Enhancing the Harris and Crighton Particle-in-Cell (PIC) Stress Model with Bayesian Learning

NATIONAL ENERGY TECHNOLOGY LABORATORY

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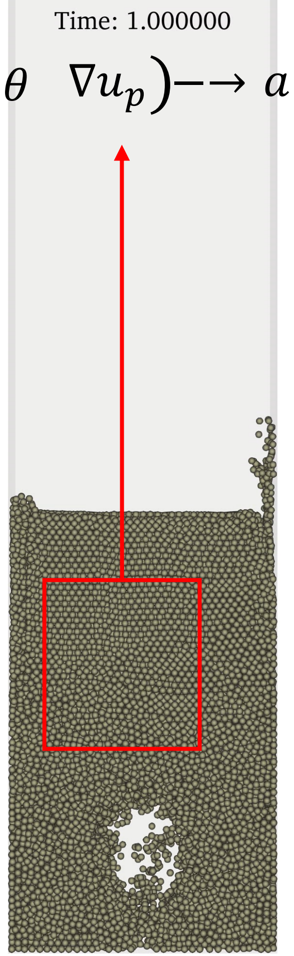
Motivation

Harris and Crighton (1994) model:

- Simplistic and cannot directly predict the possibility of particle clustering
- "Phenomenological" and does not have a physical basis
- The model is low dimensional in the feature space

Sampling Data from DEM Simulations

$$f(\varepsilon \quad \nabla\varepsilon \quad \theta \quad \nabla u_p) \dashrightarrow a = \left\langle \frac{d\tilde{u}_p}{dt}_{collision} \right\rangle$$

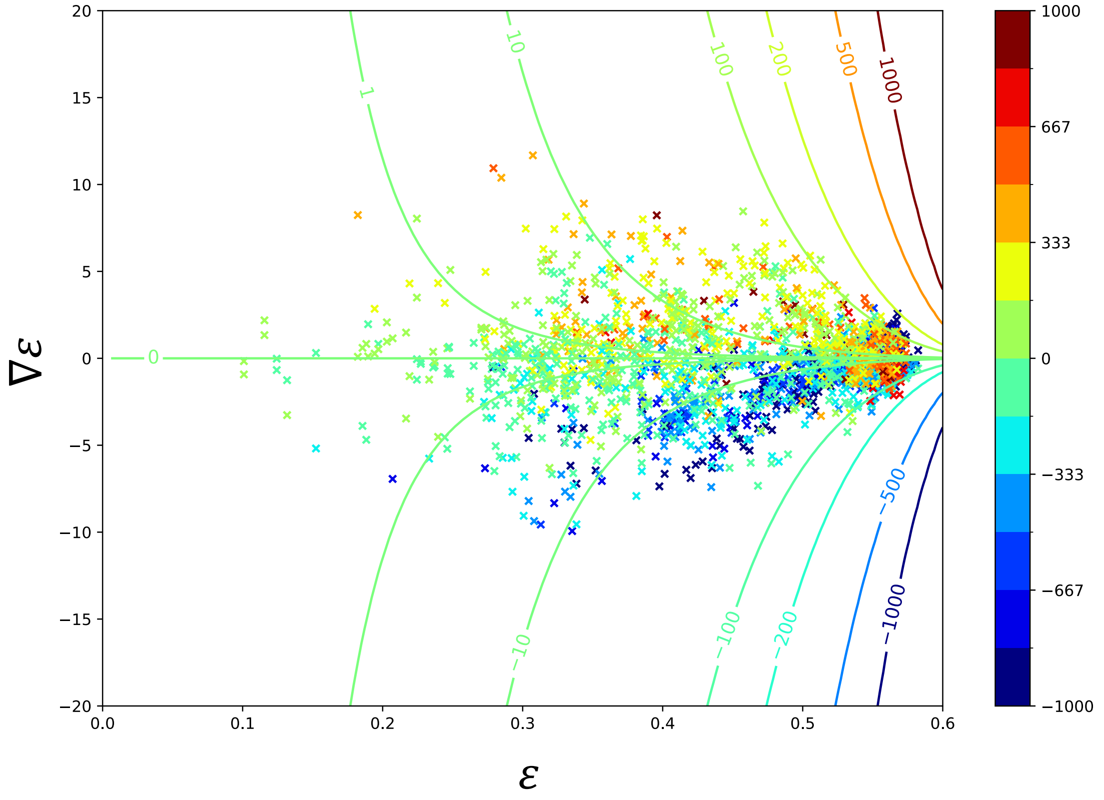


- Discrete Element Method (DEM) simulations are performed for a two-dimensional (2D) fluidized bed configuration with different inlet velocities
- A 2D window of size 5 cm x 5 cm is used to spatially sample average particulate properties such as volume fraction (ε), gradient of volume fraction ($\nabla\varepsilon$), granular temperature (θ), particle velocity gradient (∇u_p), and the deceleration due to collisions (a)
- Temporal averaging of the spatially sampled data is performed over 50 DEM timesteps

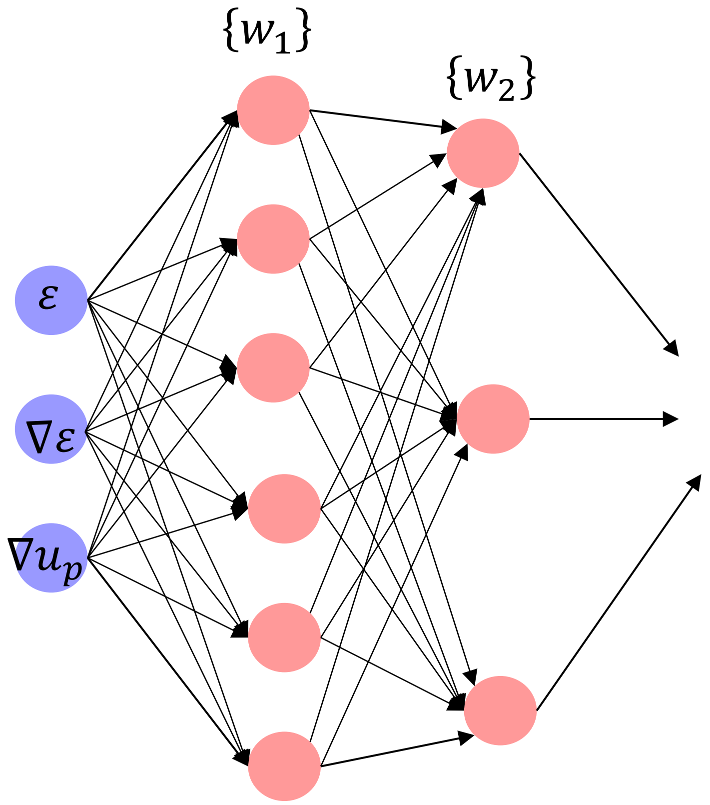
Sampling Data from DEM Simulations

- Distinct dense and dilute regimes are observed
- Compaction of particles and high deceleration magnitudes are observed in the dense regimes
- The DEM sampled data is observed to be sparse and highly "mixed" in the parametric space
- The DEM sampled data is dependent on a higher dimensional input space as compared to the Harris & Crighton criteria

$$a = \left\langle \frac{d\tilde{u}_p}{dt}_{collision} \right\rangle$$



Need for an Informative Prior



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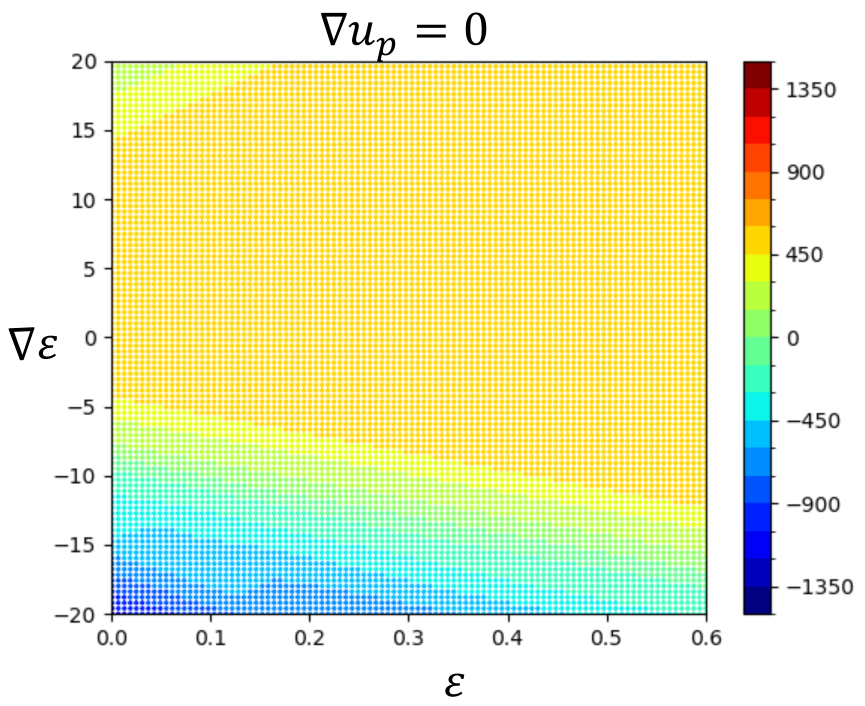

- A simple feed forward neural network (FNN), with dimensionality reduction, overfits the data
- There are no physics-based constrains to regularize the data loss (PINNs)

Bayesian Neural Network (BNN) Model

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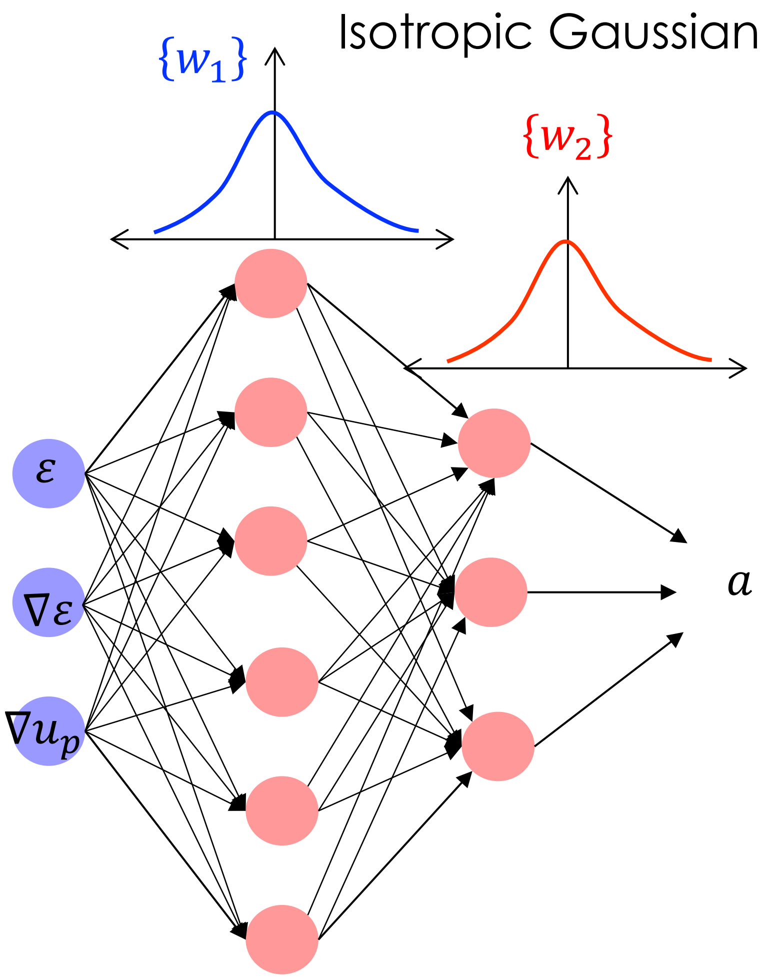
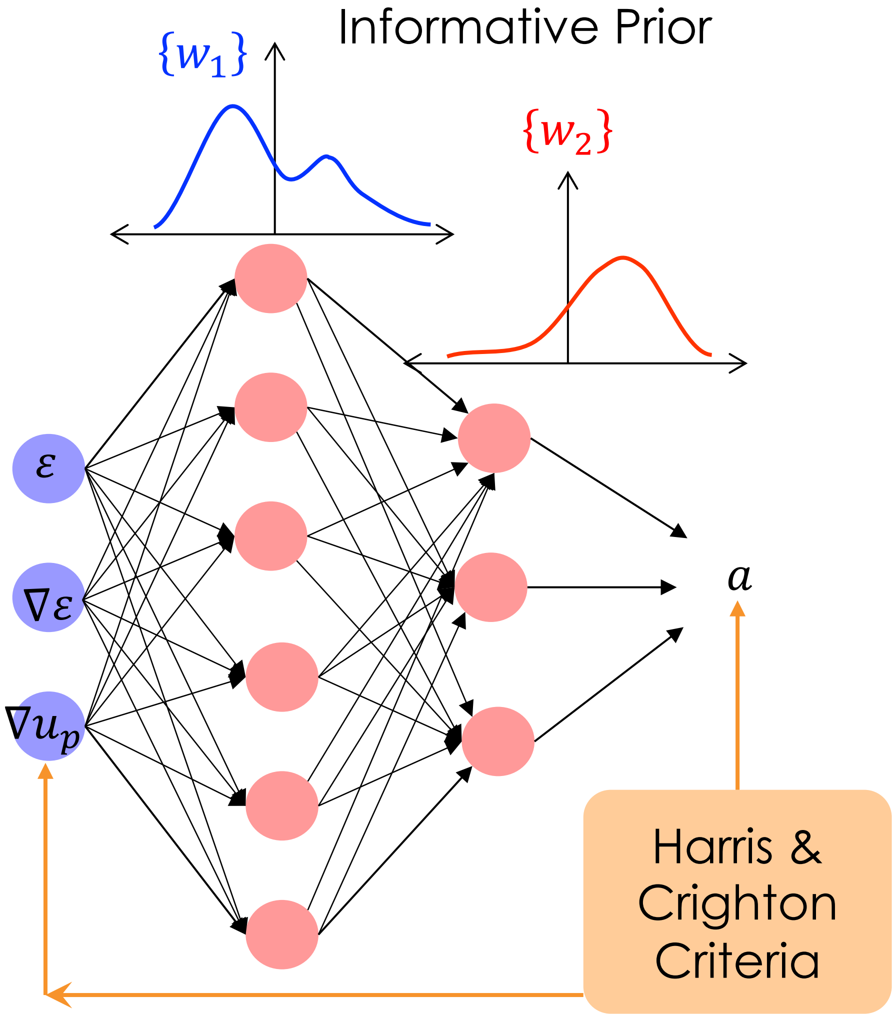


- Bayesian neural network (BNN) weights are probability distributions contrary to deterministic weights in FNNs
- Isotropic Gaussian probability distributions are used as the initial weights for the BNN

Bayesian Neural Network (BNN) Model

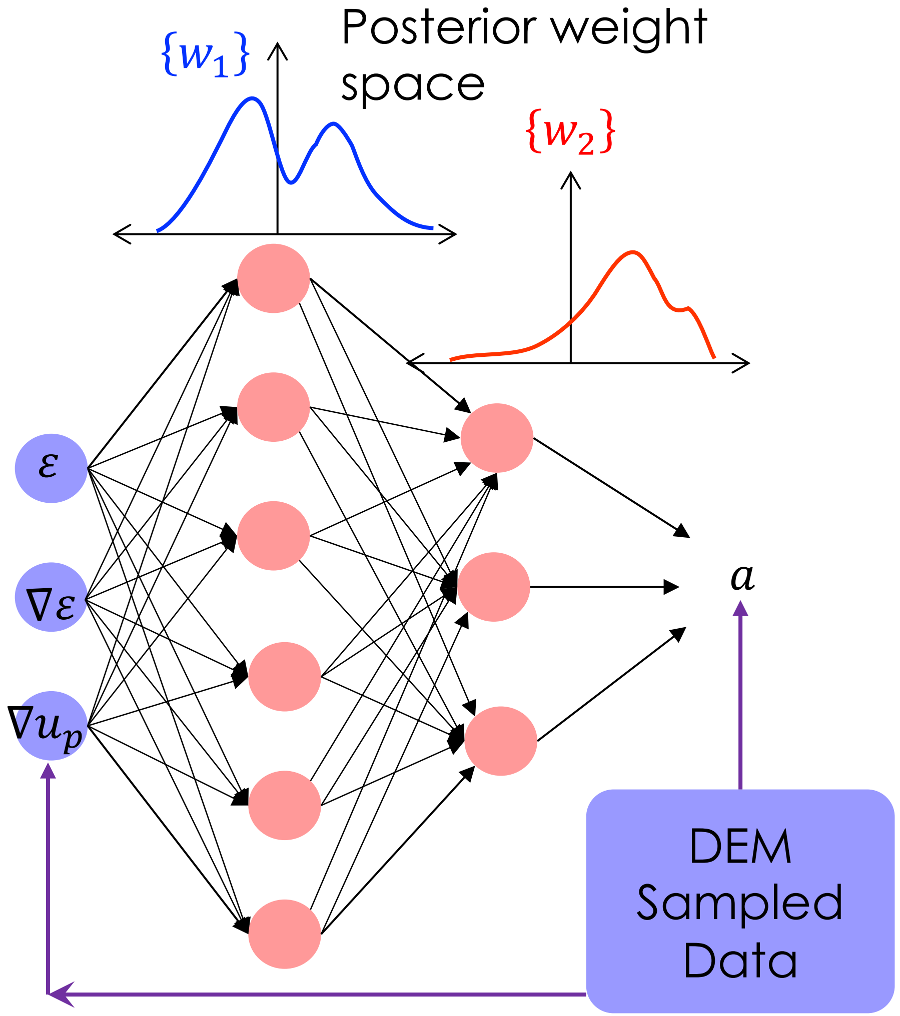


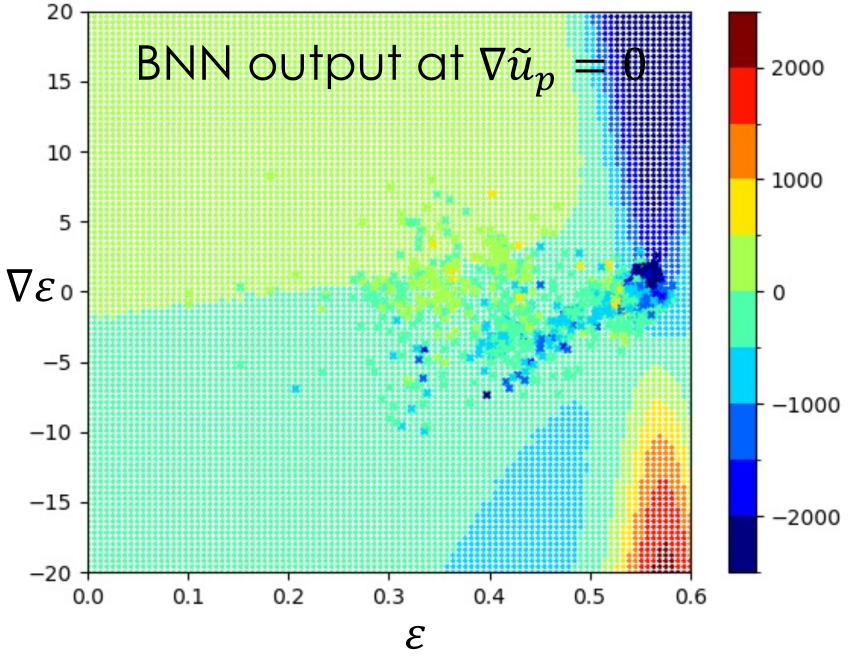
- BNN weights are probability distributions contrary to deterministic weights in FNNs
- Isotropic Gaussian probability distributions are used as the initial weights for the BNN

STAGE 1

- ❑ Introduce the Harris & Crighton criteria as the base and adjust the weight space
- ❑ This modified weight space called the informative prior incorporates the constraints required to improve the generalizability of the model

Bayesian Neural Network (BNN) Model





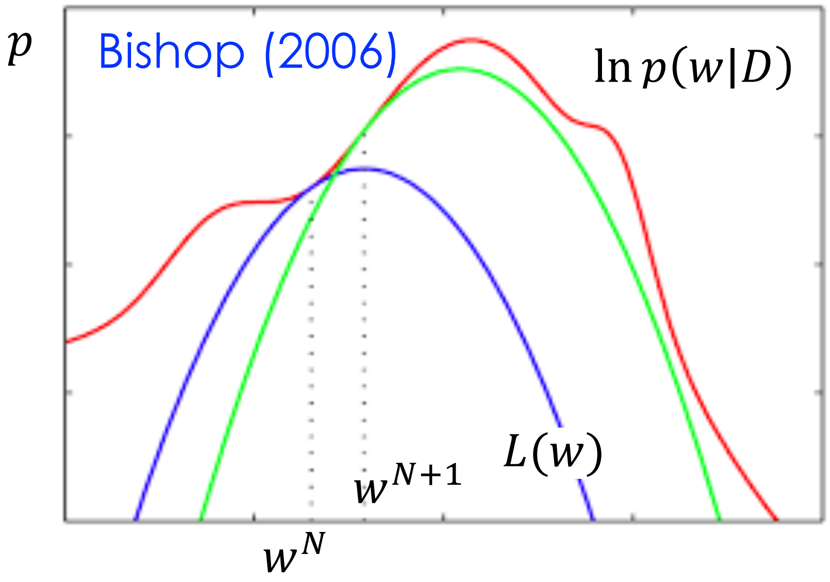
STAGE 2

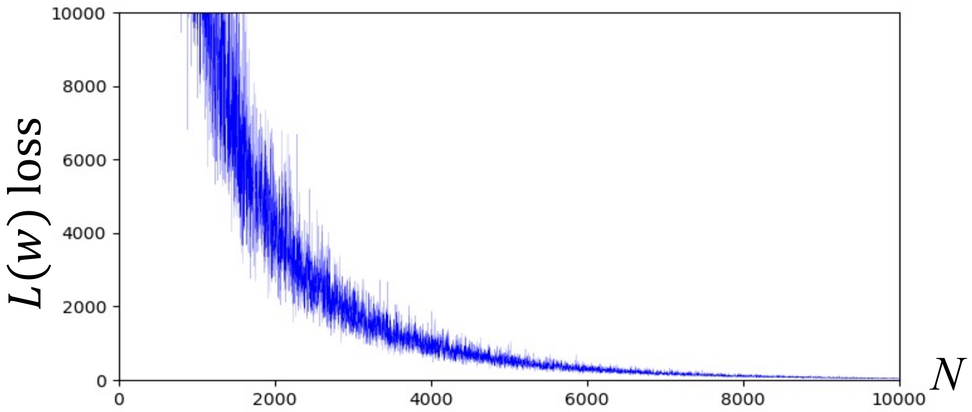
- Introduce DEM sampled data
- Re-train the network with informative prior weight initialization

Training BNNs

- Approximate the true posterior weight space using a joint Gaussian distribution
- Use Stochastic Variational Inference (Pyro library) to maximize the Evidence Lower bound (ELBO)
- Iteratively "move" the informative prior weight space to approximate the posterior weight space

$$p(D) = \int q(w)\, \ln\left\{\frac{p(D,w)}{q(w)}\right\} dw - \int q(w) \ln\left\{\frac{p(w|D)}{q(w)}\right\} dw$$





Incorporating ML Model in MFiX (Work in Progress)

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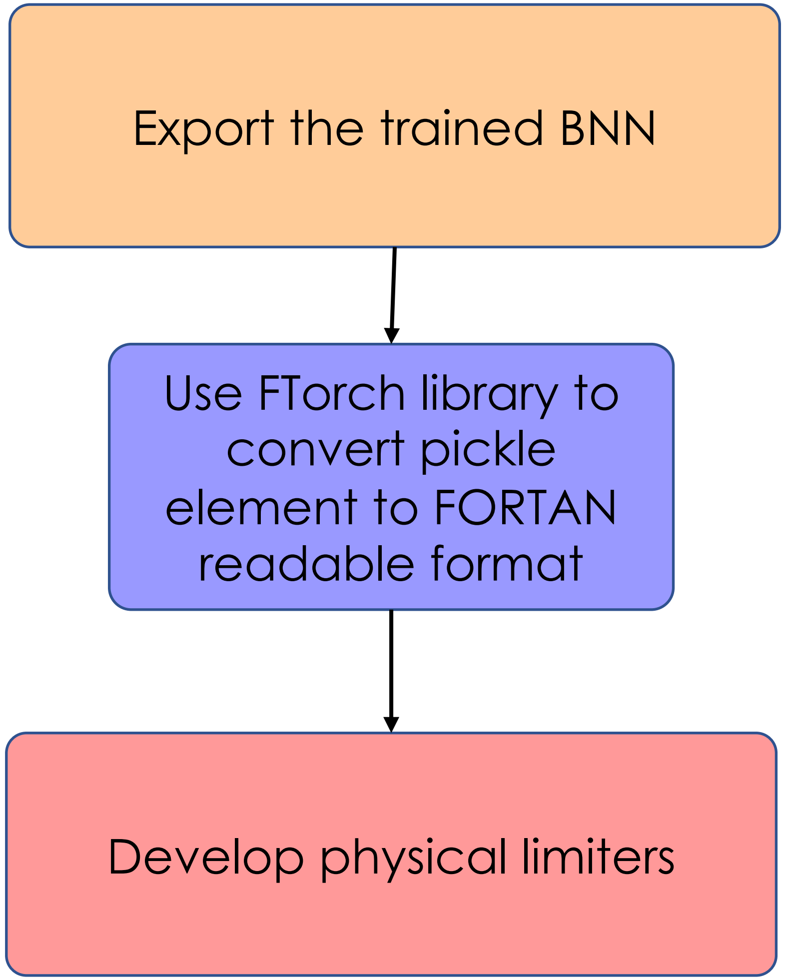
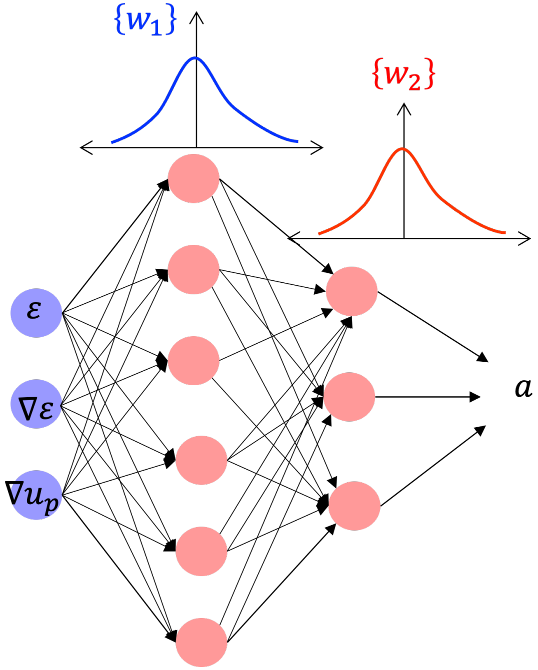
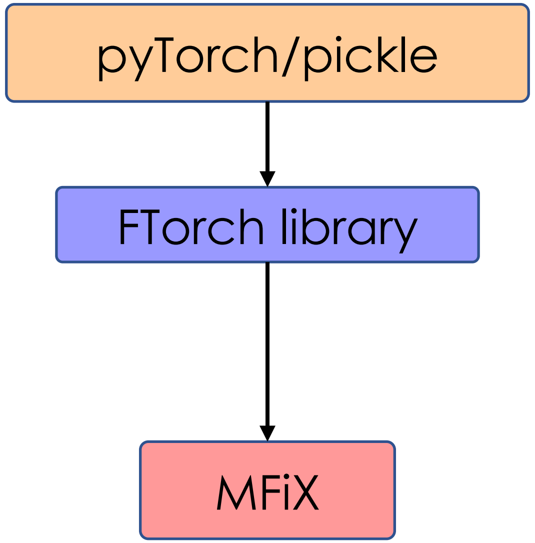
- Export the trained BNN model as a pickle element (Python)
- Use FTorch library to convert the Python model to a FORTRAN readable format
- Design User Defined Functions (UDFs) to compute model input arguments for the model and link the model output to the original MFiX solver
- Develop physical limiters for computational stability of the new model



Summary





1) Sampling spatially and temporally averaged data from DEM simulations

2) Combining Harris & Crighton criteria with sampled datapoints using Bayesian approach

3) Incorporating trained BNN model in MFiX code

References

- Harris and Crighton (1994) Solitons, solitary waves, and voidage disturbances in gas-fluidized beds. Journal of Fluid Mechanics 226, 243-276
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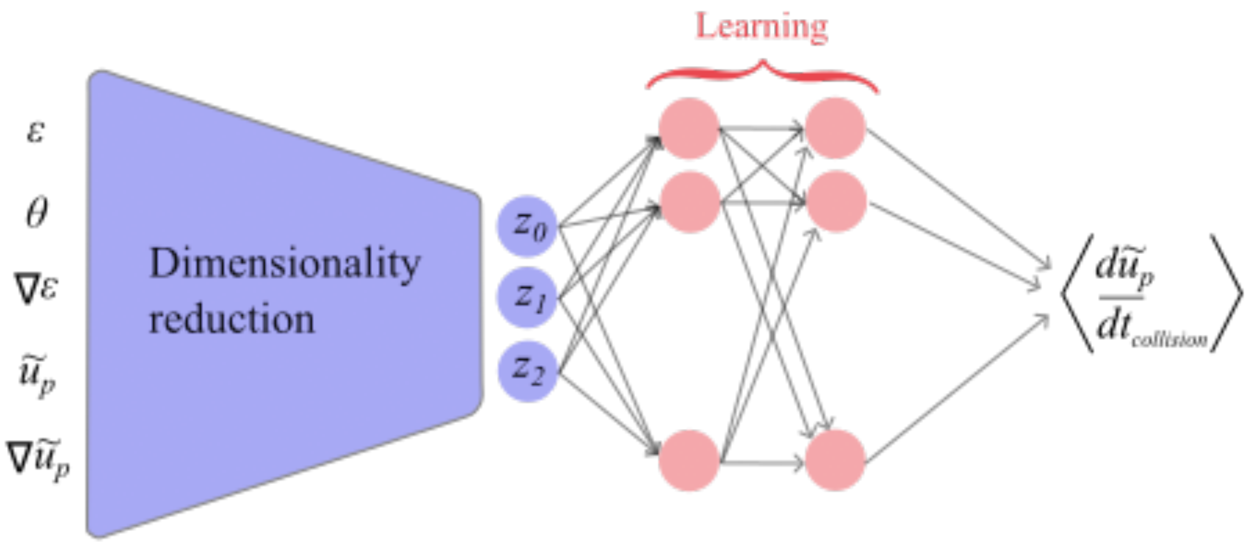
Backup Slides: Network Model

- The neural network architecture has two sections. Dimensionality reduction is used to map the high-dimensional parametric space to a lower dimensional representation in the latent space. This dimensionality reduction improves the convergence of the feed-forward network in the second stage.



Stage 1: Input space dimensionality reduction

Linear/Non-linear latent space

Stage 2: Non-linear mapping from latent space to target term

Backup Slides: Dimensionality Reduction

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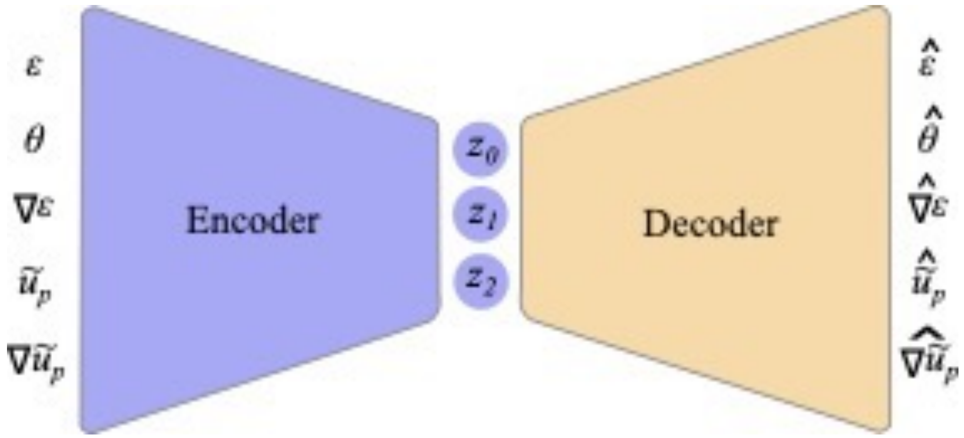
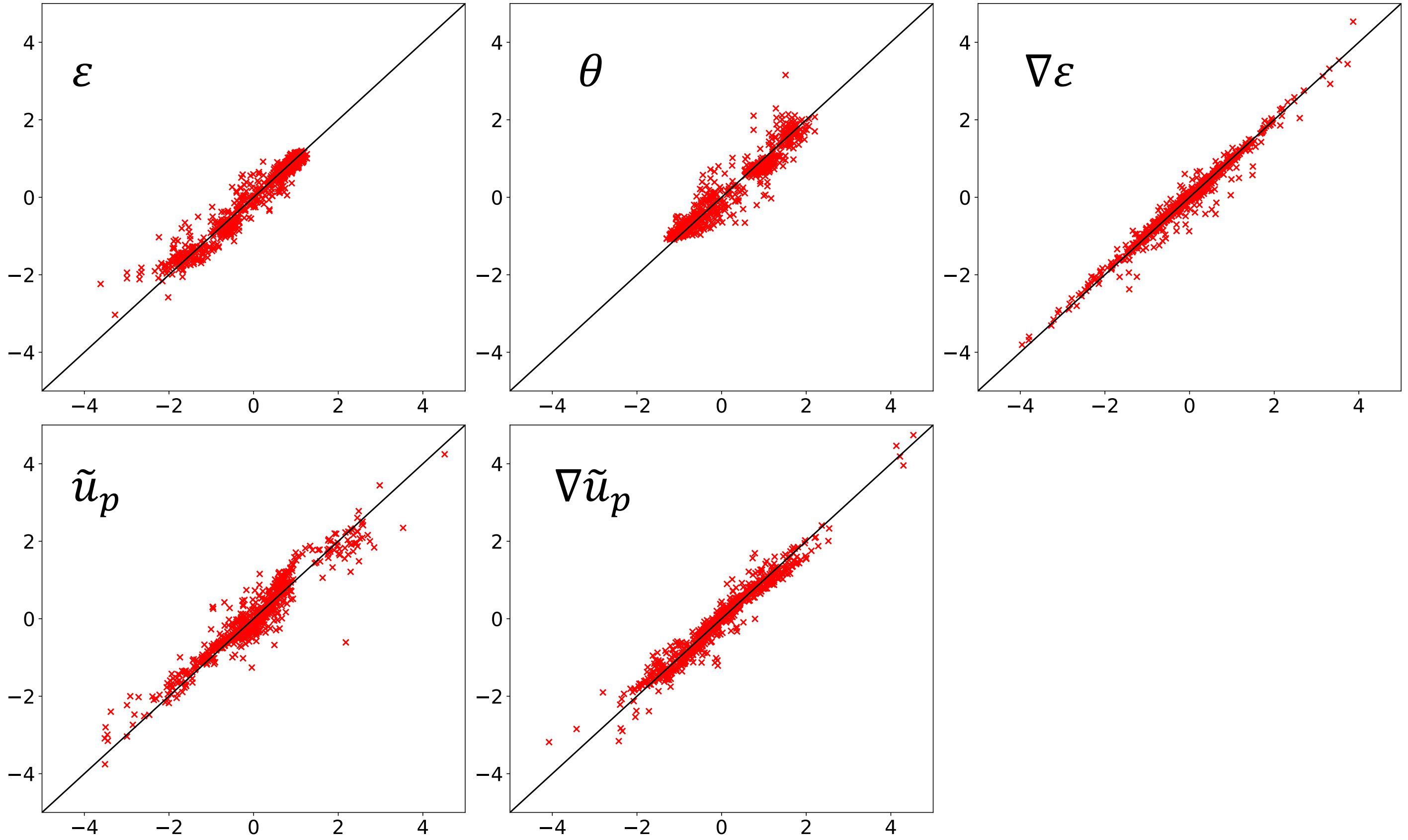
An auto-regressor architecture is used to map the scaled high dimensional parametric space to a non-linear latent space (z) of three-dimensions. The encoder-decoder architecture represents the input data with ~ 88% accuracy and hence the lower dimensional latent space is a reasonable representation of the high dimensional input space.

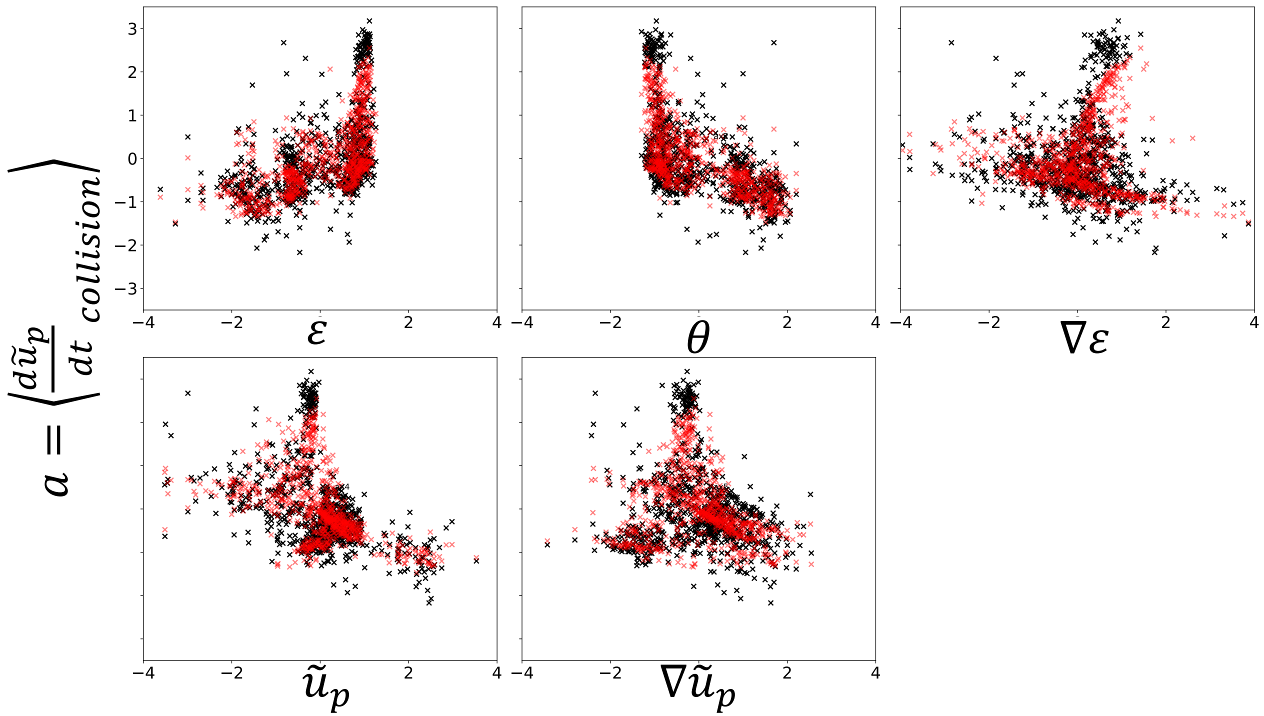


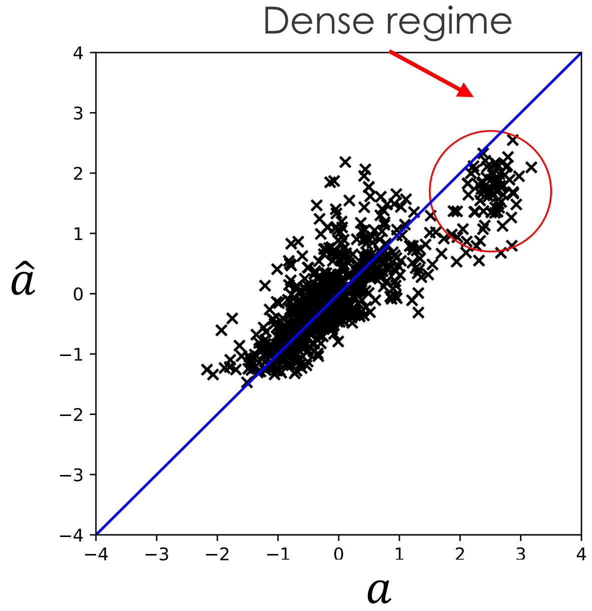
Mapping of the input space to non-linear latent space using auto-regressor

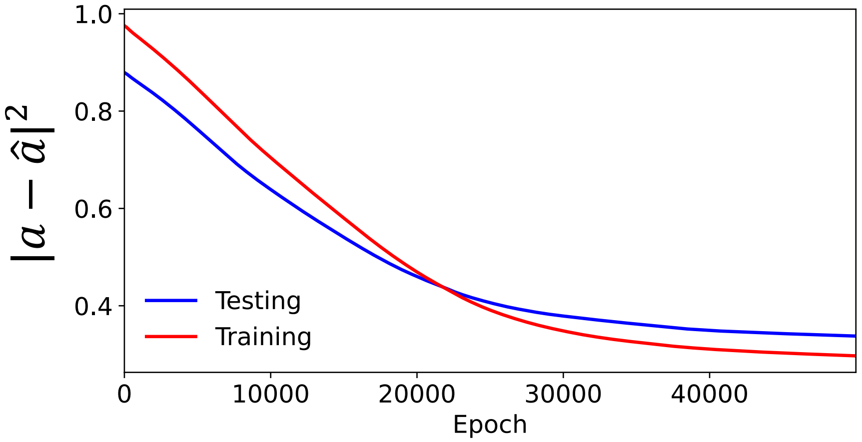


Backup Slides: Learning

- Better predictability than directly applying a feed-forward neural network on the "raw" data
- Underpredicts the dense/compact regime collision term







Backup Slides: Mapping BNN Weights onto a "Deterministic" Network

- The weight space in a BNN is probabilistic represented by a joint pdf
- We have used guides or approximations to represent the weight space as a combination of multiple uncorrelated Gaussians
- This facilitates the use of two parameters **mean $\boldsymbol{\mu}$ and standard deviation $\boldsymbol{\sigma}$** (X # of weights) to represent the entire weight space
- Since FTorch library is not compatible with a probabilistic network, we have to convert the BNN as a deterministic network by **mapping the mean** $\boldsymbol{\mu}$ of the BNN weight space