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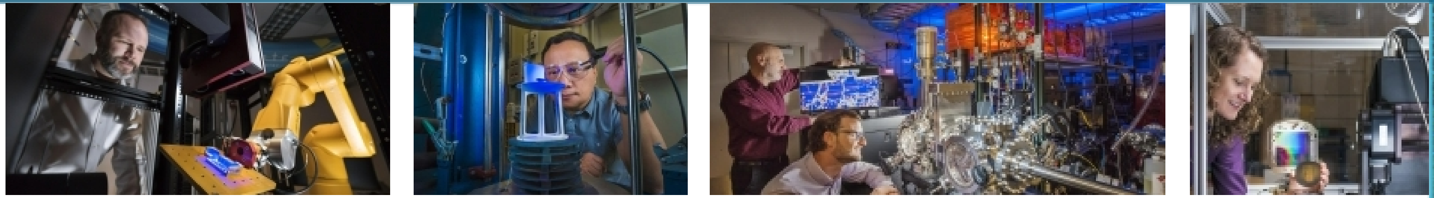
Sandia National Laboratories

Estimating Uncertainty of Neural Network Predictions for Inelastic Mechanical Deformation using Coupled FEM-NN Approach

MATERIALS SCIENCE & ENGINEERING



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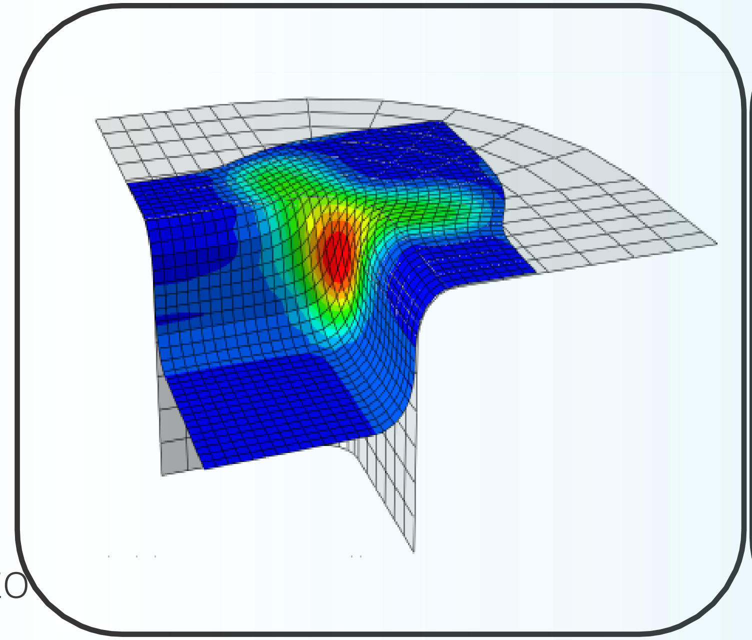
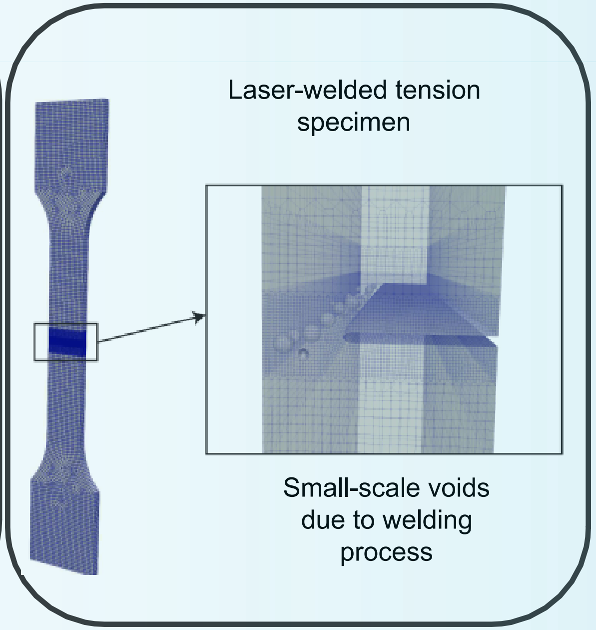
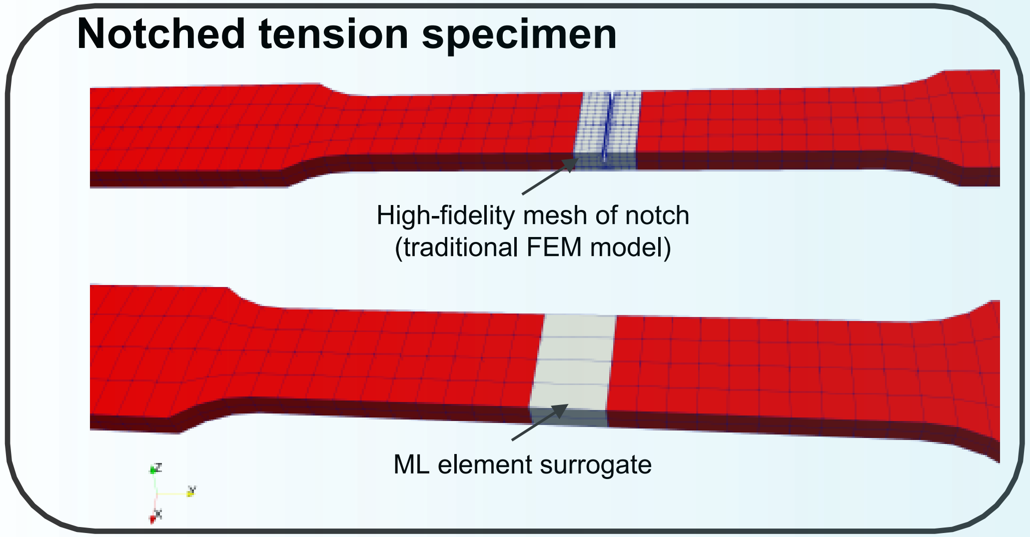
Accelerated and Accurate Results: The need for a coupled FEM-NN Approach

1. FEM iterative nature and need to solve complex non-linear equations require significant computational power and time.
2. System wide and large component simulations have complex/intricate geometry that is note easily meshed/discretized (memory constraints) and requires significant time to obtain a response.

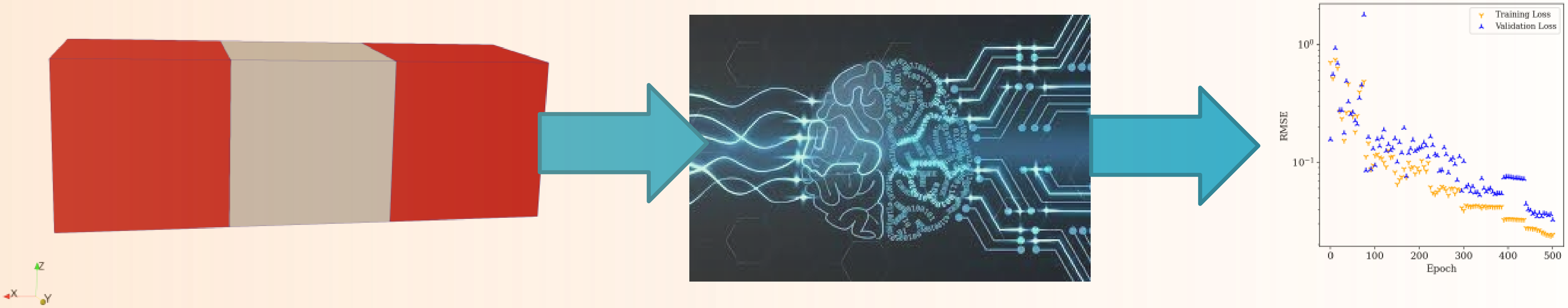


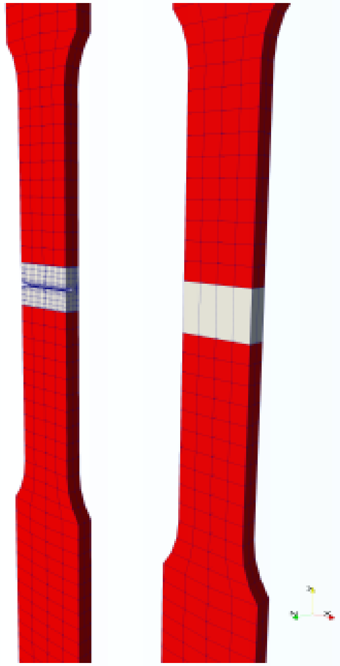


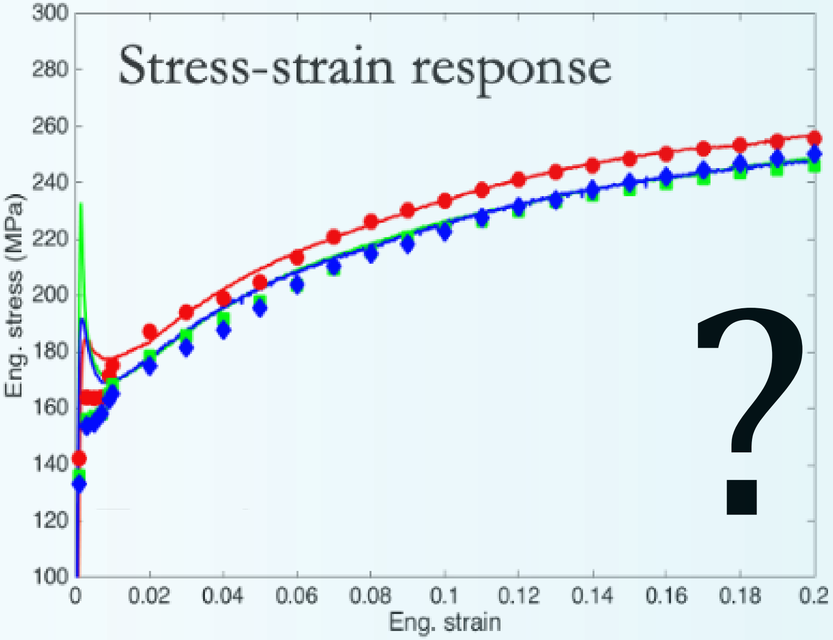
- There is a critical need for a data-driven approach to account for fine-scale features without directly incorporating them in a simulation.
- Neural networks are a viable surrogate to approximate the forces/deformations that occur at these fine scale features and the rest of the model.
- NN-FEM elements are trained to set of training data and can be used to provide accurate predictions for new/unseen geometries and loadings.

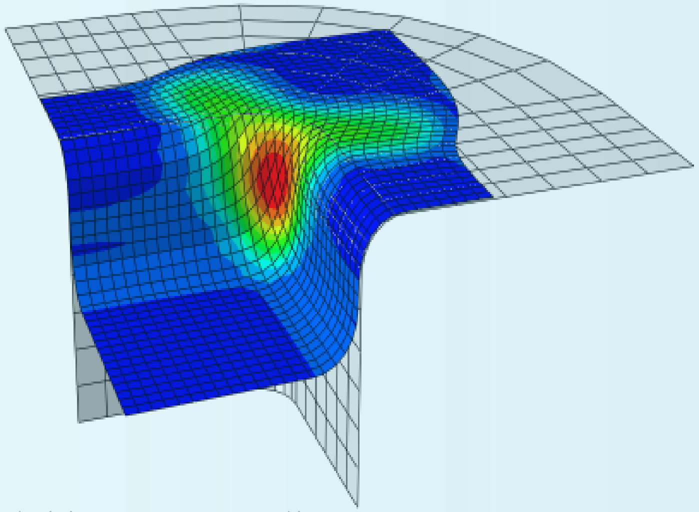


How can you trust the answer of the model?

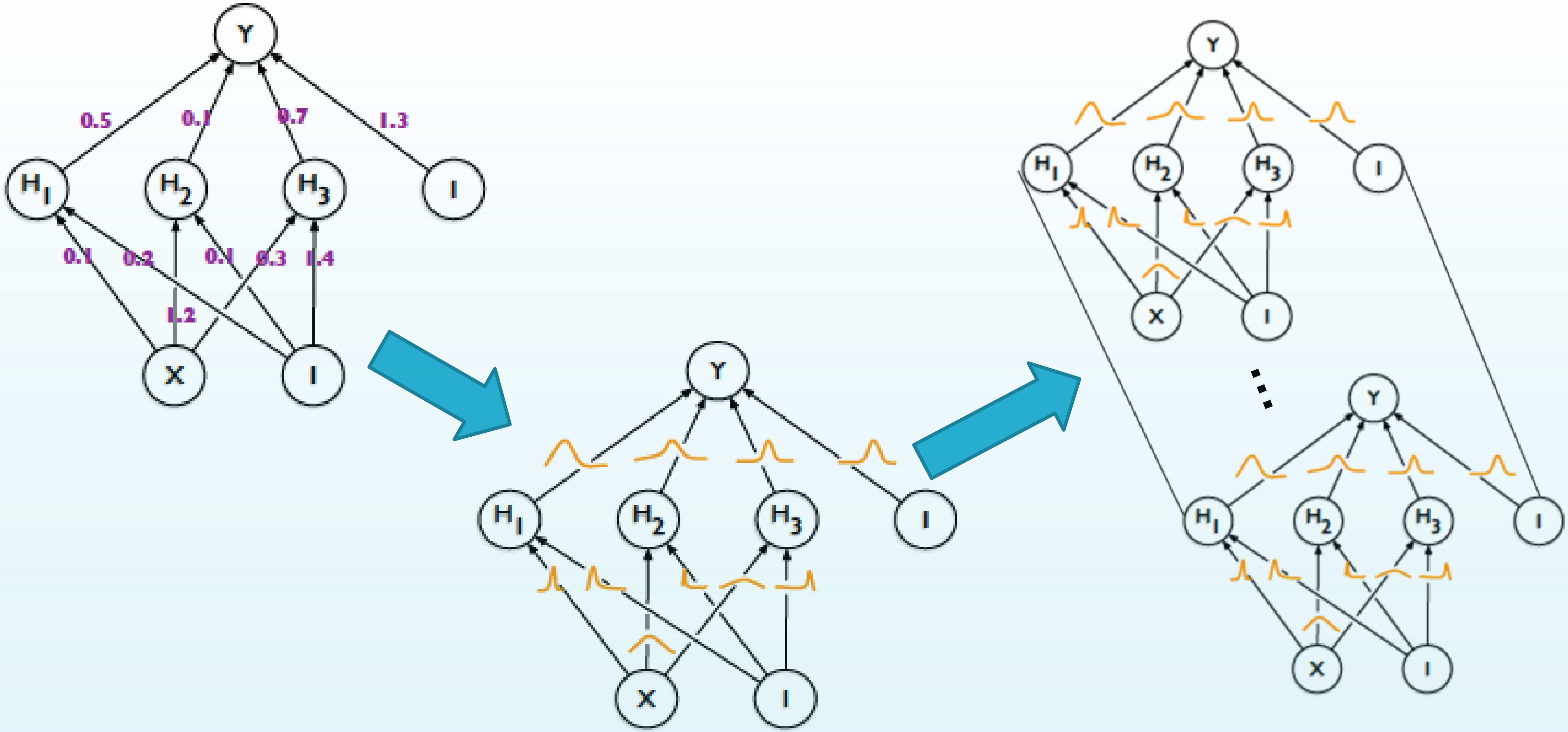




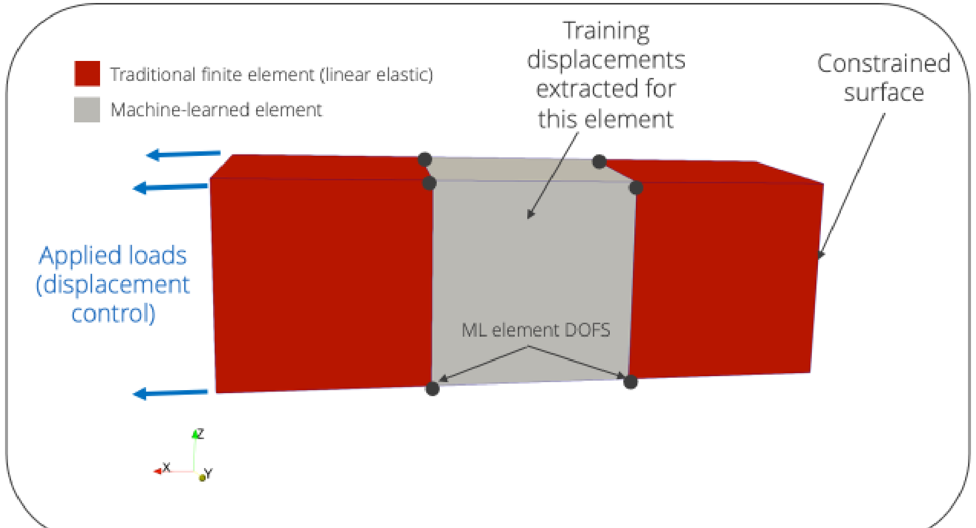


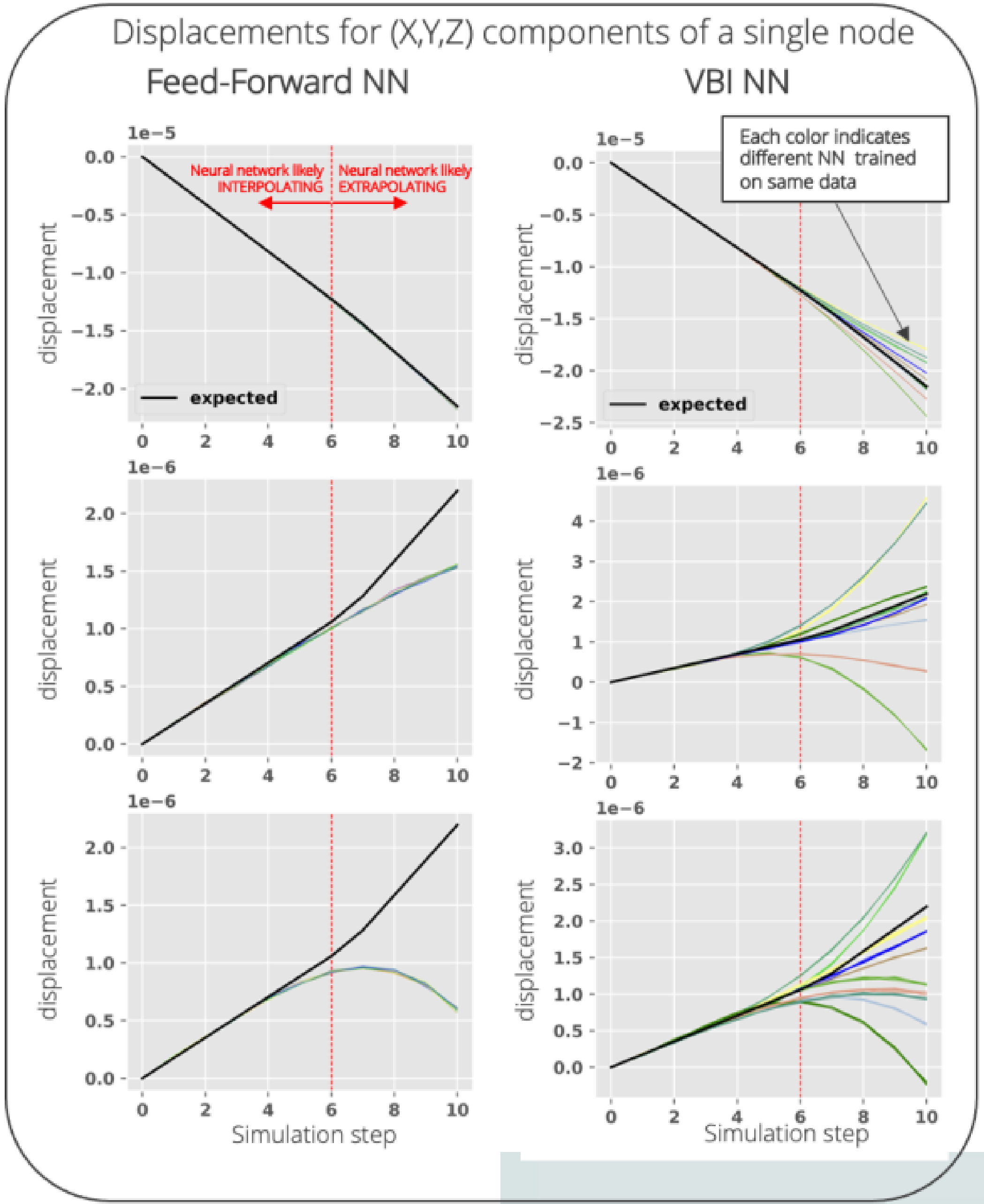


Make a model say "I don't know": Uncertainty Quantification in Deep Learning Models



Make a model say "I don't know": Example in Coupled FEM-NN Model





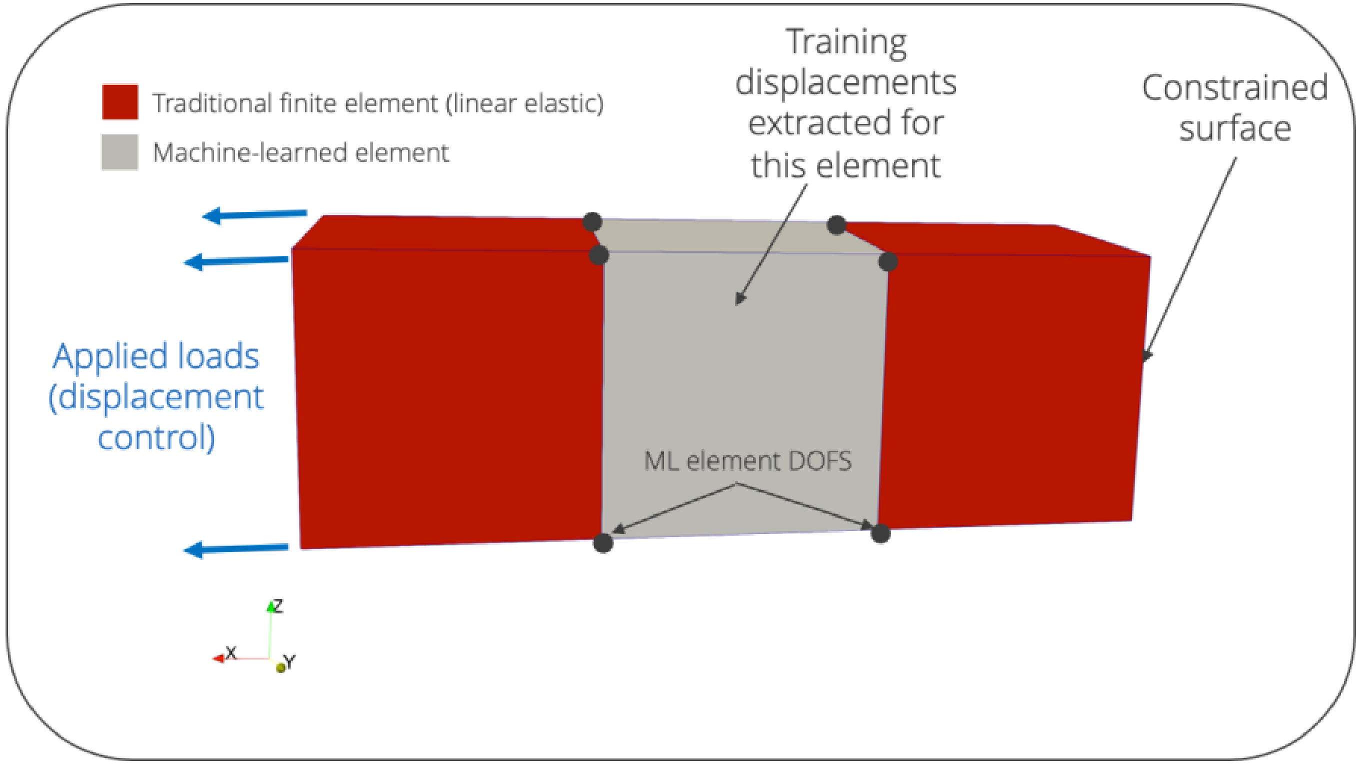
- Three element example being deformed axially to a small amount of plasticity.
- Using a traditional Feed-Forward NNs one obtains consistent (biased) responses but using an ensemble of VBI-NNs we obtain a distribution of responses.

Goal:
Use the variability in the responses from the ensemble of VBI-NNs to establish a robust protocol for quantifying the uncertainty from FEM-NN models.

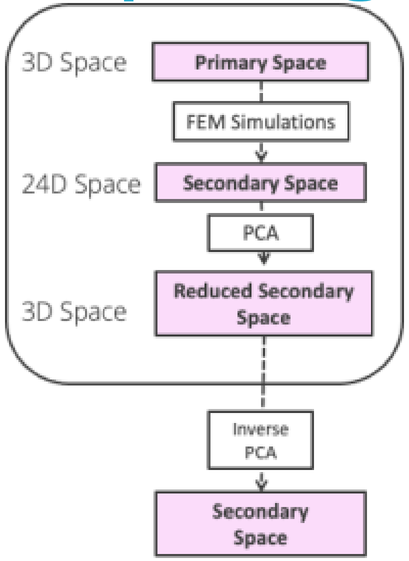
Incorporating UQ into FEM-NN Models: General Approach

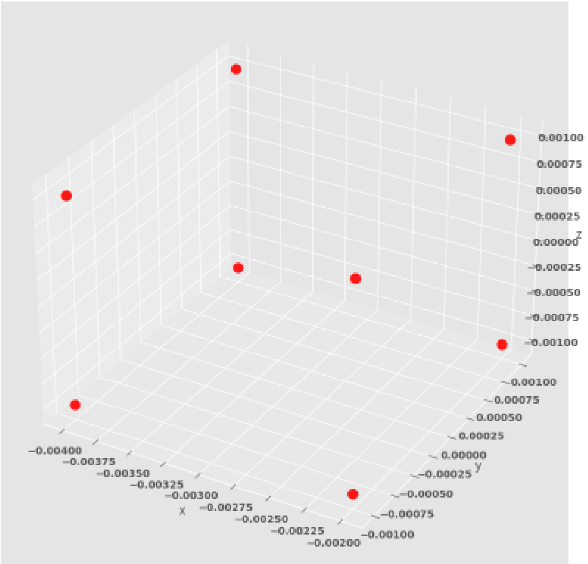
1. Generate training data from relevant BCs/loads
2. Train multiple neural networks (ensemble)
3. Test relevant BCs/loads in FEM-NN simulations
4. Extract QOIs and compute uncertainty metrics

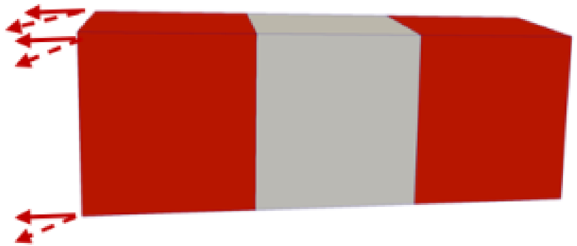
Three Element Model Set-Up



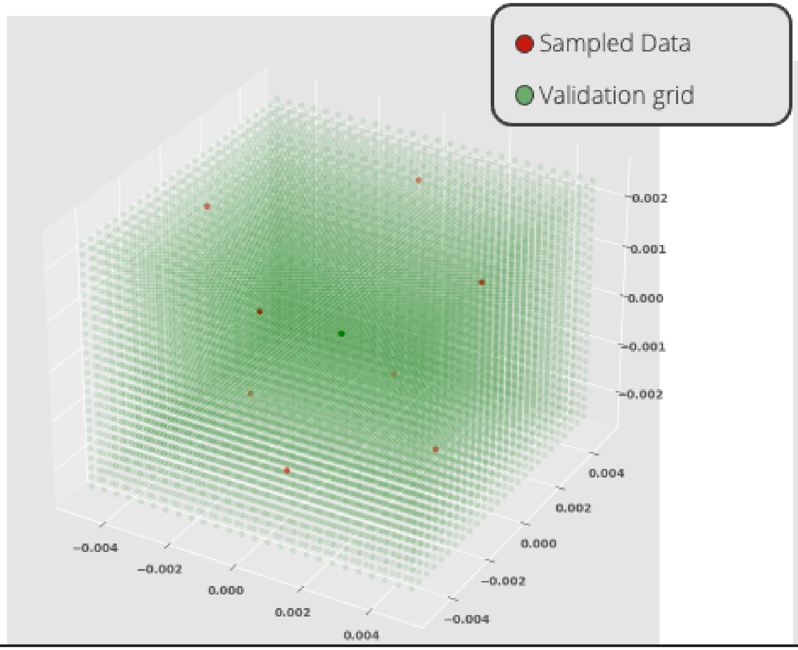
Incorporating UQ into FEM-NN Models: Generating a diverse dataset.



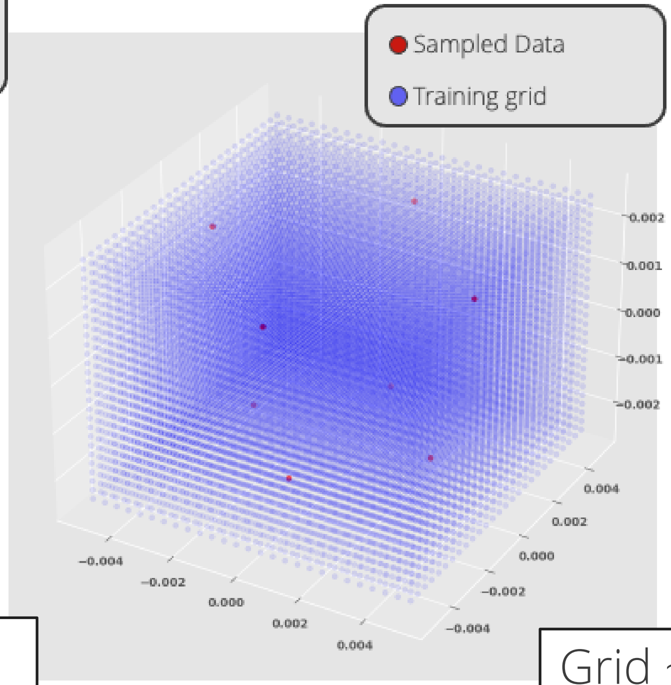




- The primary space is 3D cartesian space where we define a 2x2x2 grid (8 load cases).
- After running the FEM simulations of our initial grid we extract the nodal values which are in a 24D space (8 nodes with 3 DOF each) which we denote as Secondary Space.
- This is the space we need to adequately sample (not trivial).
- Therefore, we use PCA to sample a set of training and testing data in a reduced dimensionality space.
- Using the inverse PCA transformation we transform the sampled points back in Secondary Space and compute the output forces.



Grid ~20k validation points in PCA space

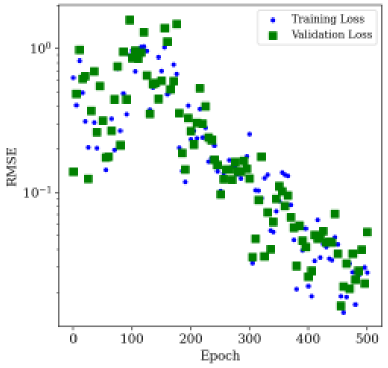


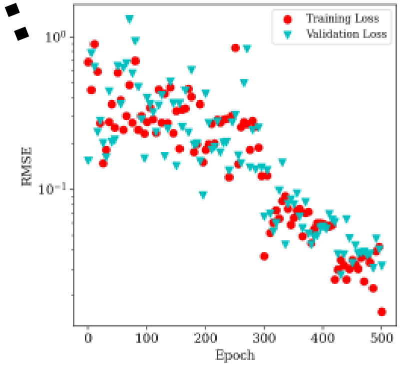
Grid ~20k training points in PCA space

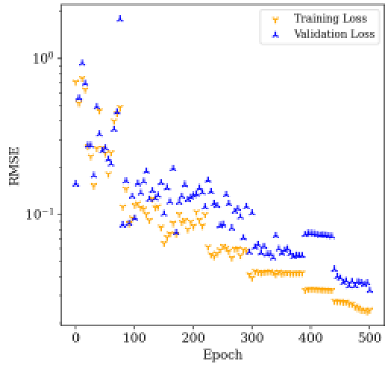
Incorporating UQ into FEM-NN Models: Training the Ensemble.

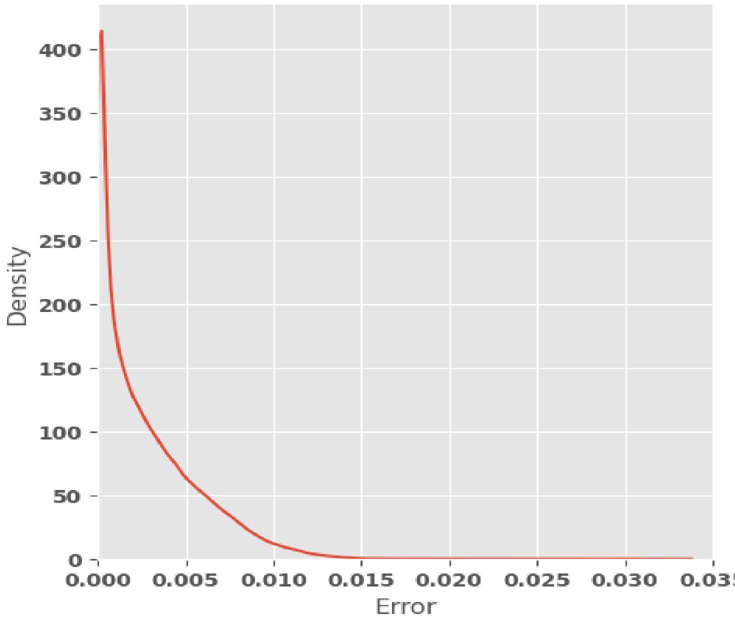
- Train 20 VBI-NN to the training data, each one with unique initialization of weights.
- Architecture uses 1 hidden layer with 100 nodes to predict the output.
- Network was trained with an initial learning rate of .1 and the ADAM optimizer.
- Monte Carlo sampling of 10 samples was used to sample the distribution of the weights and thus the distribution of outputs.
- Architecture was trained for 500 epochs.

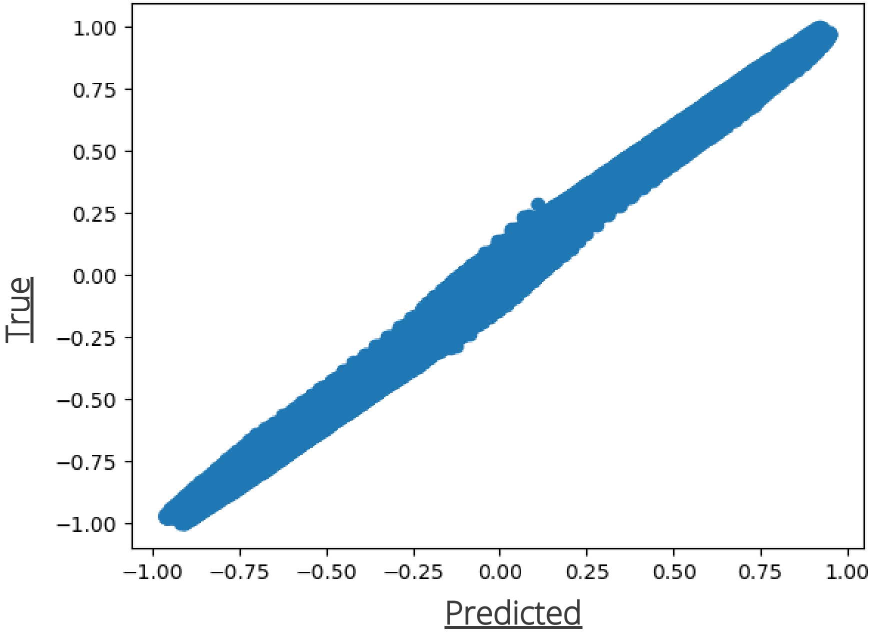
Loss evolution Curves



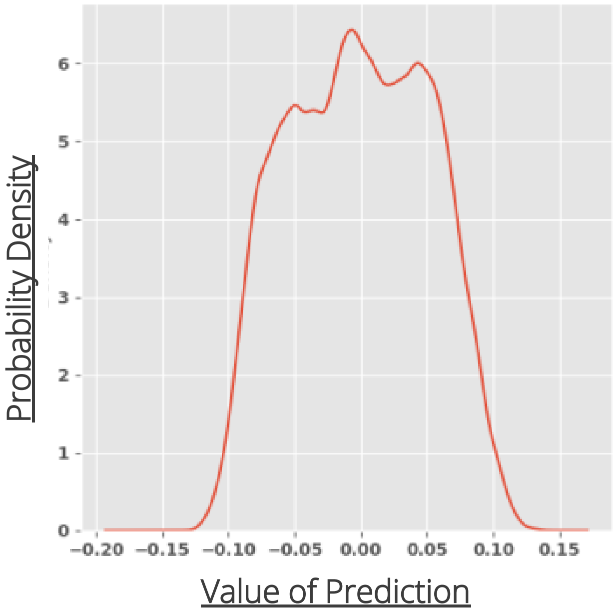


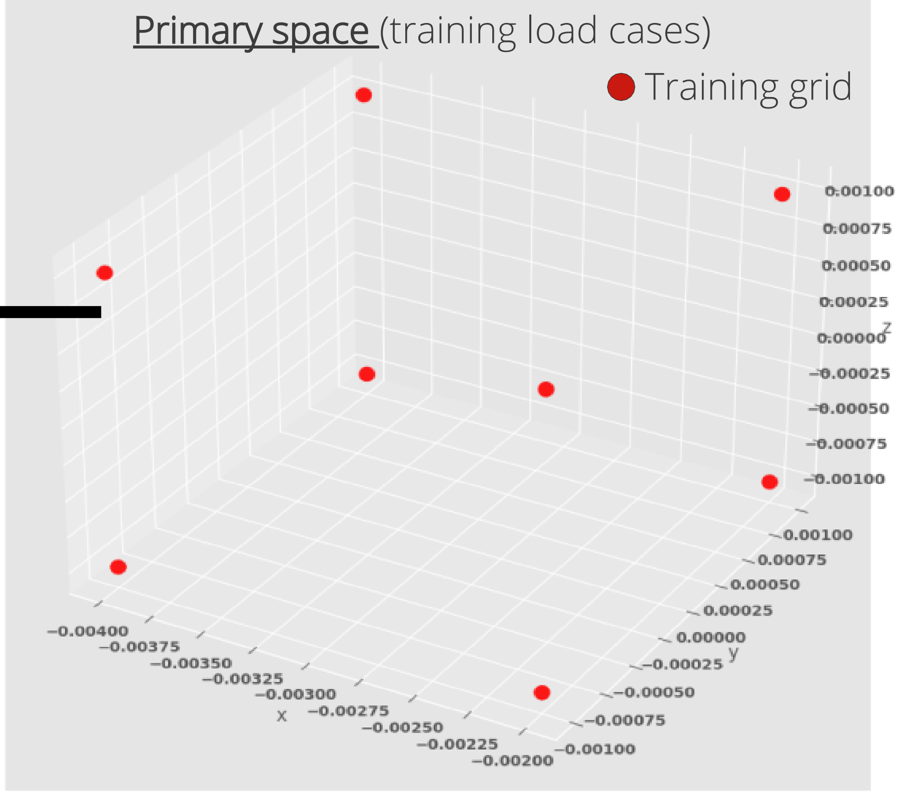






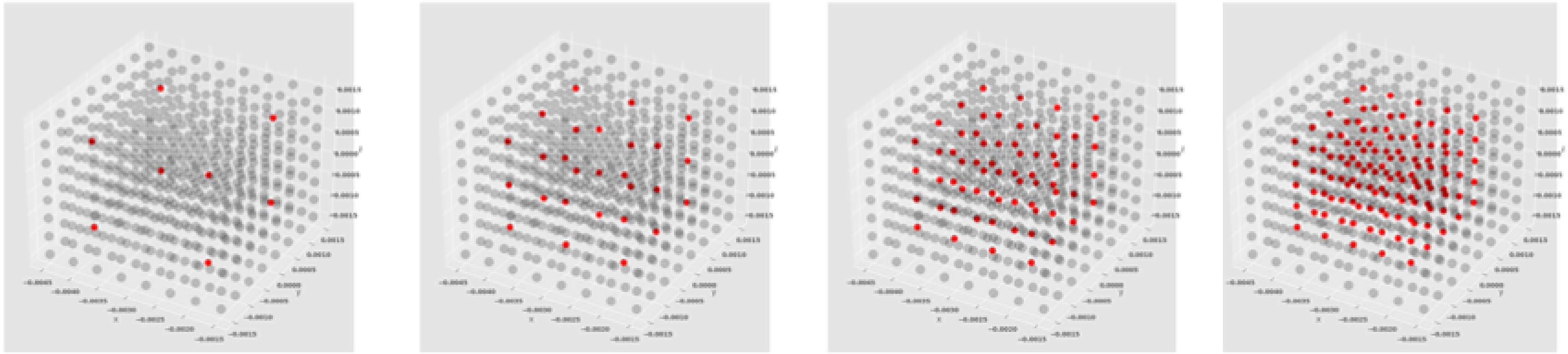
Incorporating UQ into FEM-NN Models: Using the Uncertainty Values.





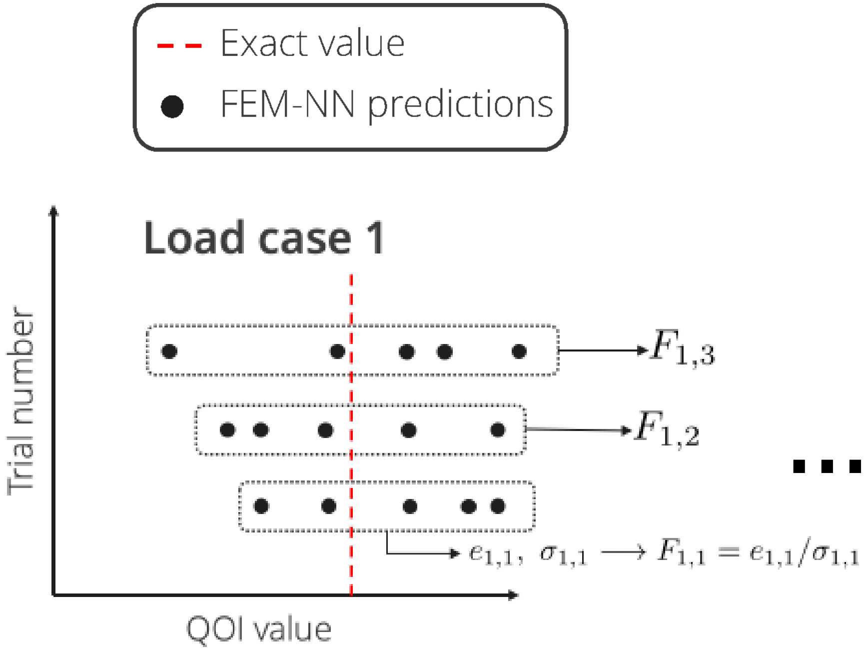
- Training grid
- Testing grid (8x8x8)

2x2x2 3x3x3 4x4x4 5x5x5

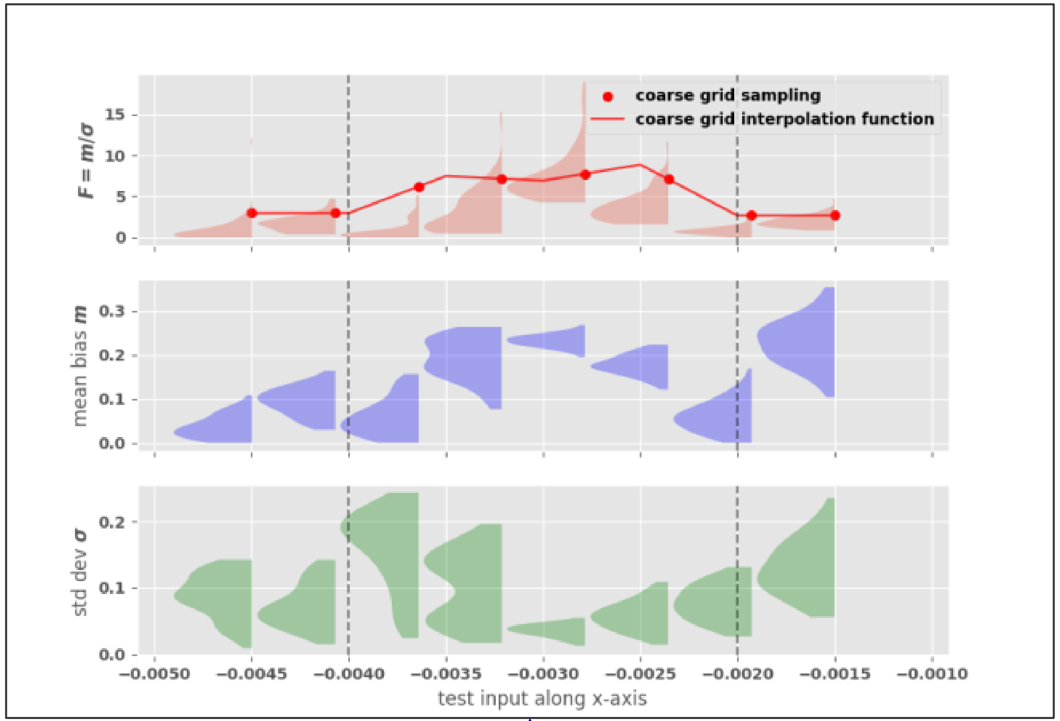


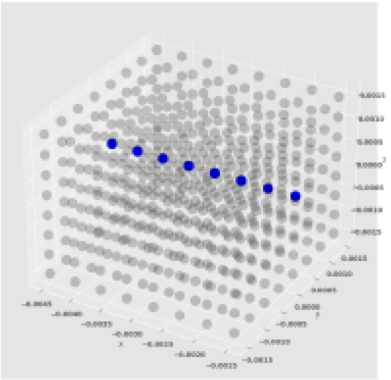
- For each one of the training cases you have distribution of predicted values, a true value to compare and an uncertainty metric.
- Calibrate the uncertainty using the training points to obtain an empirical value of the uncertainty at new/unseen loads.
- In order to calibrate our uncertainty we systematically increase the discretization of the training gird.
- Then we evaluate the uncertainty in a new testing grid in primary space.

Incorporating UQ into FEM-NN Models: QOI and uncertainty metric.



... *Etc.*





pTI distribution for loads associated with blue points shown on the right

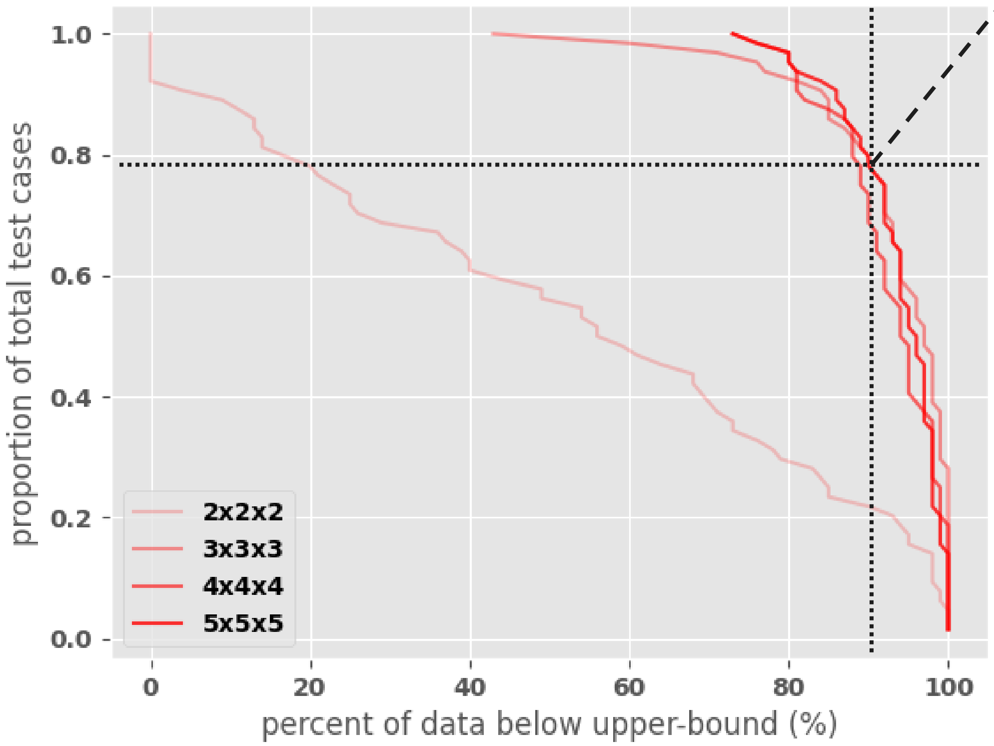
- QOI is element-averaged von Mises stress of top element.
- Randomly subsample 100 combinations of 20-choose-5 neural networks for each load case.
- Generate pseudo-tolerance intervals (pTIs) based on distribution of 100 samples.
- Calculate the F's at the training grid (all 4 of them) and the testing grid.

Incorporating UQ into FEM-NN Models: Using the calibrated uncertainty.

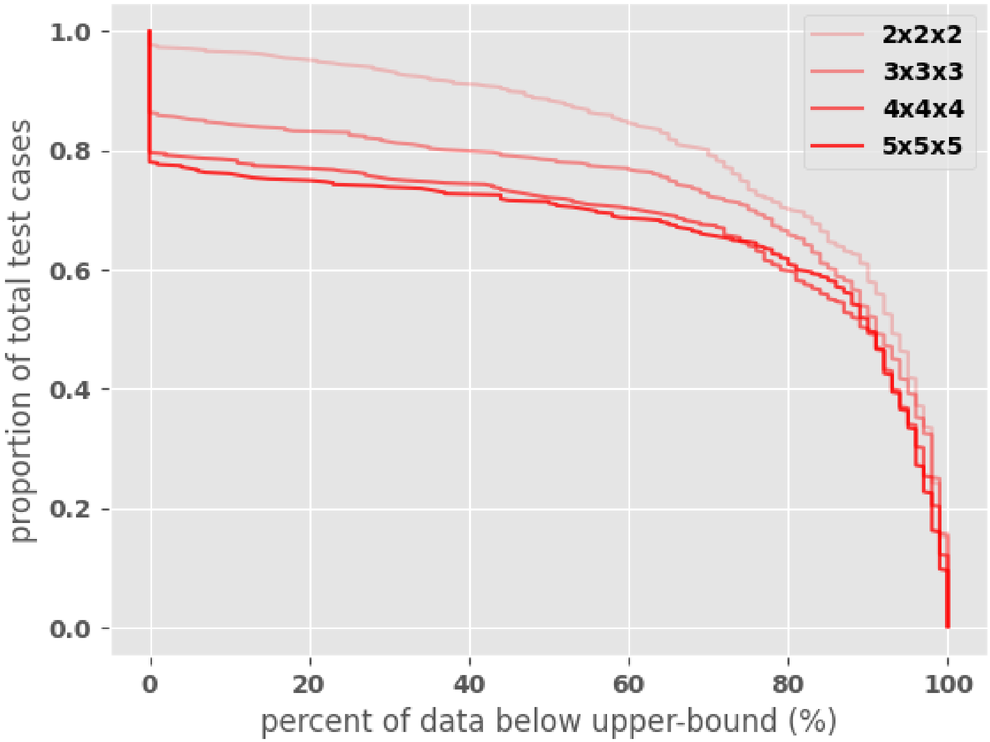
- Compare the estimated uncertainty (obtained by interpolating the F from the training grid) to the true uncertainty (obtained with the ensemble and comparing it to the true values).

For interpolation, the upper-bound approximation (95th percentile) of pTIs on a 5x5x5 grid will be conservative for approximately 80% of test load cases with 90% empirical confidence.

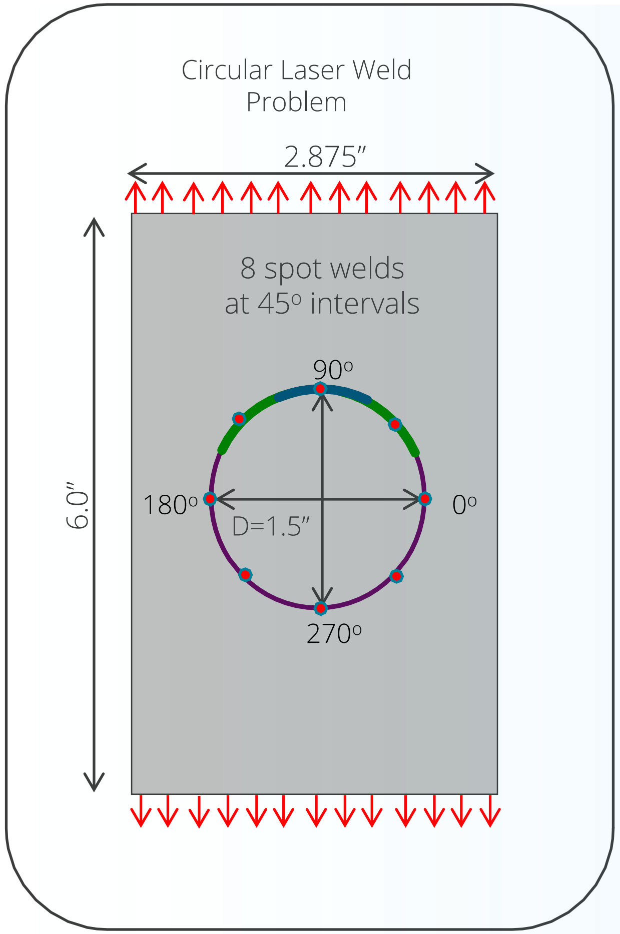
interpolation



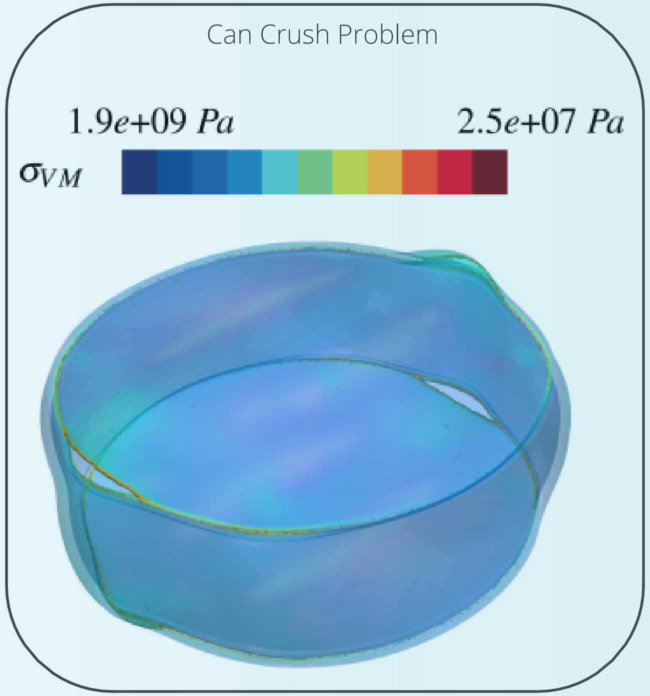
extrapolation



Conclusions:

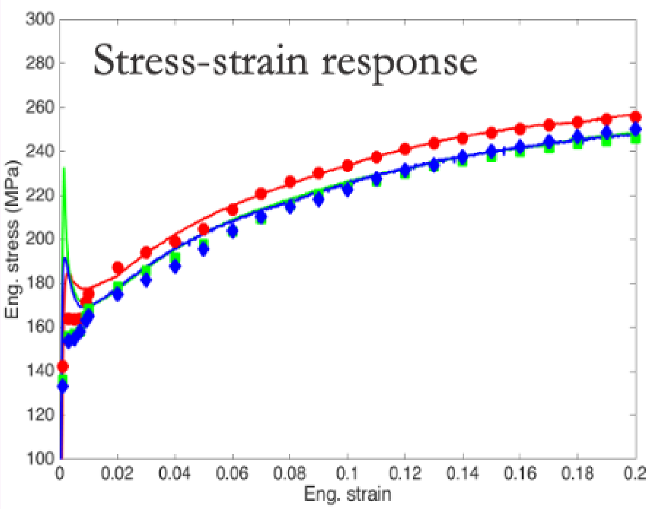


- Established a metric of the uncertainty in the prediction from the surrogate model and calibrated that value order to distill actionable knowledge from it.
- As a result, we successfully established a protocol for quantifying the uncertainty in the predictions from a FEM-NN model.



Next Steps:

- Develop frame invariant metrics to evaluate as inputs/outputs of NNs.



- Apply physics-based constraints to the NN-surrogate model to ensure physics grounded responses.

$$\mathrm{dev}(\sigma) = \sigma - \frac{1}{3}\mathrm{trace}(\sigma)I$$

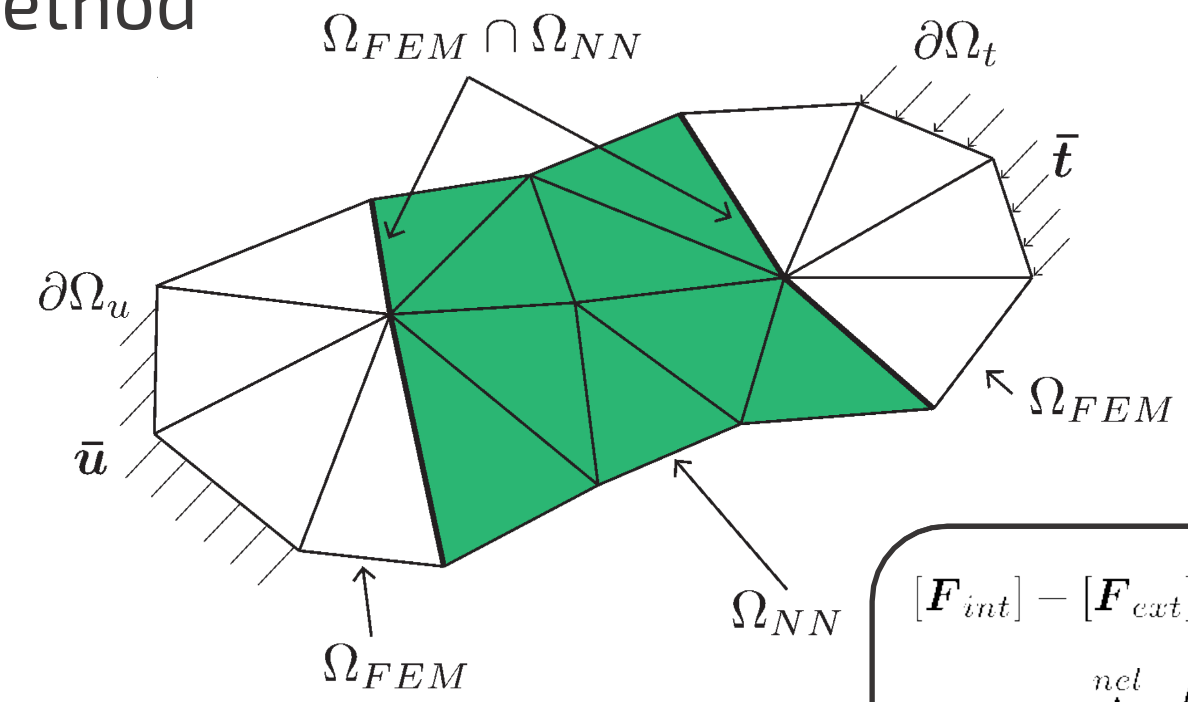
$$J_1(\sigma) = \mathrm{trace}(\mathrm{dev}(\sigma)) = 0$$

$$J_2(\sigma) = \frac{1}{2}\mathrm{dev}(\sigma):\mathrm{dev}(\sigma) = \frac{1}{3}I_1(\sigma)^2 - I_2(\sigma)$$

$$J_3(\sigma) = \det(\mathrm{dev}(\sigma)) = \frac{2}{27}I_1(\sigma)^3 - \frac{1}{3}I_1(\sigma)I_2(\sigma) + I_3(\sigma)$$

Questions?

FEM-NN Method



Equilibrium equation (local form)

$$\text{div}\ \boldsymbol{T} = \boldsymbol{0} \text{ in } \Omega$$
$$\boldsymbol{T}\boldsymbol{n} = \bar{\boldsymbol{t}} \text{ on } \partial\Omega_t$$
$$\boldsymbol{u} = \bar{\boldsymbol{u}} \text{ on } \partial\Omega_u$$

FEM (global form)

$$[\boldsymbol{F}_{int}] - [\boldsymbol{F}_{ext}] = \boldsymbol{0}$$
$$[\boldsymbol{F}_{int}] = \mathop{\mathsf{A}}_{e=1}^{nel} \int_{\Omega^e} [\boldsymbol{B}^e]^T \hat{\boldsymbol{T}}\, dv$$
$$[\boldsymbol{F}_{ext}] = \mathop{\mathsf{A}}_{e=1}^{nel} \int_{\partial\Omega^e \cap \partial\Omega_t} [\boldsymbol{N}^e]^T \bar{\boldsymbol{t}}\, dv$$

FEM-NN Approach

$$[\boldsymbol{F}_{int}] - [\boldsymbol{F}_{ext}] = \boldsymbol{0}$$
$$[\boldsymbol{F}^{e,FEM}_{int}] = \int_{\Omega^e} [\boldsymbol{B}^e]^T \hat{\boldsymbol{T}}\, dv$$
$$[\boldsymbol{F}^{e,NN}_{int}] = \boldsymbol{f}_{\boldsymbol{w}}(\boldsymbol{u})$$

Variational Bayesian Inference

$$w \sim N(\mu, \sigma)$$

Distribution for each weight

Schematic of training data generation