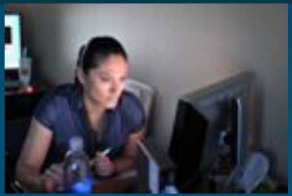
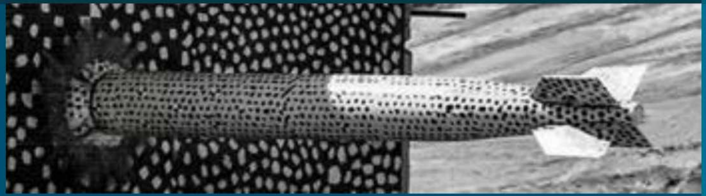
Sandia National Laboratories

SAND2020-7482C

A New Paradigm for Materials Science Failure Prediction Using Deep Learning





Presented by:

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Kyle Johnson (1558) (LDRD PI), Matthew Smith (9323), Carianne Martinez (9323), and John Emery (1558)

U.S. DEPARTMENT OF ENERGY NNSA

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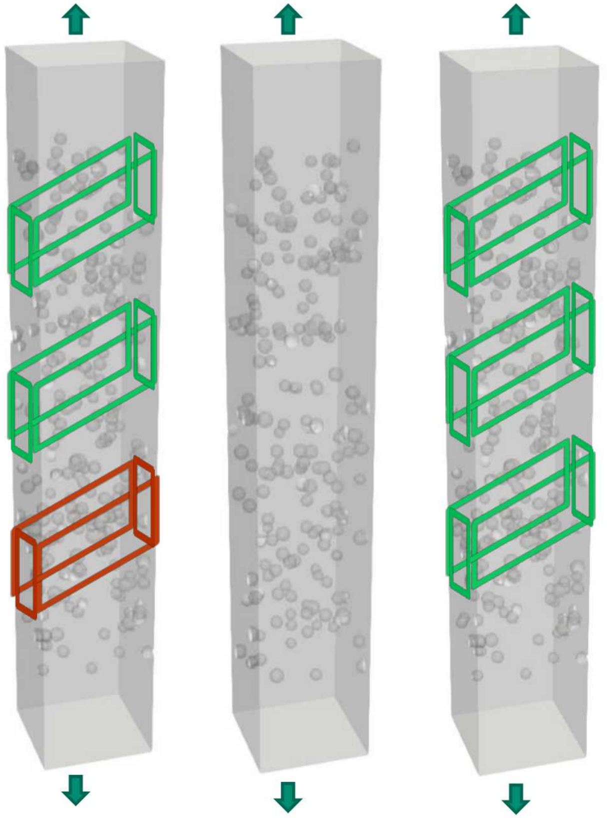
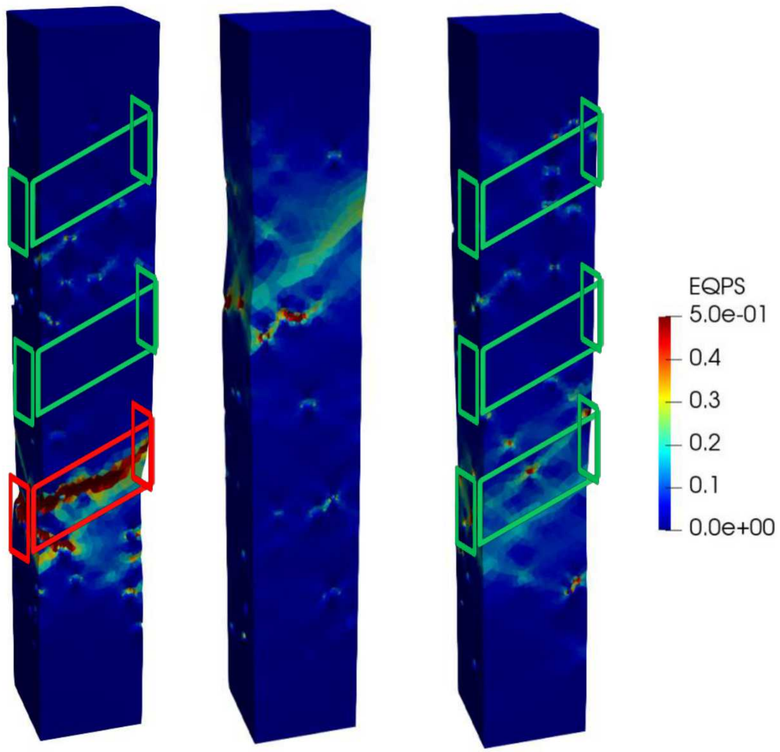
Numerical methods

Currently: Numerical simulations allow for “failure” prediction of mechanical behavior of a tensile bar.



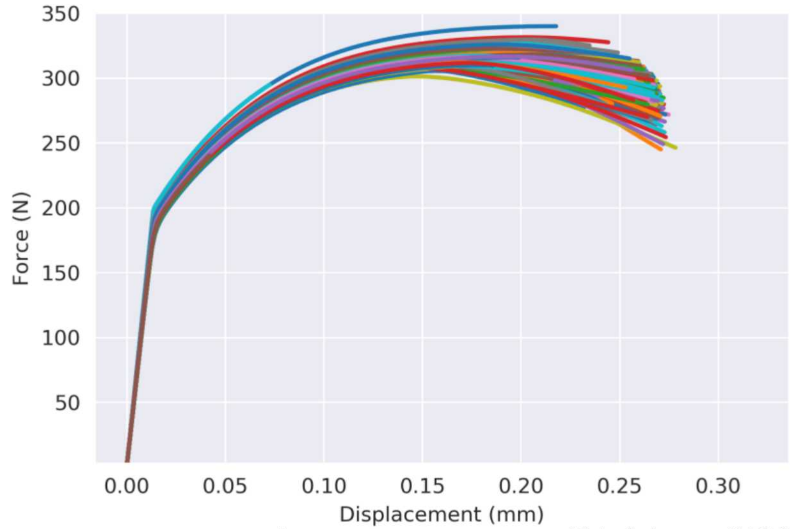
Kyle Johnson (1558)

Voids in Geometric microstructure



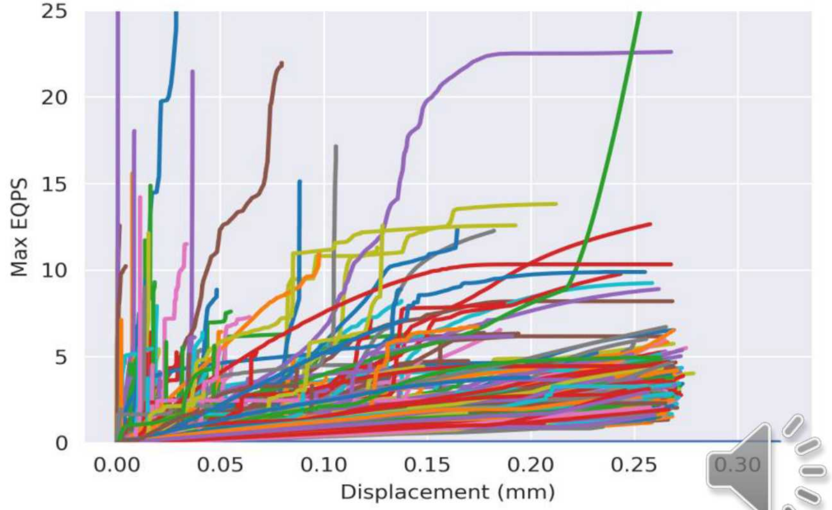
Kyle Johnson (1558)

Tensile bar with tetrahedral elements



Force vs Displacement

Kyle Johnson (1558)



EQPS vs Displacement

Kyle Johnson (1558)

Numerical methods

Currently: Numerical simulations allow for "failure" prediction of mechanical behavior of a tensile bar.

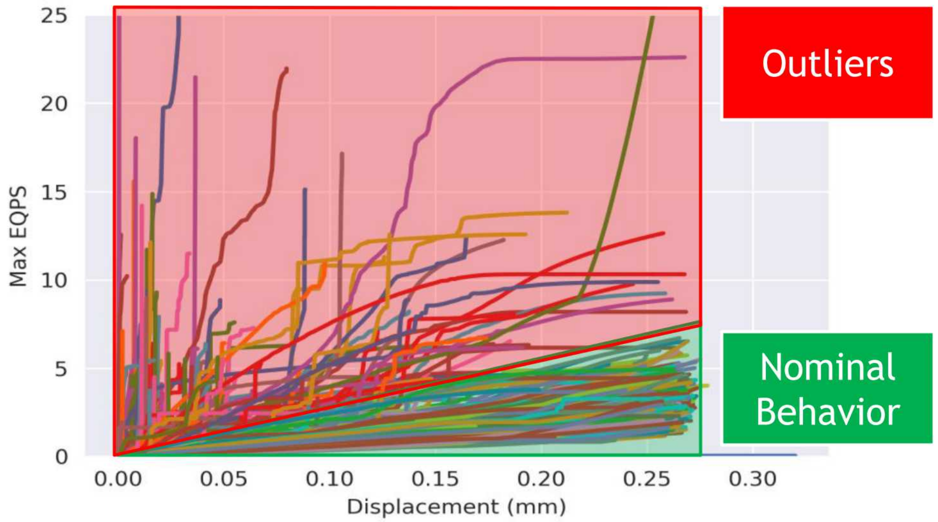
"Failure": The inability of a sample to reach a required load.

Failure Metrics include:
- Critical Equivalent plastic strain (EQPS) before meeting required load

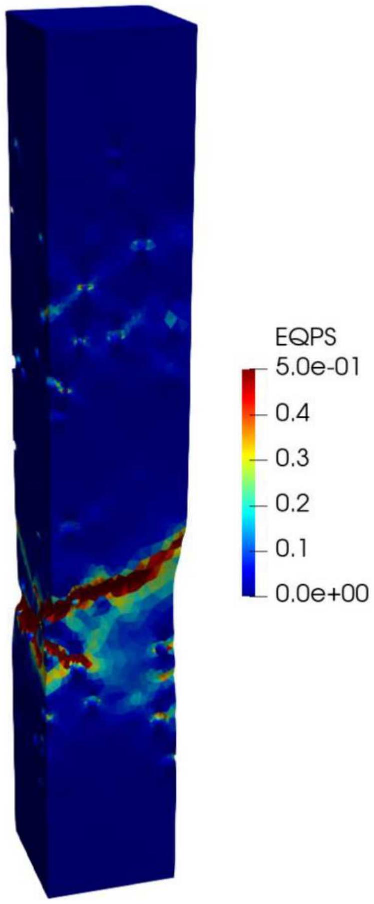
- Critical Equivalent plastic strain before meeting required Displacement

- Reaching a required load

- Reaching a required displacement



EQPS vs Displacement

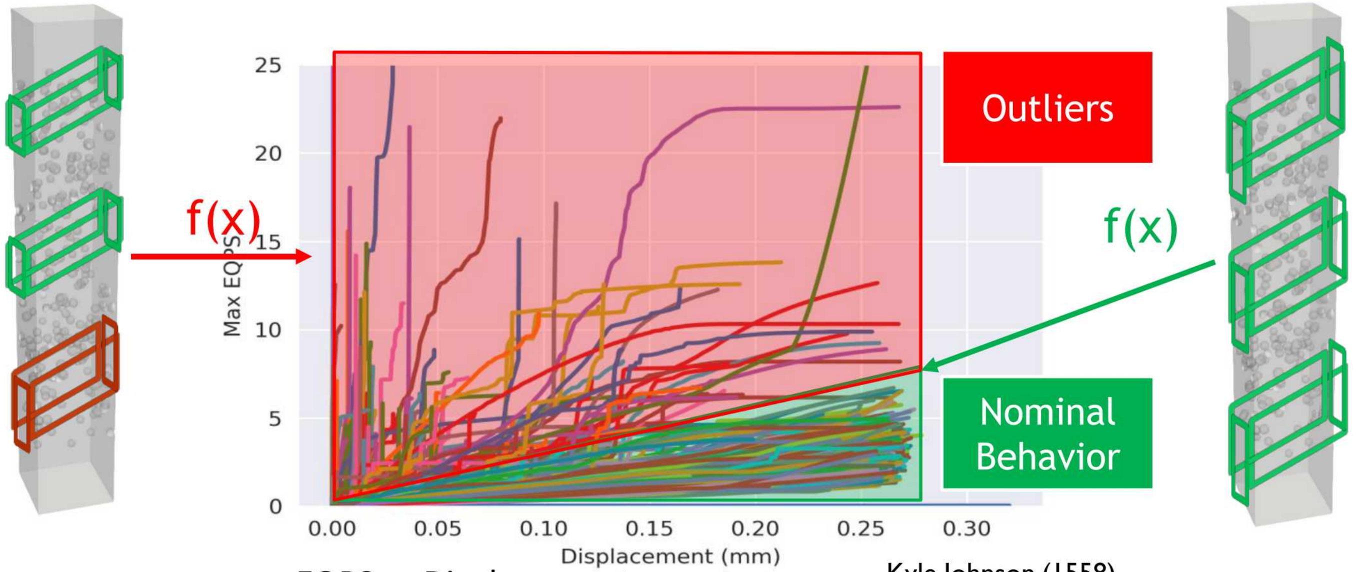


Tensile bar

This is great, but can we do better?

Simulation Time: 88 minutes on 216 CPUs of a CTS-1 cluster

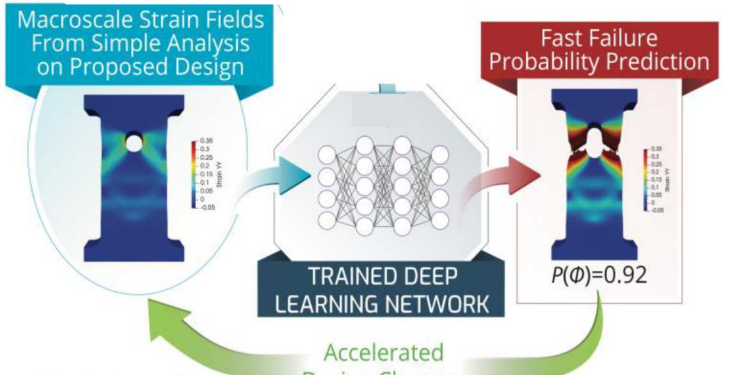
So, why Deep Learning?



EQPS vs Displacement

Kyle Johnson (1558)

- Mechanical performance measured from these square bars is a function of defect structure
- Neural networks are universal function approximators!
- In this case, we hope to approximate void structure -> Mechanical performance



Training Cycle

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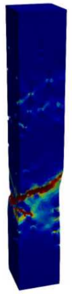
- Cost is the initial training time for DL (~1.5 days), but then inference in milliseconds!
- If keeping the same microstructure domain, we may be able to predict over similar macrostructures!



This is not a true replacement for numerical methods, but can be used to rapidly sample the design space of materials components!

DL Architecture

We used a model that was pretty close to out of the box:

"Diagnosis of Alzheimer's Disease via Multi-modality 3D Convolutional Neural Network"

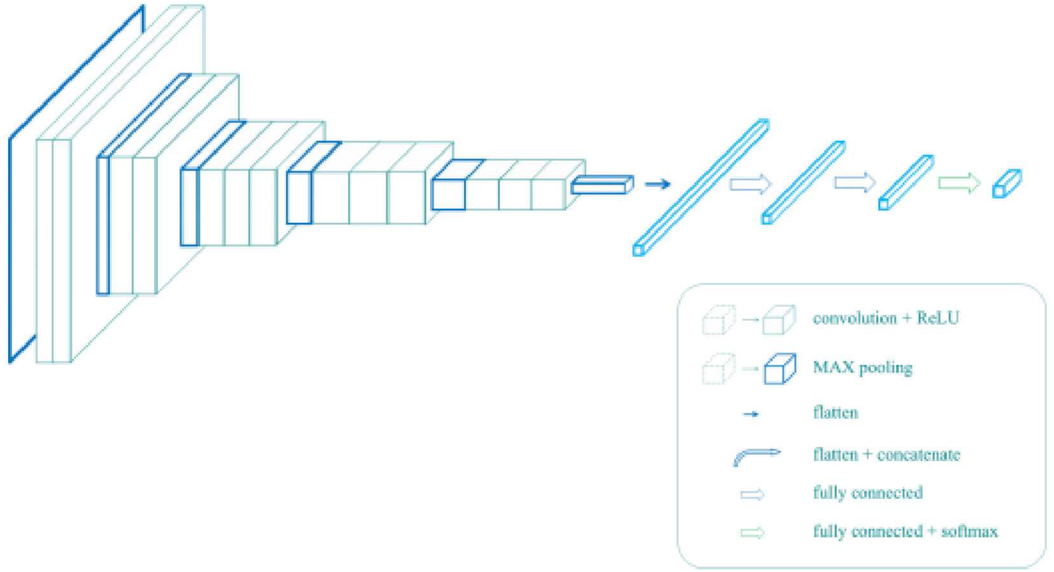
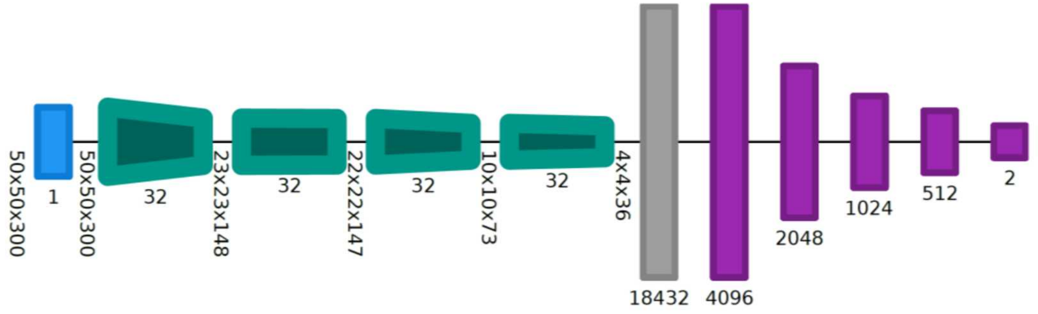


Figure 1 VGG16, which is a very deep network consisting of 13 convolution layers, 5 max pooling layers and 3 fully connected layers. Several convolution layers are followed by max pooling layer, reducing the dimensionality. In this figure, the original image with pixel size 224 × 224 formed a feature map of size 7 × 7 × 512 after multiple convolutions and pooling layers, obtaining classification result after fully connected and Softmax layers.

arXiv:1902.09904 **[cs.CV]**

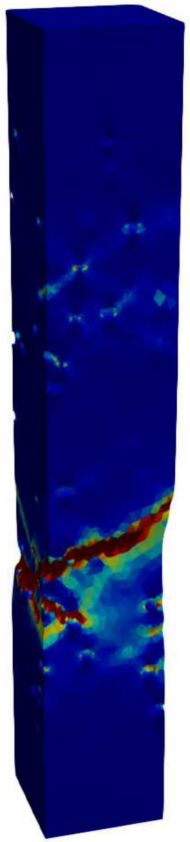
Our Model:



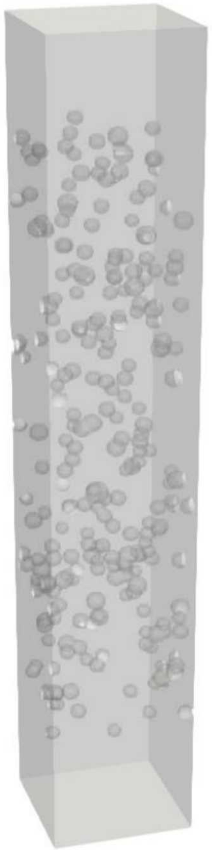
Steve Sleder (9323)

Data to Architecture

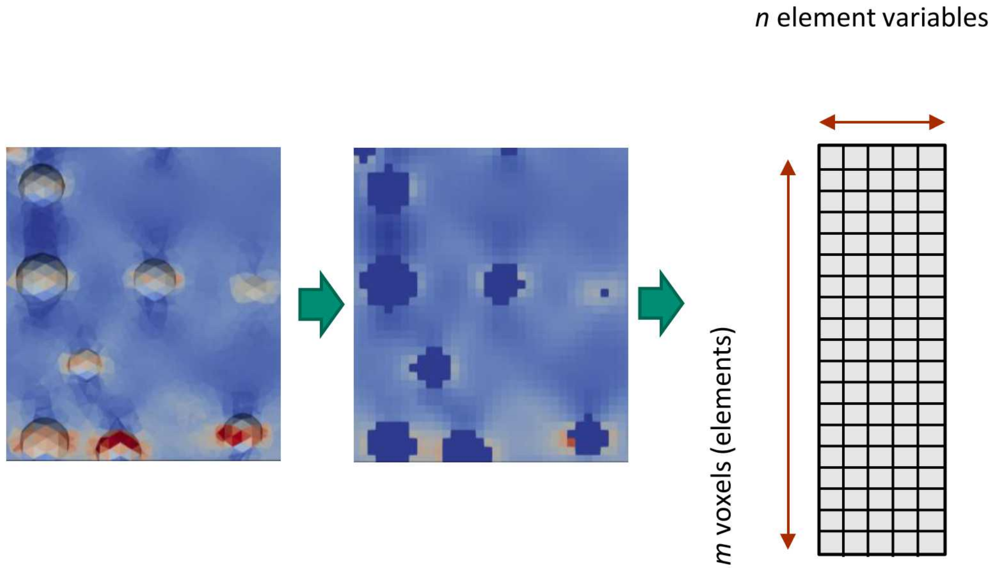
The architecture was close to off-the-shelf, as the goal of the project was to rapidly explore microstructure to mechanical performance mapping. The input data was converted to match the format of the architecture in the interest of time.



Tensile bar with tetrahedral elements



Voids in Geometric microstructure



Tets

Voxels

Array

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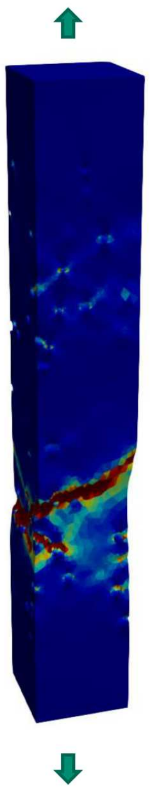
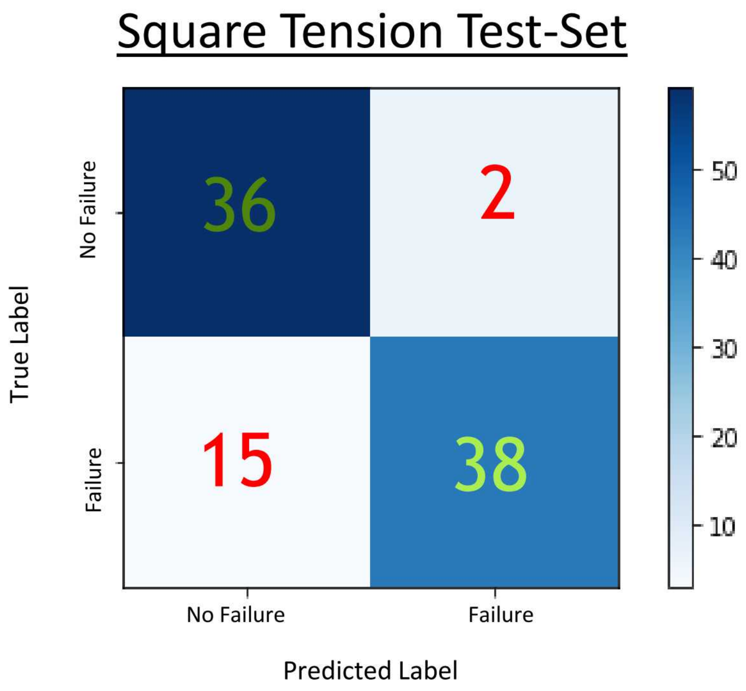
Square data results

Results of the held back test set over **reaching a required load** using the square tension bars.

Failure Metrics include:
- Critical Equivalent plastic strain (EQPS) before meeting required load
- Critical Equivalent plastic strain before meeting required Displacement
- Reaching a required load
- Reaching a required displacement



Tensile bar with tetrahedral elements



Test: Accuracy: **84.7%**

Speedup

The cost of training the network is large, but after the network is trained, we see a huge decrease in per-sample estimation time.

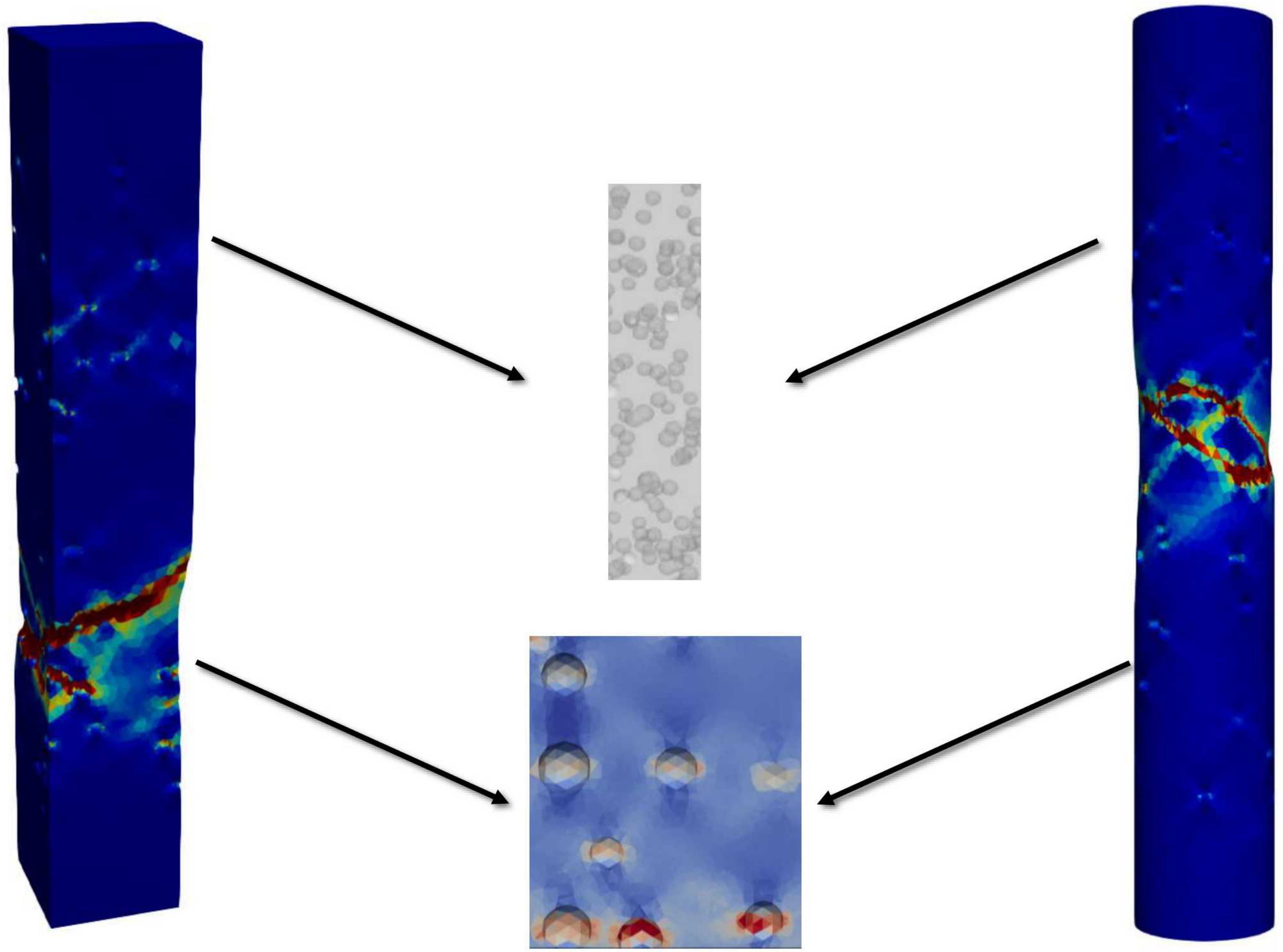
FEA Simulation Time: 88 minutes on 216 Ghost CPUs

DL Network Inference Time: 20 milliseconds on 2 GPUs

Speedup: **264000x**

More applications

We currently believe the microstructure geometry and mechanics are explicitly driving the DL prediction.
Because of this, we believe there is potential for classifying the mechanical performance of different macrostructures given the microstructure is in the same domain

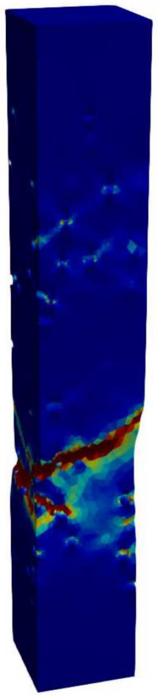


Tensile bar

Cylindrical tensile rod

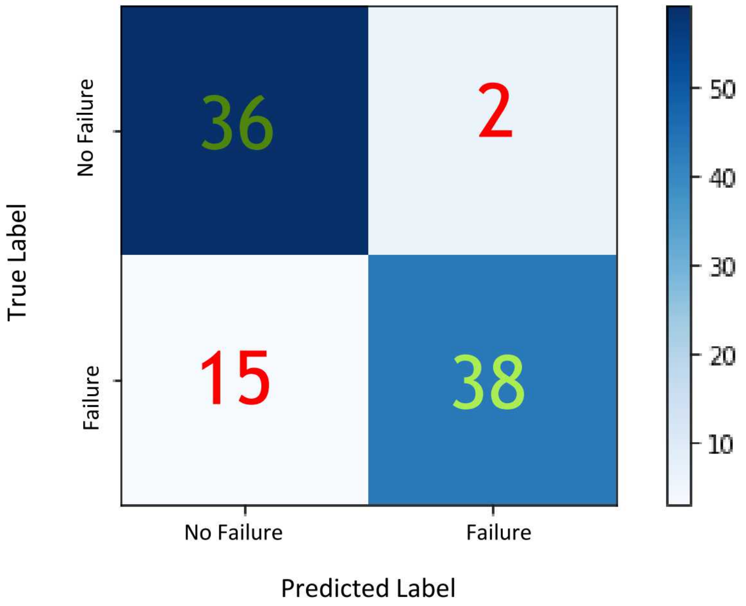
More Applications

Results of reaching a required load over cylindrical tension bars.

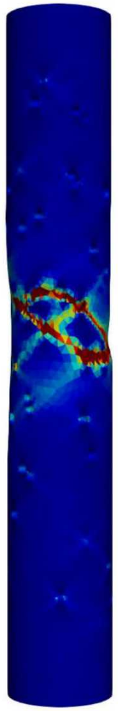


Square Tension Test-Set

(trained over square tension data)

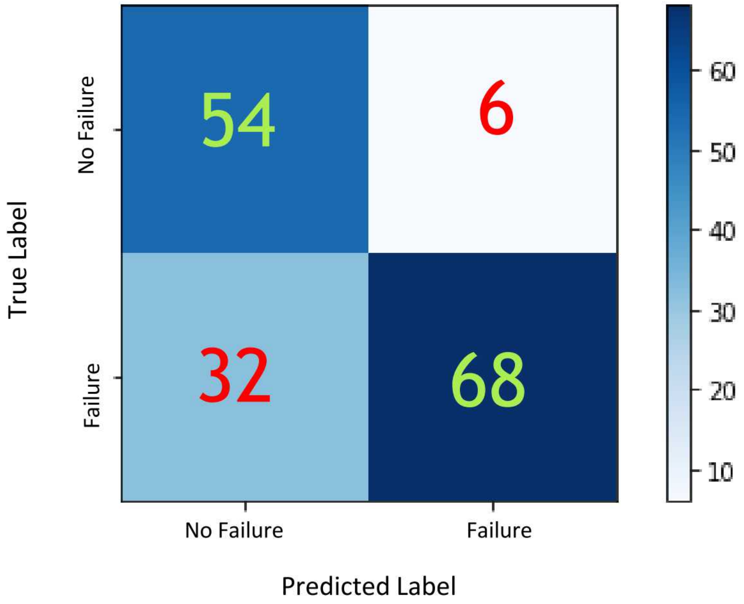


Test: Accuracy: **84.7%**



Cylindrical Tension Test-Set

(trained over square tension data)

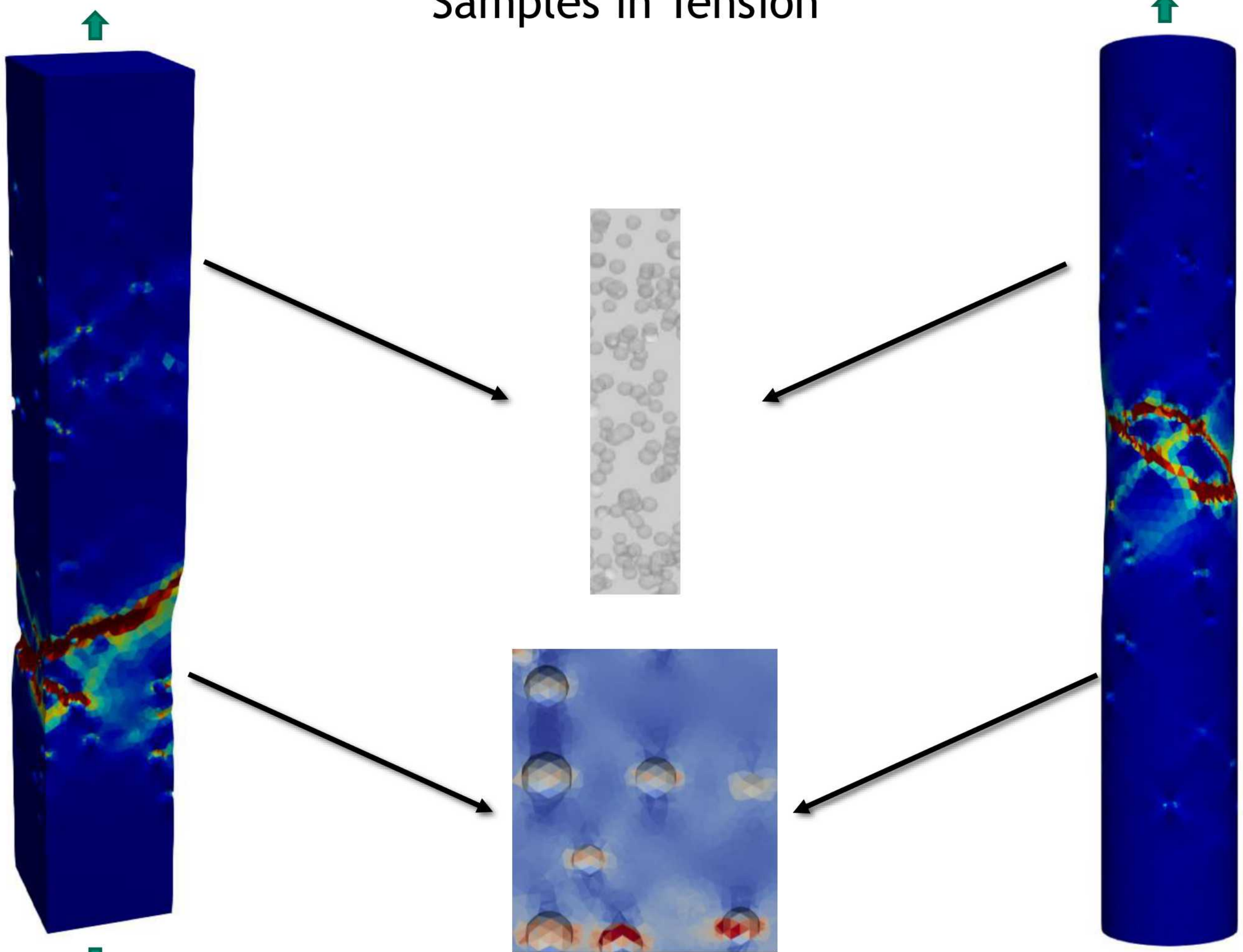


Test: Accuracy: **76.2%**

More Applications

We've run our failure prediction DL model over different macrostructures in tension. If we were to apply a different force such as compression to the macrostructure, are we going to see the same results?

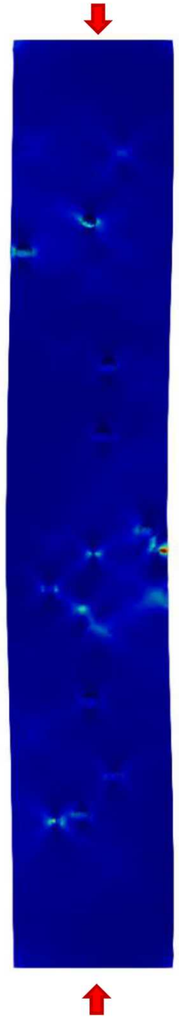
Samples in Tension



Tensile bar

Cylindrical tensile rod

Samples in Compression



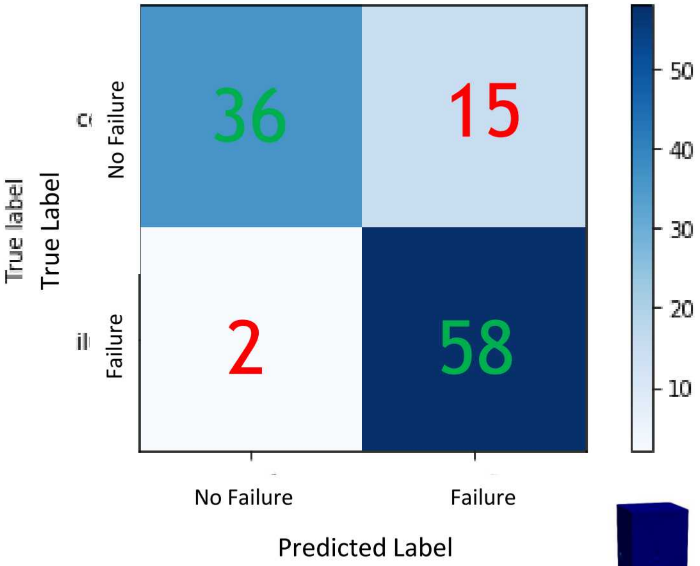
Compressive bar

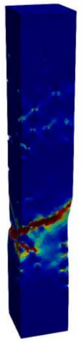
More Applications

Ultimately yes, due to the forces over the microstructure of the material. This provides some level of confidence that the algorithm is truly learning the classification of a curve relative to that materials simulation in this domain.

Required load examples:

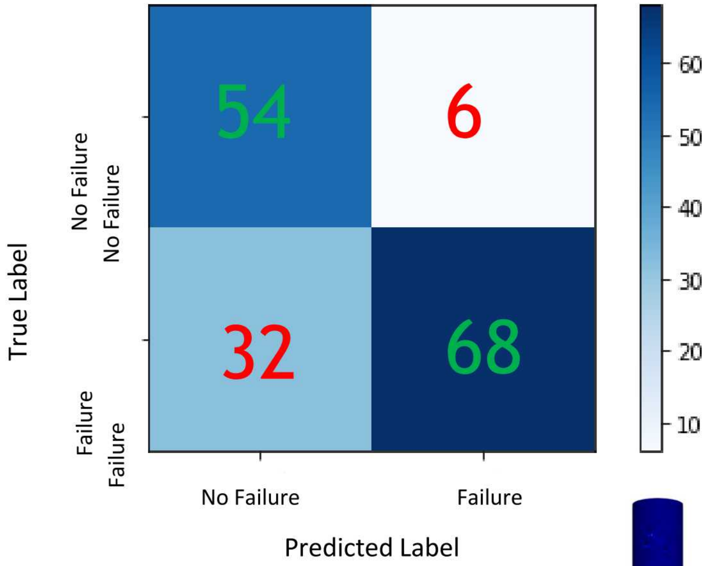
Square Tension Test-Set
(trained over square tension data)

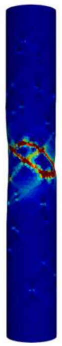




Test: Accuracy: **84.7%**

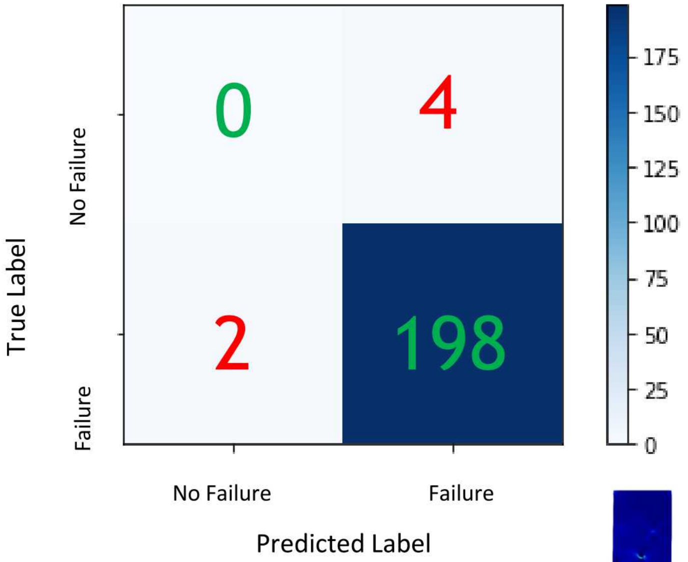
Cylindrical Tension Test-Set
(trained over square tension data)

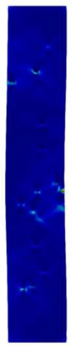




Test: Accuracy: **76.2%**

Square Compression Test-Set
(trained over square tension data)

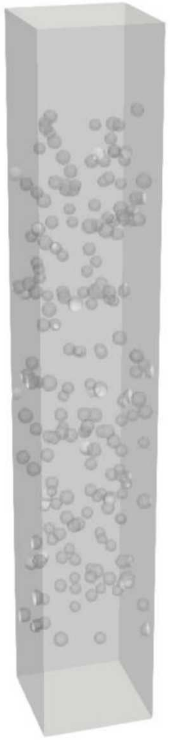




Test: Accuracy: **97.1%**

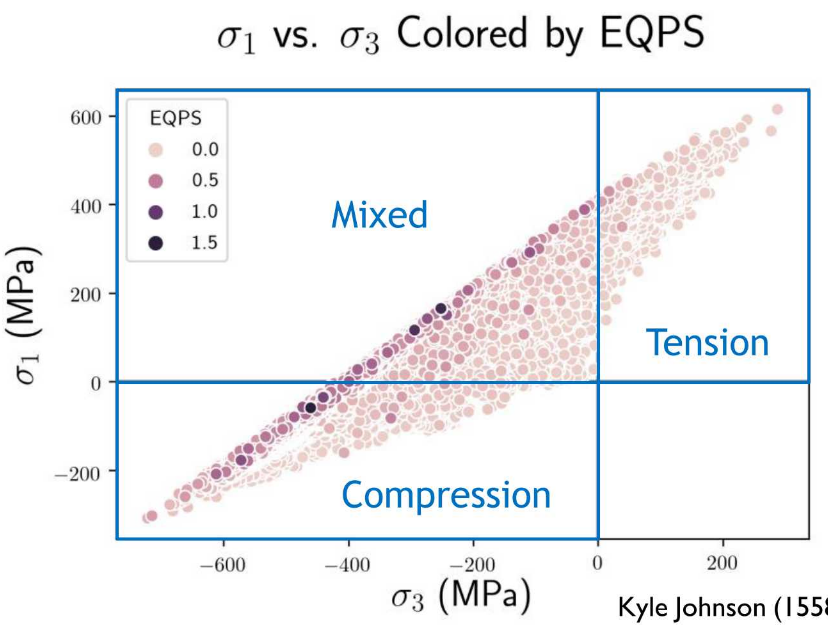
More Applications

Ultimately yes, due to the forces over the microstructure of the material. This provides some level of confidence that the algorithm is truly learning the classification of a curve relative to that materials simulation in this domain.



Voids in Geometric microstructure

In Compression



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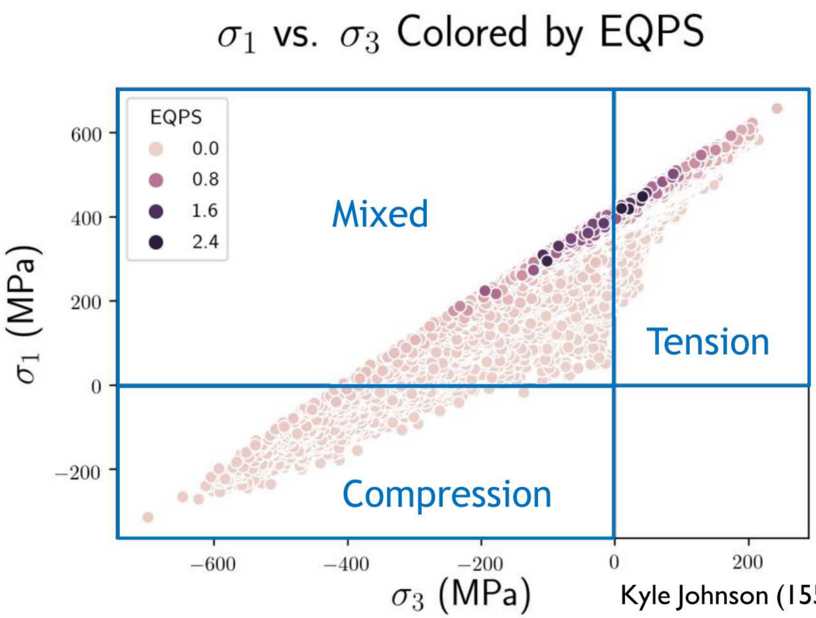
In Tension



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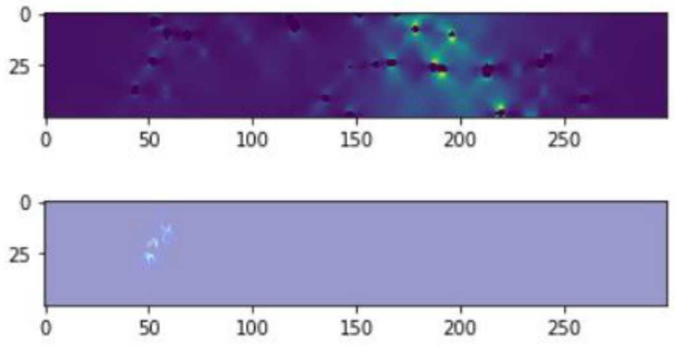
Future work

- Test more forces (now working on triaxiality)
- Start looking into activation visualizations
- Publish work
- Not a 3 year LDRD; These results were generated with seed funding in 8 months.

Activation map visualizations



Top: EQPS Results
Bottom: Activation Map of internal layer