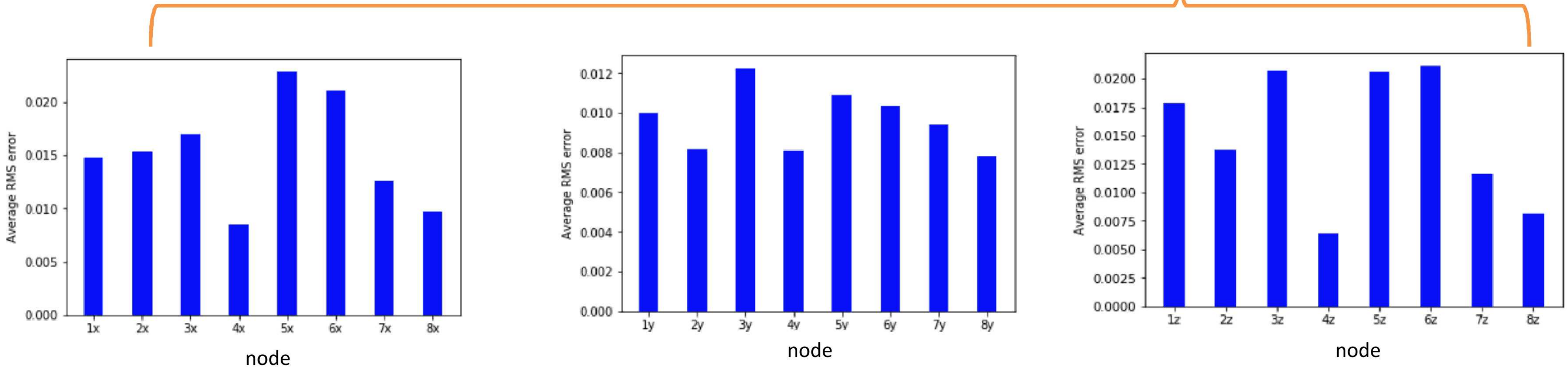
Results post-process

- Force values are invariant of translation
- To obtain everything back in global frame,

$$F_g = R^T F_{pred}$$

- Validation results by running new cases from $U_g \longrightarrow F_g$

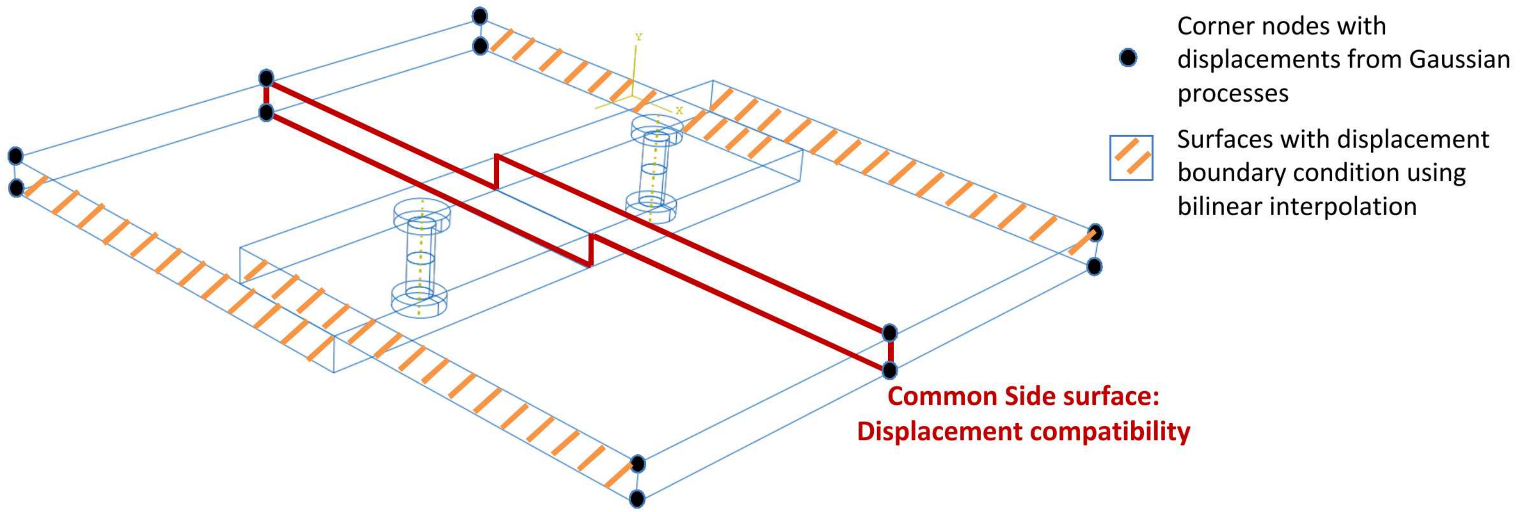
$$\frac{1}{samples}\sum_{i=1}^{samples}\left(\frac{1}{max(Fa_j)}\sqrt{\frac{1}{len}\sum_{j=1}^{len=100}(Fa_j - Fp_j)^2}\right)$$



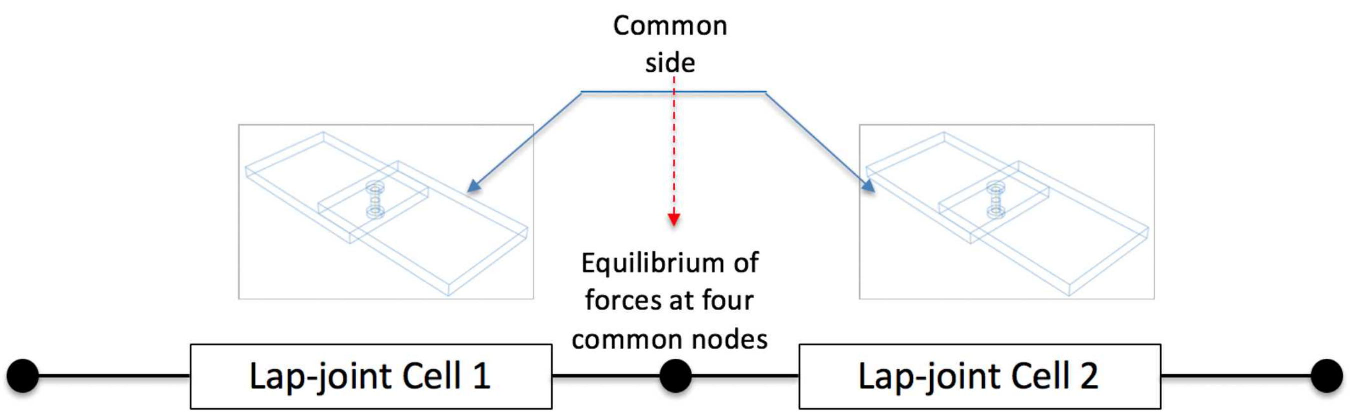
Avg. RMS error in plastic strain is 0.0015

Assembly of two lap-joints
SET UP (work in progress)

FEA set-up:



ML representation:



FEM PROBLEM SCHEMATICS:
bilinear interpolation (boundary condition)

- For accurate interpolation to cover account for entire side surface, we assume a bigger (rectangular) space
- Interpolation formulation:

$$f(x_1,y) = \frac{y_2 - y}{y_2 - y_1} f(Q_{11}) + \frac{y - y_1}{y_2 - y_1} f(Q_{12})$$

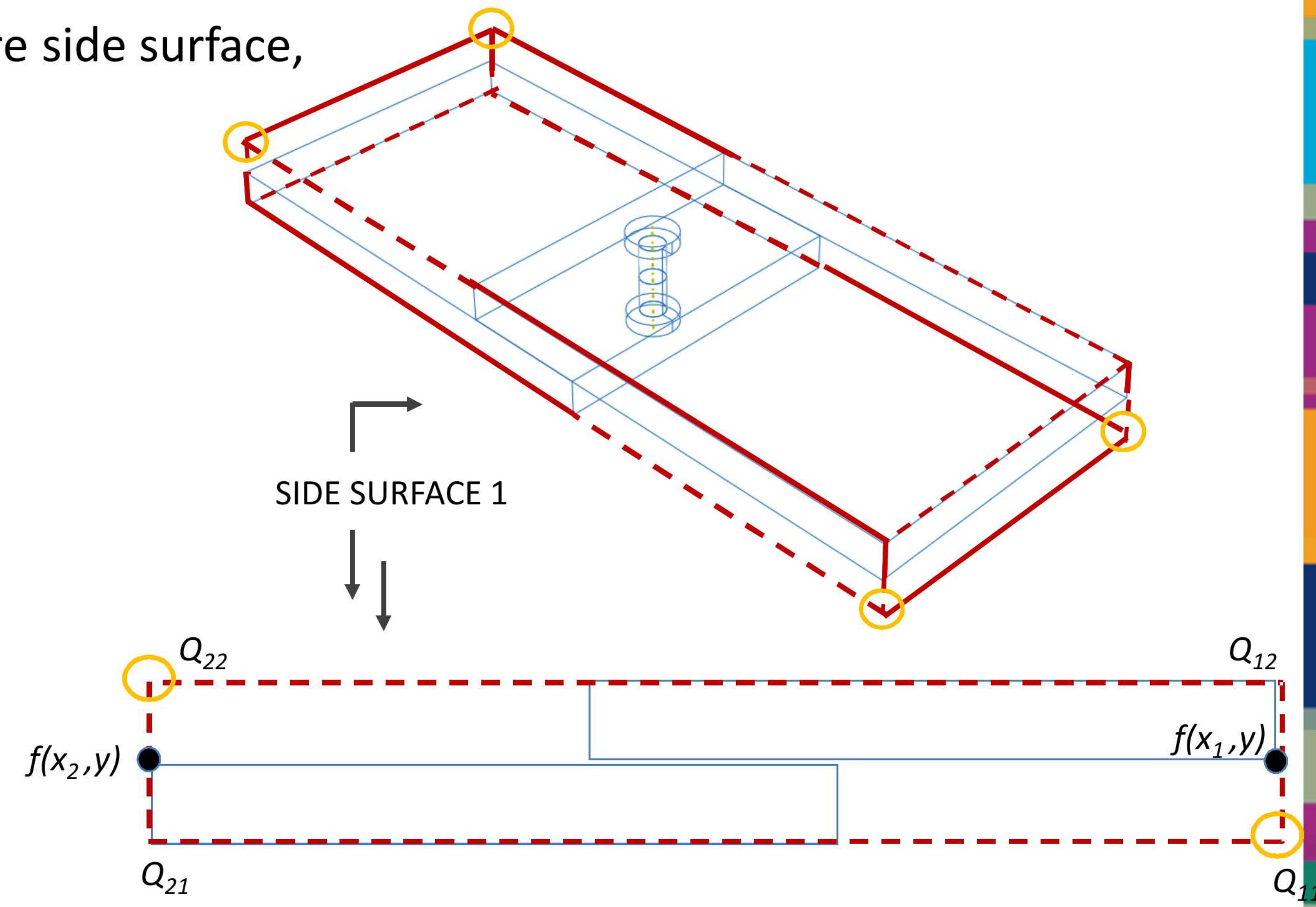
$$f(x_2,y) = \frac{y_2 - y}{y_2 - y_1} f(Q_{21}) + \frac{y - y_1}{y_2 - y_1} f(Q_{22})$$

$$f(x,y) = function\ of\ x\ and\ y\ (\ displacement\ )$$

$$x, y = nodal\ co - ordinates$$

(green circle) → Known values of displacement from Gaussian processes

(orange circle) → Unknown values computed using above formulation



- The obtained Q_{11} and Q_{22} are used in above formulation for computing $f(x,y)$ for all nodes on defined boundary surfaces

Open questions / future directions

- Productionize (make it usable)
- How to choose calibration dataset?
- Reduce network size and memory?
- Enforce more known mechanics?

Machine learning the constitutive response for foam RVEs

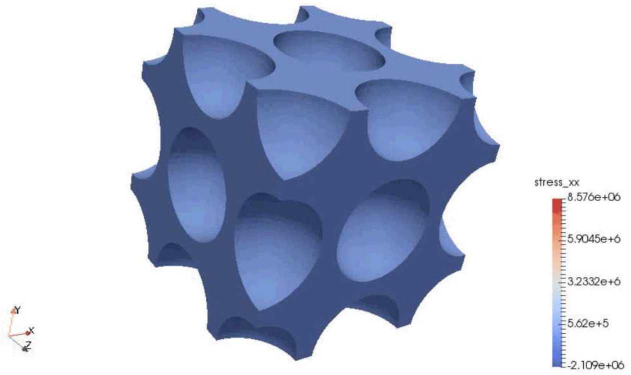
Dan Bolintineanu, Kevin Long, Sharlotte Kramer. Sandia National Laboratories

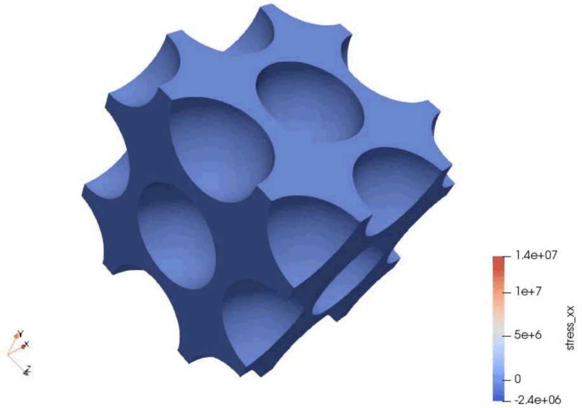
ML on BCC RVEs

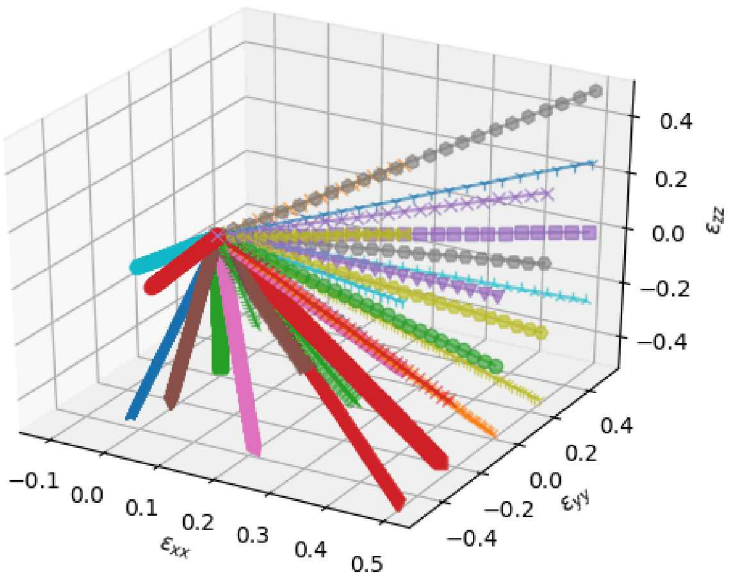
Input:
Microstructure, **3D strain**
(later add history, strain rate…)

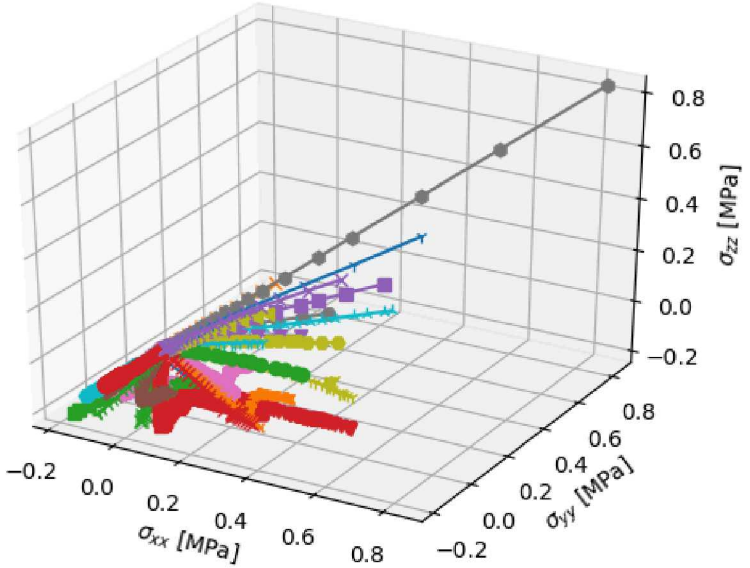
→ **ML model** →

Output:
3D stress state









Brute force approach: sample

$$\epsilon_{xx}, \epsilon_{xy}, \epsilon_{xz}, \epsilon_{yy}, \epsilon_{yz}, \epsilon_{zz}$$

However, assuming isotropy, only need to sample in principal space:

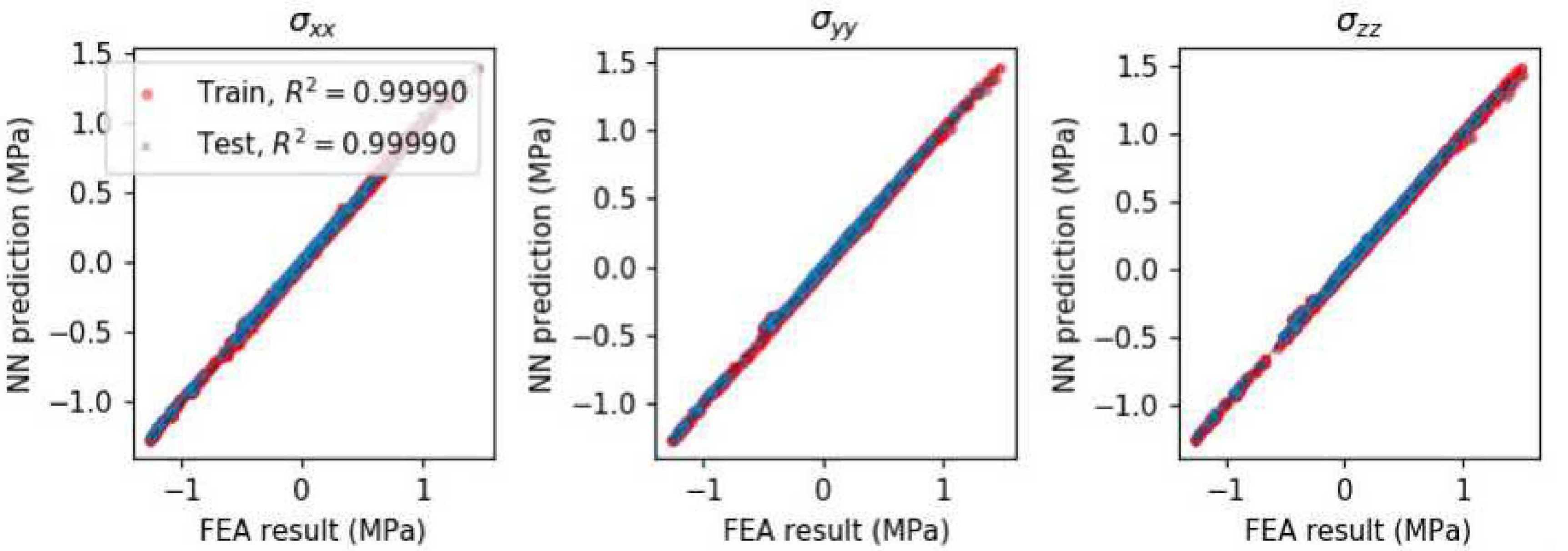
$$\hat{\epsilon}_{xx}, \hat{\epsilon}_{yy}, \hat{\epsilon}_{zz}$$

Furthermore, axes are symmetric, only need to sample space where

$$\hat{\epsilon}_{xx} \leq \hat{\epsilon}_{yy} \leq \hat{\epsilon}_{zz}$$

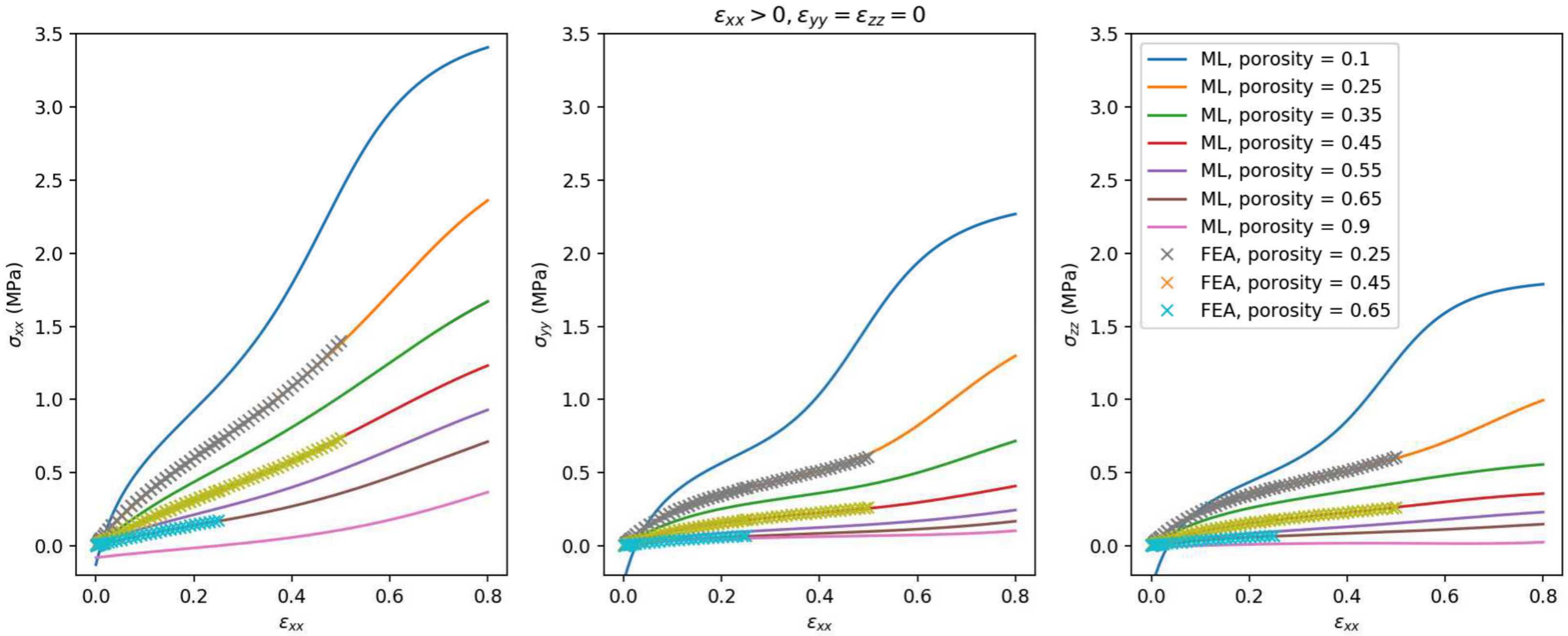
Convincing calibration

ML model: simple 3-layer fully connected neural net



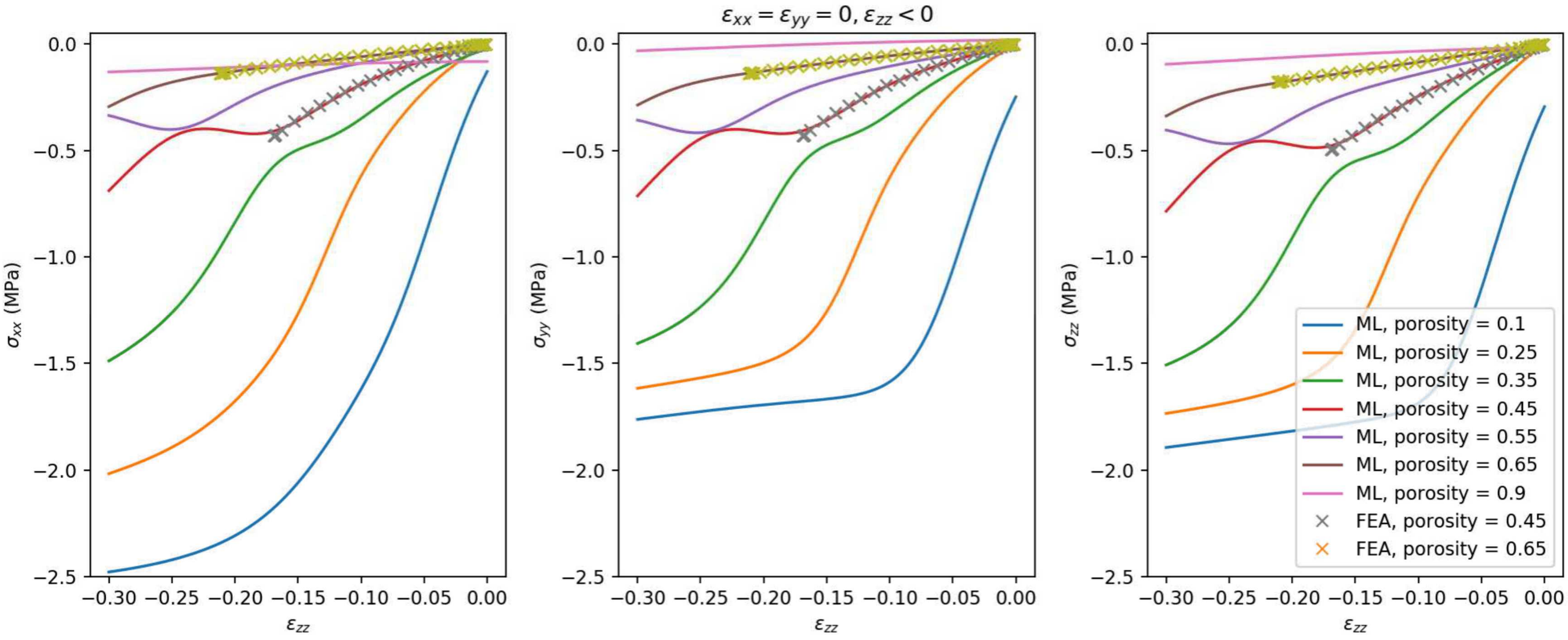
Boundary value problem test using ML model

Uniaxial strain: tension



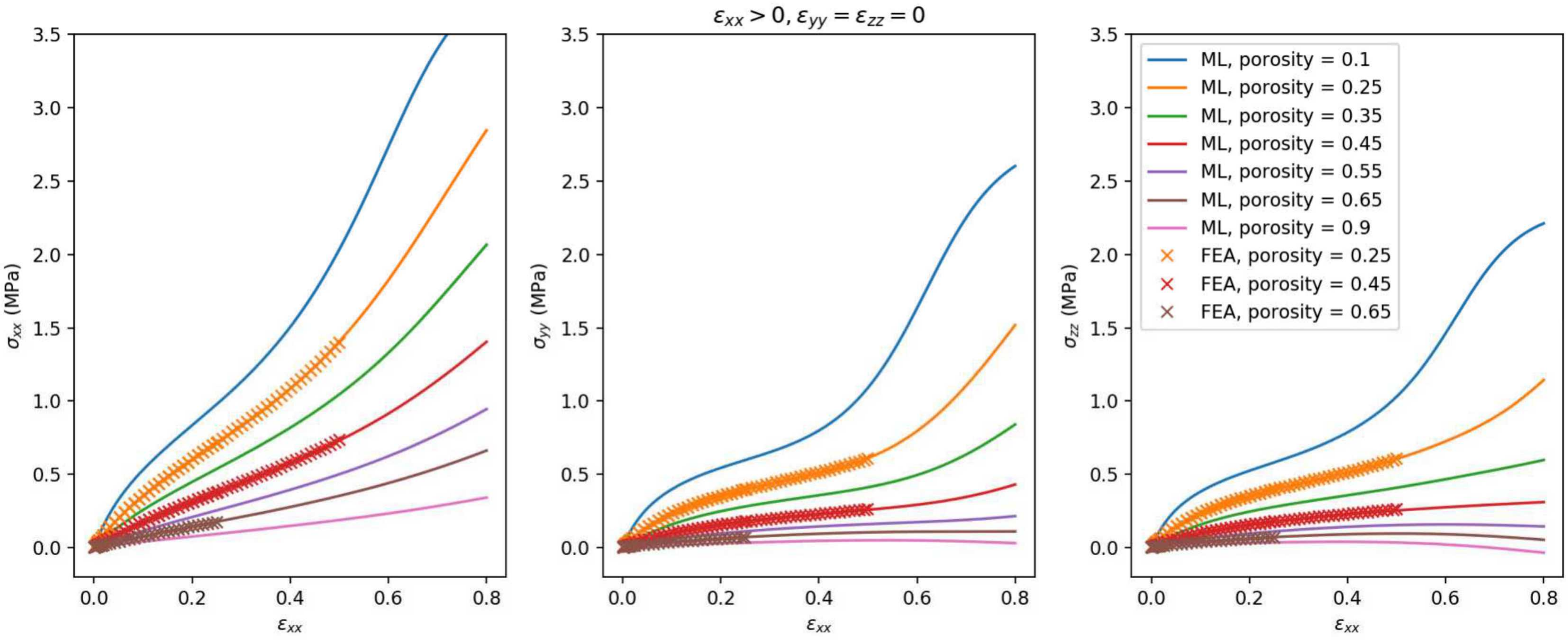
Boundary value problem test using ML model

Uniaxial strain: compression



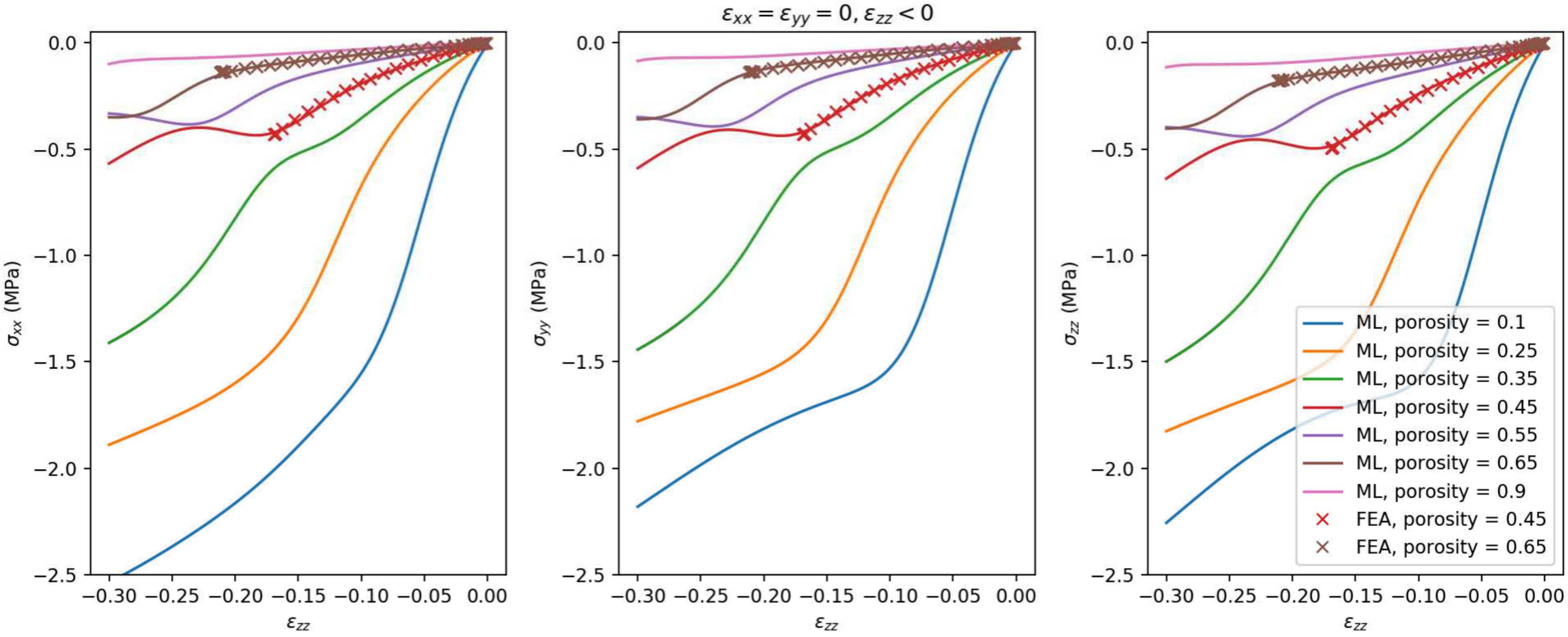
Boundary value problem test using ML model

Uniaxial strain in tension



Boundary value problem test using ML model

Uniaxial strain in compression



Future considerations

- Alternative regression models (Gaussian processes, boosted gradient regression trees); likely minimal improvement, since $R^2 > 0.9999$ for current neural net, but GPs provide uncertainty bounds

- Additional approaches to physical constraints (e.g. ‘soft’ via loss function penalty, or ‘hard’ via changes to network architecture)

- Expand space of training data and dimensionality of model:
  - More porosities, loading states
  - Other microstructural variations besides porosity, e.g. anisotropy
  - Variations in solid polymer parameters (e.g. lock-up)

Nonlinear multiscale homogenization

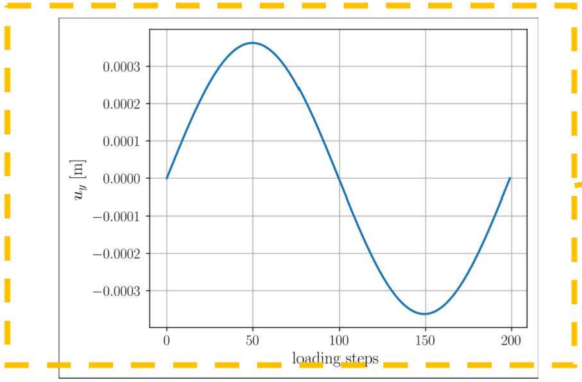
- Multiscale analysis
- Plane strain problem

MAIN IDEA:
Solve a quasi-static multi-scale problem using:

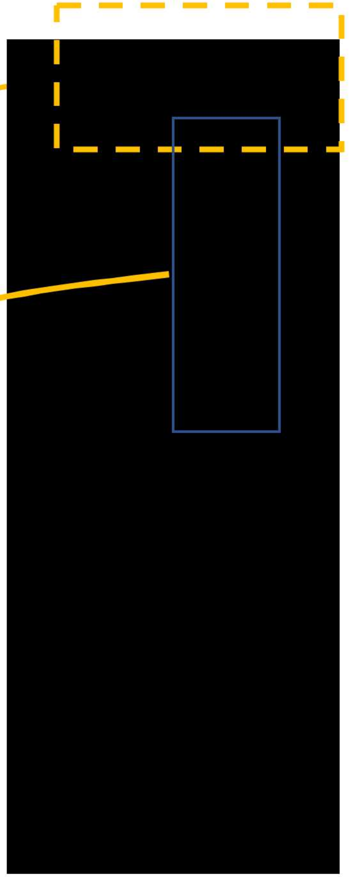
- **High-fidelity** result **(from a concurrent multiscale model)**
- Data-Driven result (from a Smart Constitutive Law (SCL)

GOAL

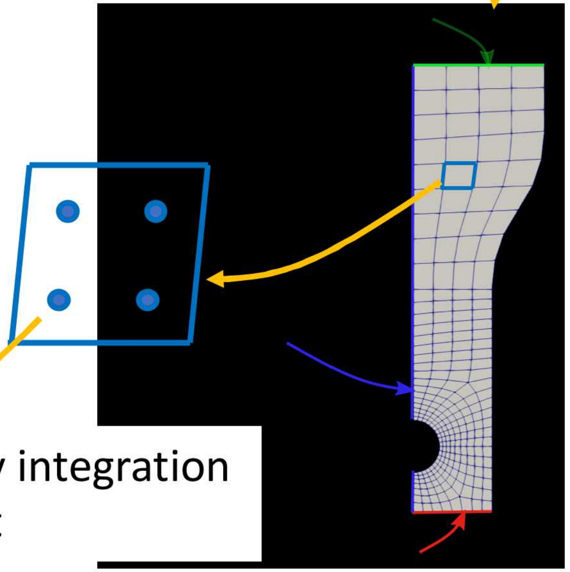
Find an efficient method to reduce computation time in real life applications



Quasi-static displacement

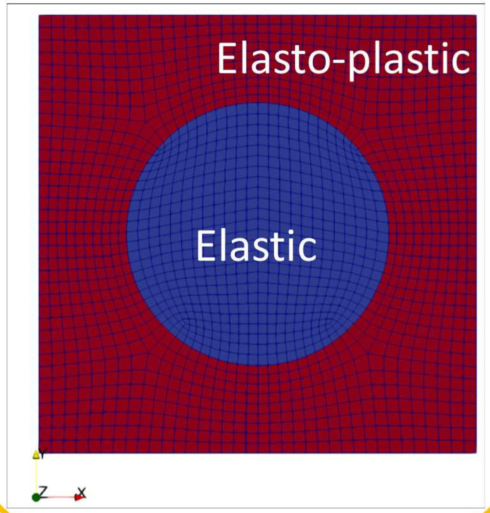


FE of the macro-scale



Every integration point

Microestructure



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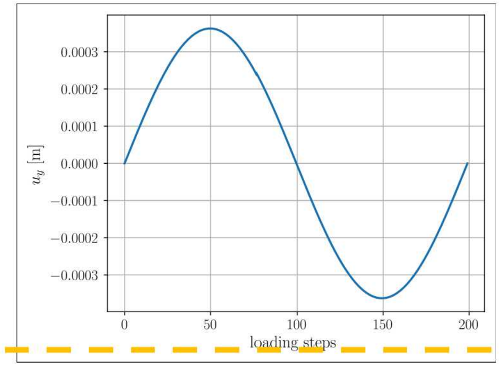
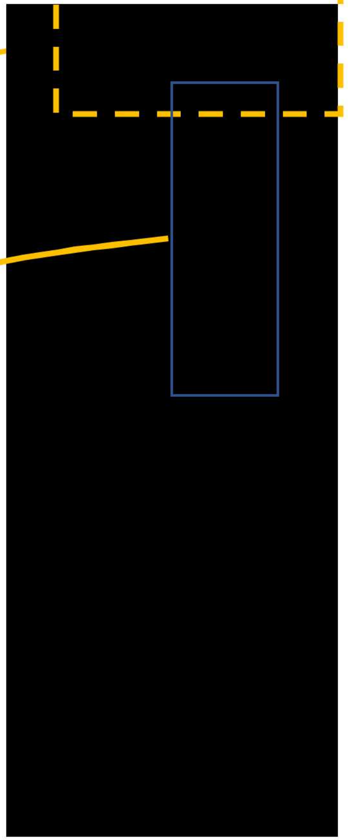


Quasi-static displacement



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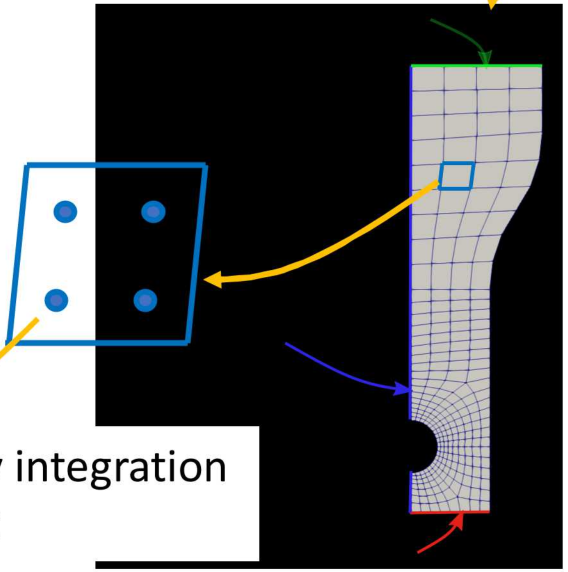
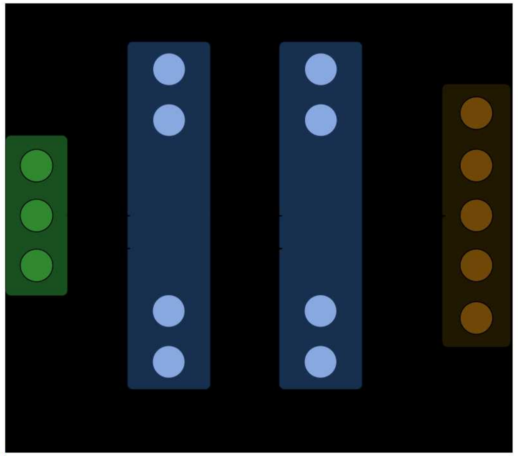
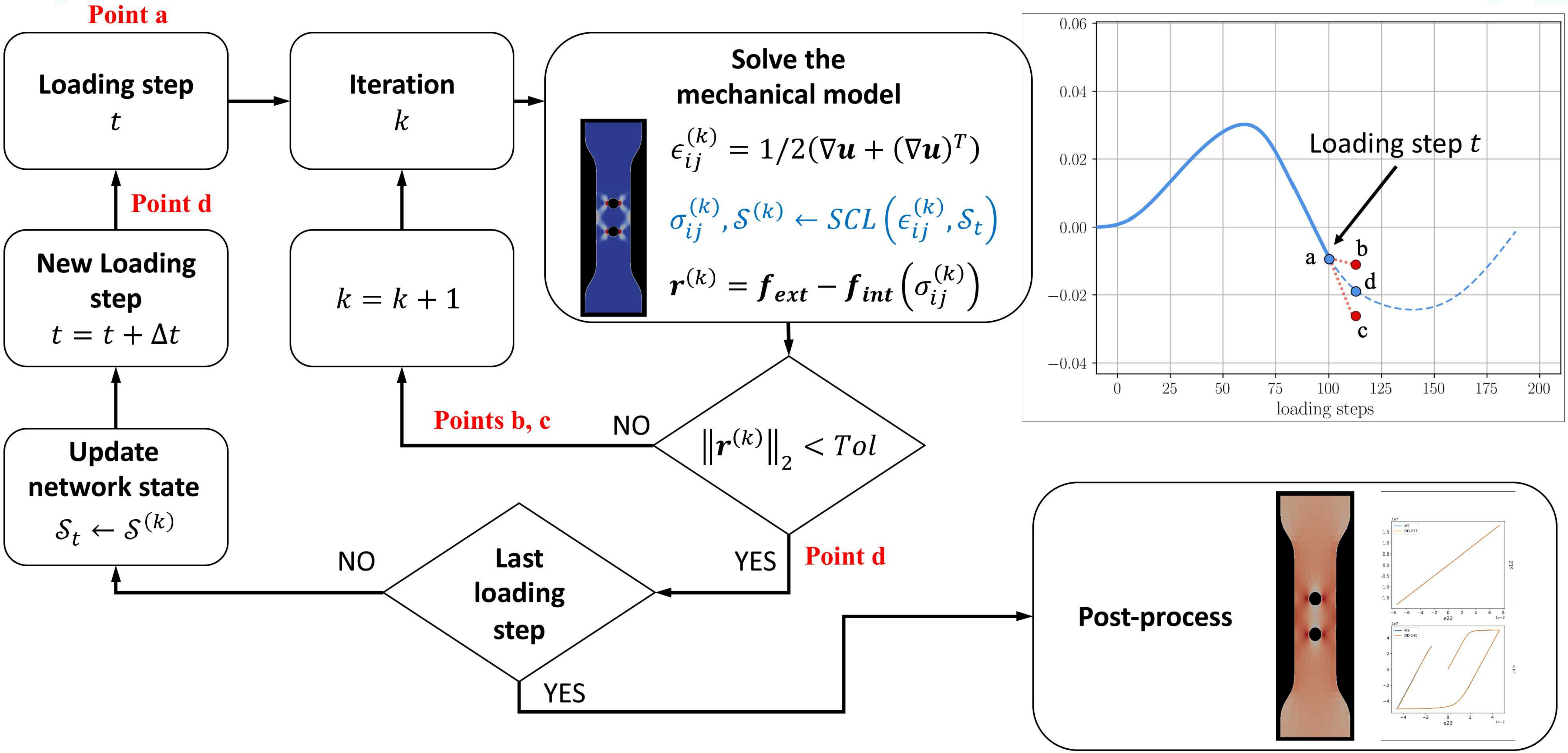


Every integration point

Neural Network





Point a
Loading step
t
Iteration
k
Solve the
mechanical model
$\epsilon_{ij}^{(k)} = 1/2(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T)$
$\sigma_{ij}^{(k)}, \mathcal{S}^{(k)} \leftarrow SCL\left(\epsilon_{ij}^{(k)}, \mathcal{S}_t\right)$
$\boldsymbol{r}^{(k)} = \boldsymbol{f}_{ext} - \boldsymbol{f}_{int}\left(\sigma_{ij}^{(k)}\right)$
Point d
New Loading
step
$t = t + \Delta t$
$k = k + 1$
Points b, c
NO
$\left\|\boldsymbol{r}^{(k)}\right\|_2 < Tol$
YES
Point d
Update
network state
$\mathcal{S}_t \leftarrow \mathcal{S}^{(k)}$
NO
Last
loading
step
YES
Post-process
Loading step t
a
b
d
c
0.06
0.04
0.02
0.00
−0.02
−0.04
0
25
50
75
100
125
150
175
200
loading steps

Presentation Outline

- Sandia National Laboratories Overview
- Brief Examples of ML in Mechanics of Materials at Sandia
- Deep Dive Example of ML for Polymer Foam Mechanics
- Discussion Points on Use of ML for Mechanics of Materials

What is Machine Learning?

"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks T, as measured by P, improves with experience E."

- Tom Mitchell, *Machine Learning*, 1997

How Does Machine Learning Work?

Data / Experience

$X = \{x_1, x_2, \ldots, x_n\}$		Y

Model

$$Y=f(x)$$

Loss Function

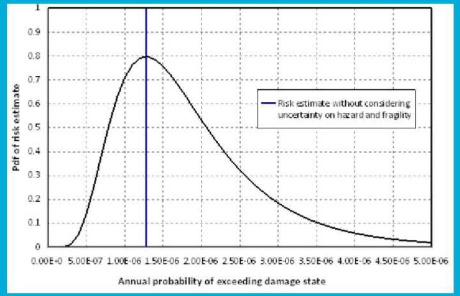
$$\varepsilon = \frac{1}{N}\sum_{i=0}^{n} g(f(x_i) - Y_i)$$

Learning Algorithm

Parameterized Model

$$f(x) = \theta_1 x_1 + \theta_2 x_2 + \cdots$$

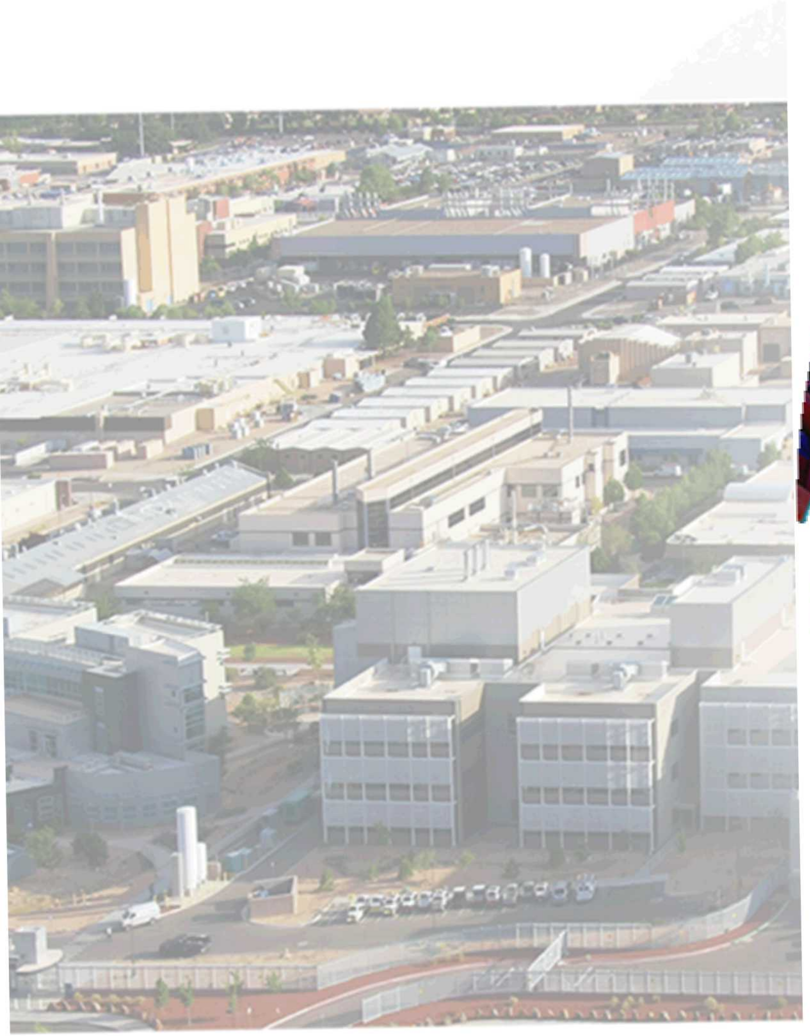
Predictions & Evaluation

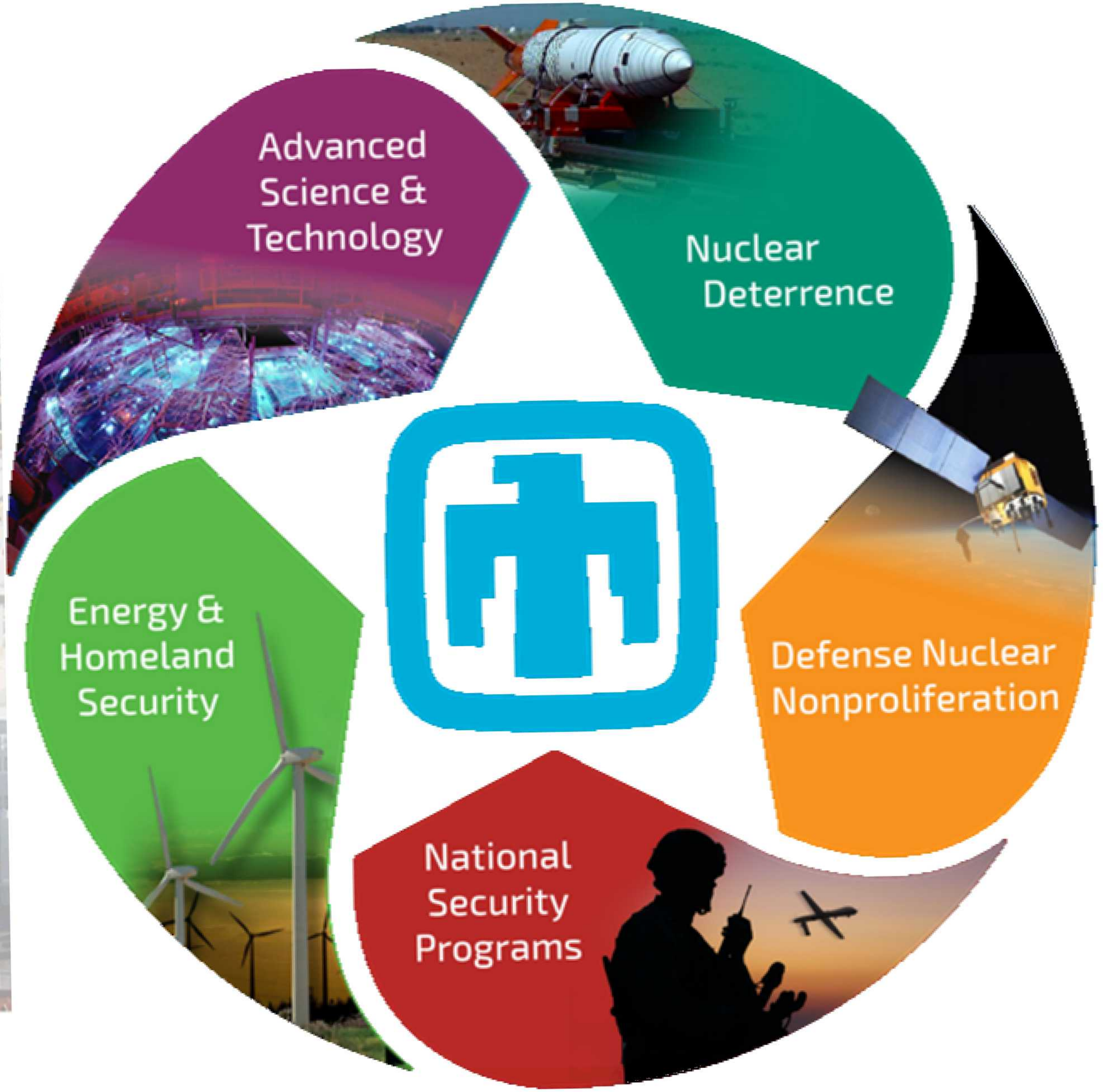


Other Potential Features:

- Uncertainty Quantification
- Domain Knowledge

Sandia Has Five Major Program Portfolios

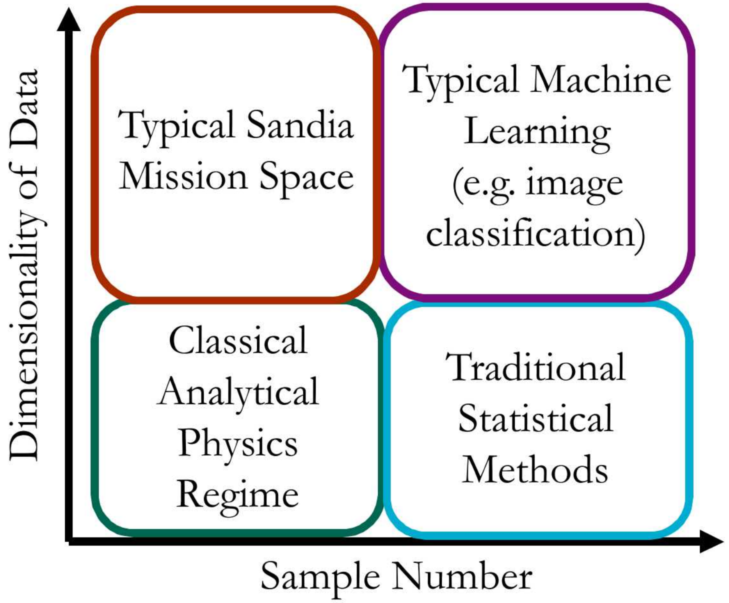




Sandia's Mission Needs

- High-consequence decisions
  - Typically designing to **very high reliability requirements**
  - Need to **assure trust** in our solutions
  - Need to **characterize & communicate uncertainty** of decisions
  - Algorithms need to be **interpretable and explainable**

- Challenges:
  - Often have **limited, unknown, or no ground truth** (no labeling and little to no positives)
  - **High dimensionality** can lead to extremely **sparse datasets**
  - National security missions can require decisions to be made in a very **short time frame** (milliseconds to minutes)
  - Many applications require methods to adhere to or account for **first principle physics**
  - Need to account for **potential adversarial issues**



Connecting Mechanics of Materials and Machine Learning

Mechanics of Materials Today

- Complex relationships and multi-scale mechanics
- Potential for spatially and/or temporally dense data
- New and advanced materials
- High cost of experiments → low sample numbers
- Sometimes high-consequence applications
- Traditional human-in-the-loop methods lacking the ability to cope with "big" and "sparse" data

How Machine Learning May Help

- Dimensionality reduction of data
- Connections between disparate data types
- Model improvement with more data
- Efficiency of trained model
- Physical intuition present in the model *sometimes*
- Opportunities of uncertainty quantification – relative confidence in decisions based on ML models

Machine Learning Challenges Upfront

- ML model may not provide new physical intuition
- Extrapolation beyond training space is tenuous
- Sometimes laborious model training process

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

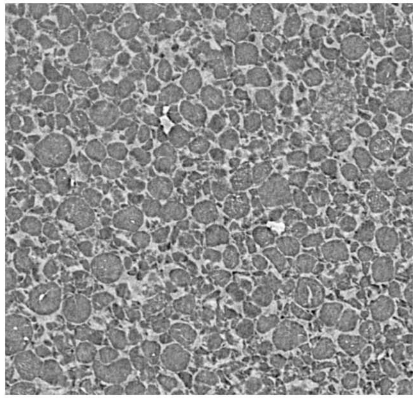
Examples of Machine Learning for Mechanics of Materials

Machine learning for 3D tomography to computational meshes

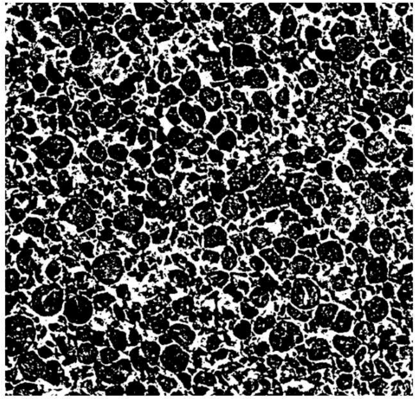
PI: Scott Roberts

Goal: Credible Automated Meshing of micro-CT Images

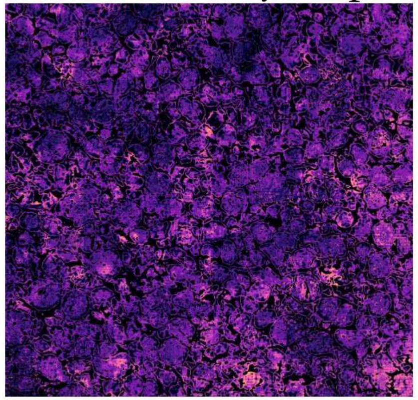
CT scan slice



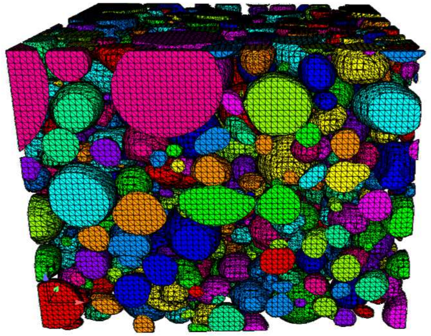
ML segmentation

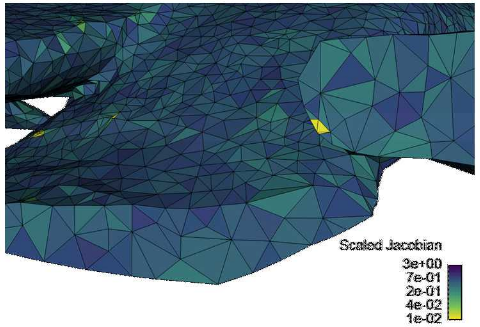


Uncertainty map



CNNs for image segmentation and uncertainty quantification for very large 3D materials datasets from XCT, FIB/SEM, etc.

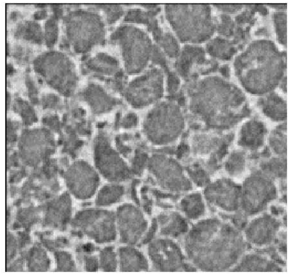




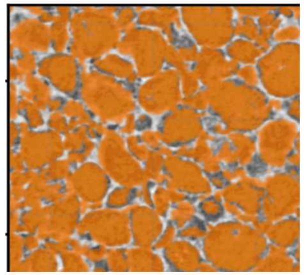
Automated meshing techniques from ML output of a Bayesian CNN, propagating UQ through to physics predictions.
Exemplars: Battery materials, woven composites, laser welds.

Incrementally trained Deep-Learning (DL) model segments to high accuracy, higher than human labels in some cases

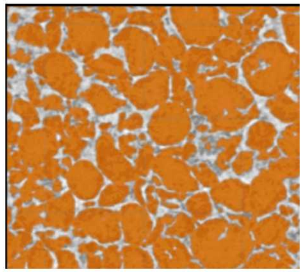
DL inferences takes minutes on GPU vs. hours to days manually!



Slice from CT image of graphite electrode



Human label (orange) overlaid on CT scan of battery



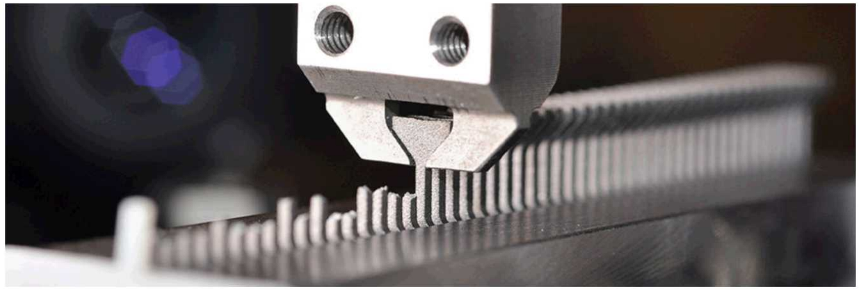
Deep learning label (orange) overlaid on CT scan of battery

This work proves DL models are capable of flexible and accurate image segmentation with rigorous per-voxel UQ estimates (but still requires labor-intensive training data).

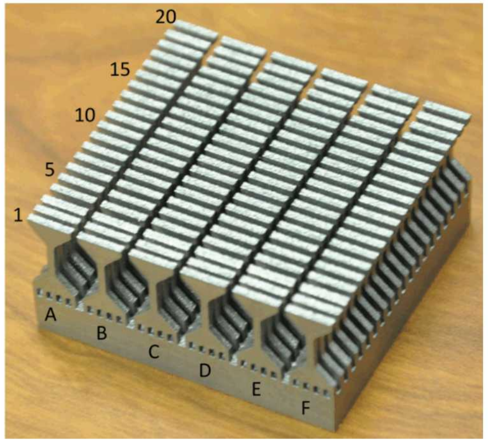
Mechanical Properties Mapping to AM Build Plate Location

PI: Laura Swiler

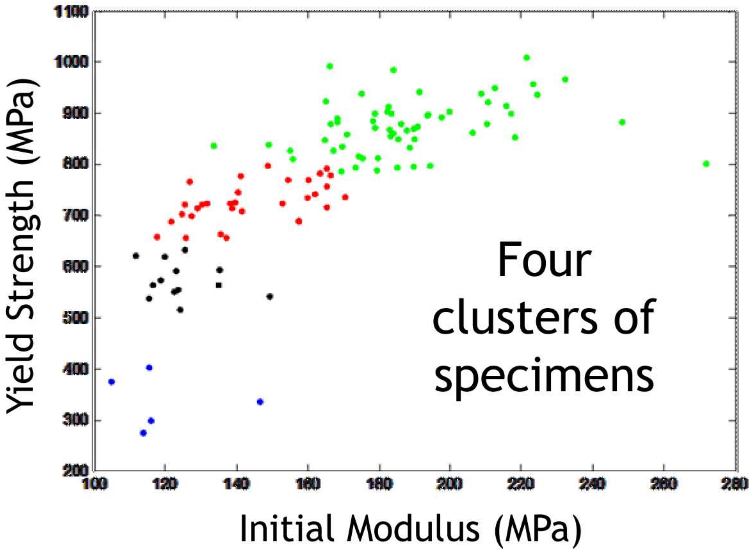
Goal: Correlating many material properties together with AM build plate location



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



- High-throughput testing for many replicates of tensile tests, here for additively manufactured stainless steel.
- Use of k-means clustering to identify sets of feature values correlated to location on the build plate
- The four clusters identified over 15 material properties are projected onto two of the material properties showing a delineation of the clusters. The four clusters were mapped onto the build plate, showing some correlation of clustering with respect to build location.



	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

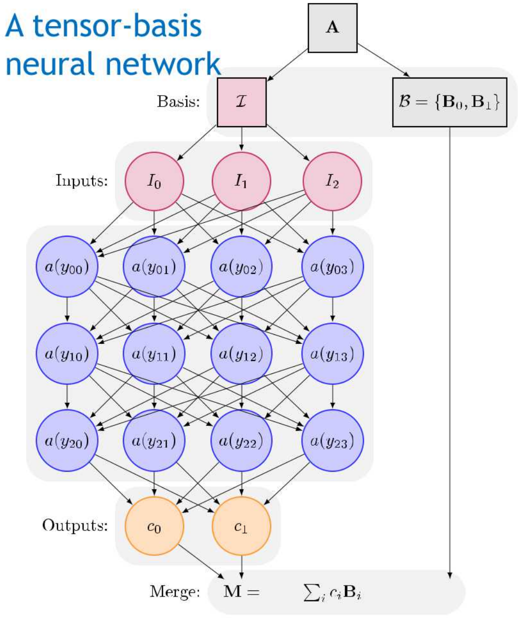
ML methods can correlate many specimens across several mechanical properties.

Neural network models of plasticity for metals with microstructure

PI: Reese Jones

Goal: Utilize crystal microstructure to predict deformation

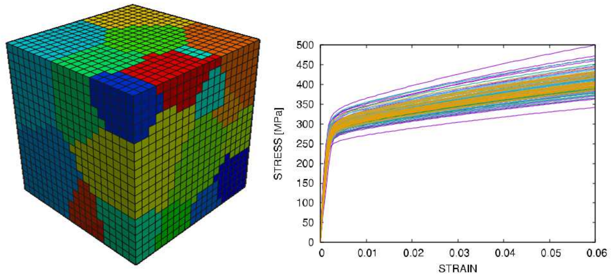
A tensor-basis neural network

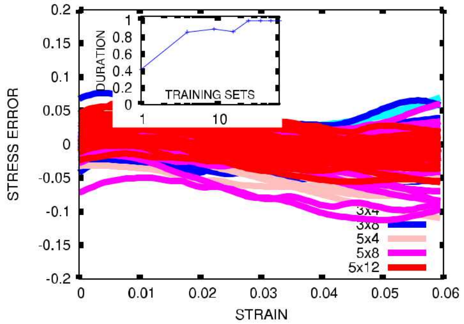


This research involved design of novel neural networks to model plastic flow of metals with microstructure

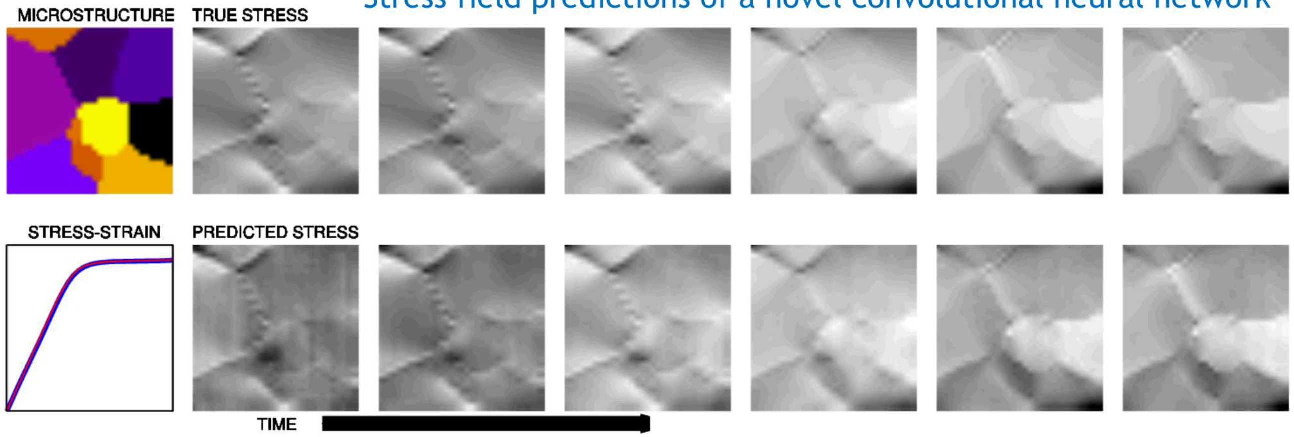
- Employing traditional representation theory allows the networks to **preserve** symmetries and physical constraints exactly instead of learning them imperfectly [1].
- Convolutional layers allow the models to **discover** what features in the initial microstructure are needed to predict the mechanical

Synthetic data based on crystal plasticity simulations from 4 grain structures (grouped by color in stress-train plot) with varied grain orientations





Stress field predictions of a novel convolutional neural network



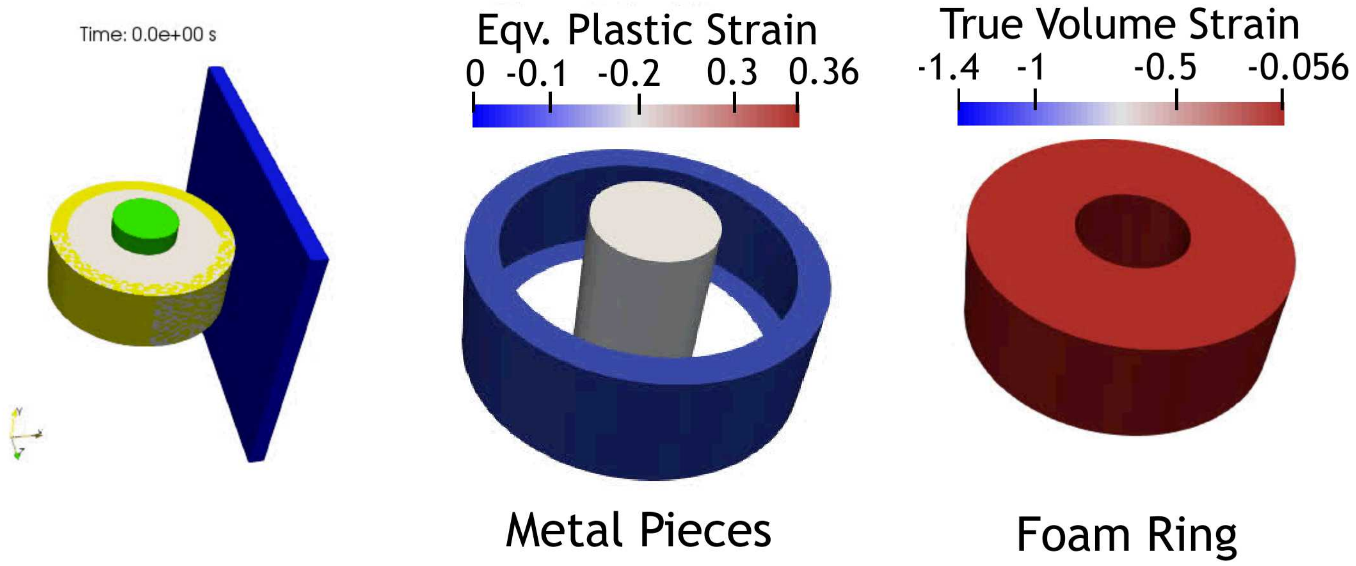
[1] Jones, RE et al. "Machine learning models of plastic flow based on representation theory.", *Comp.Mod,Eng.Sci.,* 2019
[2] Frankel, A et al. "Predicting the mechanical response of oligocrystals with deep learning." *Comp.Mat.Sci.,* 2019
[3] Frankel, A et al. "Prediction of the evolution of the stress field of polycrystals undergoing elastic-plastic deformation with a hybrid neural network model." *arXiv,* 2019

Two different ML methods were developed/applied to model homogenized and local stress responses based on synthetic crystal plasticity data.

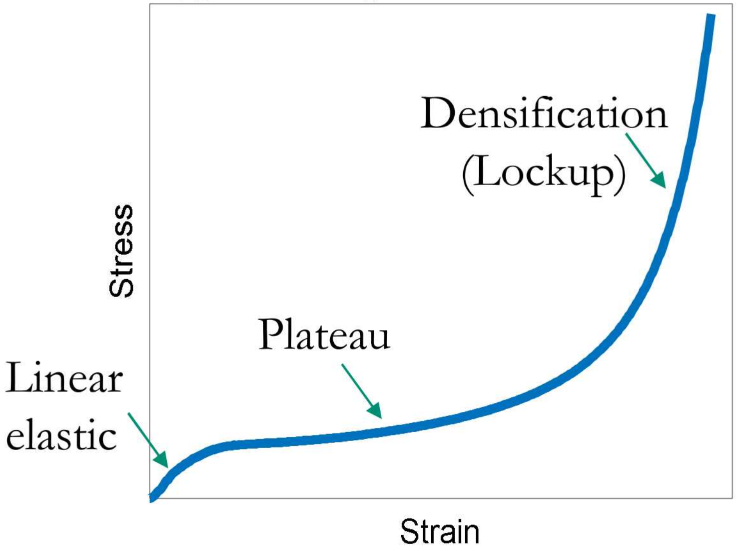
Machine Learning for Polymer Foam Mechanics

Extreme Deformation of Foams

Inspiration: Crash Scenario at 65 mph



Typical σ-ε profile for PU foam



Modeling Approaches:

- Phenomenological empirical fits generally, with a few micromechanics-based models for low-density foams
- Lacking microstructural understanding generally
- Lacking solid polymer physics understanding

Foam Research Areas:

- Fundamental understanding of role of microstructure in large deformation mechanics for all densities
- Utilization of full-field experimental data to inform development of new models and calibration of them

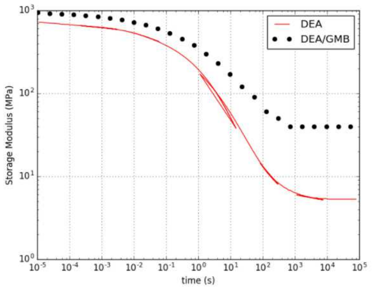
There is little literature on large deformation of polymer foams, particularly of moderate density. Current models are cumbersome and require calibration for every density.

Technical Approach

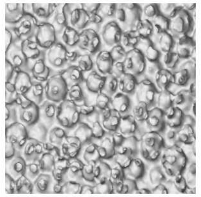
Project Objective: Discover how the large deformation behavior in polymer foams is governed by the interplay of foam microstructure and solid polymer behavior

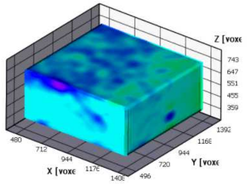
Experiments

Solid Polymer

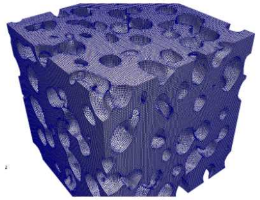


Foam (Flexible PU)

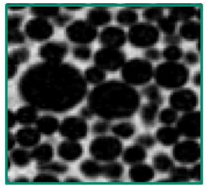


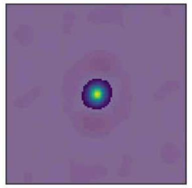


RVE Simulations



Microstructural Analysis / Unsupervised Machine Learning

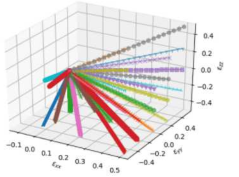


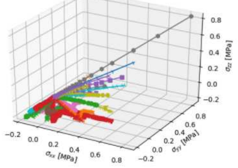


Machine-Learned Model

INPUTS → OUTPUTS

$\phi, \epsilon_{xx}, \epsilon_{yy}, \epsilon_{zz}$ → $\sigma_{xx}, \sigma_{yy}, \sigma_{zz}$



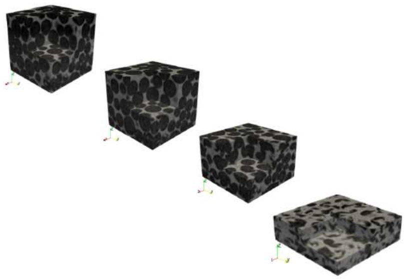


Constitutive Model

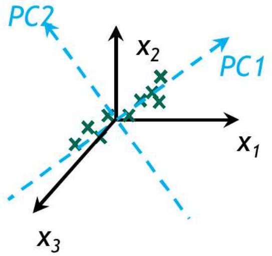
$$\Psi_{\text{foam}} = \Psi_{\text{foam}}\left[\mathbf{E}, \Theta, \Psi_{\text{solid}}, \frac{\rho_{\text{foam}}}{\rho_{\text{solid}}}, \xi_1, \xi_2, \ldots\right]$$

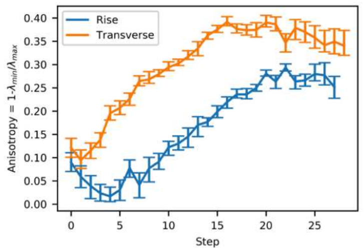
Machine Learning Tools for Foam Mechanics

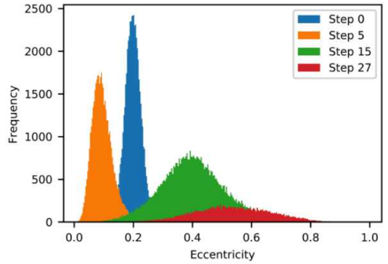
Goals: (1) Discover the important microstructural metrics and their evolution with deformation
(2) Develop a constitutive model given a set of microstructural descriptors



Spatial Statistics, PCA, etc.







INPUTS

Microstructure, strain state, history

$\phi, \epsilon_{xx}, \epsilon_{yy}, \epsilon_{zz}$

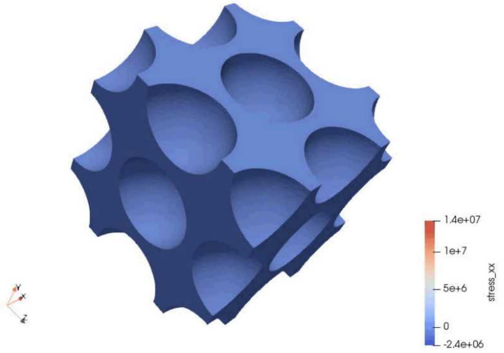
→ ML model →

OUTPUTS

Stress state

$\sigma_{xx}, \sigma_{yy}, \sigma_{zz}$

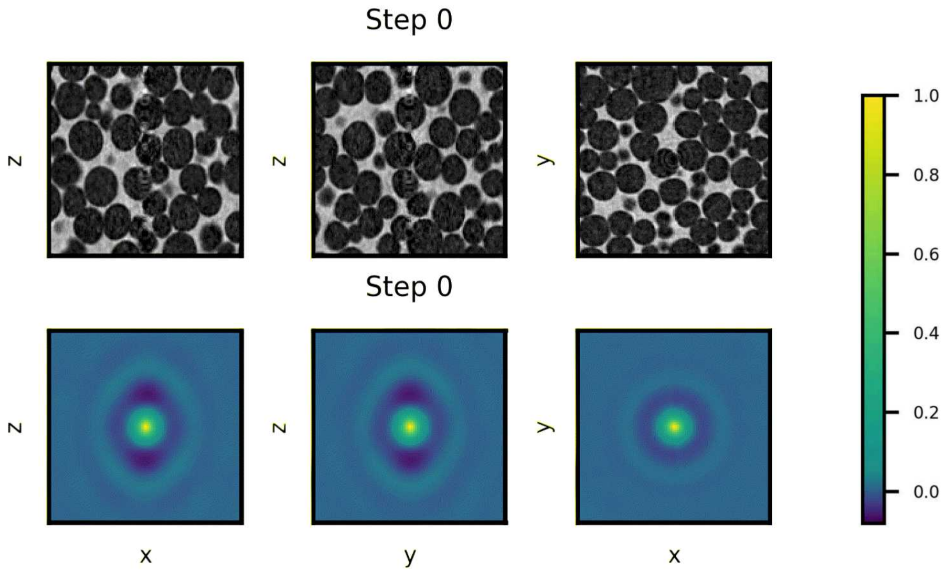
Body-Centered Cubic 2x2x2 Periodic Structure
0.25, 0.45, and 0.65 Initial Porosity
Gent Matrix (Sylgard 184) with a fixed shear mod and lockup



Microstructural Analysis: Spatial Autocorrelation and Anisotropy

Strength of correlation between two points separated by vector **r**

$$A(\mathbf{r}) = \frac{\langle I(\mathbf{x}+\mathbf{r})I(\mathbf{x})\rangle - \langle I(\mathbf{x})\rangle^2}{\langle I(\mathbf{x}) - \langle I(\mathbf{x})\rangle\rangle^2}$$

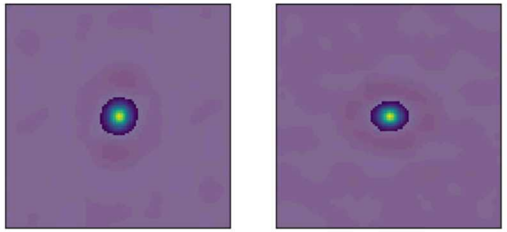


Microstructure and ACF for 15-pcf PU Foam in Three Orthogonal Orientations

- Moment of inertia (MOI) tensor of level set of ACF
- Anisotropy = 1- (λ_{min}/ λ_{max}), where λ_{min}, λ_{max} are the min and max eigenvalues of the MOI tensor
- This method is not sensitive to level set choice and does not require image segmentation

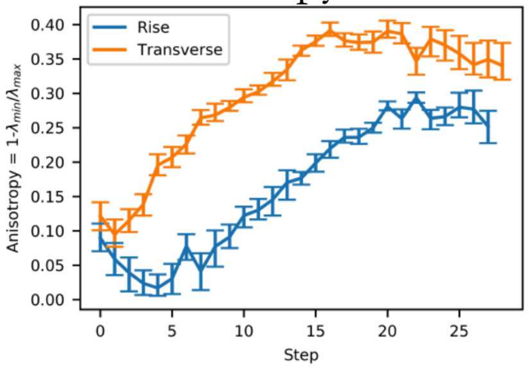
Level Set of ACF

Undeformed ~28% strain

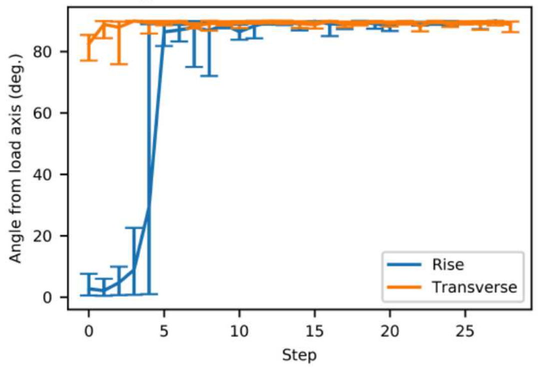


15 pcf PU, rise direction
Compression is along vertical direction

Anisotropy Ratio



Angle From Load Axis



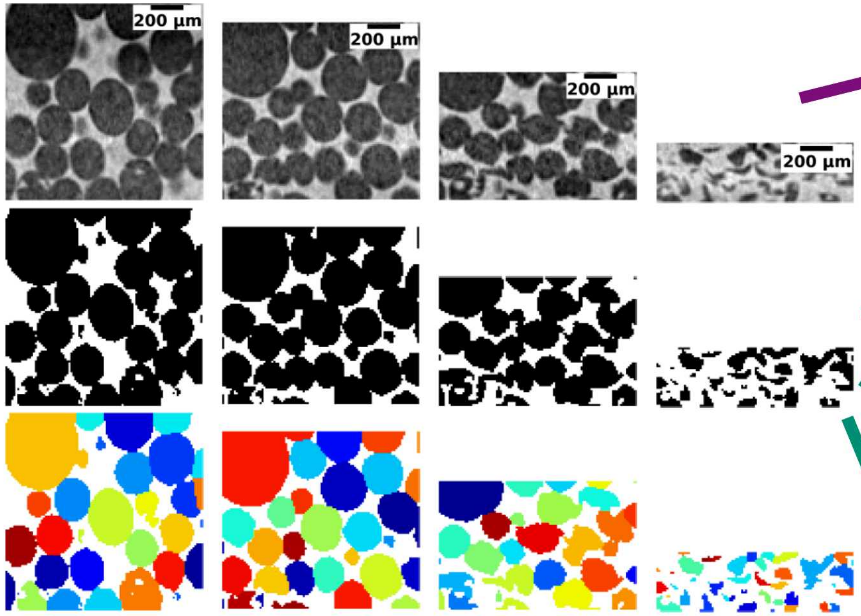
The ACF and MOI analyses allow for physical insight regarding evolution of anisotropy with deformation and for dimensionality reduction.

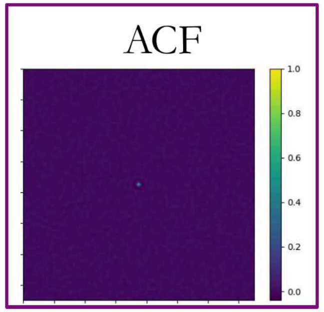
Segmentation

Original grayscale data: does not directly distinguish pore/solid phases

Binarized data: separate pore/solid (thresholded data / semantic segmentation)

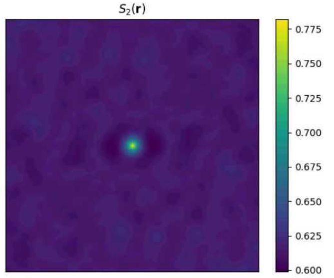
Labeled data: separate individual pores (instance segmentation)



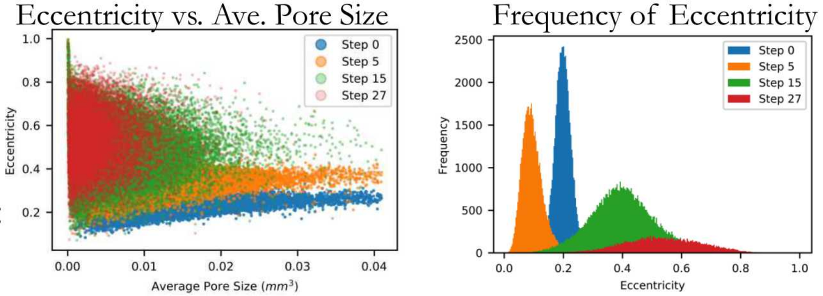


Two-Point Correlation (S_2)

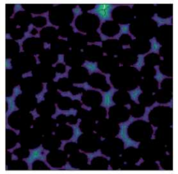
Probability two points are in the pore phase



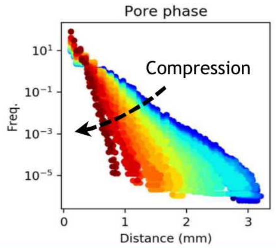
Statistics of individual pore size, shape, etc. with deformation:



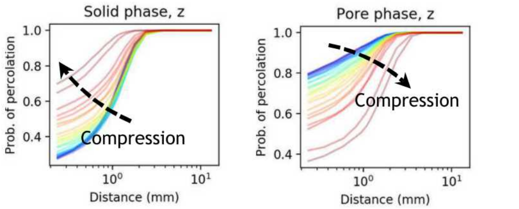
Distance transform at medial axis of solid phase: connect to evolution of distance between pores



Distribution of solid phase 'thickness'

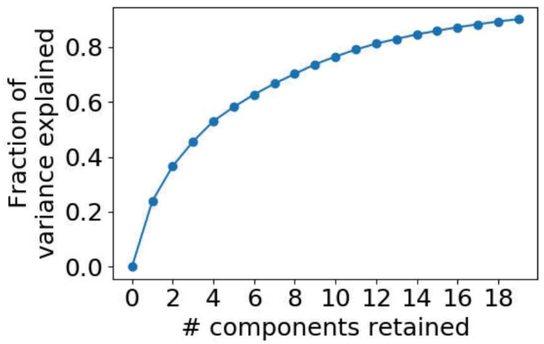


Measures of topology/connectivity, e.g. probability of percolation as a function of subvolume length scale:



Segmentation is standard in quantitative image processing, but can also be thought of as 'data preparation/pre-processing'. It enables more physically intuitive metrics.

Automated Feature Extraction with Principal Components Analysis (PCA)



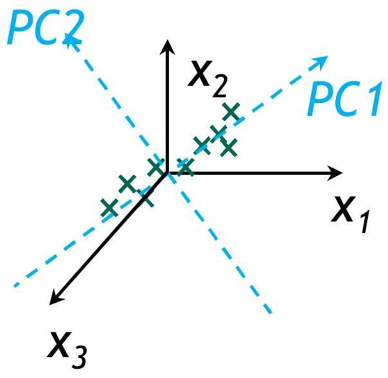
20+ components required to explain variance (better than 500^3)

Challenge

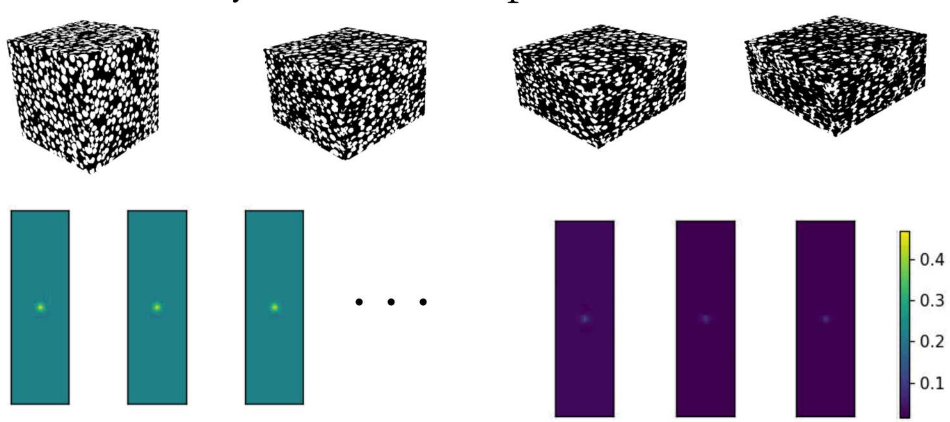
Systematically discern/describe differences between multiple structures due to:

1. high dimensionality of metrics
2. potentially subtle differences between metrics across structures

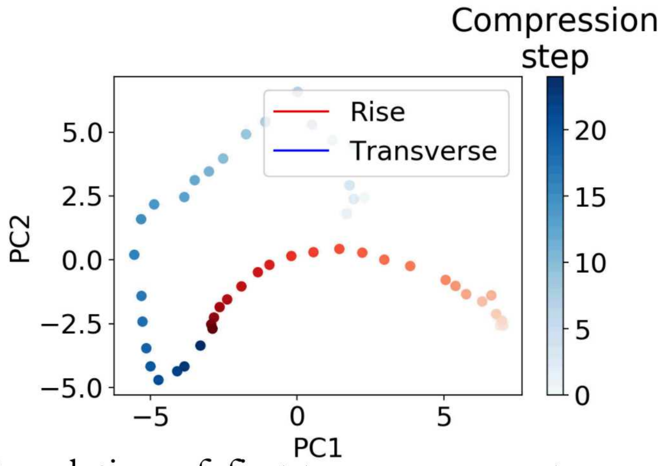
Principal components analysis (PCA) of ACF* :



Polyurethane compression scans



*Method from Kalidindi et al, *JOM* 63.4 (2011), Choudhury et al, Acta Mat 110 (2016)



Correlation of first two components are different for rise and transverse orientation of foams relative to compression

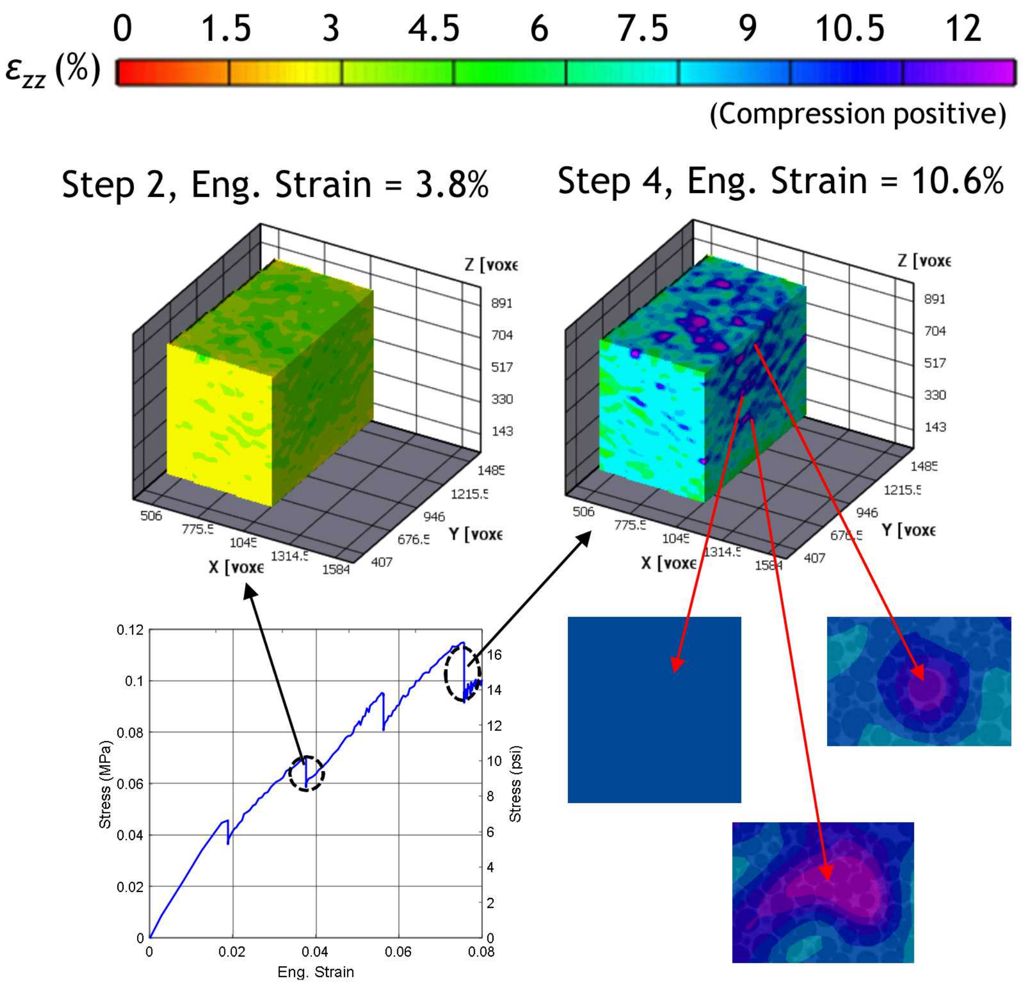
PCA can help order the relative magnitude of effect of principal components on mechanical response, but connecting the principal components to microstructural feature is nontrivial.

Future Work and Challenges for Unsupervised Learning on Foam

- **Future Work**:
  - Comparison of X-ray CT scans/DVC with RVE simulations
  - Deep learning/CNN model to predict local strains given undeformed scan
  - Variational auto-encoder (VAE) for dimensionality reduction/feature extraction of CT scans

- **Challenges**:
  - ACF/S_2/PCA → lots of "**needles in the haystack**" that may not link to physical quantities
  - **Little/no physical intuition** from reduced dimensionality features at face value
  - Need for a **copious amount of data** for different boundary value problems, requiring reliance on simulations that are difficult at large deformations
  - Unknowns of **how key microstructural descriptors evolve with generalized motion**, not just the boundary value problems tested

Example of DVC Data From *in situ* XCT Scans



Unsupervised learning techniques support dimensionality reduction, but interpretation of the results are nontrivial and difficult to connect to physical quantities to build new insights.

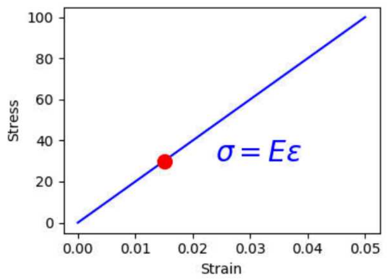
Mechanics Modeling Approaches

Physics-Based Constitutive Modeling

- Typically relatively few parameters, in principle measurable from very few simple experiments
- Extrapolates beyond calibration data (but can fail if assumptions of physics-based model are broken)
- Accuracy tied to quality of physical model as well as calibration data
- UQ more challenging due to model form error

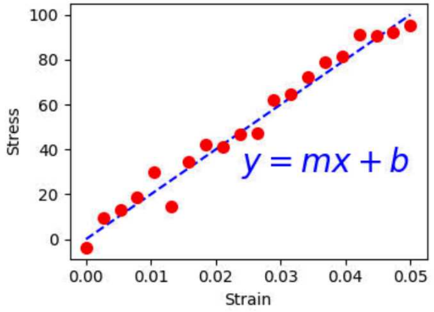
Phenomenological Modeling

- Utilizes experimental data to drive the form of the model, requiring extensive data for a comprehensive model
- Requires mechanics constraints be met (usually)
- Extrapolation beyond the calibration data is tenuous
- Assumptions (like isotropy, etc.) can lead to poor fitting of the data
- UQ challenging due to model form error



Data-Driven Machine Learned Modeling

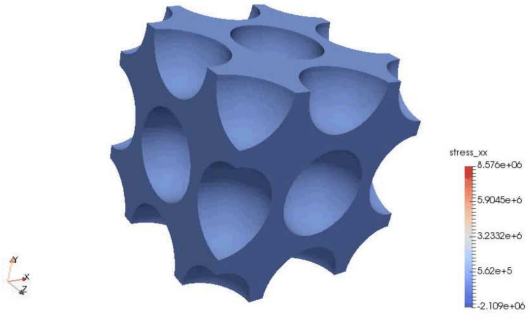
- Potentially very large numbers of parameters, require large datasets
- Extrapolates poorly beyond measured data
- Accuracy relies solely on measured data, thus bias and measurement errors can lead to errors in the model
- UQ potentially more tractable

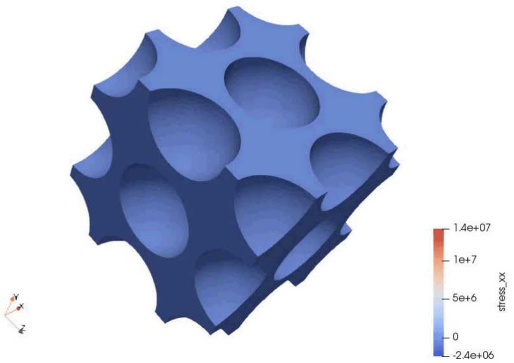


Modeling Moving Forward: Each regime can be improved by the other – more physics in data-driven methods and more data in traditional methods.

Proof of Concept: RVE Simulations and Use of Physical Insight

RVE Simulations (Microstructure + Polymer Physics) Seeding Machine-Learned Modeling

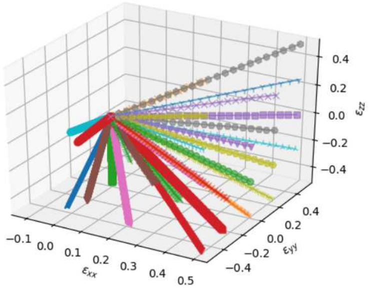


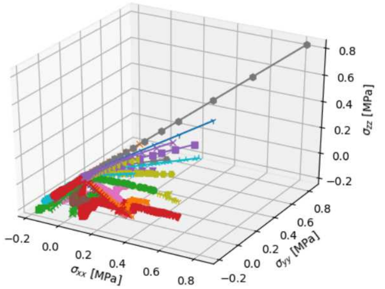


INPUTS → ML model → OUTPUTS

$\phi, \epsilon_{xx}, \epsilon_{yy}, \epsilon_{zz}$ → ML model → $\sigma_{xx}, \sigma_{yy}, \sigma_{zz}$

Exploit Material Symmetry: Work In Principal Space



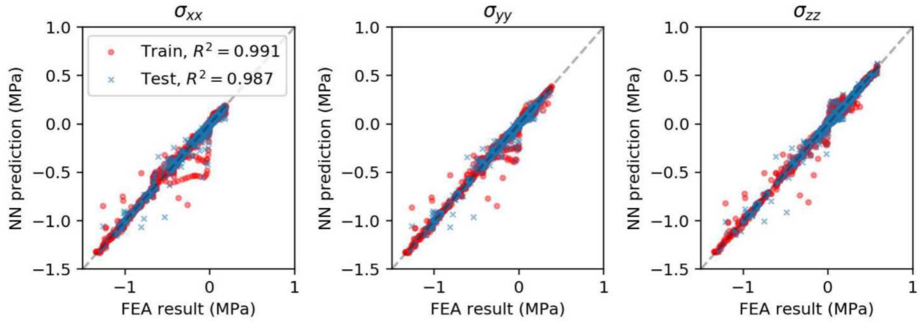


Preliminary Results

- Tried simple, fully connected neural networks with 1-3 hidden layers
- Data with excessively large stresses are excluded
- 80% of data used for training, 20% held out for testing
- Loss function modified in all cases to minimize total *relative* error:

$$\sum_{i=1}^{N}\left(\frac{y_{predicted} - y_{actual}}{y_{actual}}\right)^2$$

- Results for all pairings of porosity, stress → strain



- NN fits to data are encouraging, but even simple loadings (BVPs) give unphysical results

The first attempt at ML modeling here demonstrates that simple ML modeling provides results with relatively low errors, but sometimes unphysical stresses, requiring improvements in our approaches.

Future Work for Modeling on Foam

Input:
Microstructure, **3D strain**
(later add history, strain rate…)

→ ML model →

Output:
3D stress state

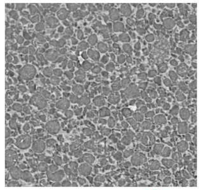
- Expand space of microstructure beyond porosity (e.g. anisotropy, correlation length scale, material thickness)
- See about Gaussian process models to provide uncertainty of prediction
- Incorporate history via e.g. recurrent neural networks
- More realistic microstructures for training data
- Augment training data with experimental data, investigate different weightings to reflect different relevance of experimental and simulation data
- Incorporate insights from ML modeling into a traditional physics-based constitutive model and compare performance

Machine learning for foams in an age of high-dimensional data is natural, but modeling of the deformation behavior requires physical insight and mechanics constraints.

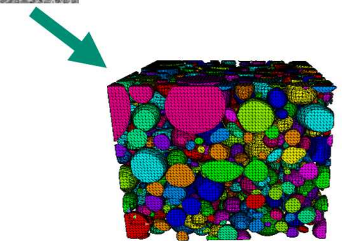
Summary and Discussion Points

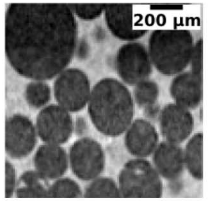
Summary: Examples of ML and Mechanics at Sandia

ML Related to Images



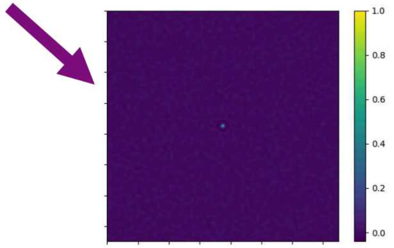
Automated Mesh Generation from CT-Scans





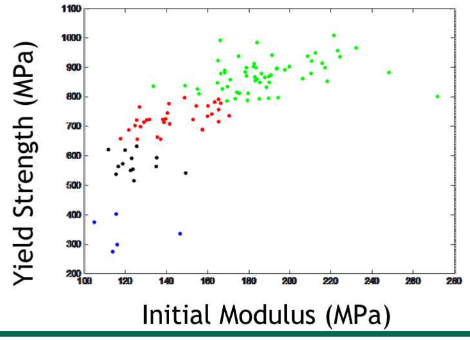
Microstructural Analysis of Polymer Foams

ACF

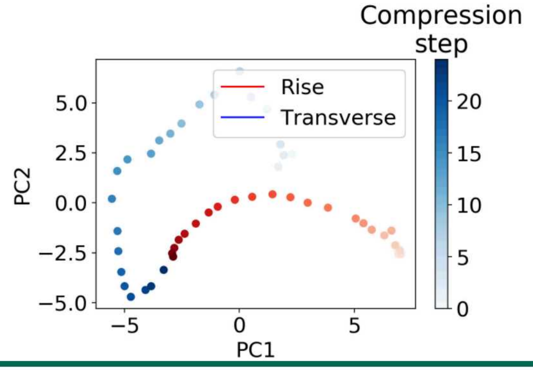


ML Supporting Connections Between Data Types

K-means Clustering of AM Material Properties

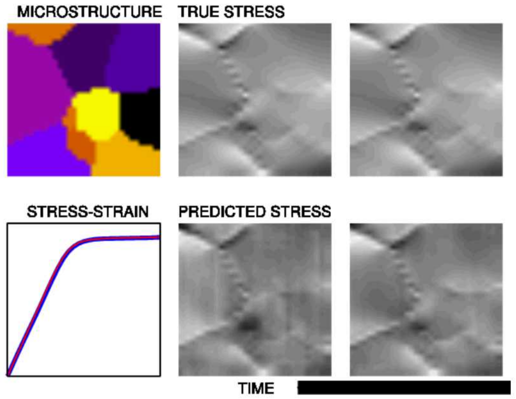


Evolution of Principal Components with Compression Relative of Material Orientation

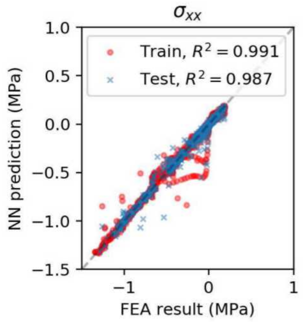


ML for Material Modeling

Use of Microstructure to Predict Plastic Behavior



Microstructure and Solid Polymer Affecting Foam Deformation Modeling



Opportunities and Challenges for ML in Mechanics of Materials

Opportunities

- Dimensionality reduction of data
- Connections between disparate data types
- New paradigm of constitutive modeling that can incorporate physical constraints, data of disparate types, and data of varying size/density (sparse, high-dimensionality, and/or vast quantities)
- Model improvement with more data
- Efficiency of trained model
- Physical intuition present in the model *sometimes*
- Opportunities of uncertainty quantification – relative confidence in decisions based on ML models
- Potential for greatly reducing human-in-the-loop at certain stages of engineering analysis (not upfront)

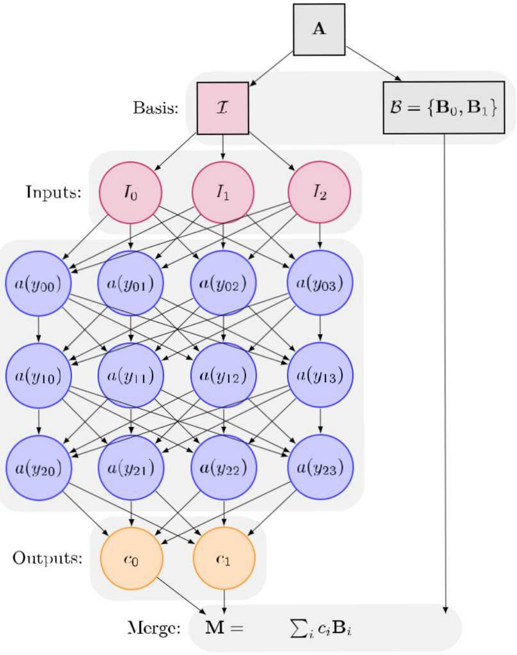
Challenges

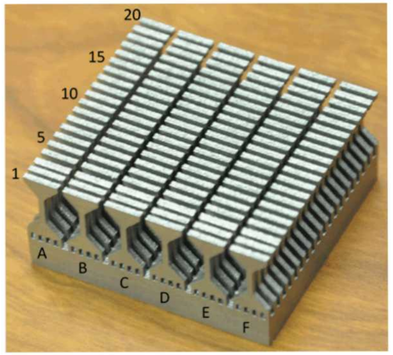
- Need for discovery of new physical intuition that can be difficult to find with many ML methods
- Credibility of ML for decision making for high-consequence applications, particularly based on sparse training data
- Use of ML to speed-up decision making that is defendable
- Need for physics-constrained models that adhere to mechanics principles
- Extrapolation beyond training space is tenuous
- Sometimes laborious model training process
- Generalizability of ML models (do new interactions dominate in generalized motion not explicitly tested in training space)
- Interpretability of UQ – what does it mean for decision making
- Education of mechanics community on appropriate use of ML methods

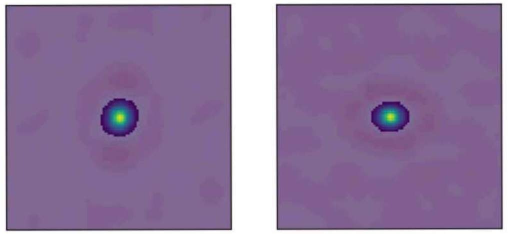
ML can be a disruptive capability in mechanics if used with care.

Summary

- Sandia Mission Space:
  - High-consequence decisions
  - High-dimensional data and low number of samples
- Examples of ML at Sandia
  - Identification of phases from micro-CT scans for automated finite element meshes
  - Clustering of mechanical behavior characteristics and AM build plate
  - Neural network models from plasticity
  - Large deformation polymer foam mechanics
    - Unsupervised learning for microstructural analysis
    - First attempts of regression ML for constitutive modeling







Modeling material variability with ML

Computational Mechanics and Physics of Solids Seminar Series,
University of Colorado, 6 March 2019, Boulder, CO USA

Image based neural networks for physical modeling

Reese E. Jones, A. Frankel
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Sandia National Laboratories

rjones@sandia.gov

U.S. DEPARTMENT OF ENERGY

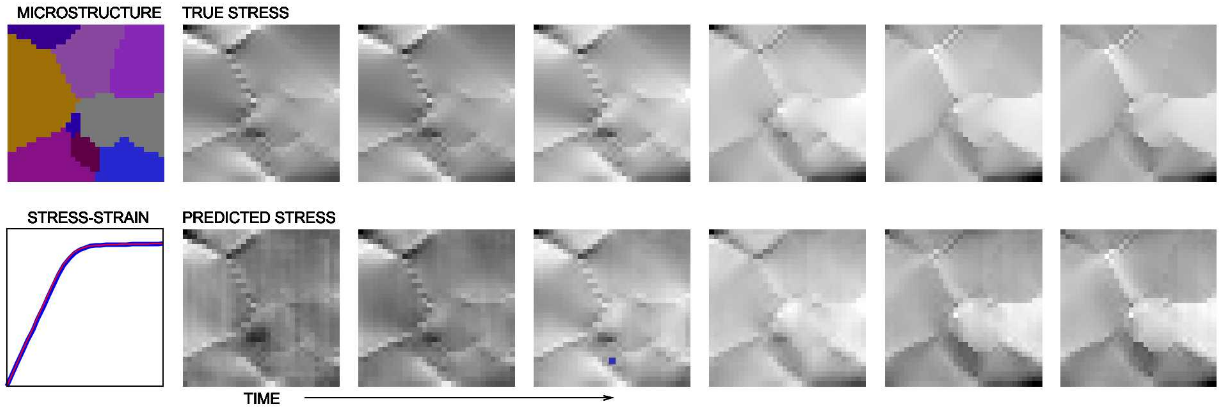

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Image based neural networks for physical modeling

Reese Jones, Ari Frankel

Outline

please ask questions as we go

Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

Objectivity and representation theory

We want to **embed** fundamental **symmetries** in the NN structure – so that they are exact and not learned.

Material frame indifference for constitutive function $\mathbf{M}(\mathbf{A})$

$$\mathbf{G}\mathbf{M}(\mathbf{A})\mathbf{G}^T = \mathbf{M}(\mathbf{G}\mathbf{A}\mathbf{G}^T) \ ,$$

for every member $\mathbf{G}$ of the orthogonal group.
Based on the spectral $\mathbf{A} = \sum_{i=1}^{3} \lambda_i \mathbf{a}_i \otimes \mathbf{a}_i$, and Cayley-Hamilton theorems

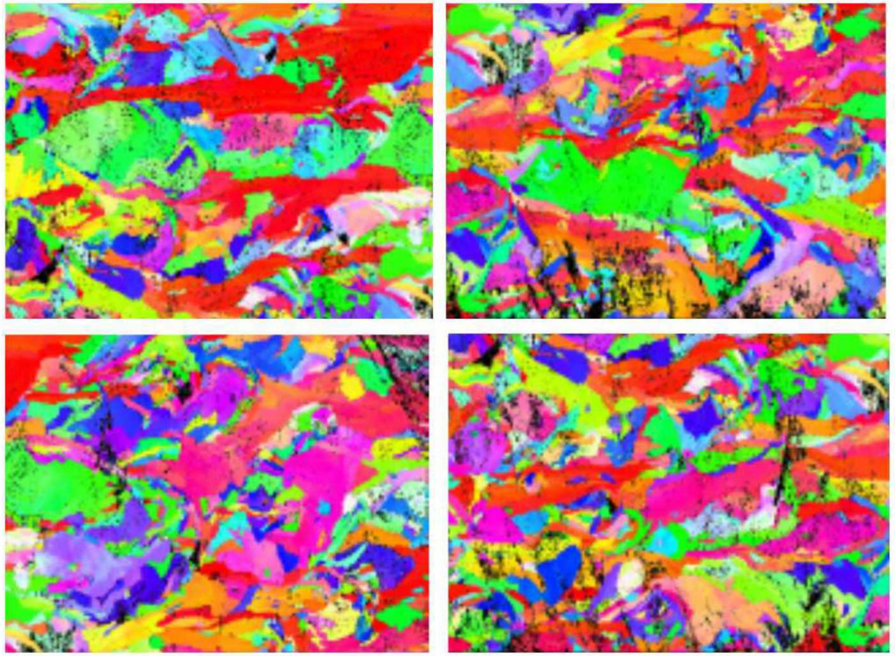
$$\mathbf{A}^3 - \mathrm{tr}(\mathbf{A})\mathbf{A}^2 + \frac{1}{2}\left(\mathrm{tr}^2\,\mathbf{A} - \mathrm{tr}\,\mathbf{A}^2\right)\mathbf{A} + \det(\mathbf{A})\mathbf{I} = \mathbf{0}$$

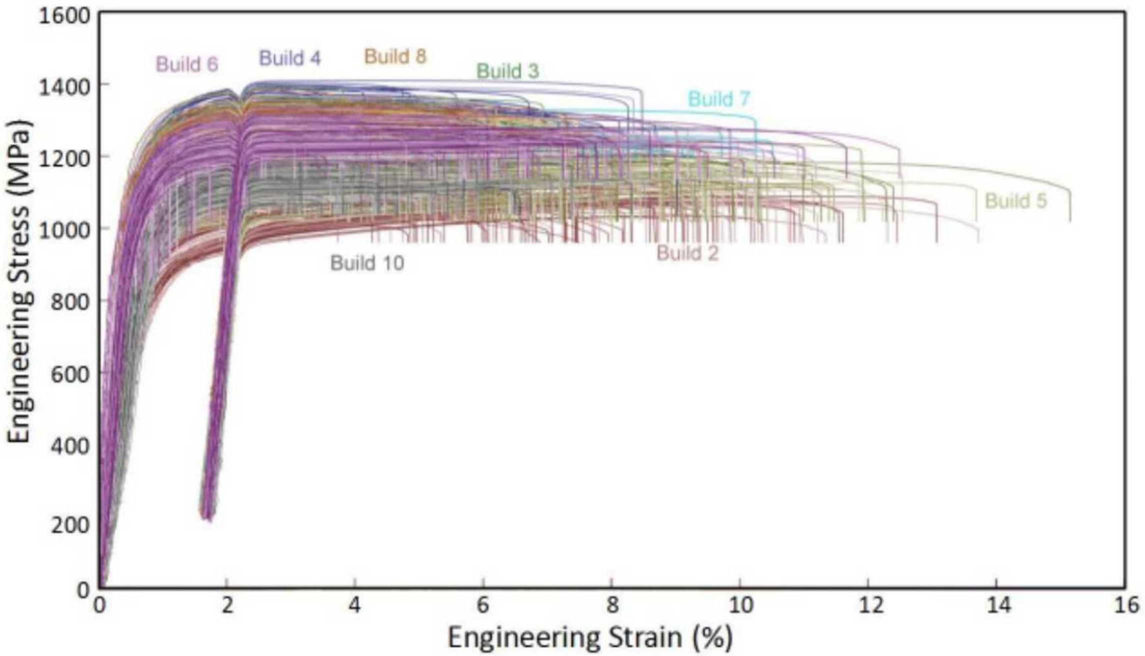
one can obtain a compact **general representation**:

$$\boxed{\mathbf{M}(\mathbf{A}) = c_0(\mathcal{I})\mathbf{I} + c_1(\mathcal{I})\mathbf{A} + c_2(\mathcal{I})\mathbf{A}^2 = \sum_i c_i(\mathcal{I})\mathbf{A}^i}$$

in form of **unknown** coefficient functions of invariants and a **known** tensor basis. Inputs: scalar invariants $\mathcal{I}$ & tensor basis $\mathcal{B}$.

If we observe **initial** microstructures and mechanical tests:

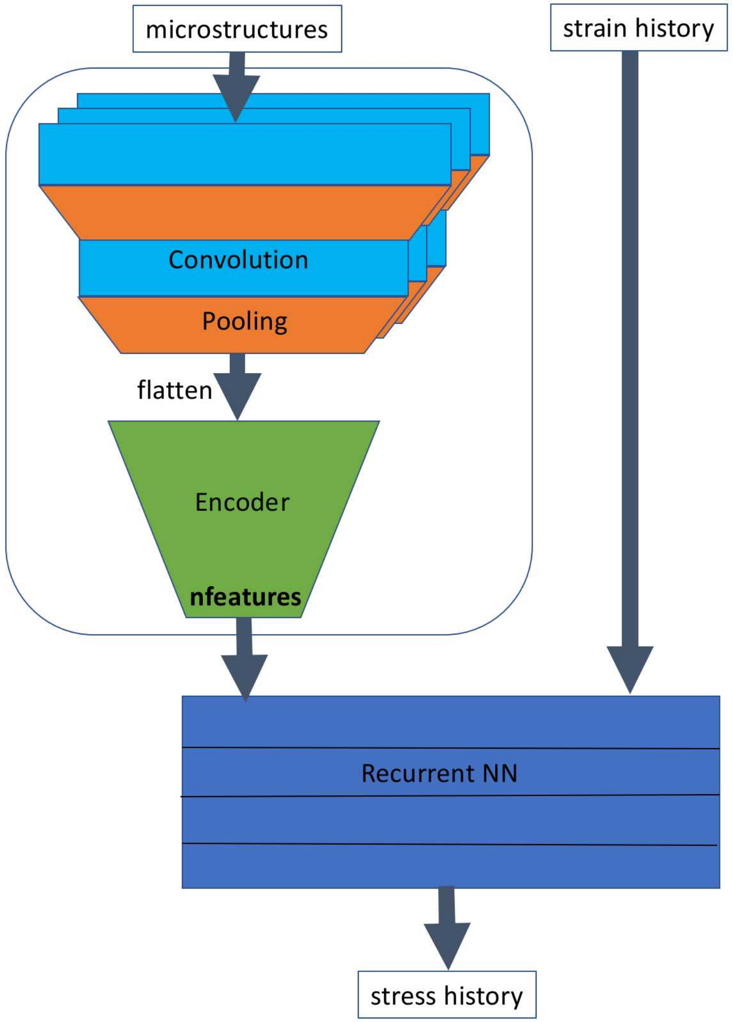




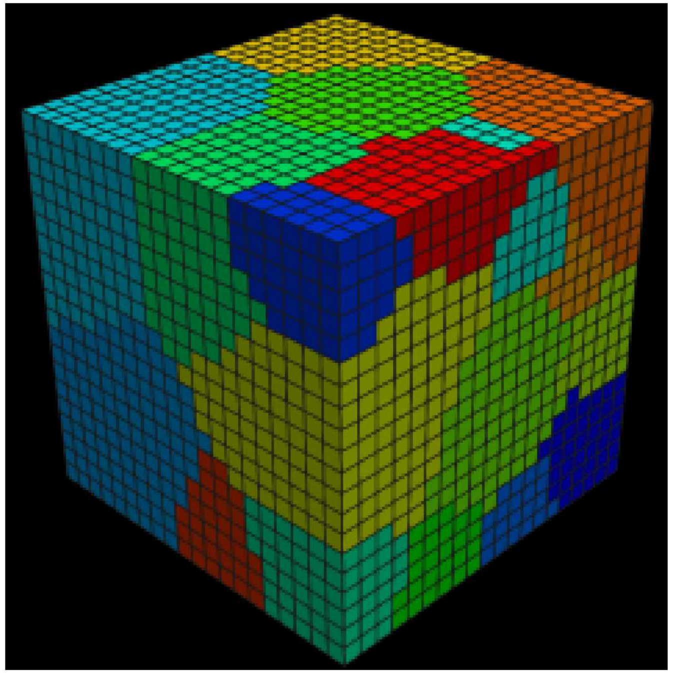
can we **predict** particular stress-strain averages or full field evolution of a polycrystalline material or a material with microstructure in general?

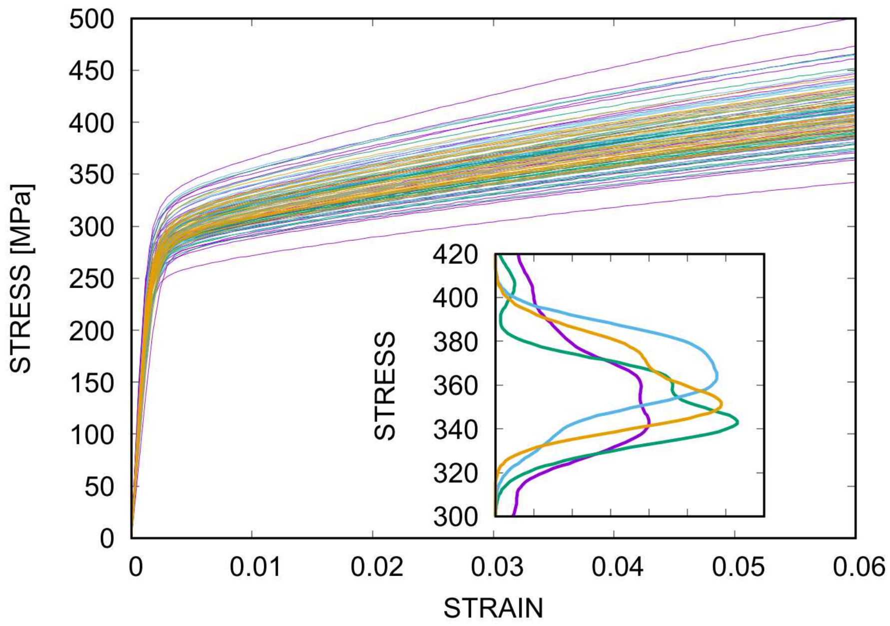
To predict the evolution of the average stress we augment the CNN with a channel that incorporates and processes the loading

The RNN is a layer that uses a causal time filter to process history information. We use a particular kind called a Long Short Term Memory (LSTM) unit which has better performance than a standard RNN.



Even with high-throughput tests we cannot current generate more that a 10^2 tests, we need about 10^4 tests.

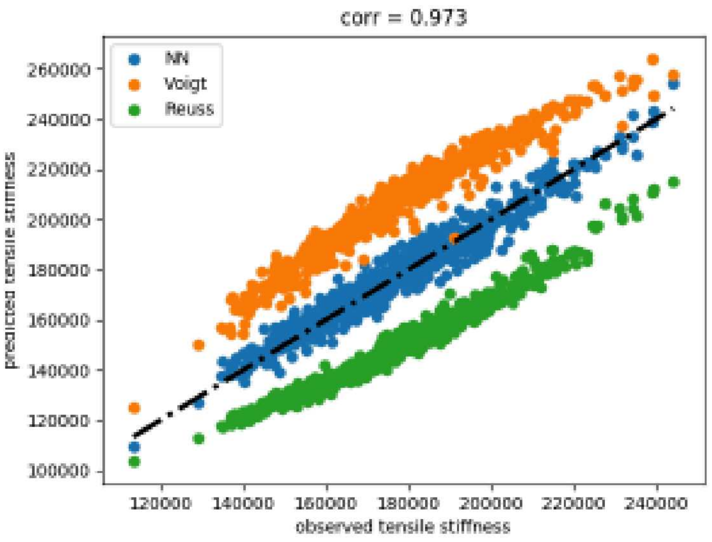




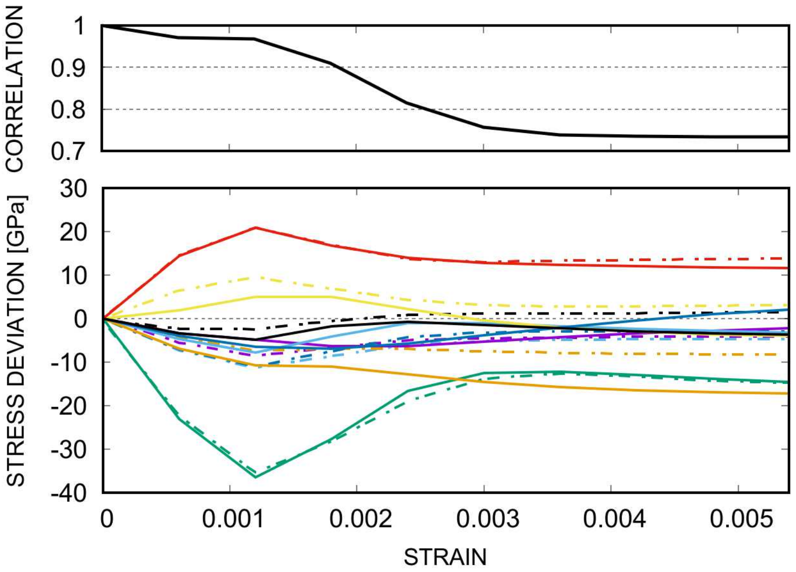
We generated realizations of oligocrystals with different textures (crystal orientations) and run crystal plasticity simulations with a variety of loadings.

Predicting the particular response to microstructure

Using data from the ensemble of polycrystals, we can make predictions of the crystal plastic mechanical response that are significantly better than traditional homogenization theory.



Correlation of elastic response (NN, Voigt and Reuss predictions), NN on par with Hill average.



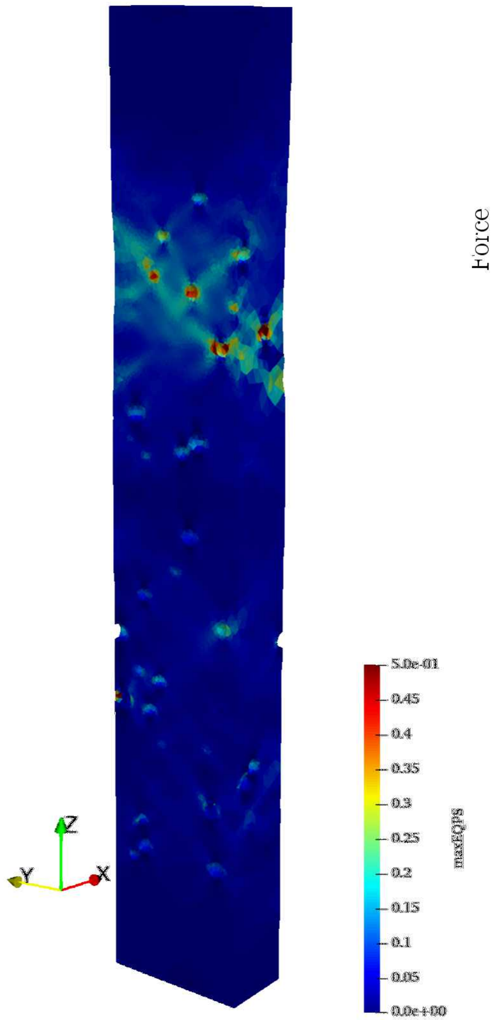
Trajectories of discrepancy from mean: solid lines data, dashed: NN prediction.

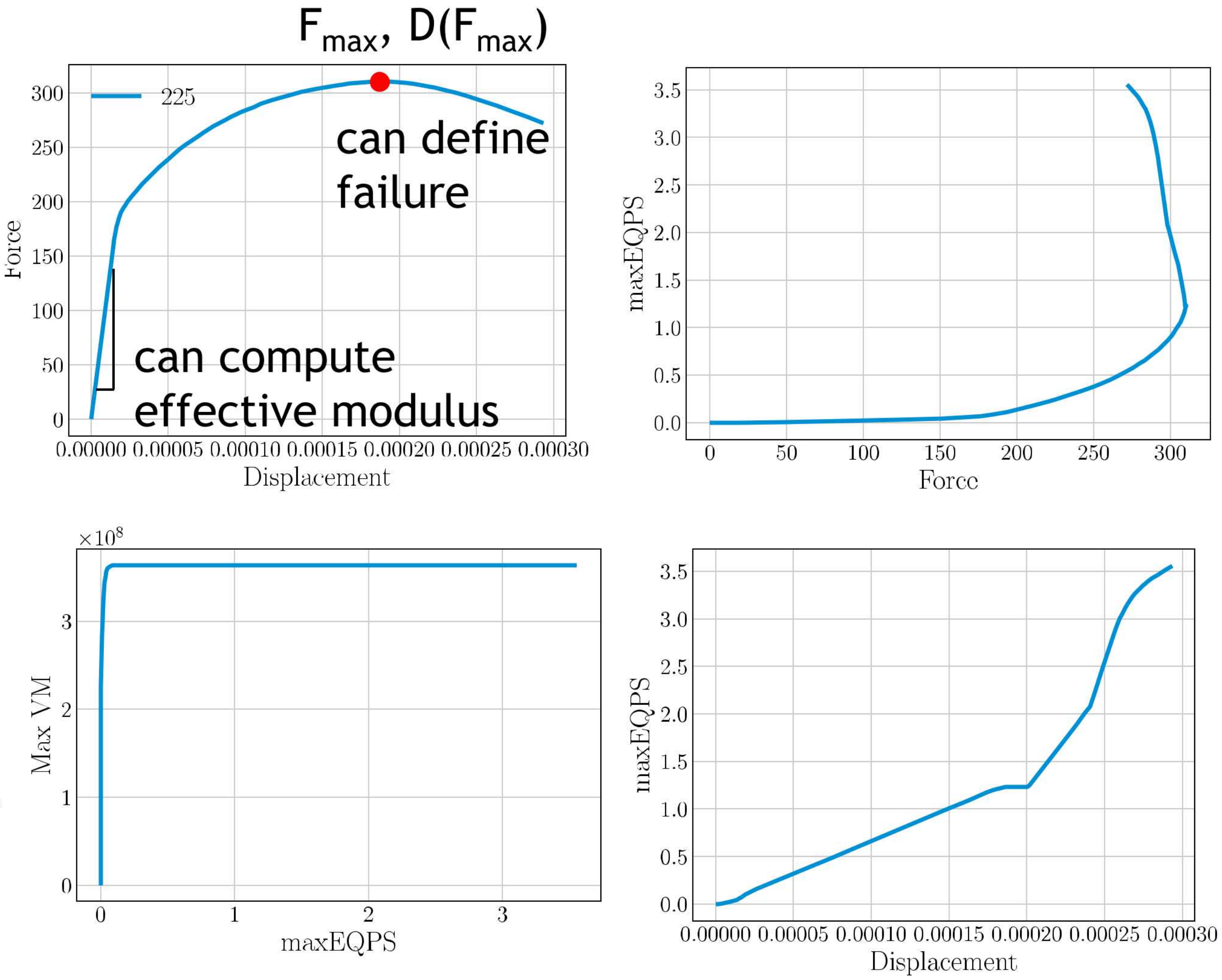
Plastic response is better than Sachs or Taylor estimates.

Machine learning for failure predictions

Kyle Johnson, John Emery, Demitri Maestas

Available data





1,000 samples available

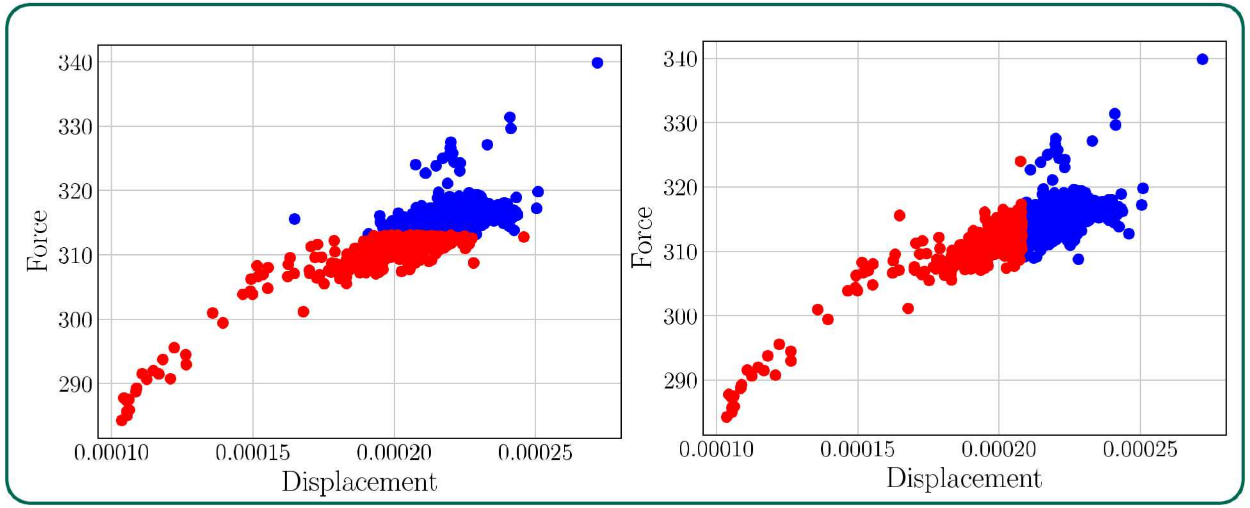
Failure

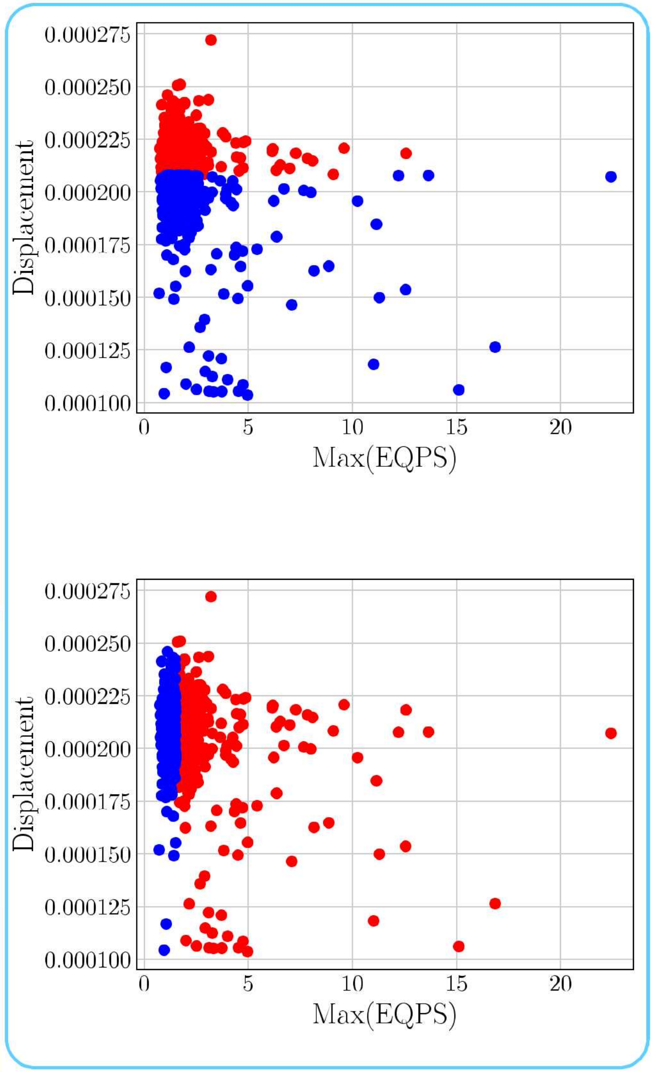
I think we can define failure like this:

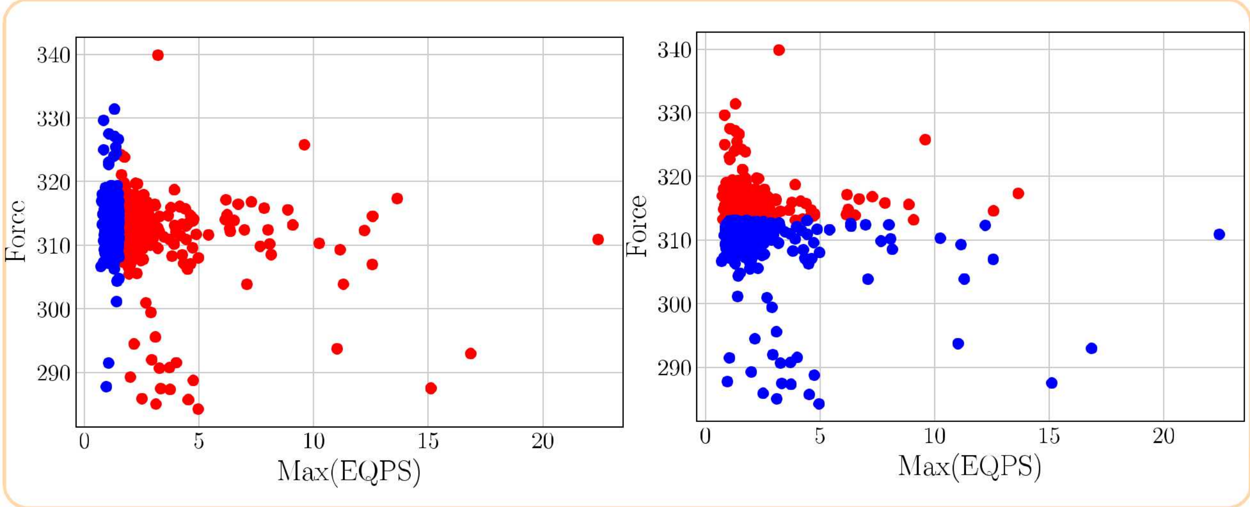
1. peak load (geometric instability) before y displacement
2. failure to carry x load
3. Failure to stay below z overall_max(EQPS) value through y displacement
4. Failure to stay below z overall_max(EQPS) value through z load

I think x load, y displacement and z overall_max(EQPS) are somewhat arbitrary for our purposes, but it seems we'd like to define them so that failure is moderately unlikely. (Demitri's preference for training is 50/50.

500 samples “failure” $\{F_{max}, D(F_{max}), maxEQPS(F_{max})\}$

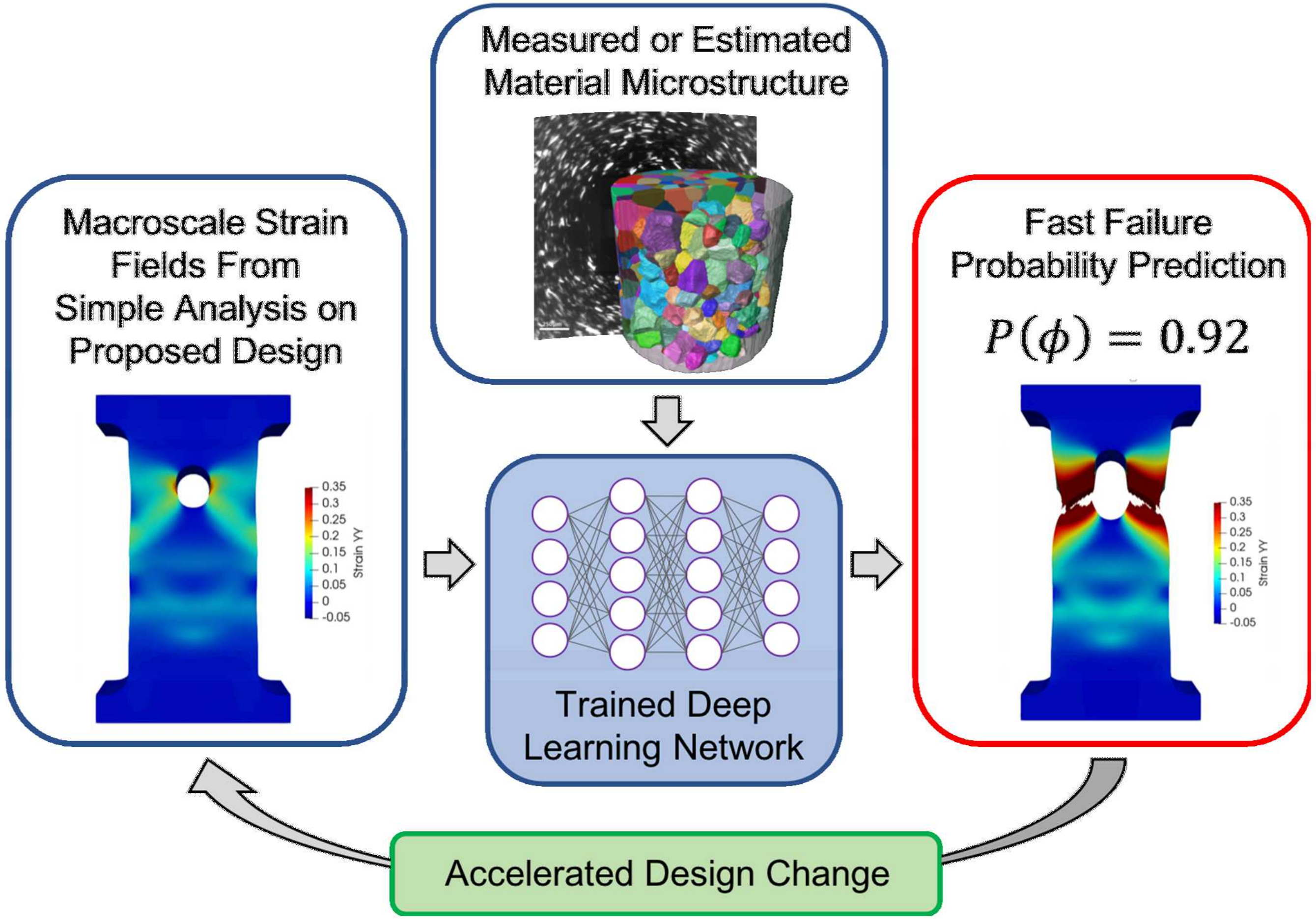




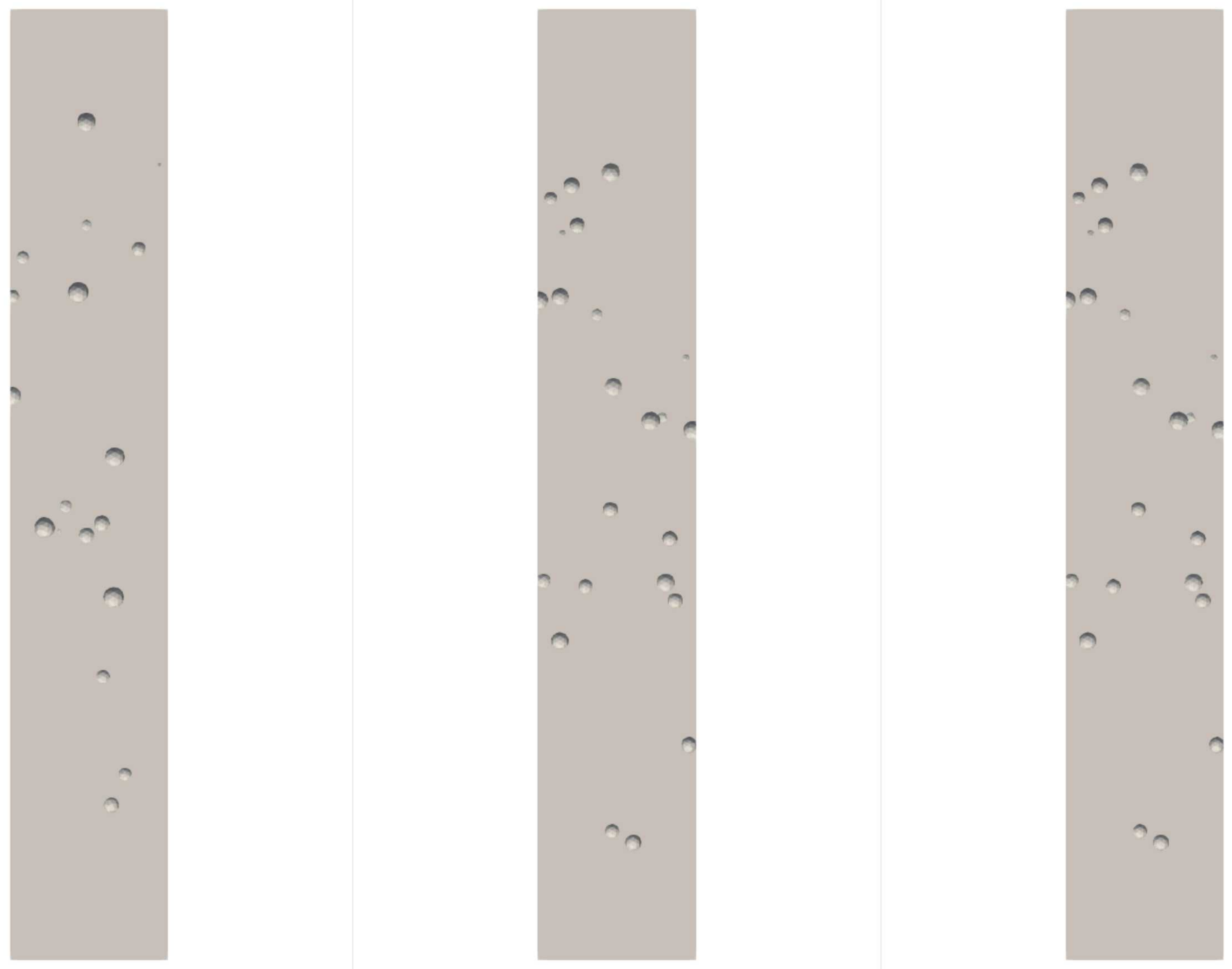


Project Overview

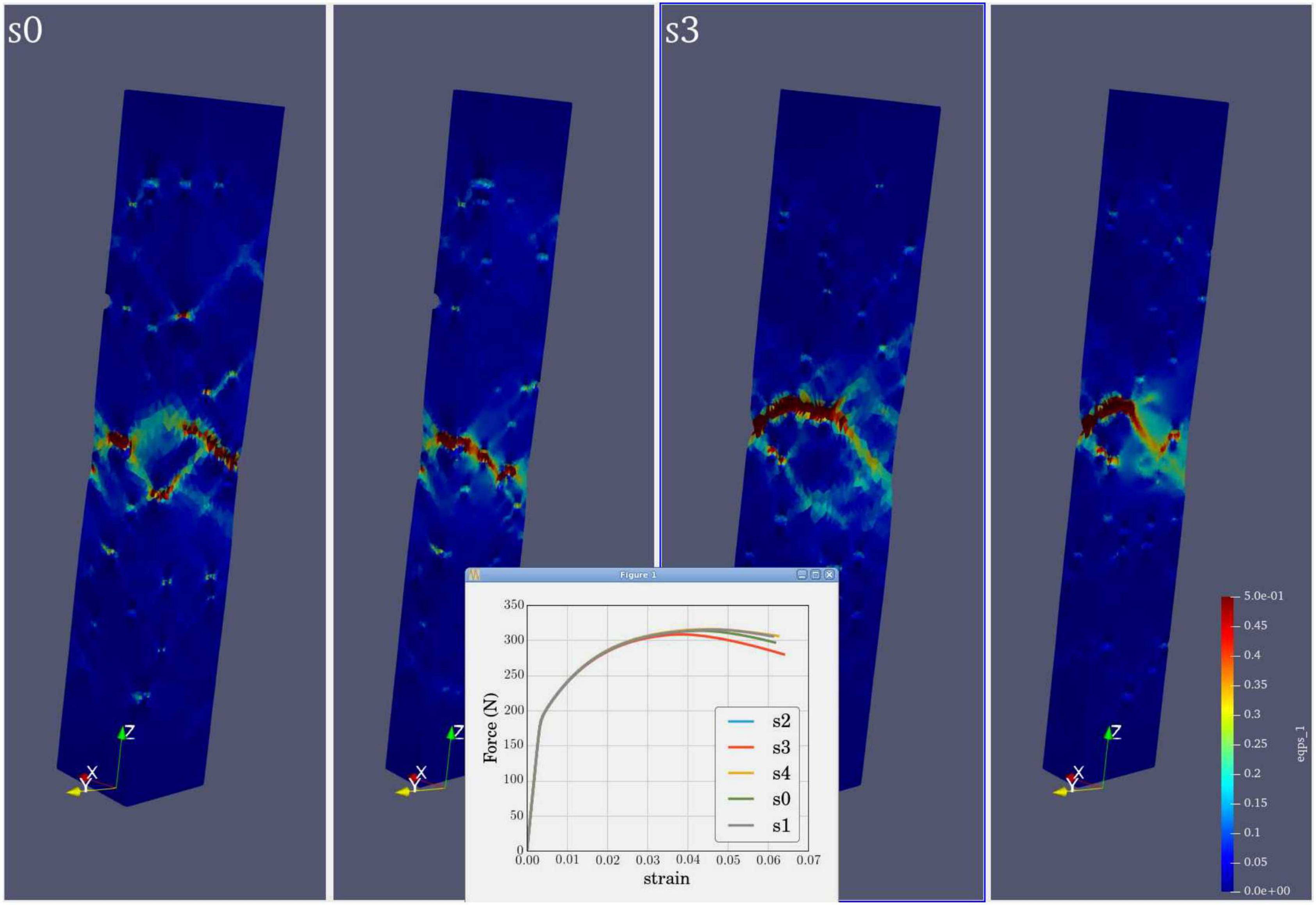
Objective: Quickly and accurately predict failure initiation in component designs using deep learning (DL) pattern recognition. For our initial study we are using Max EQPS as failure indicator.



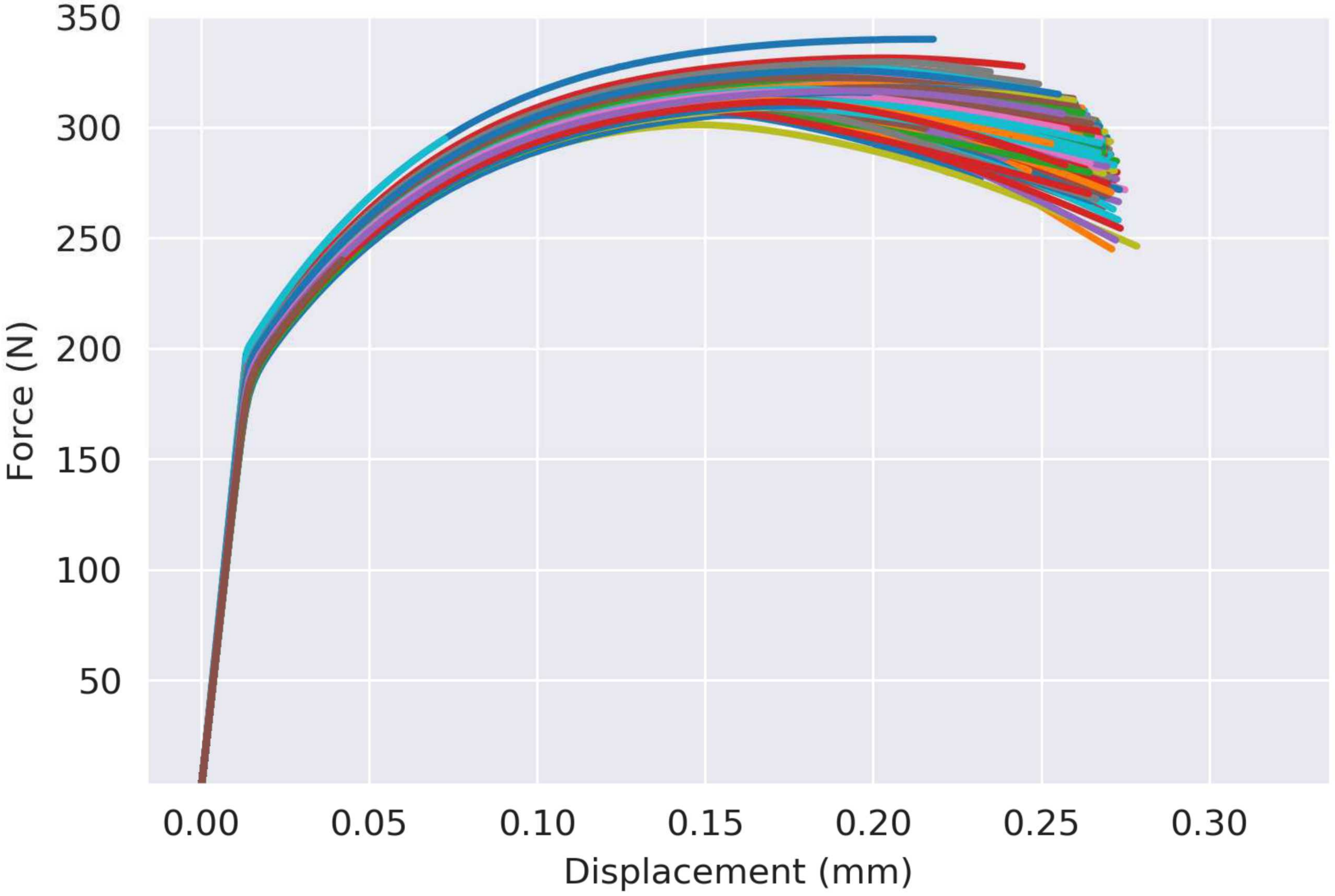
Sample Meshes Based on Porosity Distributions from Jay Carroll's LDRD CT data



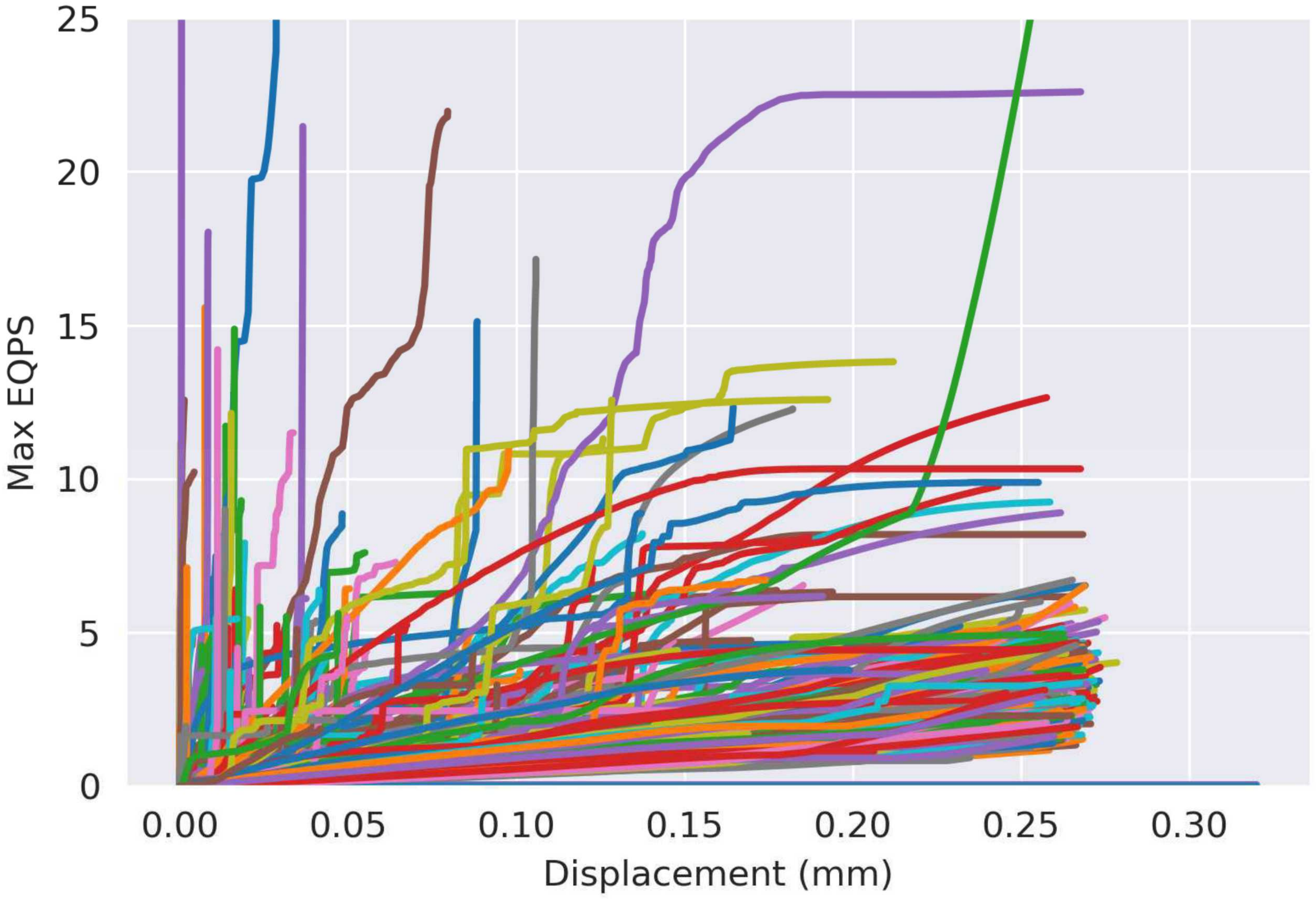
Sample Tensile Results



Approximately 900 Training Tension Simulations Have Been Run



Equivalent Plastic Strain (EQPS) Shows Large Variability



Update from Deep Learning Group

Progress has been made on three thrusts:

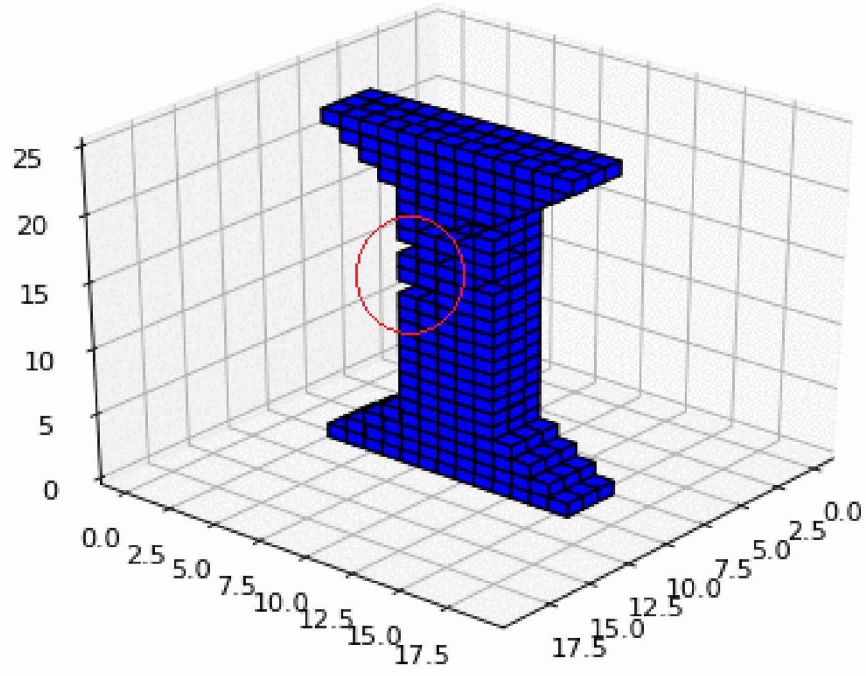
- **Synthetic data generator**
  Provides capability to mimic the converted mesh with specific properties to check performance as we add model and task complexity

- **Deep learning model implementation**
  Implementation of a 3D CNN for binary failure classification

- **Conversion tool from exodus mesh to NumPy arrays**

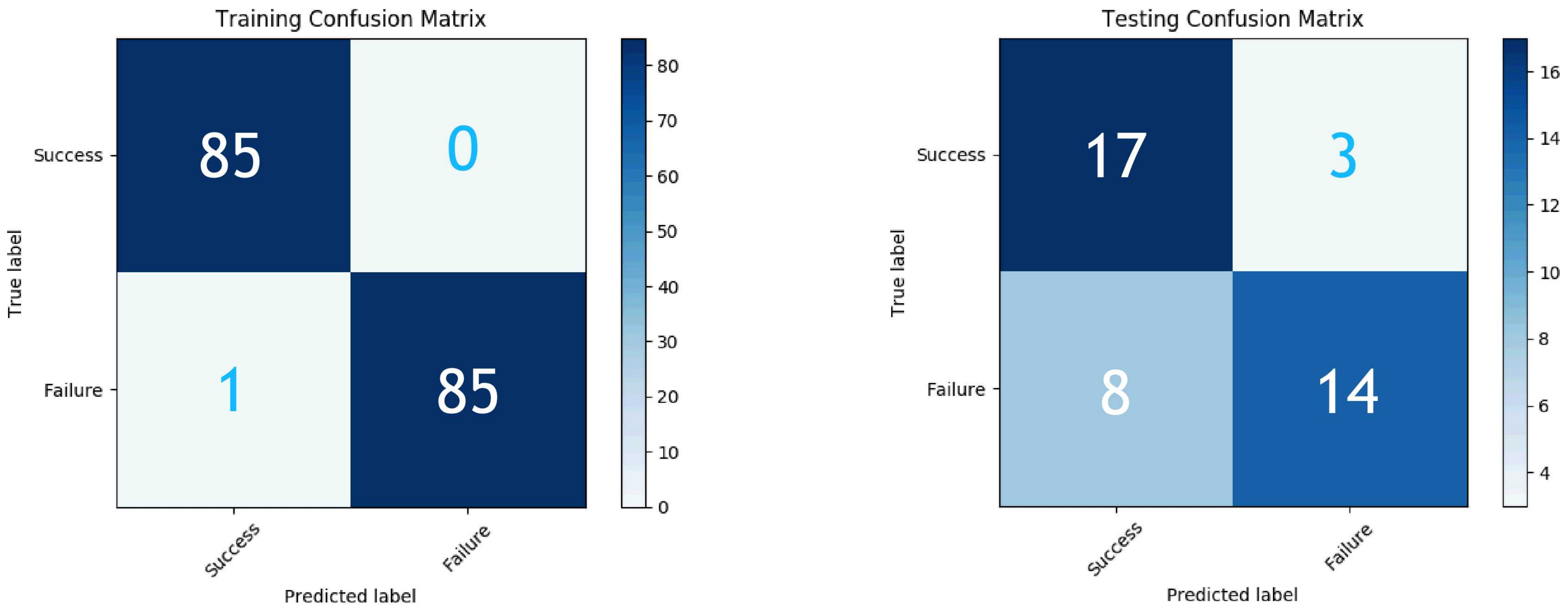
Synthetic Data Generator

- Makes 72^3 I-Beams mimicking mesh converter output
  - Allows larger kernel sizes to fit in memory
- Flaws (empty spaces) are generated in the central column of the beam to denote a failing instance
- Data generator is modular, allowing custom flaw configurations to be generated with specific distributions
- **Next steps:** Designing more configurations to mimic real data distribution



An I-Beam generated by the data generator

Trained model to run inference on real data. Below are confusion matrices for the training (99% accuracy) and held back test-set (73.8% accuracy).



Success: the part was not labelled as a failure
Failure: the part was labelled as a failure