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Predicting Mechanical Performance in Additive Manufacturing Components Using Deep Learning

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US National Congress on Computational Mechanics

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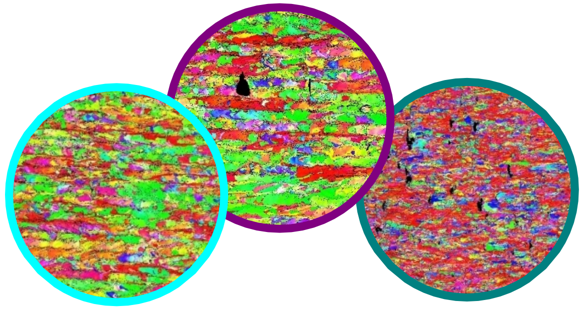
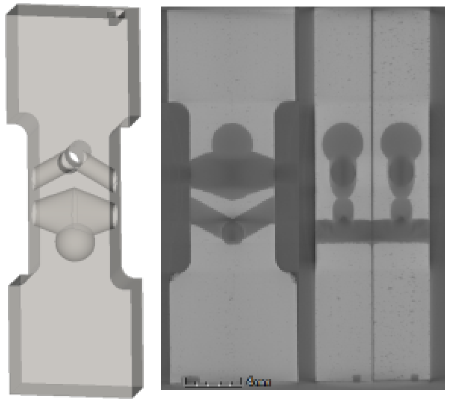
Vision: Rapid failure prediction based on microstructure, geometry, and loading conditions

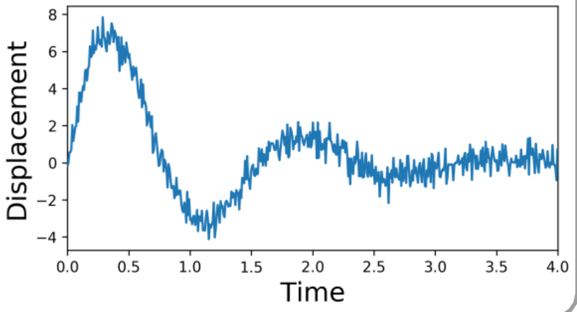
Microstructure



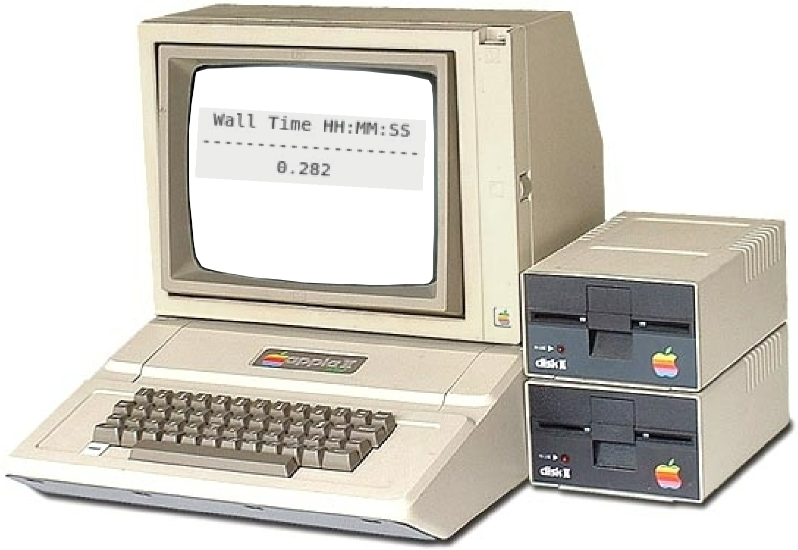
As-built Geometry

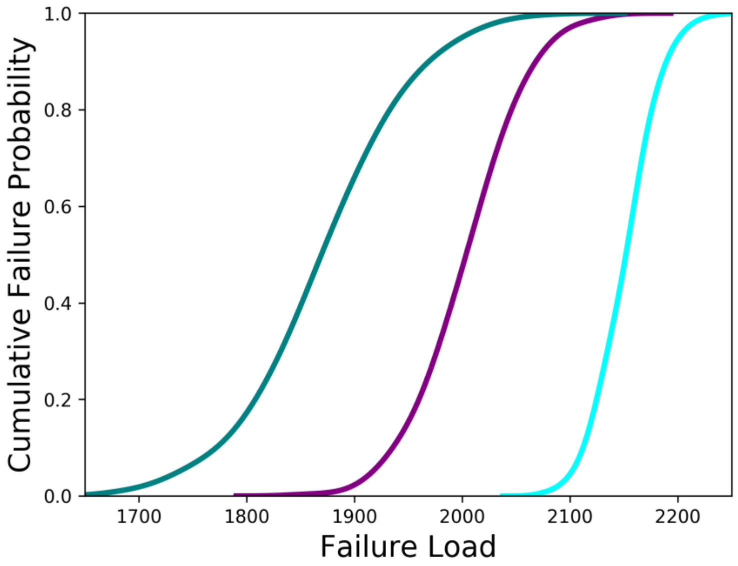


Boundary Conditions



Simulation Code



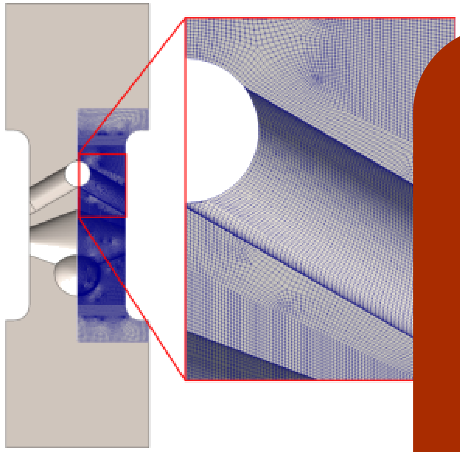


Qualification, Topology Optimization, etc.

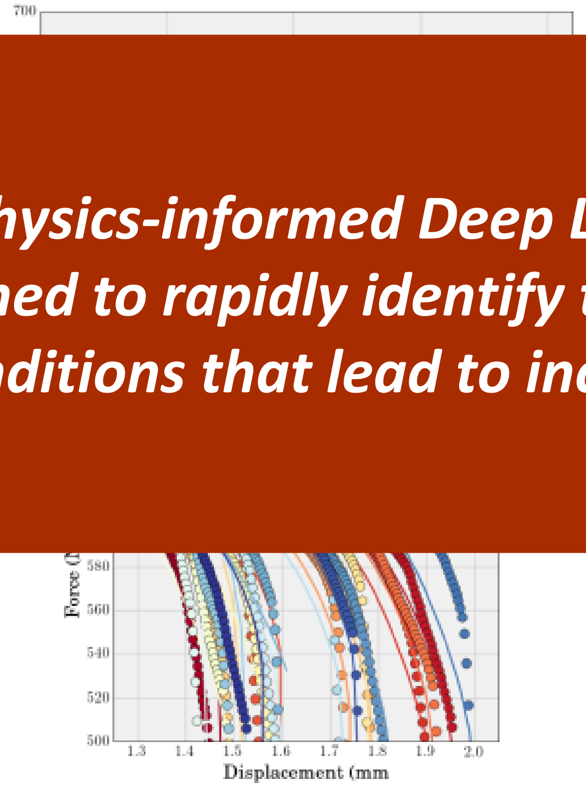
Image: oldcomputers.net

Today: Failure Prediction is Difficult and Slow Even With a Team

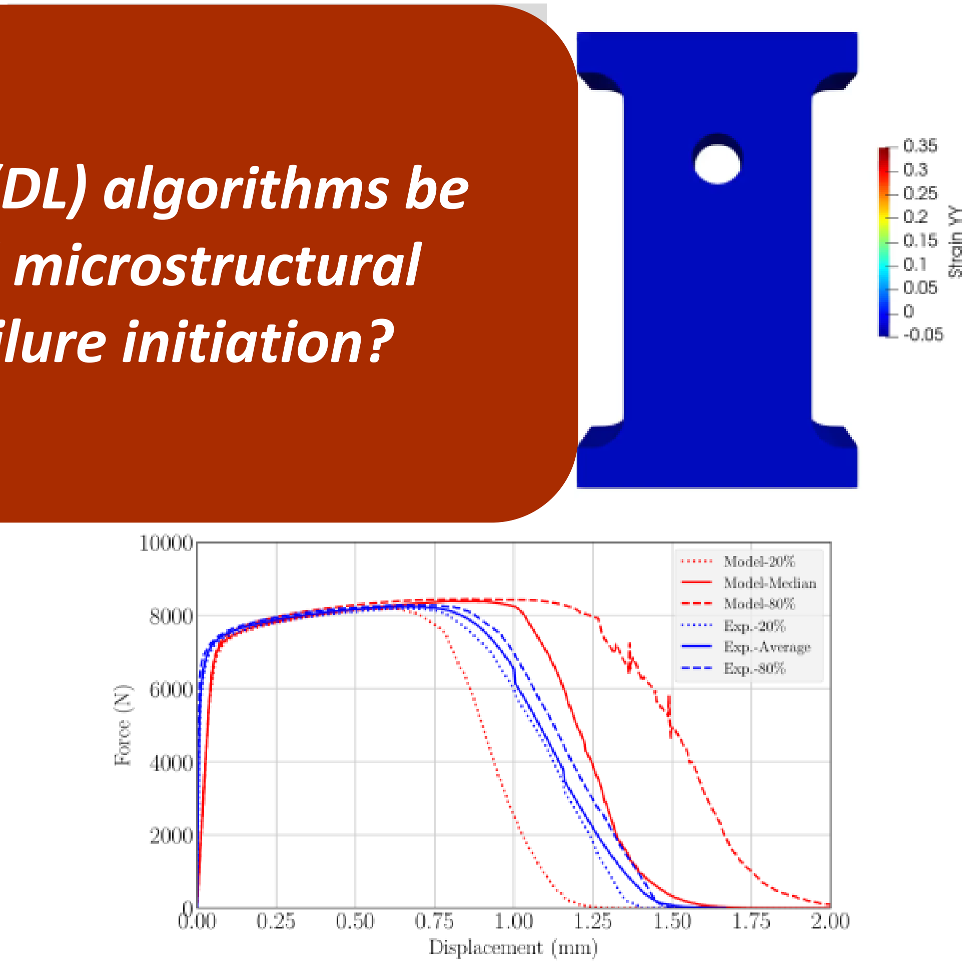
1. Create Mesh (Days-Weeks)



2. Iteratively Calibrate Material Model with Damage (Days-Weeks)



3. Run Many Large Simulations (Days-Weeks-Months)



Can physics-informed Deep Learning (DL) algorithms be trained to rapidly identify the initial microstructural conditions that lead to incipient failure initiation?

Johnson et al. *IJF 2019, Kramer, Boyce* et al., *IJF 2019*

Outline

- Part 1: Predicting AM mechanical response
  - Training data generation using porous AM material
  - Data mapping
  - Local variations in stress state
  - Deep Learning algorithm
  - Deep Learning predictions
  - Conclusions and future work

Part 1 Project Overview: Predicting AM Mechanical Response

Training Data: High fidelity model results from AM dogbones loaded in tension

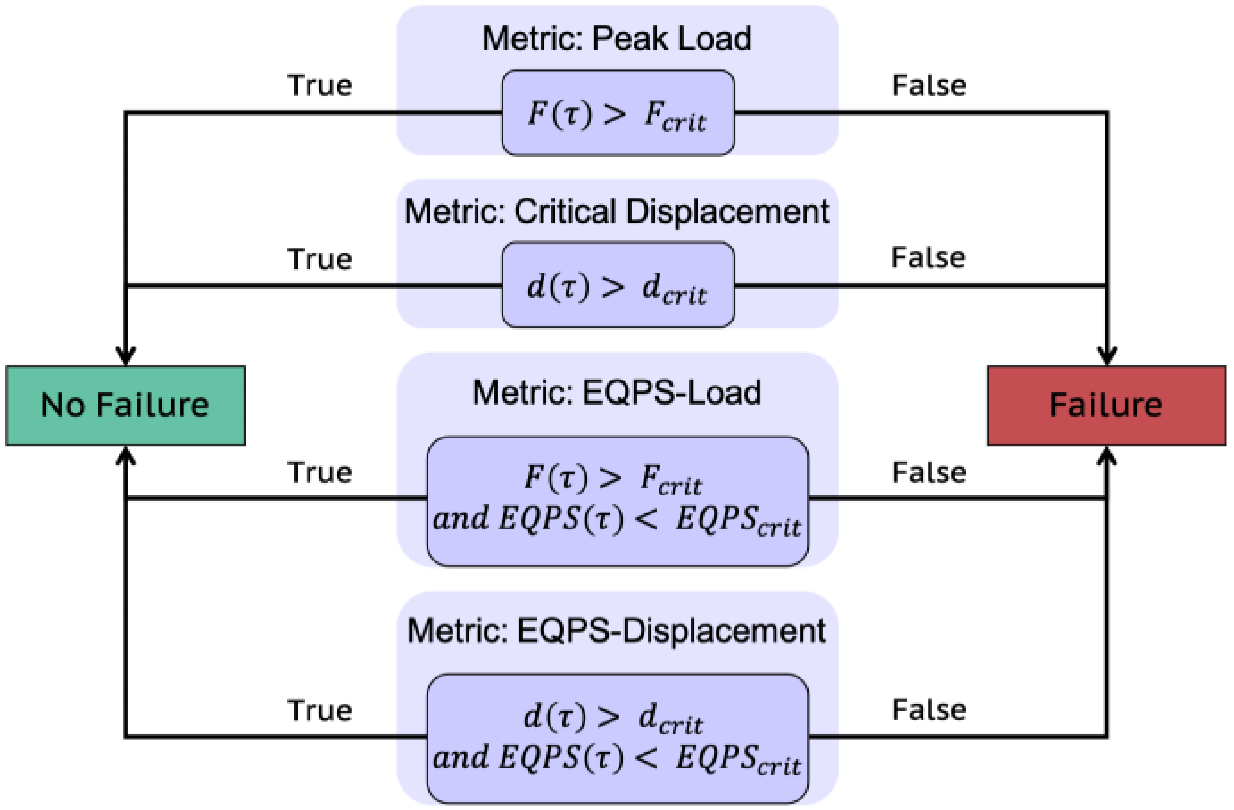
DL Model: Supervised 3D CNN

Inputs: Porosity and final state equivalent plastic strain (EQPS)

Output: Metric Classification

Submitted to: Computational Materials Science

Metrics



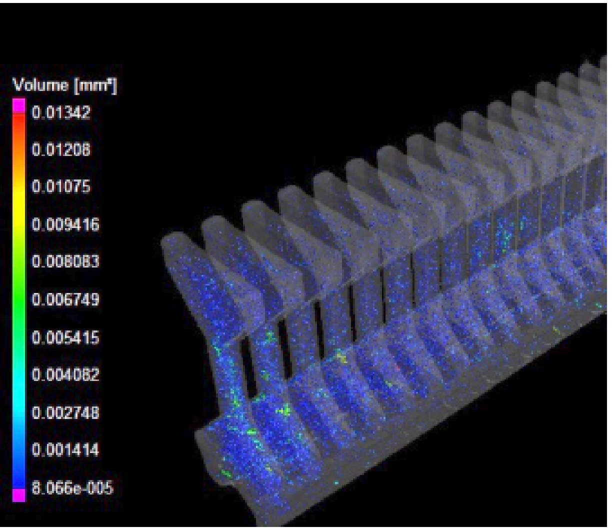
$\tau = time\ corresponding\ to\ peak\ load$

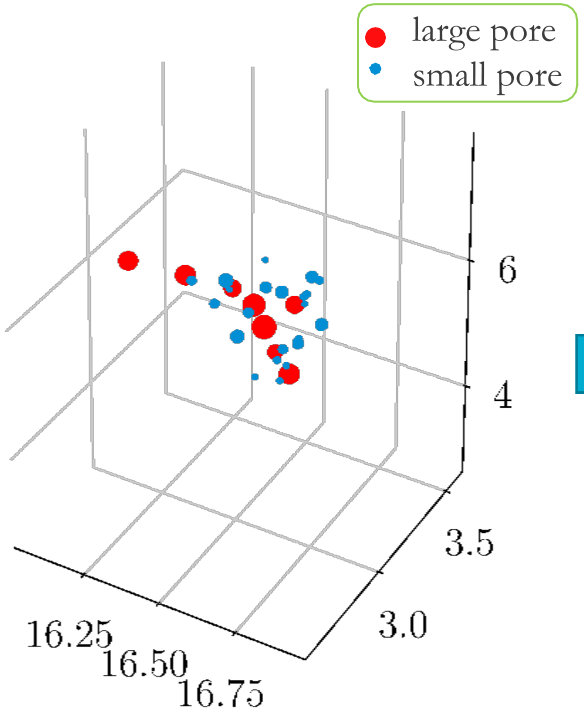
$F_{crit} = required\ load$

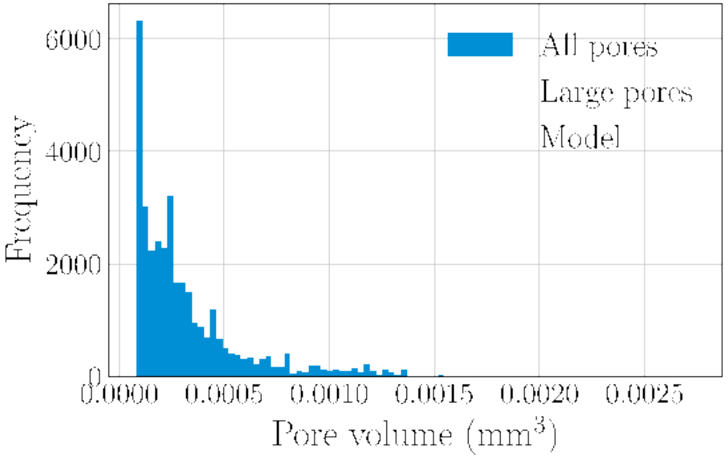
$d_{crit} = required\ displacement$

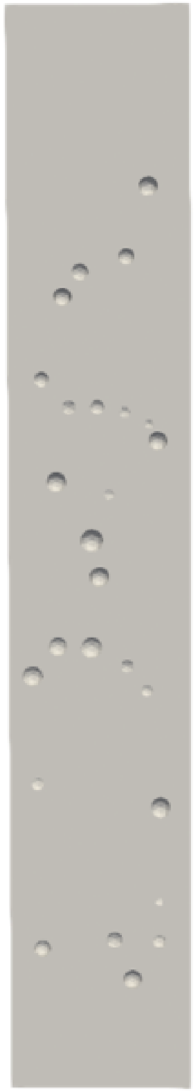
$EQPS_{crit} = required\ equivalent\ plastic\ strain$

Experimental CT measurements inform training data meshes





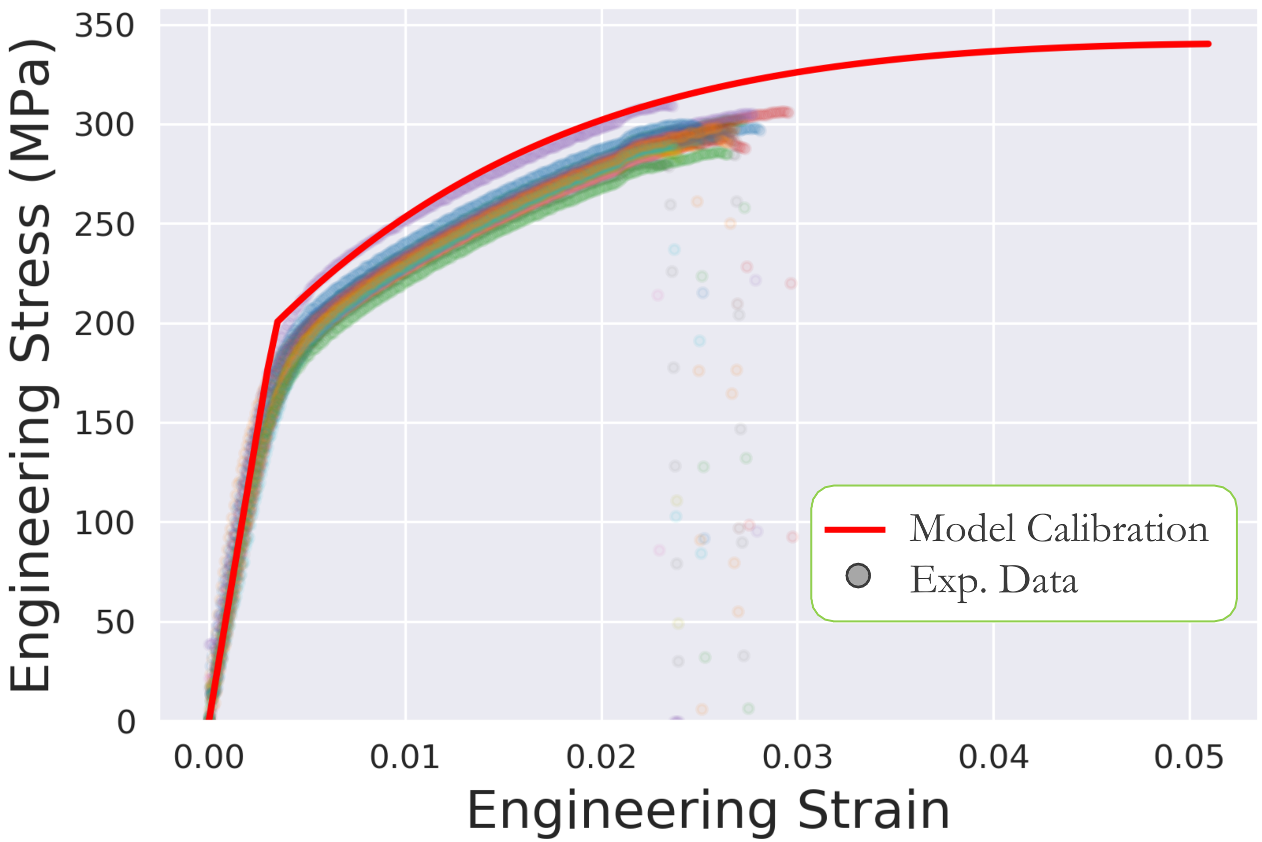




- Training data consists of dogbone gauge sections loaded in tension past peak load

CT Data: Chris Laursen, Jay Carroll

Calibration to tensile specimens

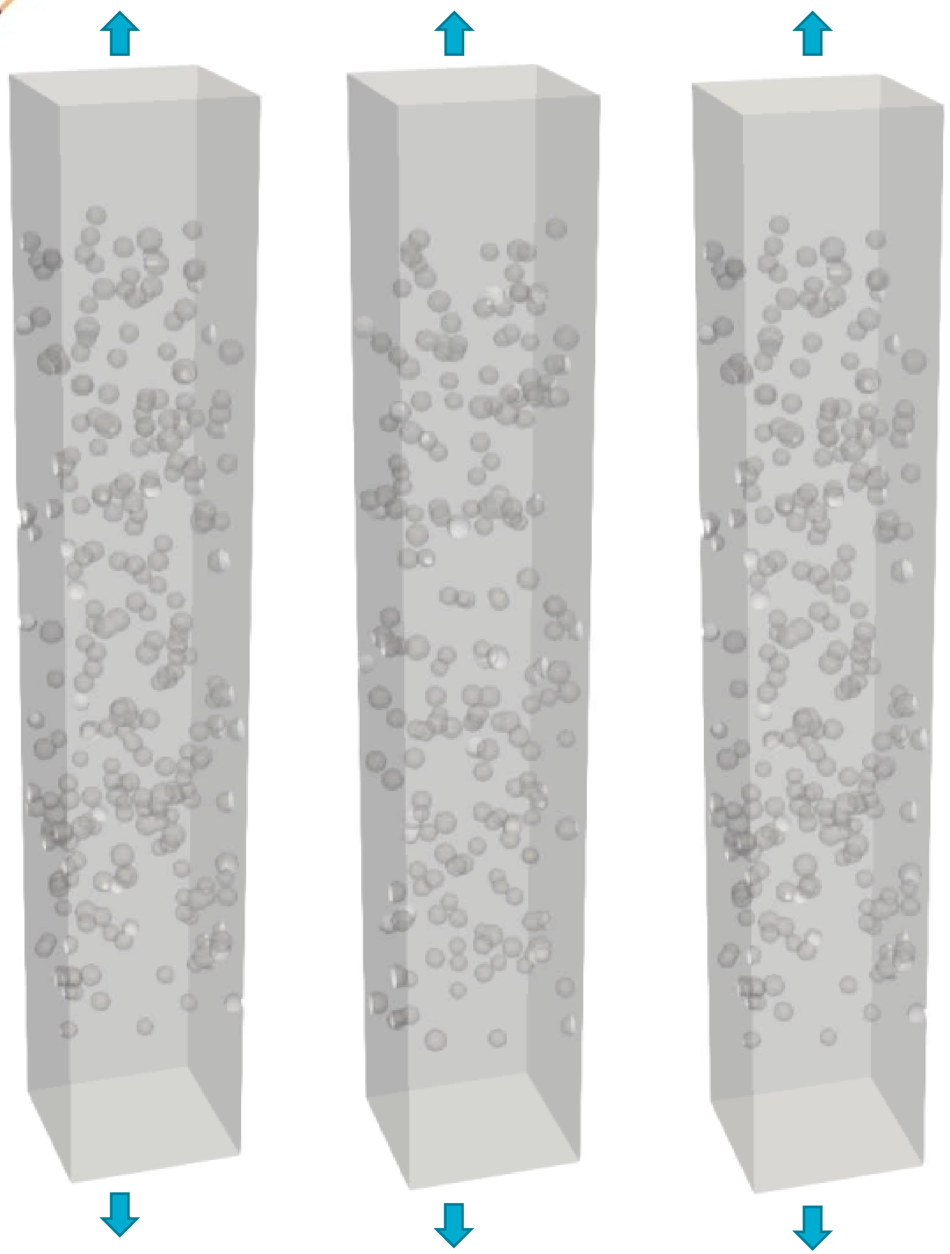


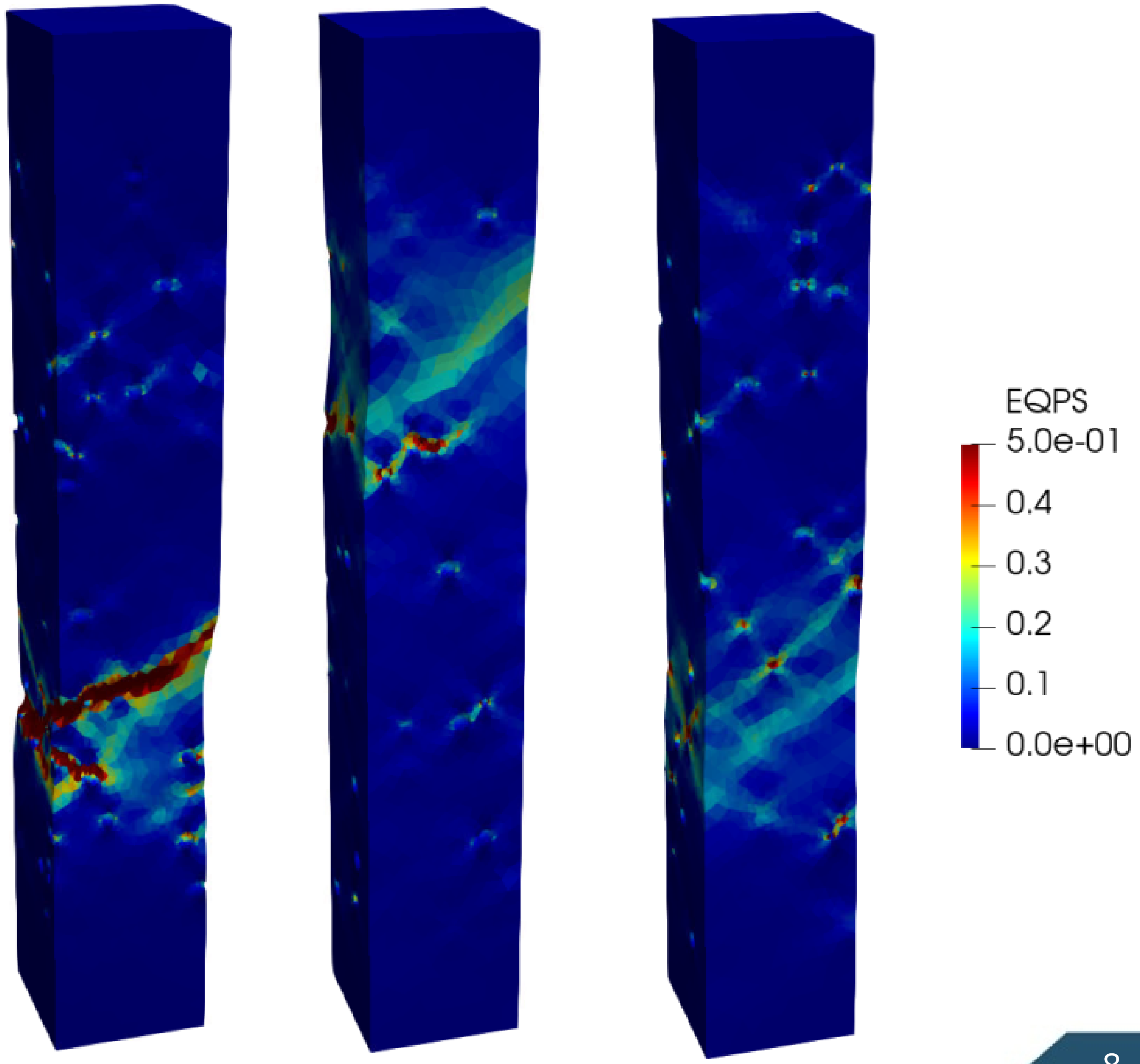
- Plasticity is captured with Voce hardening model

$$\bar{\sigma} = \sigma_y + A(1 - \exp(-n\bar{\varepsilon}^p))$$

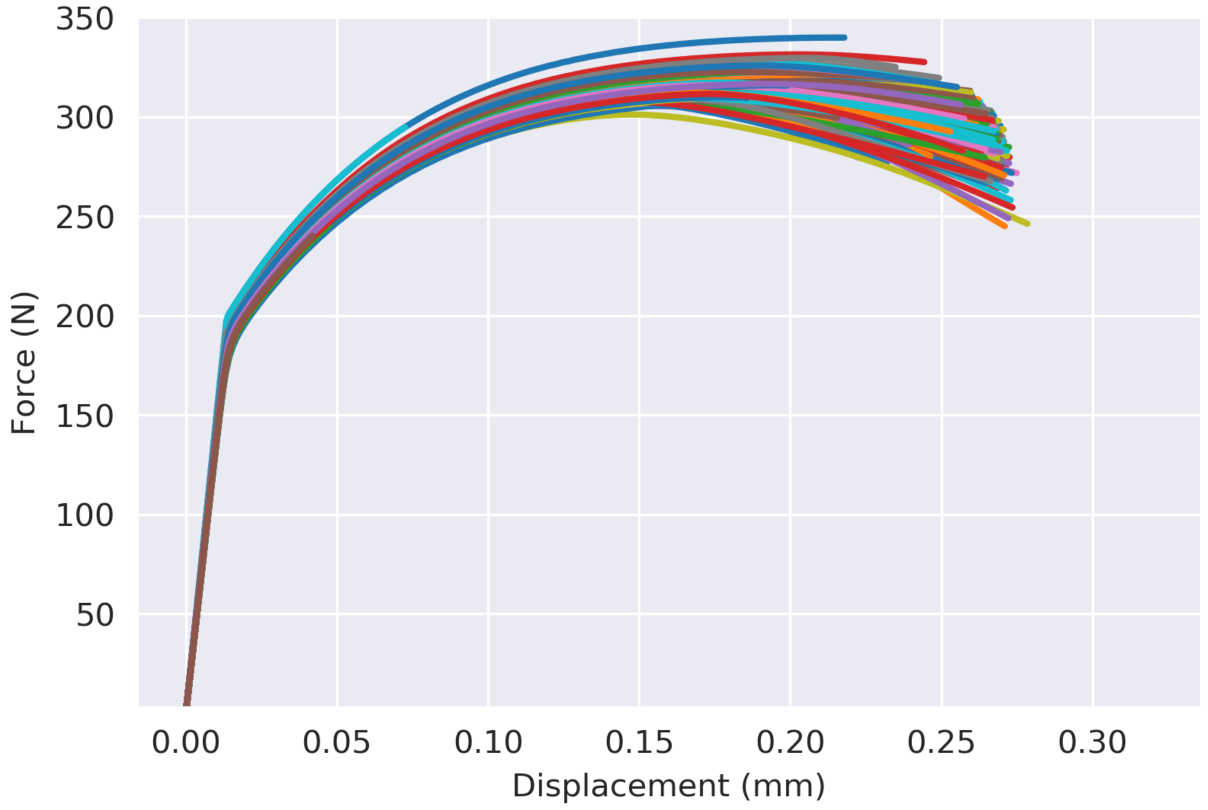
- Model calibrated using porous mesh from CT scan – captures “matrix” response

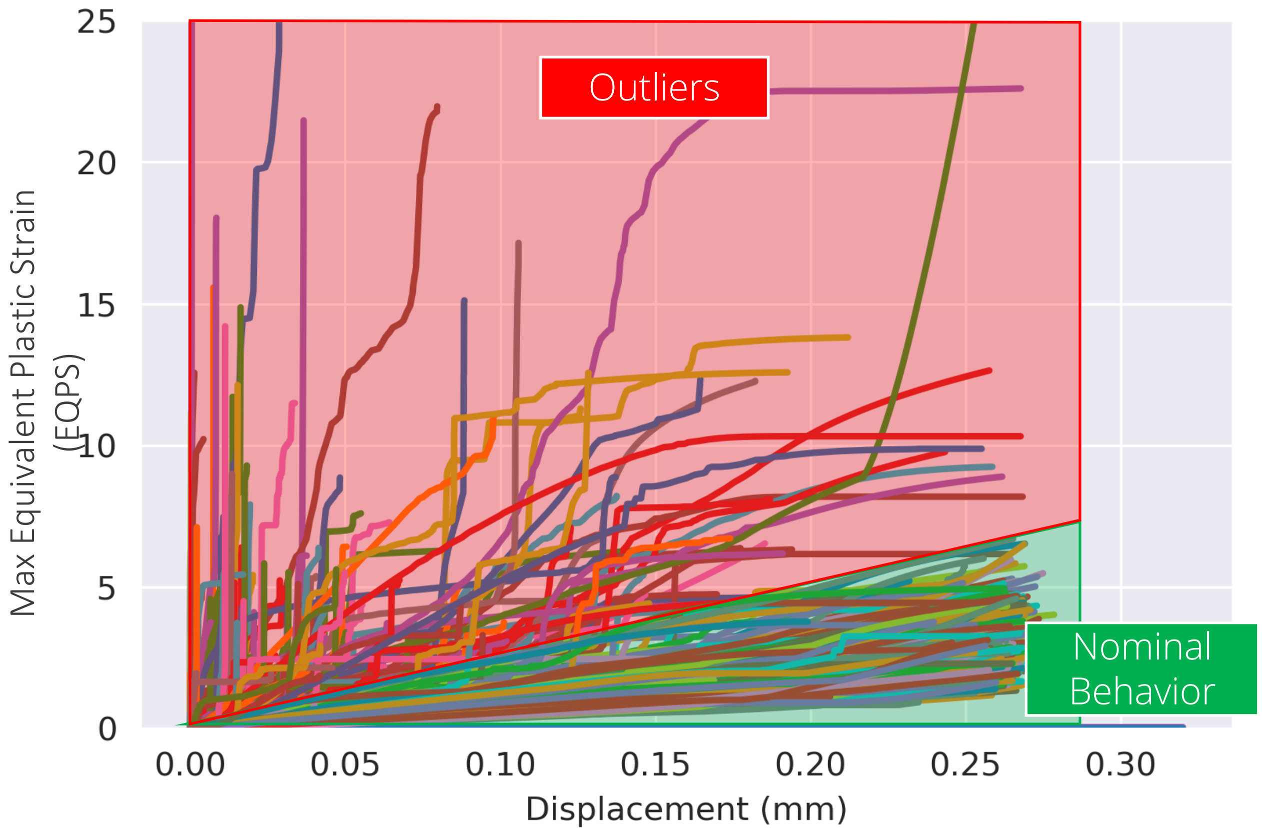
Different porosity samples lead to different local behavior



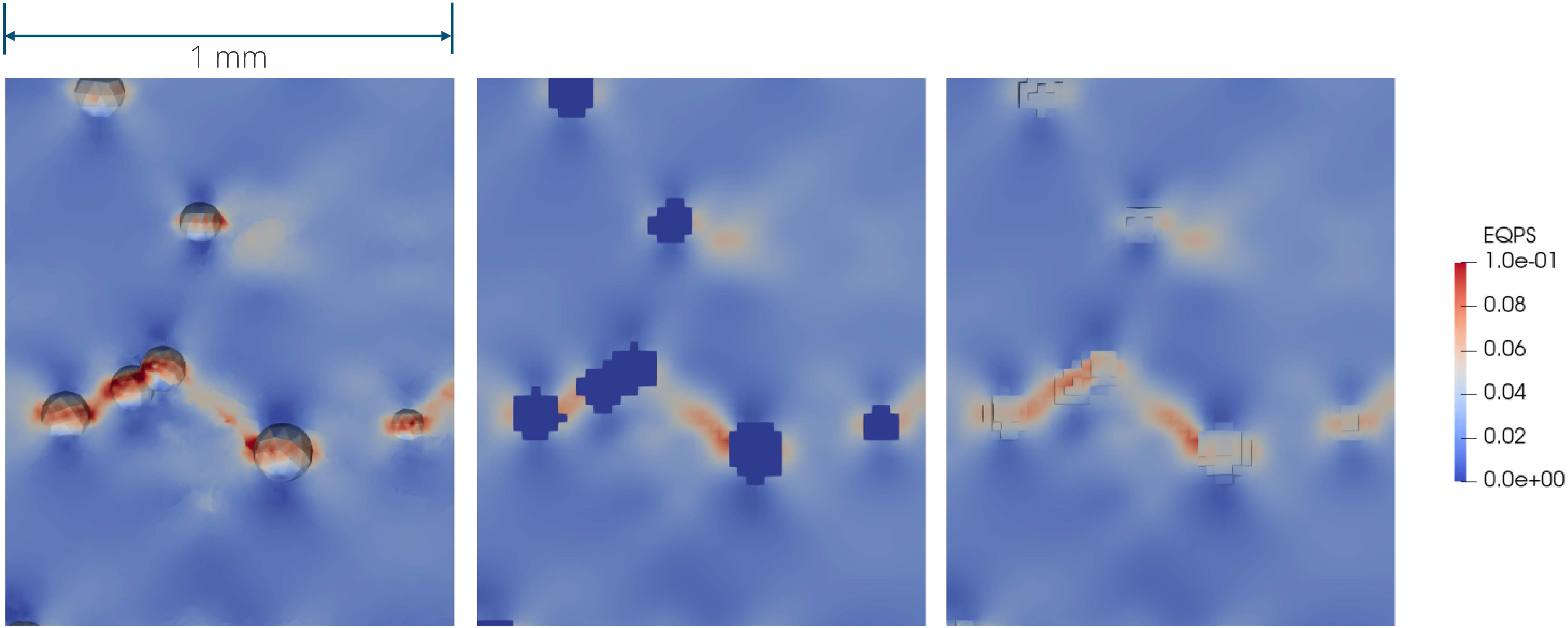


Force-displacement and max equivalent plastic strain (EQPS) show large variations due to pore structures





Deep Learning algorithm requires uniform voxel (3D Pixel) data format

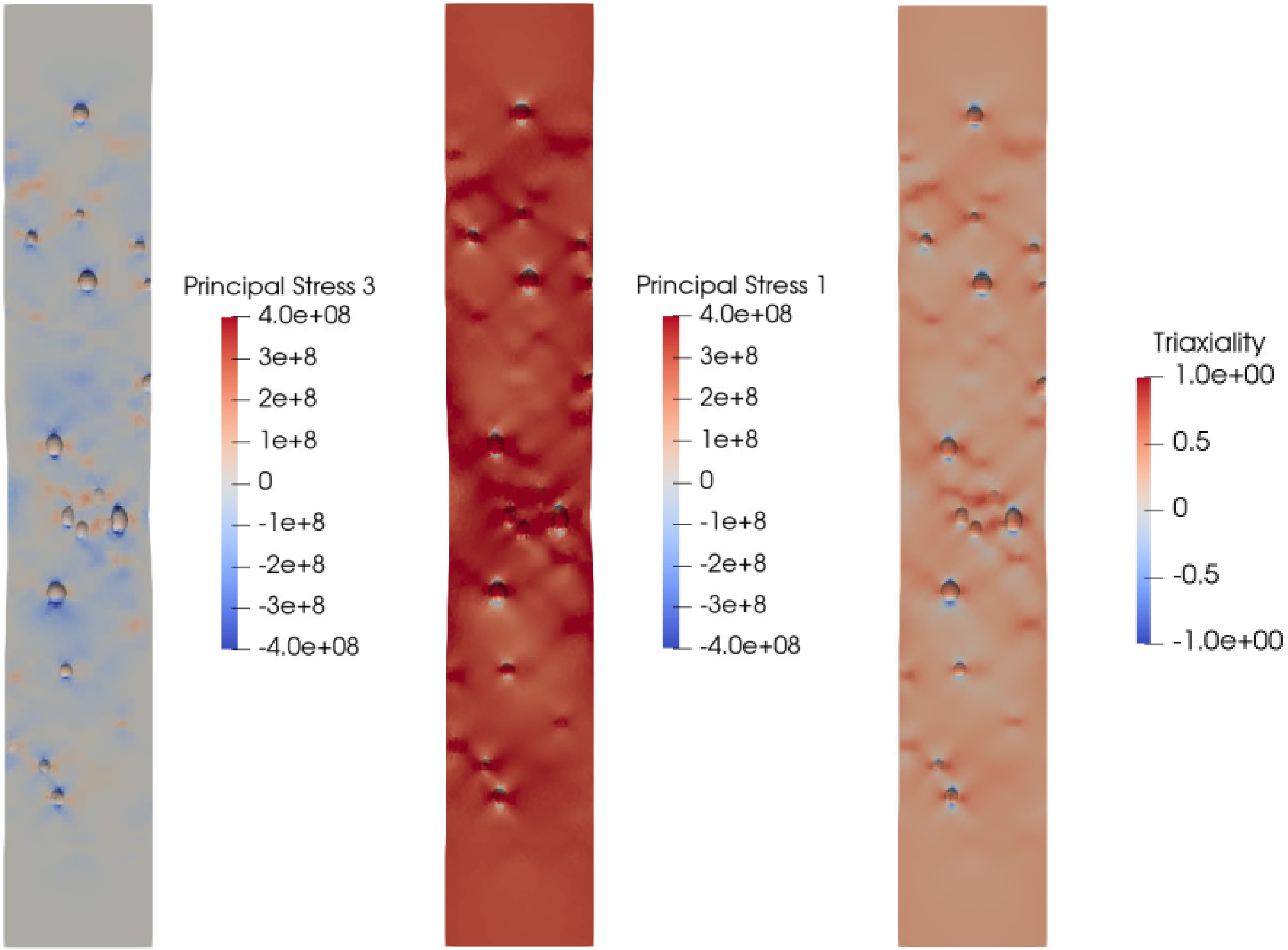


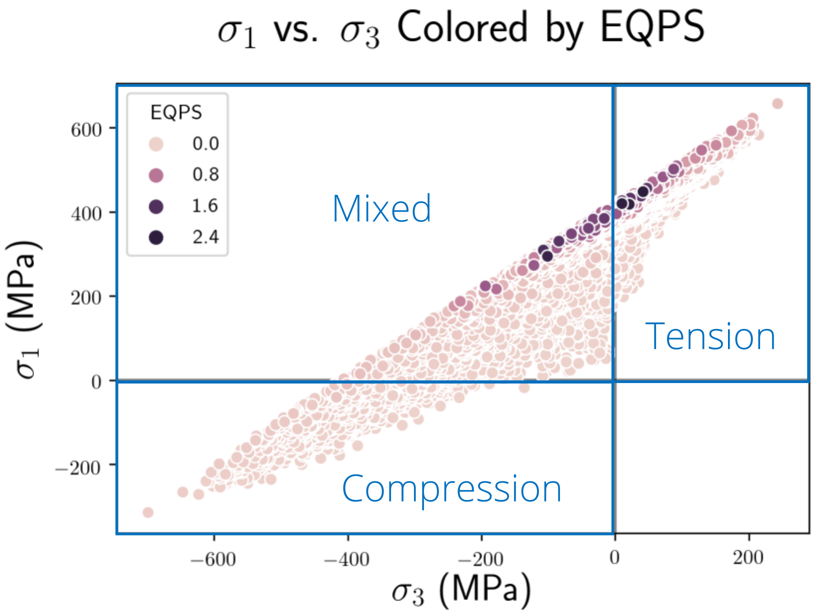
Sierra simulations results from tetrahedral mesh

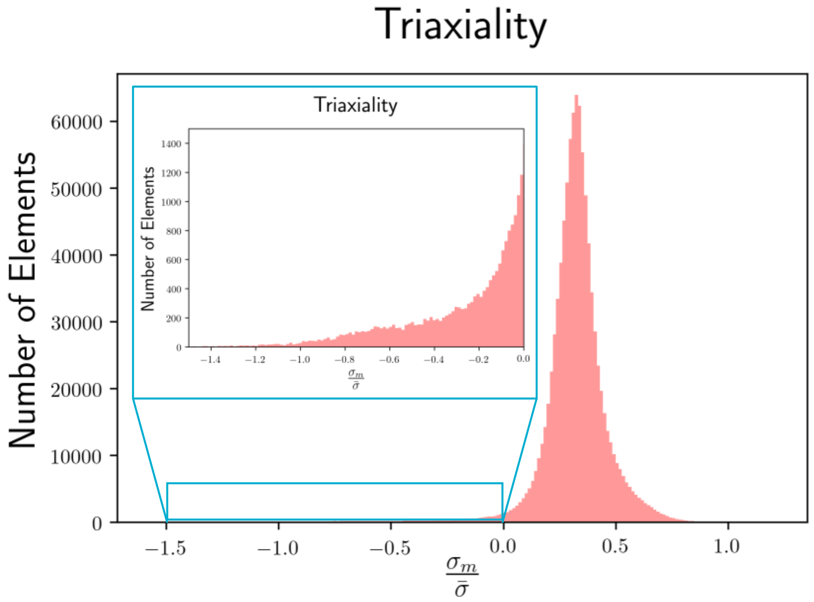
Results mapped to uniform hexahedral mesh

Hex elements in pores removed

Specimens show large local stress state variations even in nominal uniaxial tension simulations → Reduces risk of extrapolation



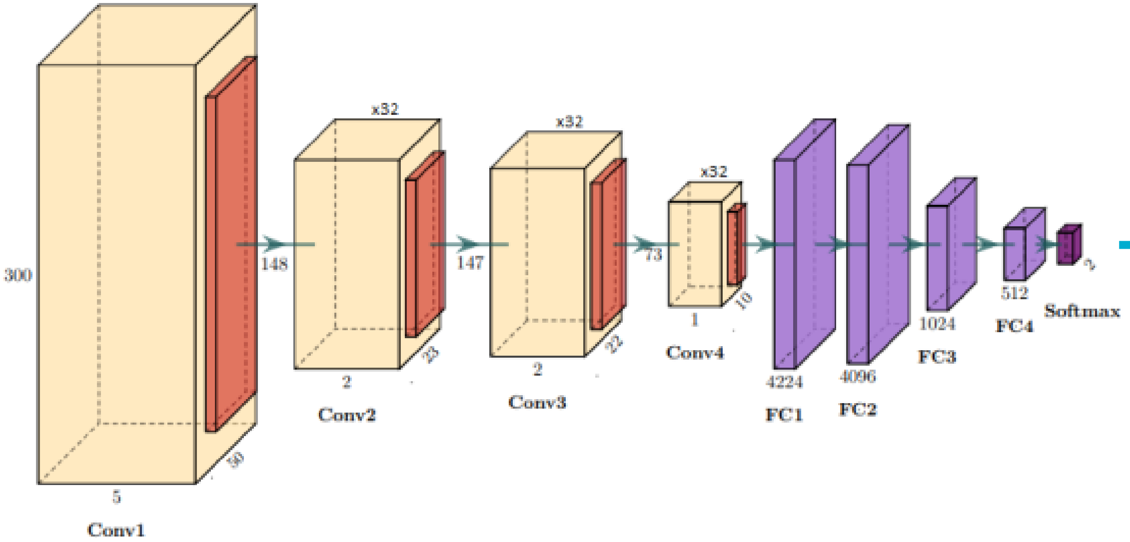




Deep Learning algorithm architecture

Model Inputs per Voxel

$$\begin{cases} EQPS_{final} & \text{if Solid} \\ 0 & \text{if Pore} \end{cases}$$



Output

Failure / No Failure

- Model architecture based on Huang et al. *Front. Neurosci*. 2019
- Output is classification – pass/fail for failure metric

Failure prediction results in test sets for network trained only on tension

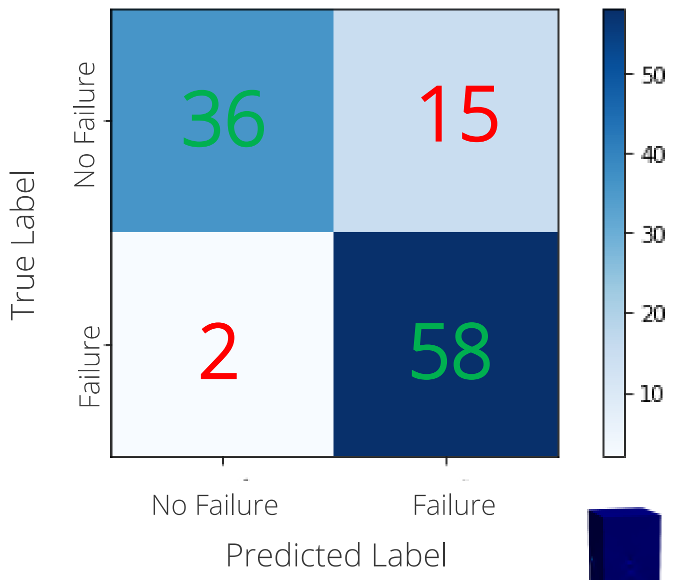
Failure Metric: Sample failed to reach a required load before onset of strain localization.

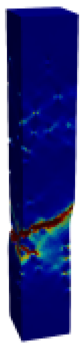
FEA Simulation Time: 88 minutes on 216 CPUs

DL Network Inference Time: 0.02 s on 2 GPUs

Speedup: 264000x

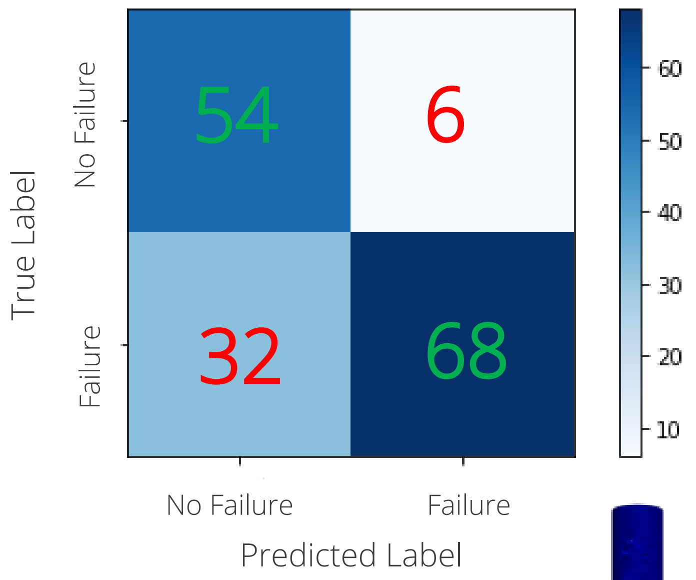
Square Tension

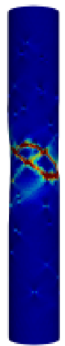




Test Accuracy: **84.7%**

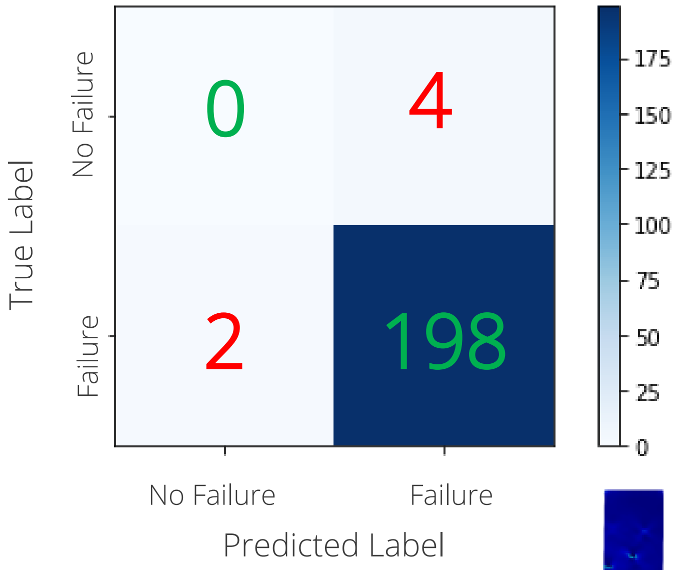
Cylindrical Tension

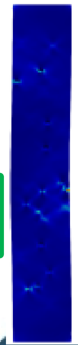




Test Accuracy: **76.2%**

Square Compression



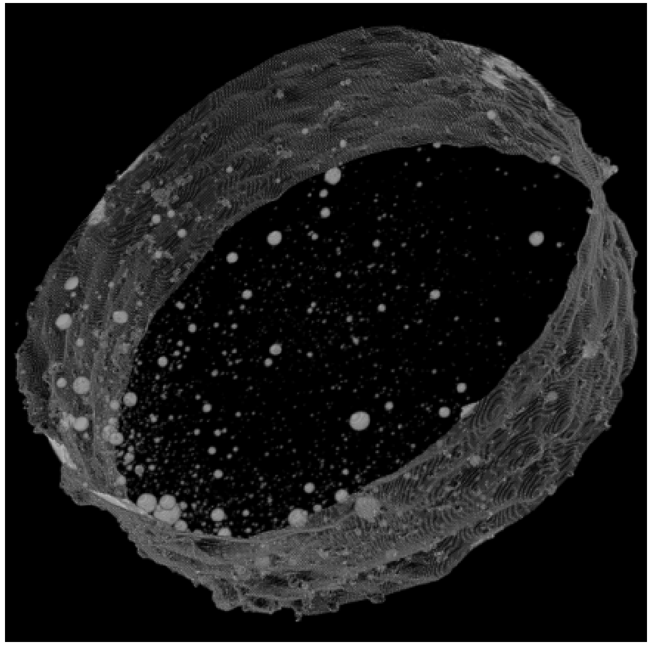


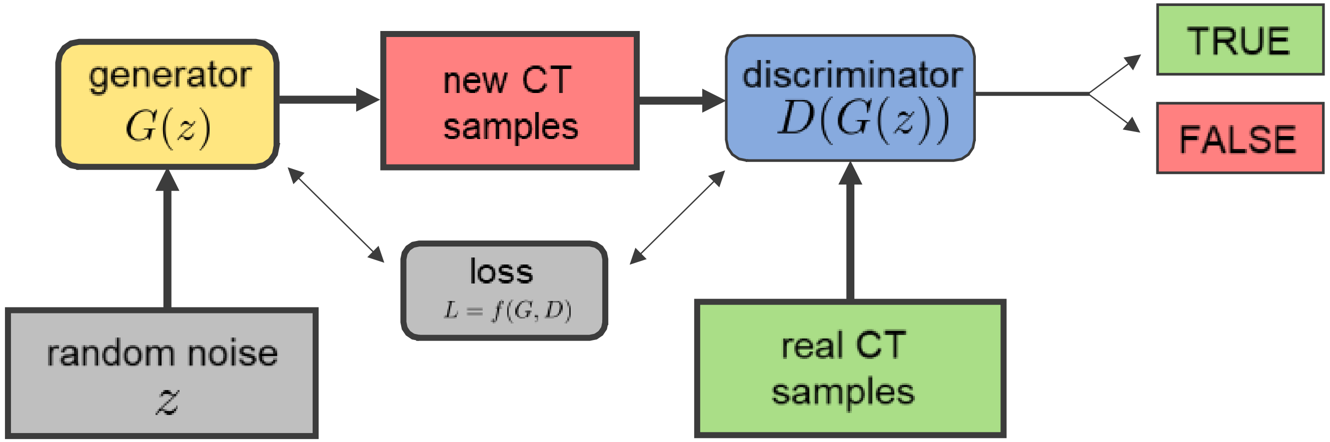
Test Accuracy: **97.1%**

Extension: Using GANs to augment CT images of AM material – Collaboration with Amir Farimani and Francis Ogoke (CMU)

- Generative Adversarial Networks (GANs) produce <u>new samples</u> from a training set while <u>preserving the underlying statistics.</u>

- GANs are trained to minimize the distance between the distribution of the training data and the generated samples.





GAN network schematic

Metric	Notes
Volume Distribution	
Nearest Neighbor Distances	
Location Distribution	
Ellipticity	$\sqrt{\frac{a^2-c^2}{a^2}}$
Moment of Inertia	
Surface Area	
Mallat Scattering Transform	$\|\|x * \psi_{\lambda_p}\| * \psi_{\lambda_{p'}}\| * \phi_J$

Project Summary

- Deep Learning was able to predict performance variation due to microstructural features 5 orders of magnitude faster than FEA (nearly instantaneous).

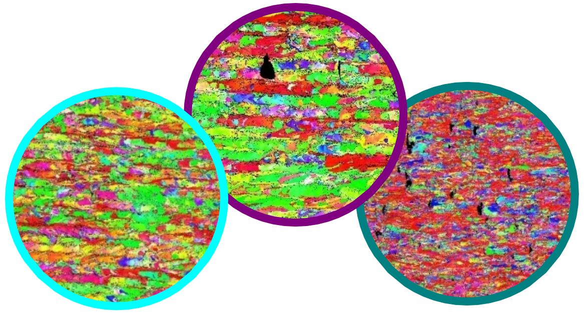
- Model maintained predictiveness in different part geometries and stress states.

- DL is able to pick up on patterns that subject matter experts cannot. Prior to this work we explored looking at stress measures to predict ductility with little success.

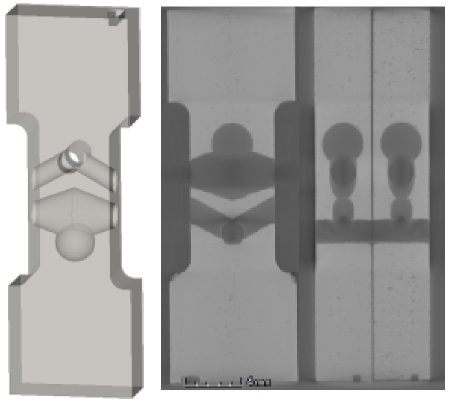
- Using large datasets for DL training, such as volumetric data used here, on GPUs is a challenge.

Vision: Rapid failure prediction based on microstructure, geometry, and loading conditions enabled by Deep Learning

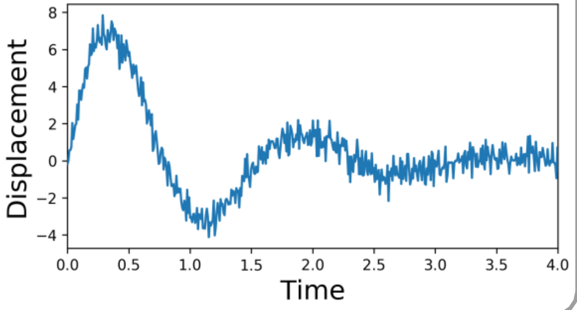
Microstructure



As-built Geometry



Boundary Conditions



Simulation Code

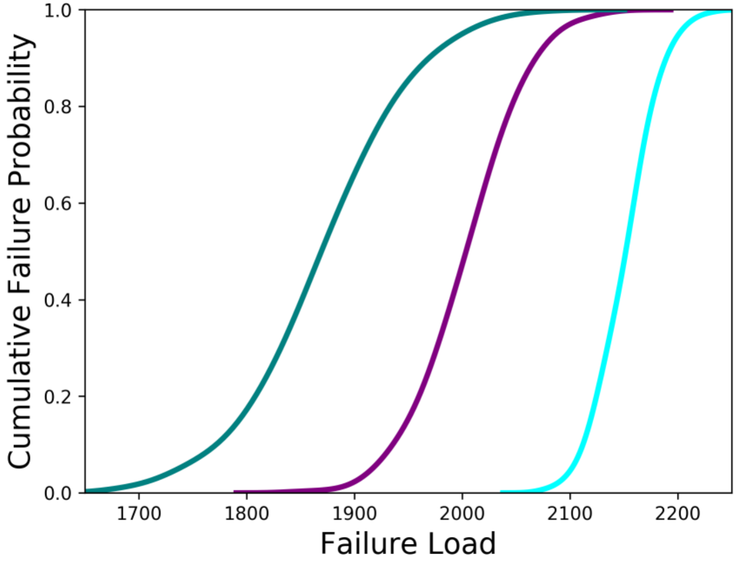
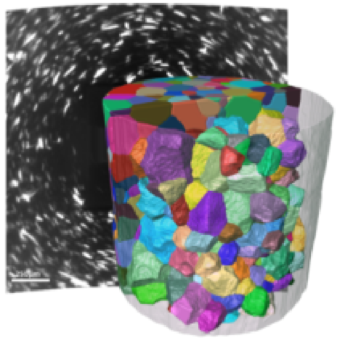


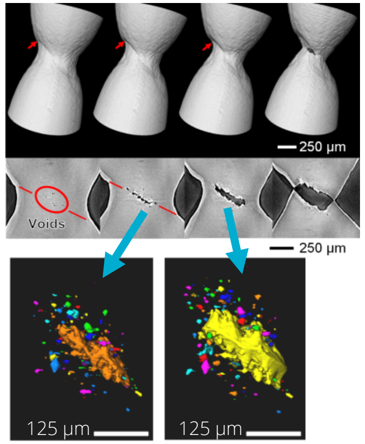
Image: oldcomputers.net

New 3-Year Project Will Combine Experimental and Computational Mechanics with Deep Learning to Predict Material Failure

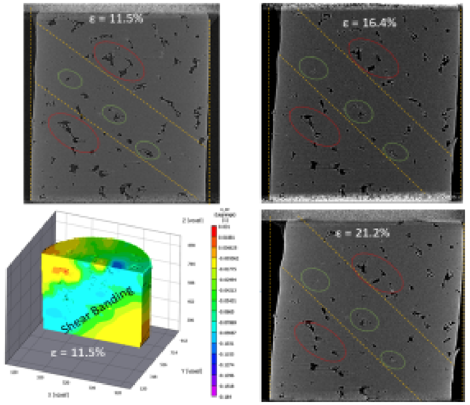
Emerging Experimental Capabilities



Diffraction Contrast Tomography (DCT)

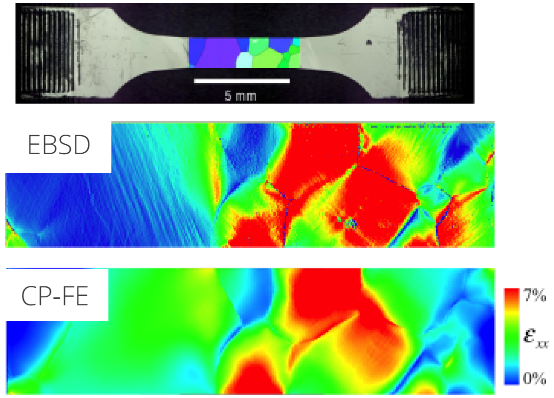


High Resolution μCT

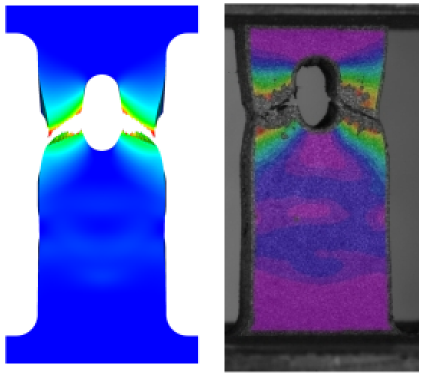


Digital Volume Correlation (DVC)

High Fidelity Modeling

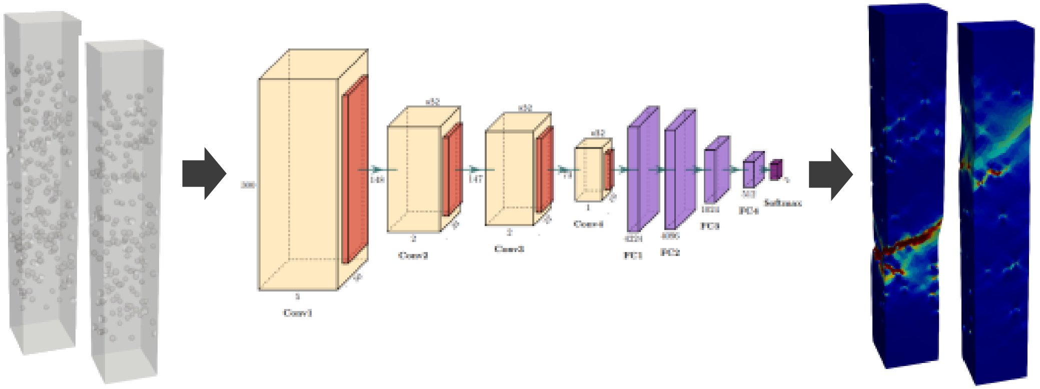


Crystal Plasticity



Continuum Plasticity and Damage Models

Large Scale Physics-Informed Deep Learning



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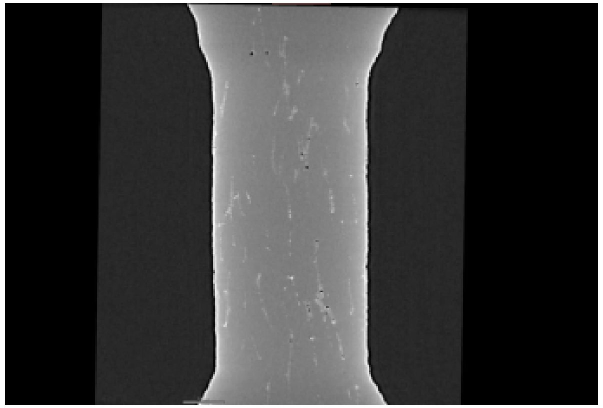
Future Work

- Multiscale coupling – mesoscale CP to macroscale continuum damage simulations
- Digital Volume Correlation (DVC) testing
- In situ micron-scale CT testing
- High Energy Diffraction Microscopy (Prof. Mike Sangid)
- Transmission Electron Microscopy for failure initiation mechanisms (Profs. Billy Oates and Brandon Krick)
- TriBeam characterization on deformed DCT+CP simulated sample
- Combining all of the above in DL model for failure predictions

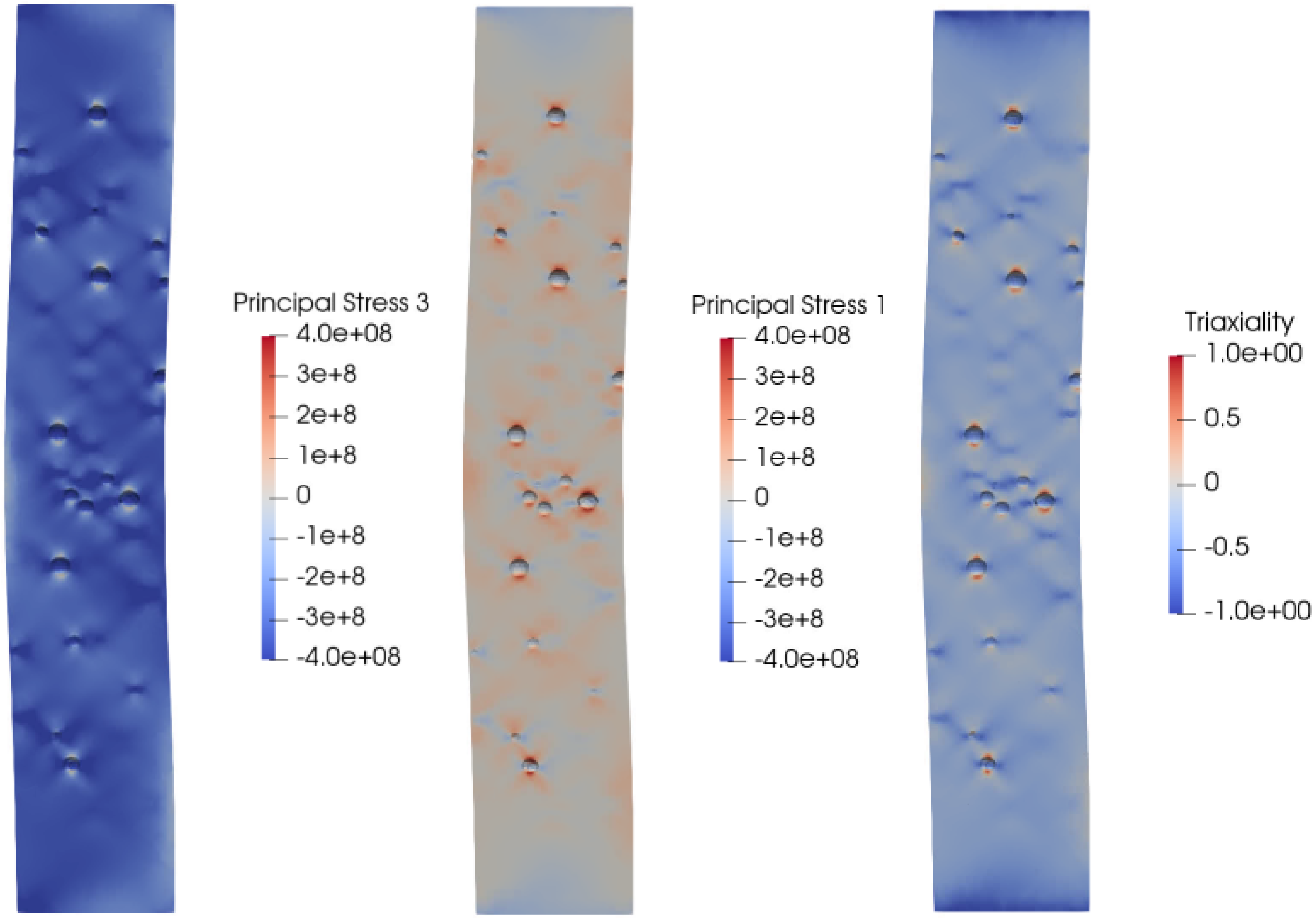


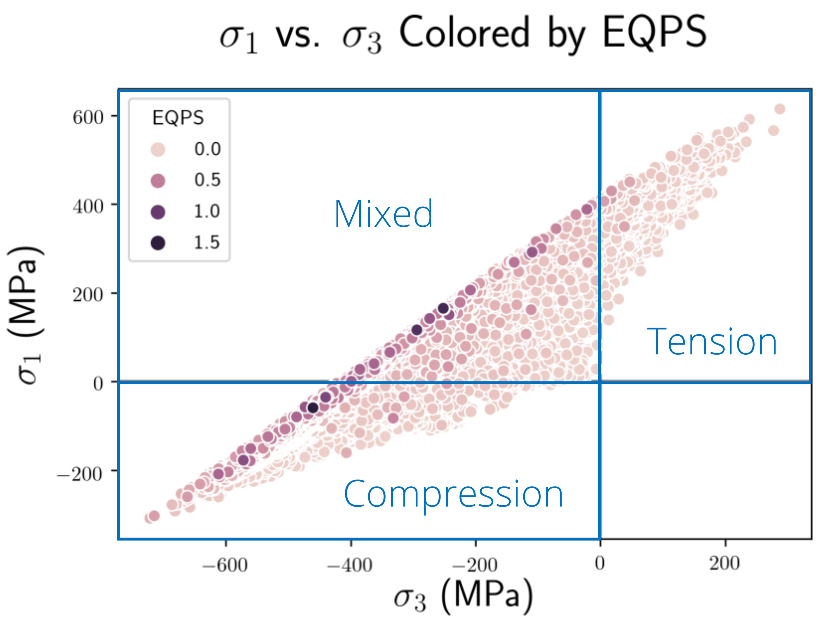
Questions?

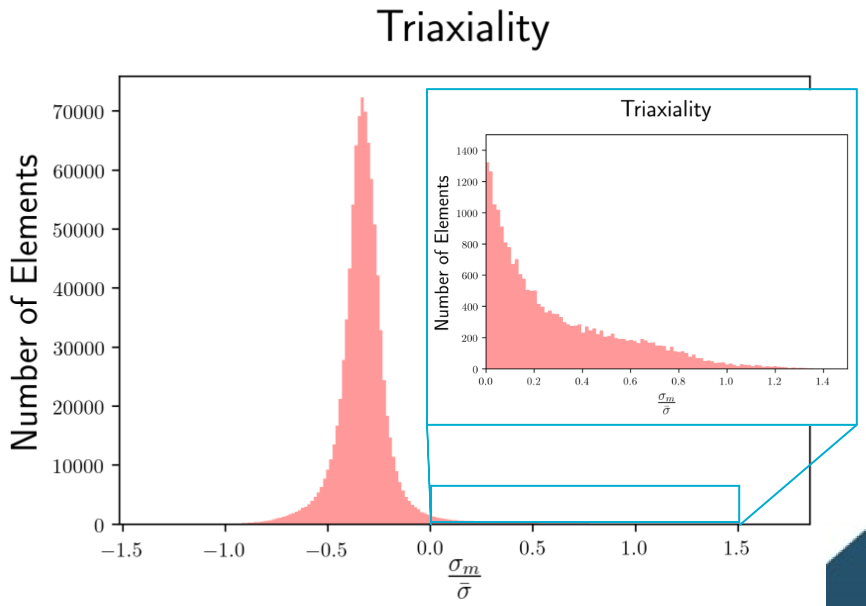
Students interested in postdoc position?

kyljohn@sandia.gov

Specimens show large local stress state variations even in nominal uniaxial compression simulations → Reduces risk of extrapolation







Failure prediction results in test sets for network trained only on tension

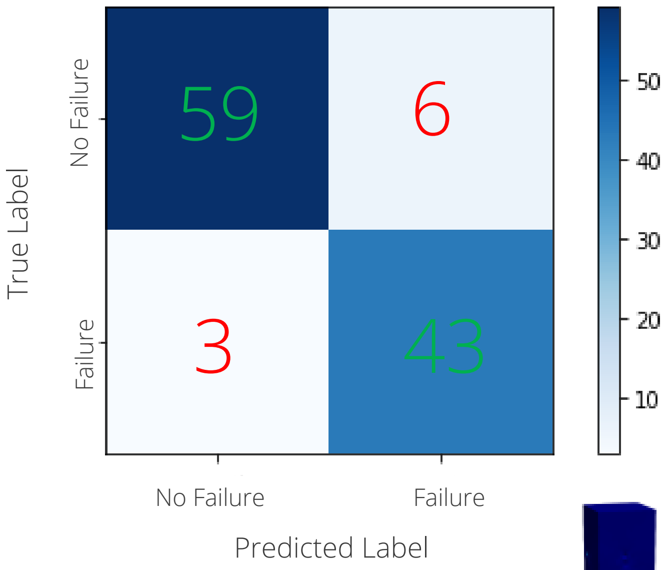
Failure Metric: Sample Max EQPS remained below critical value and displacement reached a required value at onset of localization.

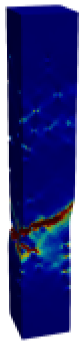
FEA Simulation Time: 88 minutes on 216 cpus

DL Network Inference Time: 0.02 s on 2 GPUs

Speedup: 264000x

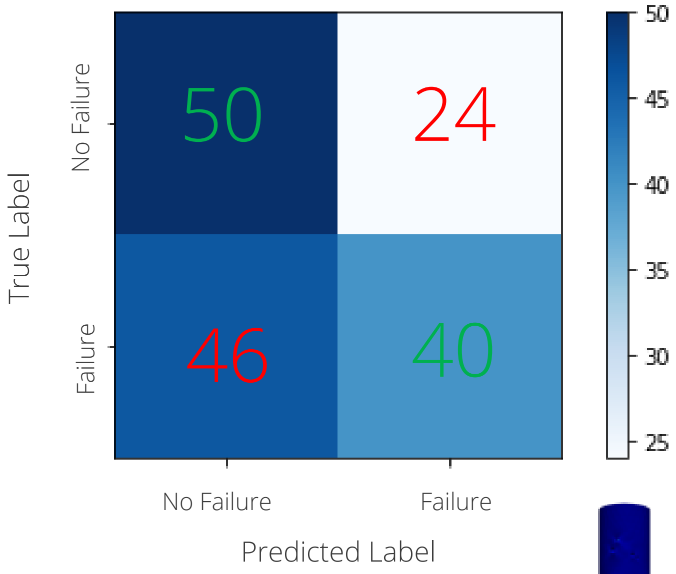
Square Tension

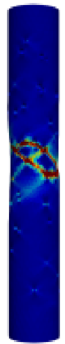




Test: Accuracy: **91.9%**

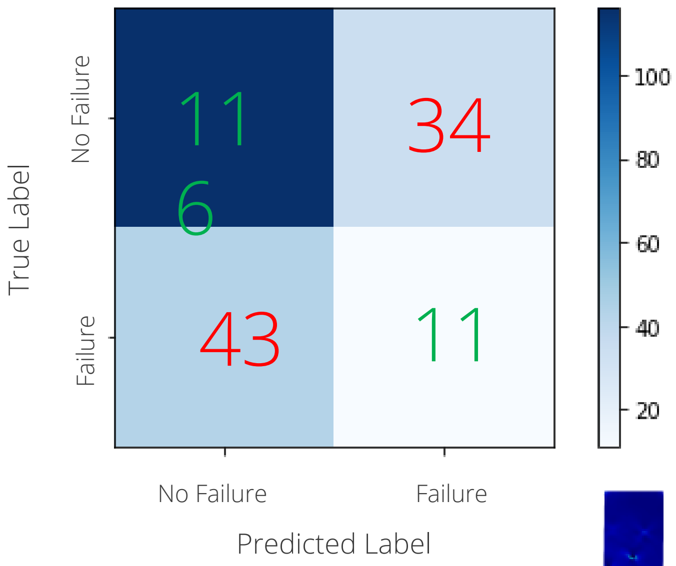
Cylindrical Tension

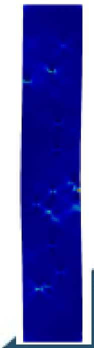




Test: Accuracy: **56.2%**

Square Compression





Test: Accuracy: **62.3%**

Failure prediction results in test sets for network trained only on tension

Failure Metric: Sample Max EQPS remained below critical value and force reached a required value at onset of localization.
FEA Simulation Time: 88 minutes on 216 cpus
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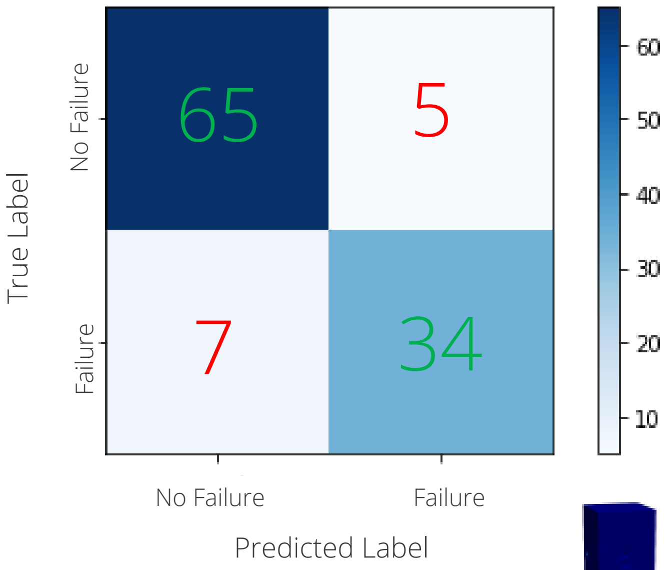
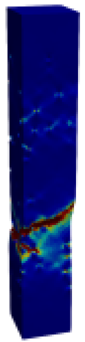
Speedup: 264000x

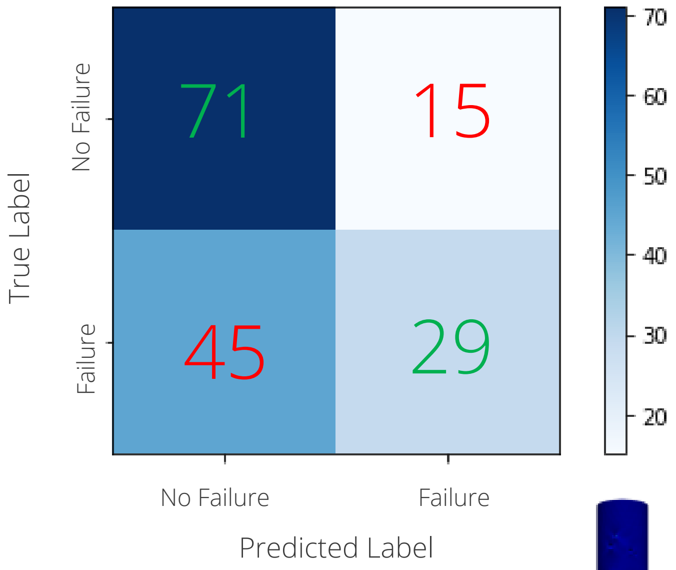
Square Tension

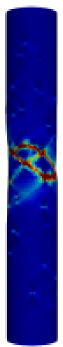




Test Accuracy: **89.2%**

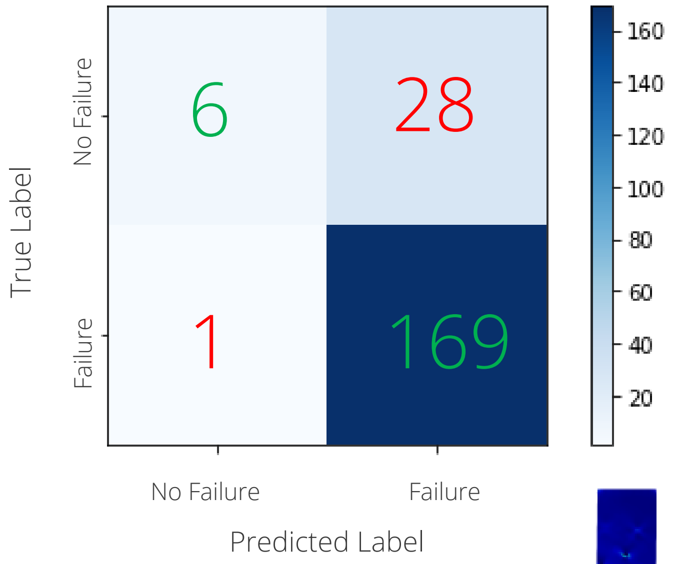
Cylindrical Tension

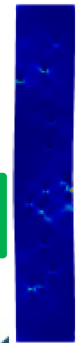




Test Accuracy: **62.5%**

Square Compression





Test Accuracy: **85.8%**

Failure prediction results in test sets for network trained only on tension

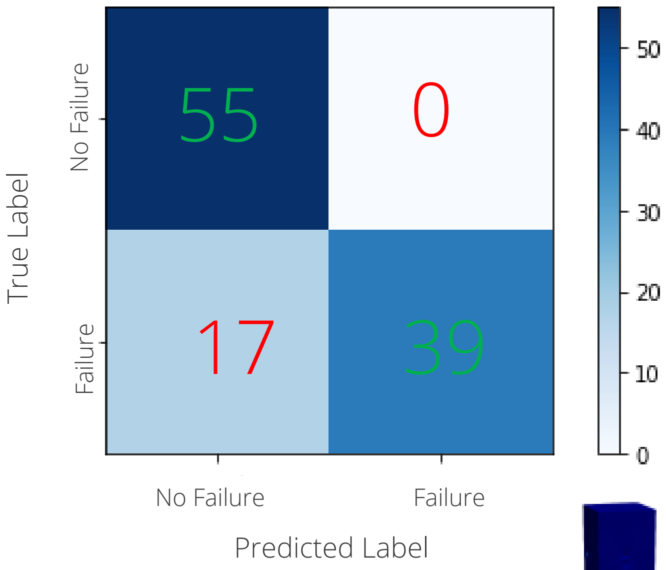
Failure Metric: Sample displacement reached a required value at onset of localization.

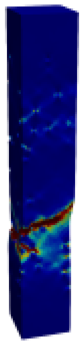
FEA Simulation Time: 88 minutes on 216 cpus

DL Network Inference Time: 0.02 s on 2 GPUs

Speedup: 264000x

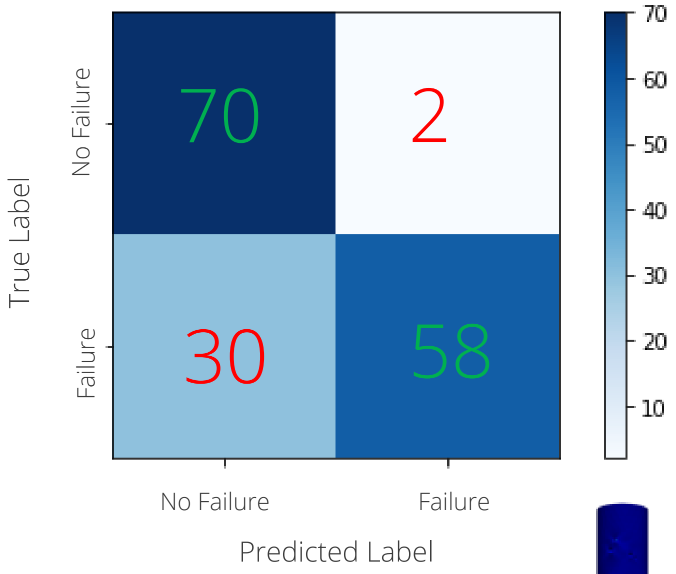
Square Tension

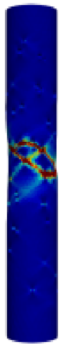




Test Accuracy: **84.7%**

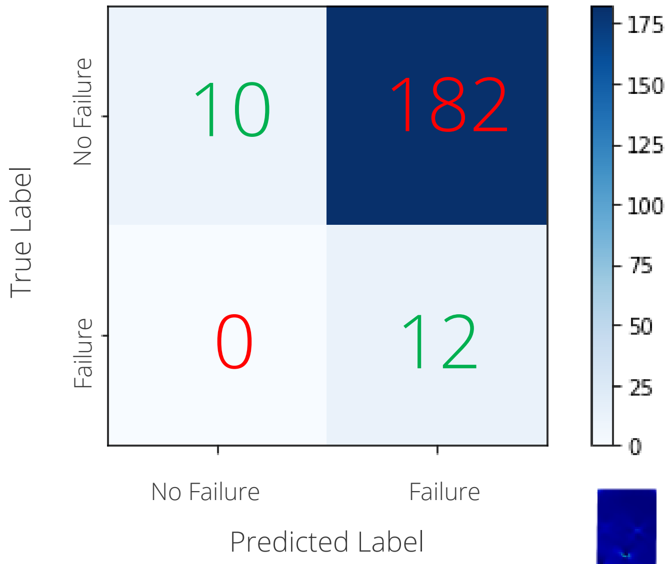
Cylindrical Tension

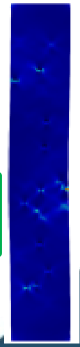




Test Accuracy: **80.0%**

Square Compression





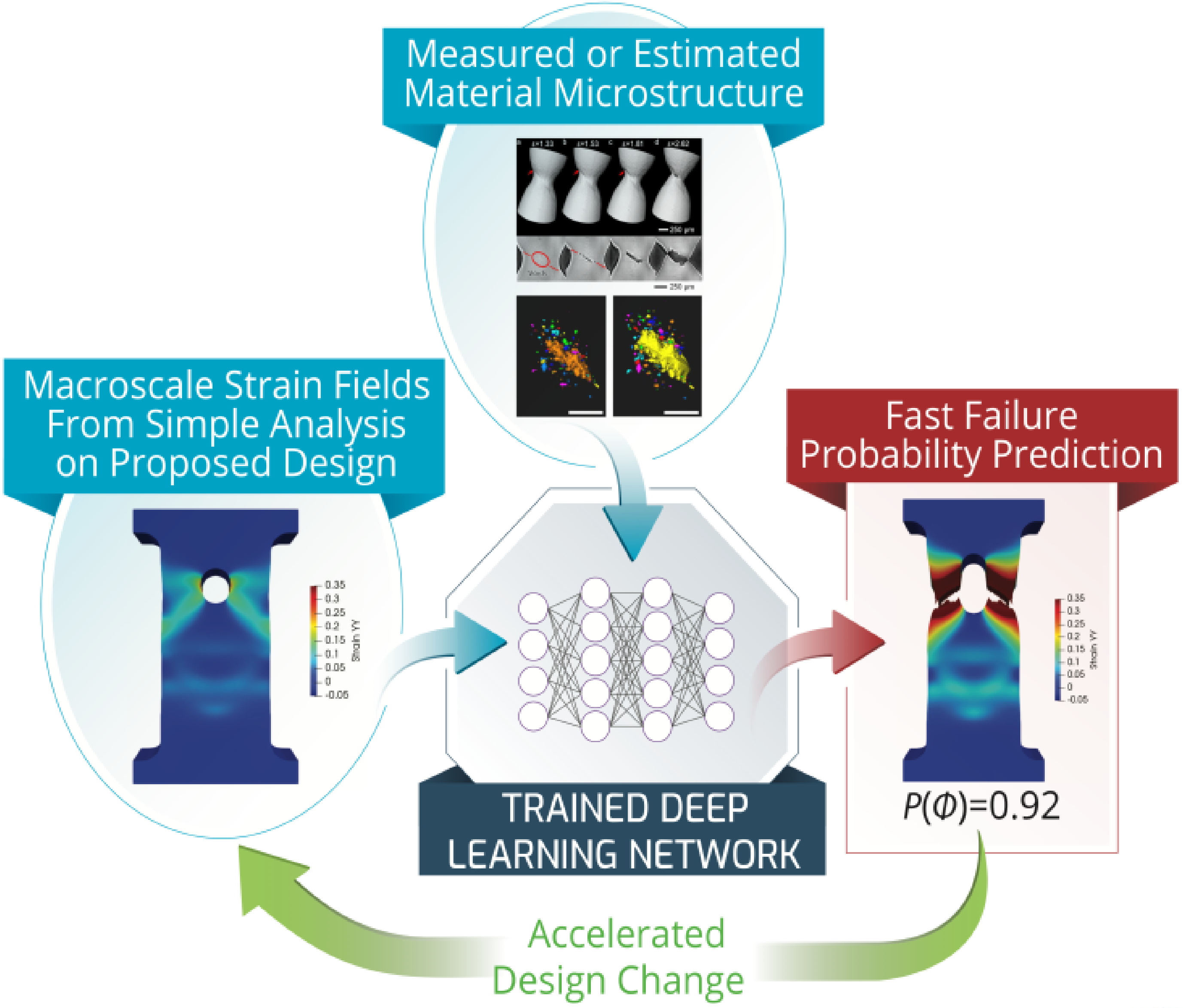
Test Accuracy: **10.8%**

Current 3-year project: Failure Prediction Using Deep Learning

- Extending approach to include Diffraction Contrast Tomography (DCT), in situ µCT, Digital Volume Correlation (DVC), crystal plasticity, and continuum damage modeling.

- Collaboration with Prof. Mike Sangid (Purdue) for High Energy Diffraction Microscopy (HEDM)

- Collaboration with Billy Oates and Brandon Krick (FAMU/FSU) for Transmission Electron Microscopy

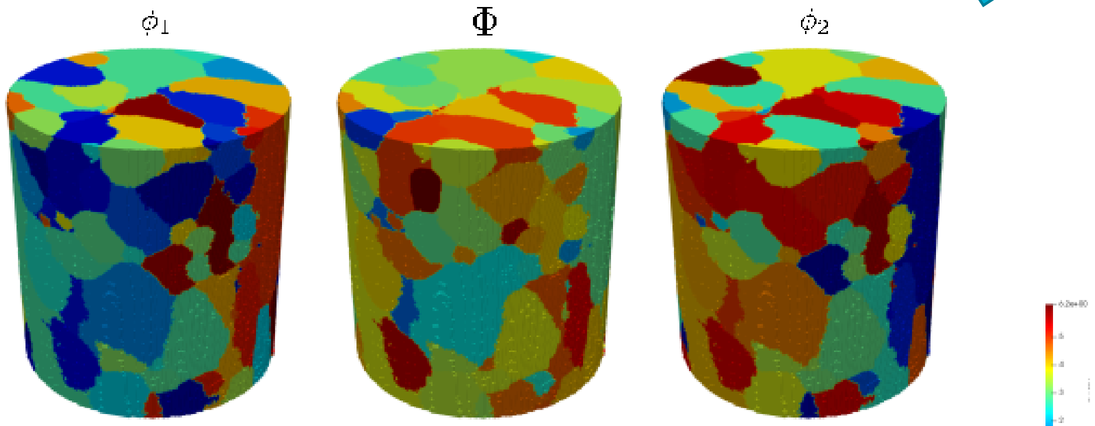


PURDUE UNIVERSITY

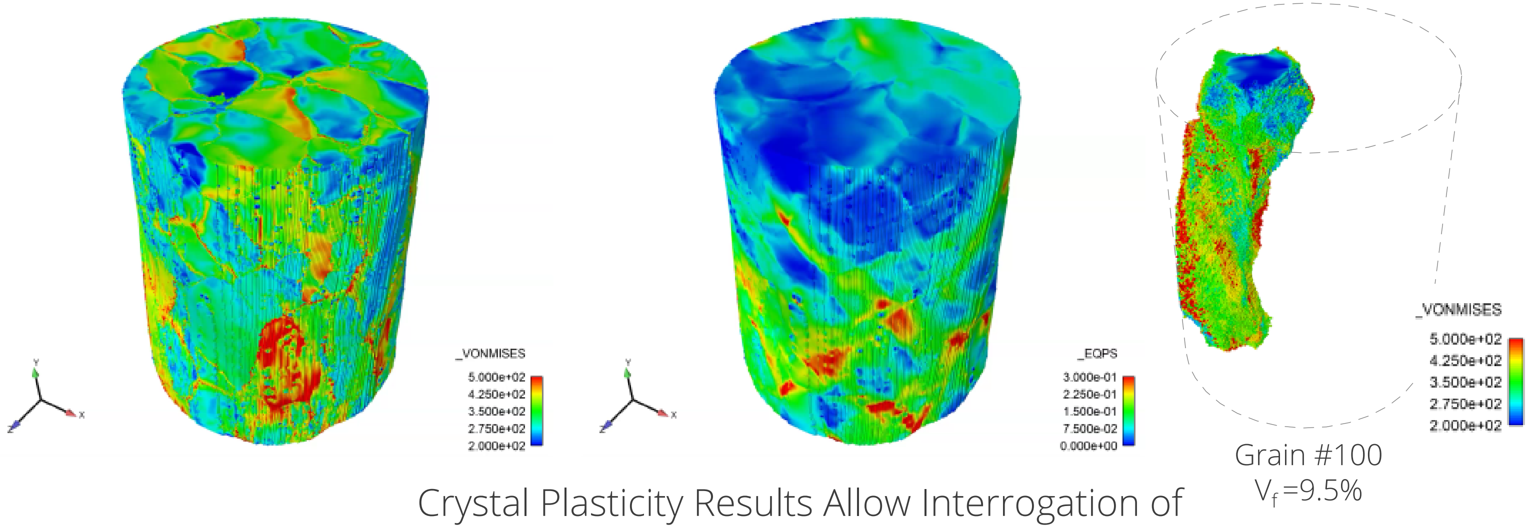
FAMU

New SNL Capability: DCT+crystal plasticity workflow successfully demonstrated

Diffraction Contrast Tomography Scan



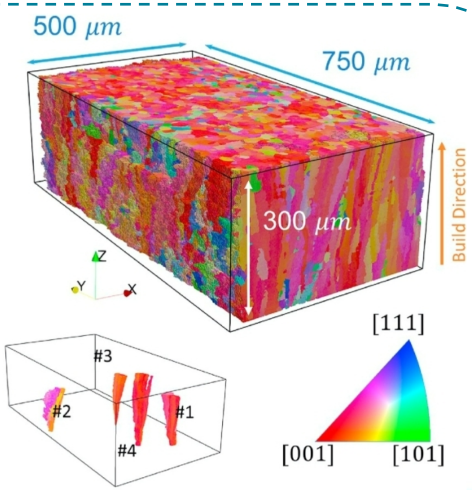
Euler Angles for Every Grain in Sample



Crystal Plasticity Results Allow Interrogation of Individual Grains

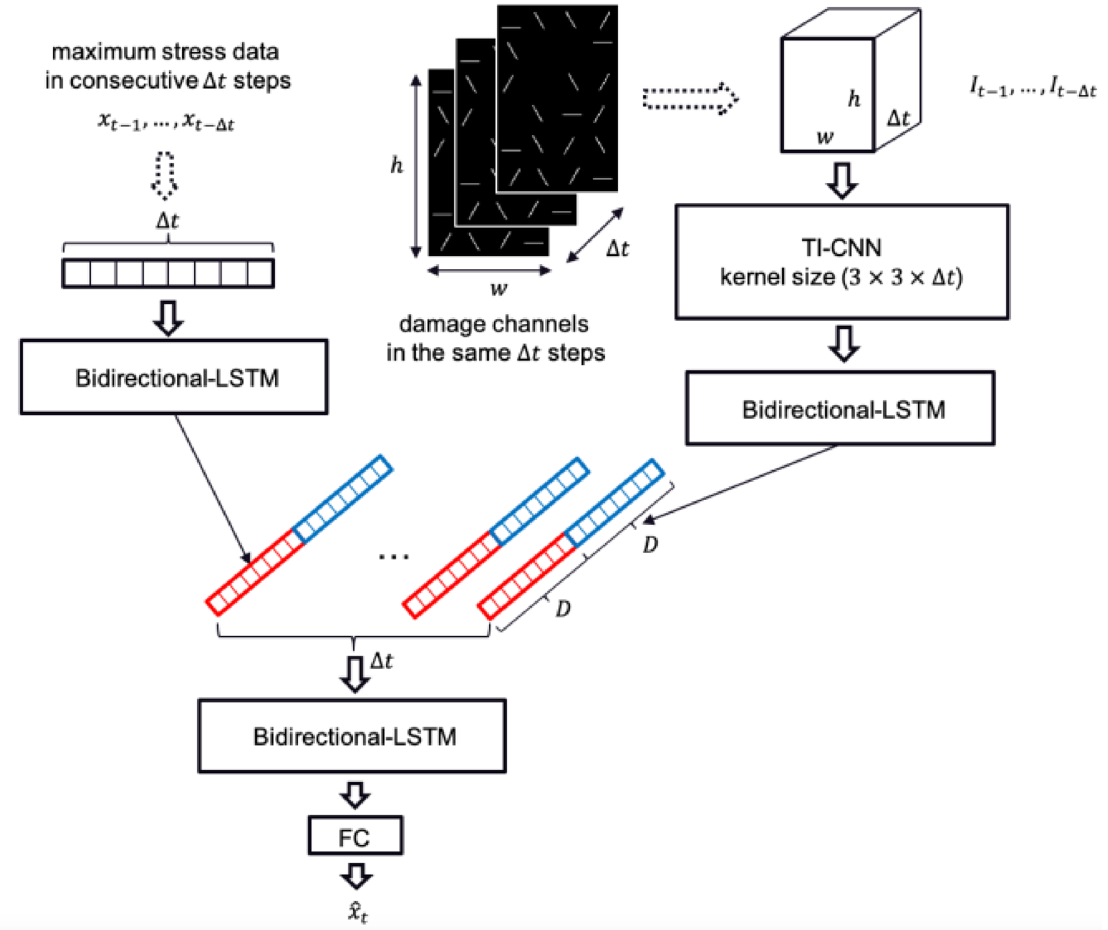
Future: TriBeam Validation

Awarded plus-up funding that will allow 3D EBSD reconstruction of sample to validate crystal plasticity predictions of DCT-characterized sample (Andrew Polonsky and Tim Ruggles)



Witzen et al., Int. J. Plast., 2020.

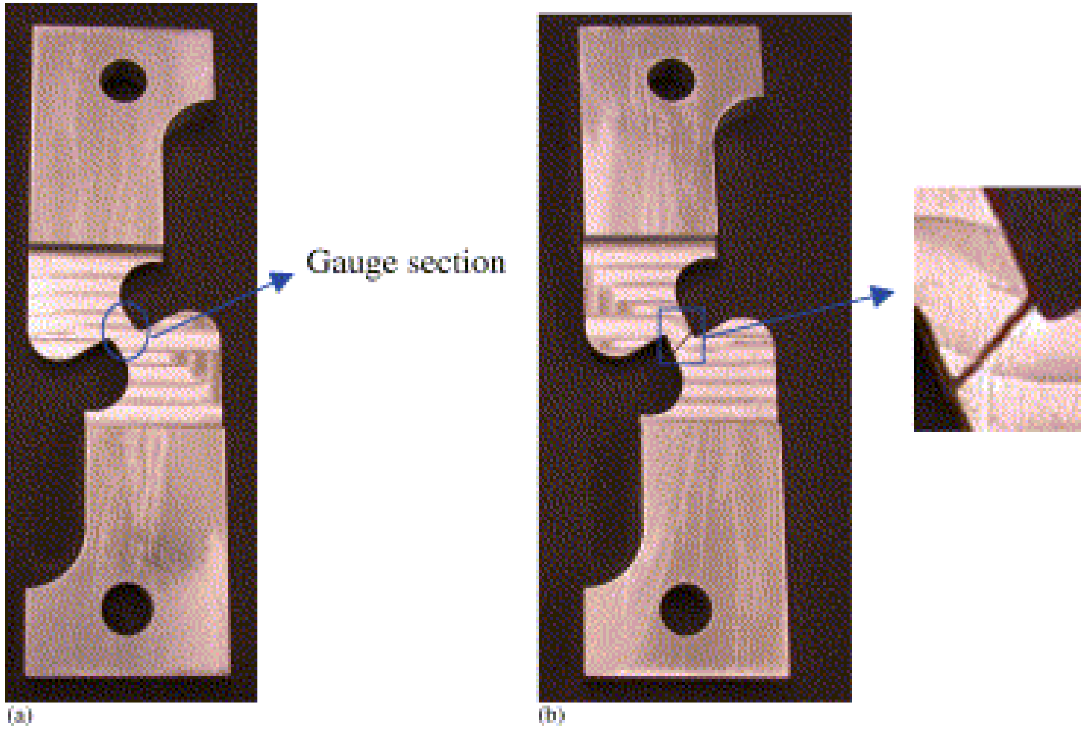
Ongoing Deep Learning Work



- Implementing and modifying StressNet[1] architecture to handle 3D, time-dependent datasets.

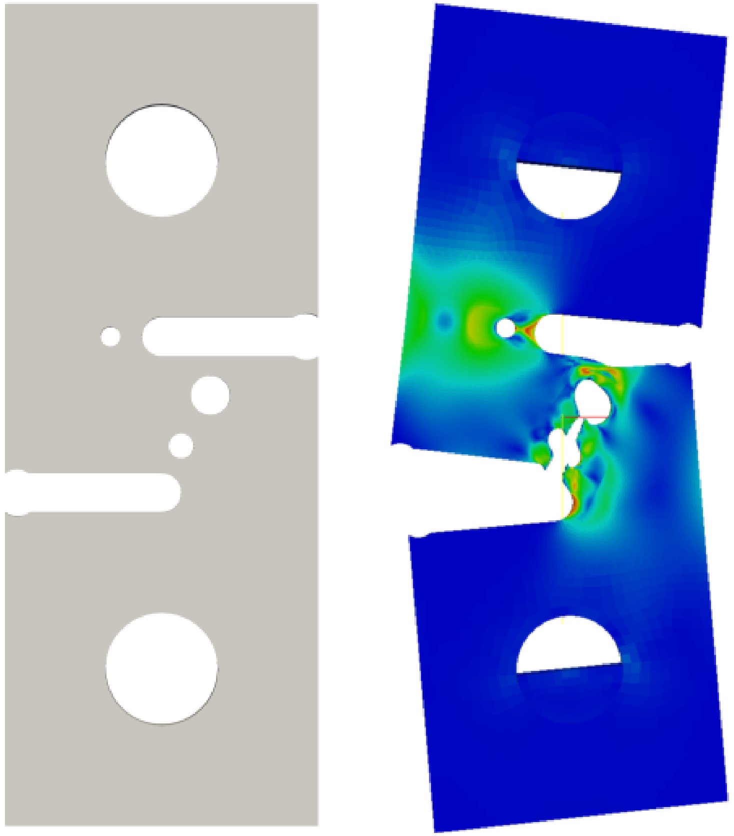
[1] Wang, Y. et al., "StressNet: Deep Learning to Predict Stress With Fracture Propagation in Brittle Materials", https://arxiv.org/pdf/2011.10227.pdf

Exemplar Designs



Combined Loading Failure Specimen

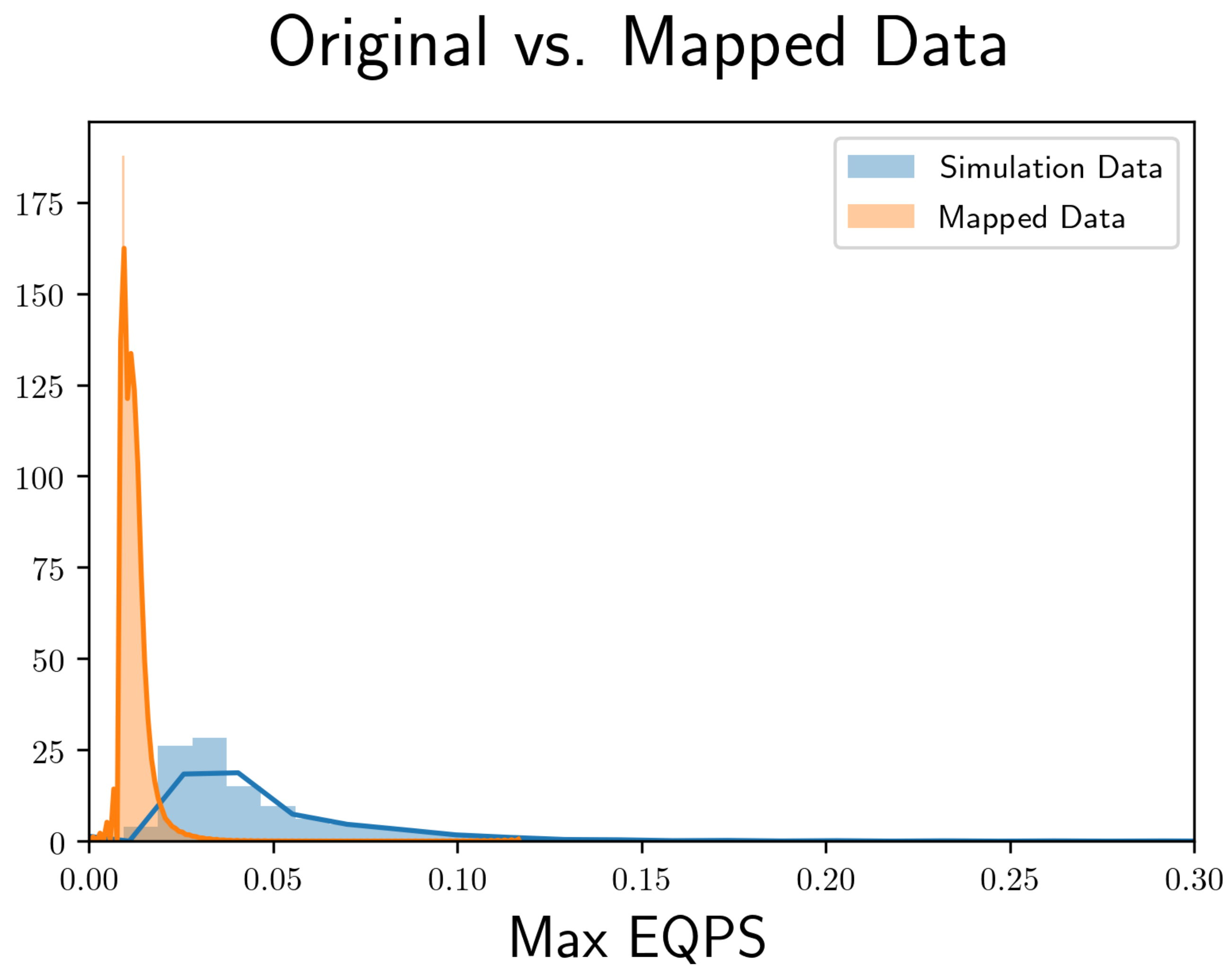
Bao and Wierzbicki, *Int. J. Mech. Sci.* 2004



2nd Sandia Fracture Challenge Specimen

Designs can be taken from different orientations of rolled plate to test anisotropy

Statistics of original data EQPS vs. mapped data EQPS illustrates smoothing



Memory management becomes an issue with large datasets

Current 3D training samples contain 750k voxels – approaching memory limits on GPU.

Multiple components of the DL process live in GPU memory simultaneously.

- DL model weights
- Activation function values
- Backpropagation update values
- 3D element values (batch of inputs)

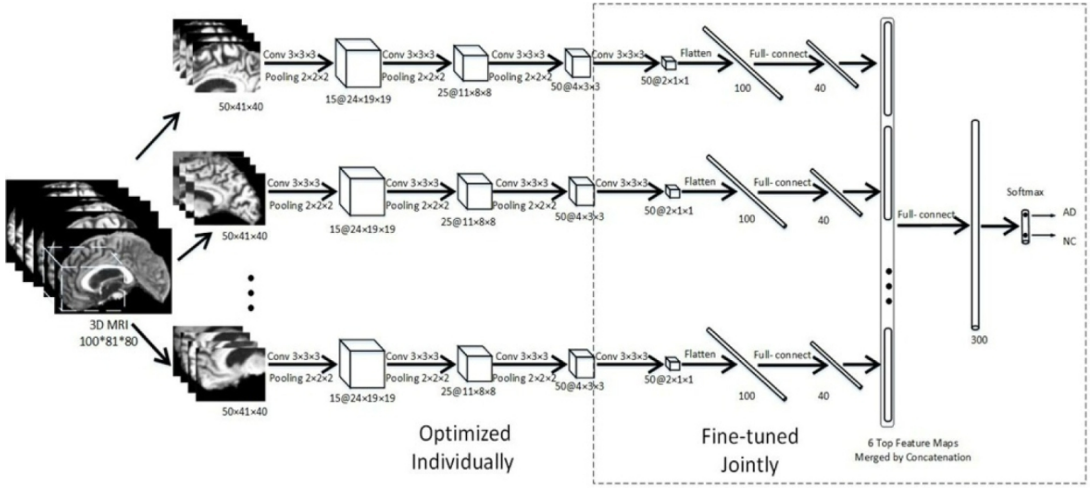
Scaling options

Increasing Complexity

- Batch size limitations
- Smaller/simpler architecture

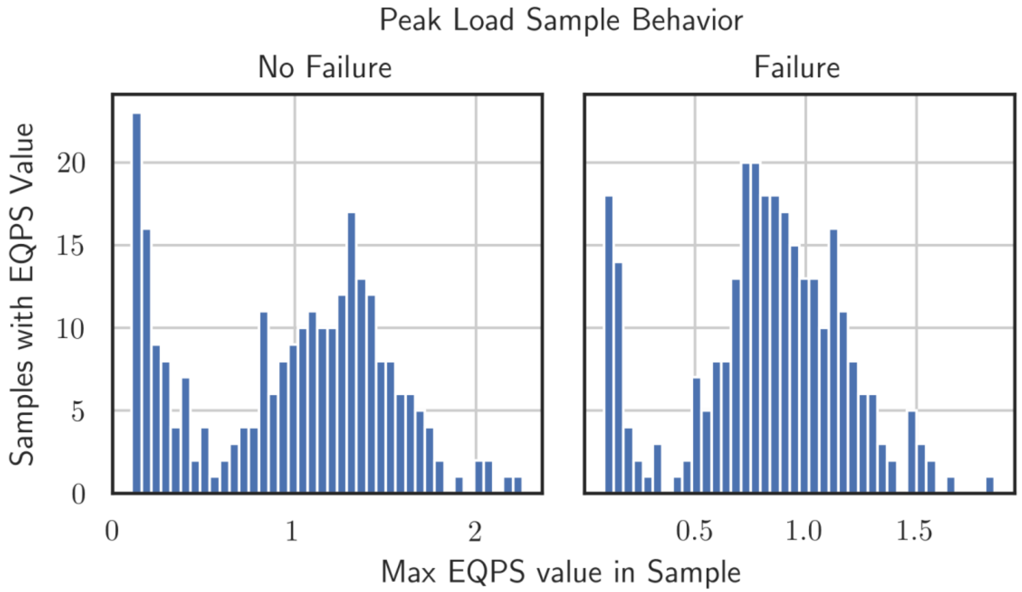
- Loading different architecture layers across GPUs
- Loading single architecture layer across GPUs

- Patch-wise CNNs
- Physics Informed Neural Networks – use physical insights to perform computations



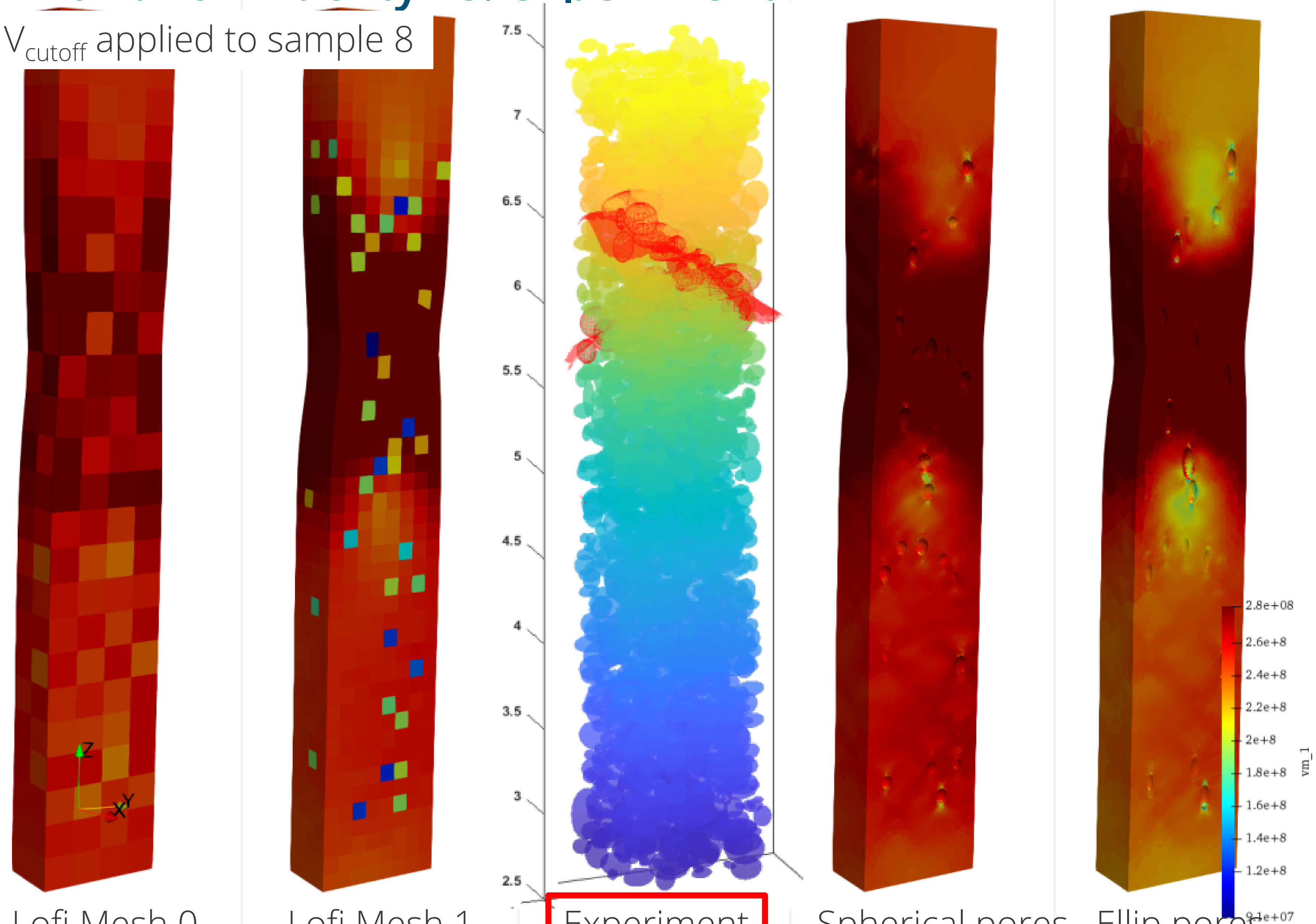
Patch-level CNN Classification (Cheng et al., ICDIP Proceedings 2017)

Algorithm is not simply ordering samples by ascending EQPS values.



Low- and full-fidelity vs. experiment

V_{cutoff} applied to sample 8



Lofi Mesh 0 | Lofi Mesh 1 | Experiment | Spherical pores | Ellip pores