Neural network-based surrogate model for multi-scale analyses

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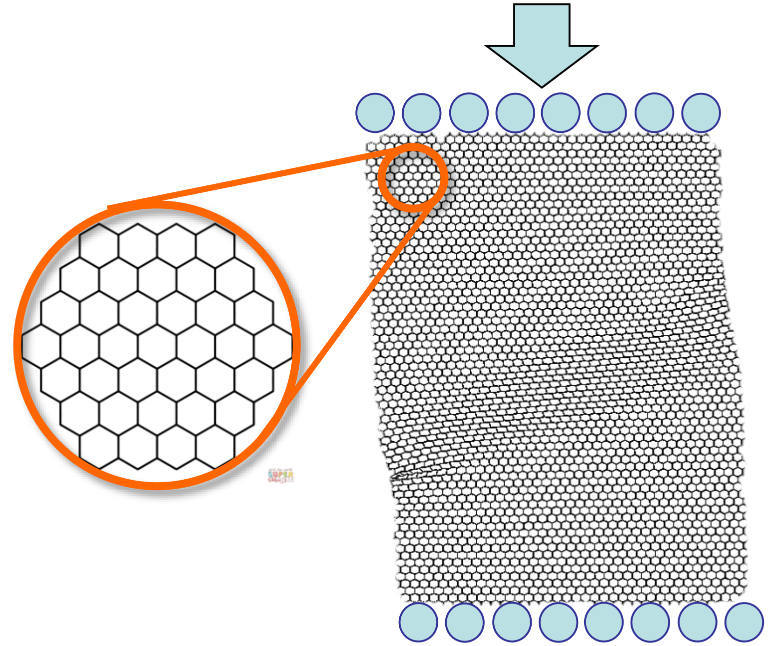
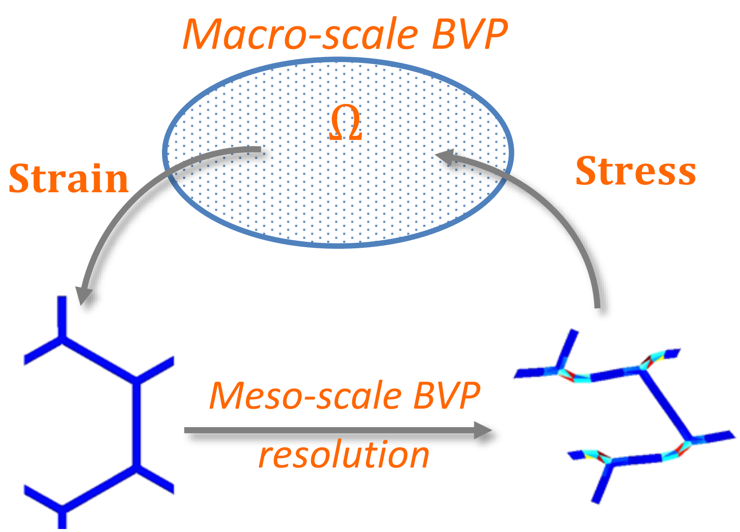
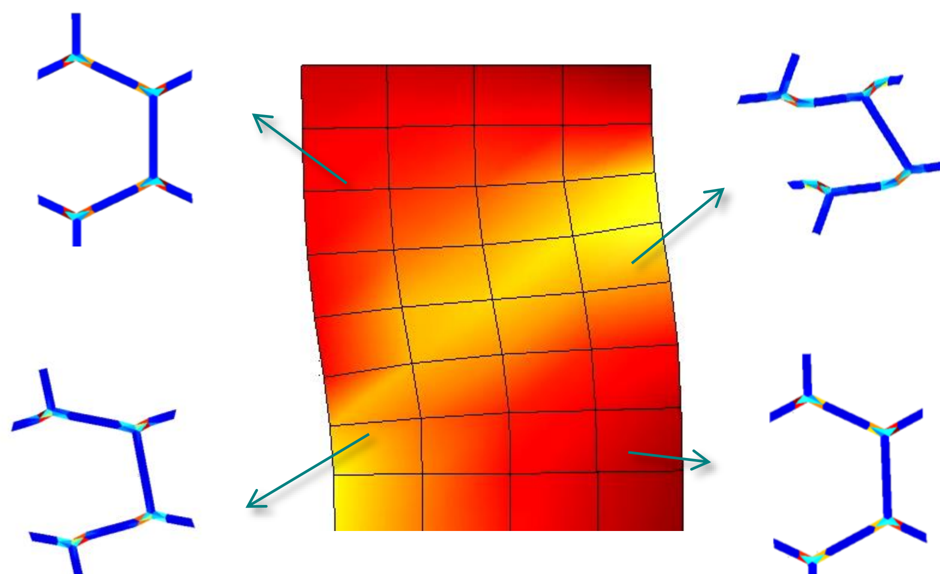
Multi-scale simulations

- Computational homogenisation (FE2)
  - Heterogeneous structures
    - Micro-scale: cell, grains, inclusions…
    - Macro-scale: seen as a continuum
  - Direct numerical simulations
    - Time consuming
  - Idea: use multi-scale strategy





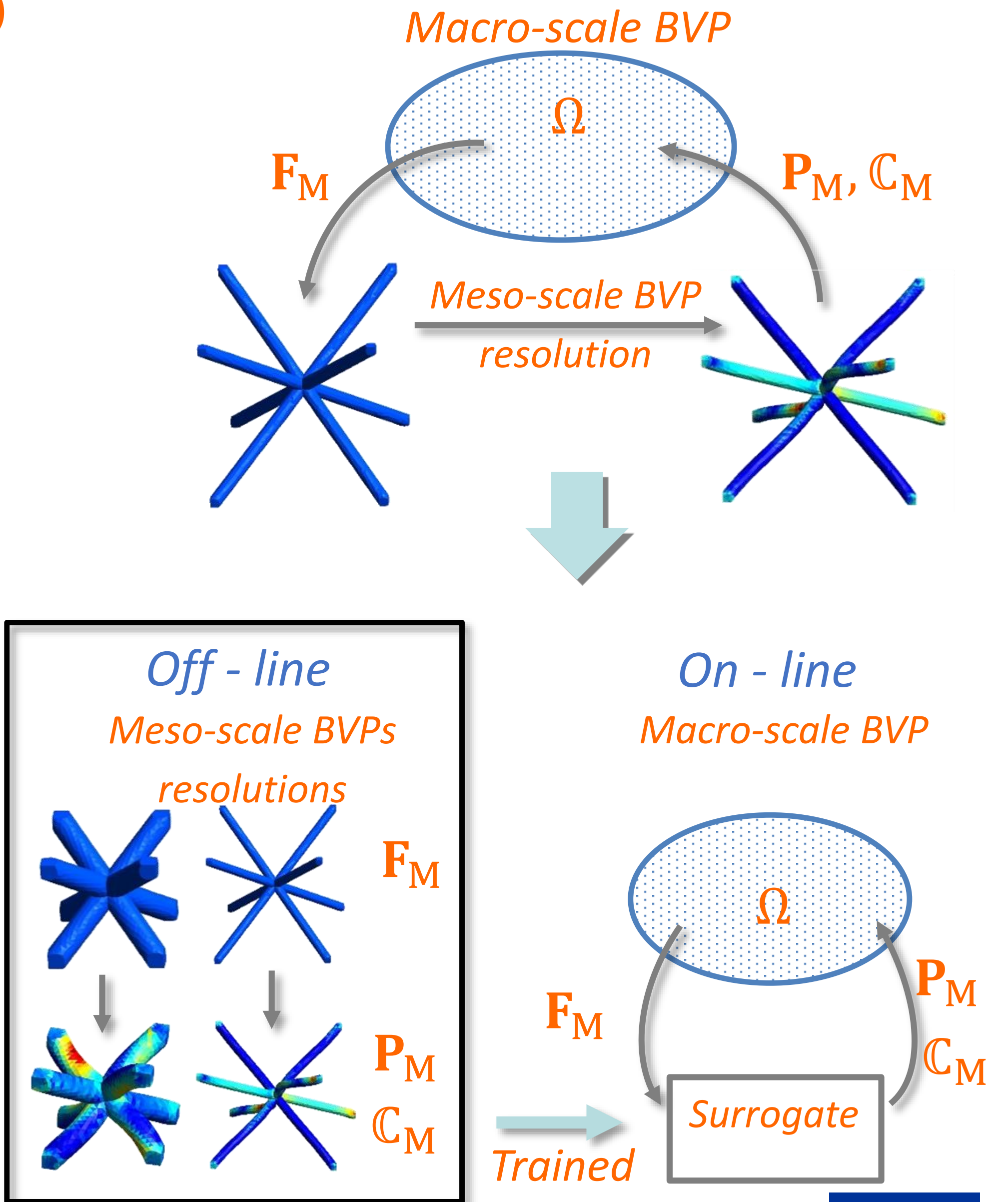


Multi-scale simulations

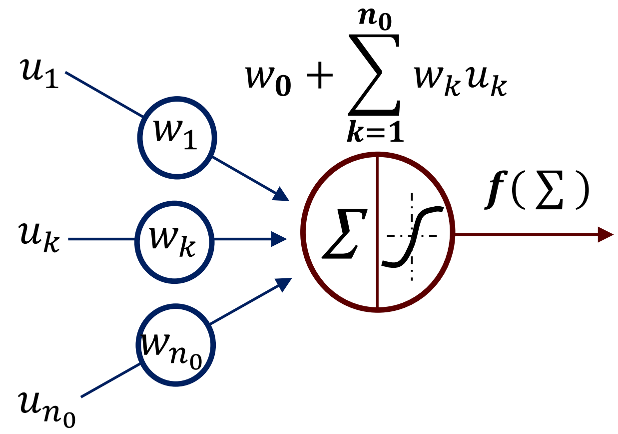
- Computational homogenisation (FE2)
  - Non-linear simulations
    - Iterations at macro-scale BVP
    - Sub-iterations at meso-scale BVP

Unaffordable

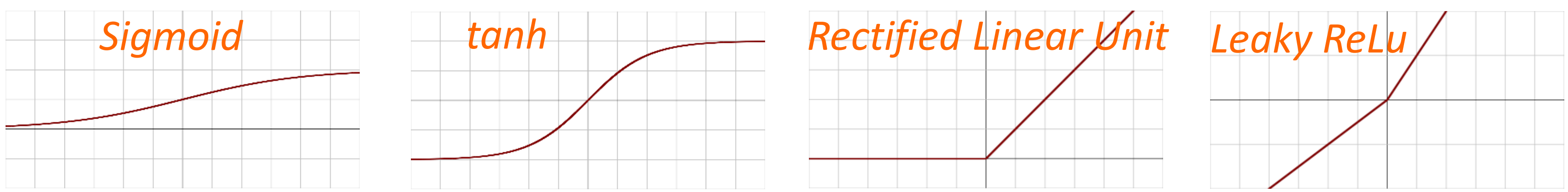
  - Introduction of data-driven approach
  - Use of surrogate models
    - Train a surrogate model (off-line)
      - Requires extensive data
      - Obtained from RVE simulations
      - Different RVE properties
    - Use the trained surrogate model during analyses (on-line)
      - Speed-up of several orders



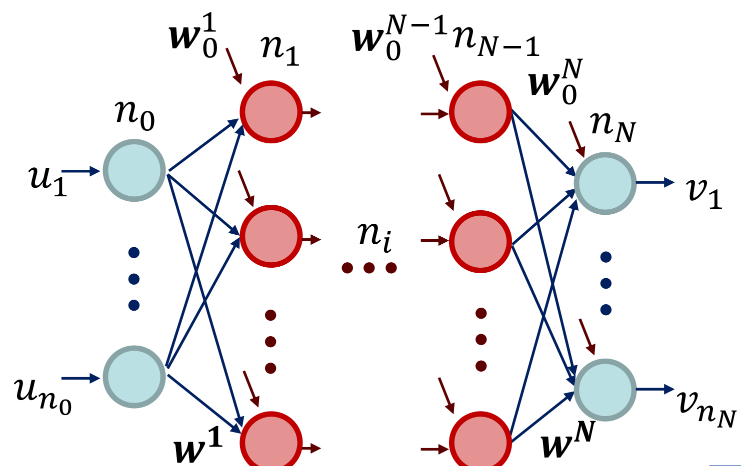
- Definition of the surrogate model
  - Artificial neuron
    - Non-linear function on n_0 inputs u_k
    - Requires evaluation of weights w_k
    - Requires definition of activation function f



  - Activation functions f



  - Feed-Forward Neuron Network
    - Simplest architecture
    - Layers of neurons
      - Input layer
      - $N-1$ hidden layers
      - Output layers
    - Mapping $\Re^{n_0} \rightarrow \Re^{n_N}: \boldsymbol{v} = \boldsymbol{g}(\boldsymbol{u})$



Artificial Neural Network

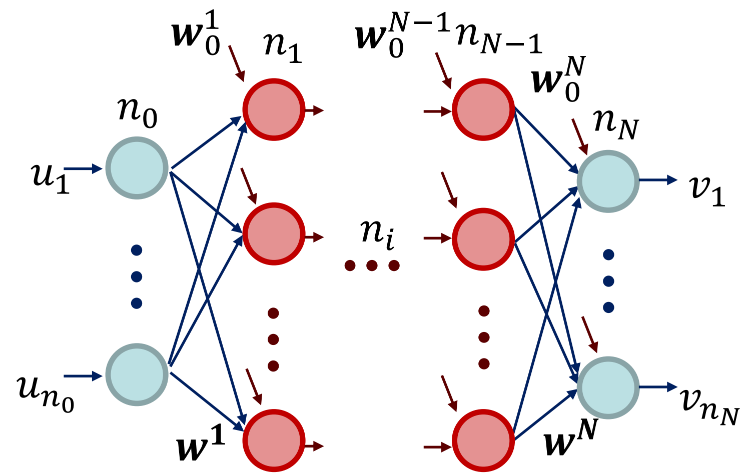
- Training
  - Use (a lot of) known data
    - Input $\boldsymbol{u}^{(p)}$ & Output $\boldsymbol{v}^{(p)}$
    - Requires normalization: $\hat{\chi} = \dfrac{\chi - \bar{\chi}}{\chi_{\max} - \chi_{min}}$
  - Evaluate
    - The weights $w_{kj}^{i}, k = 1..n_{i-1}, j = 1..n_i$
    - The bias w_0^i
    - Minimise error prediction $\boldsymbol{v}$ vs. real $\boldsymbol{v}^{(p)}$

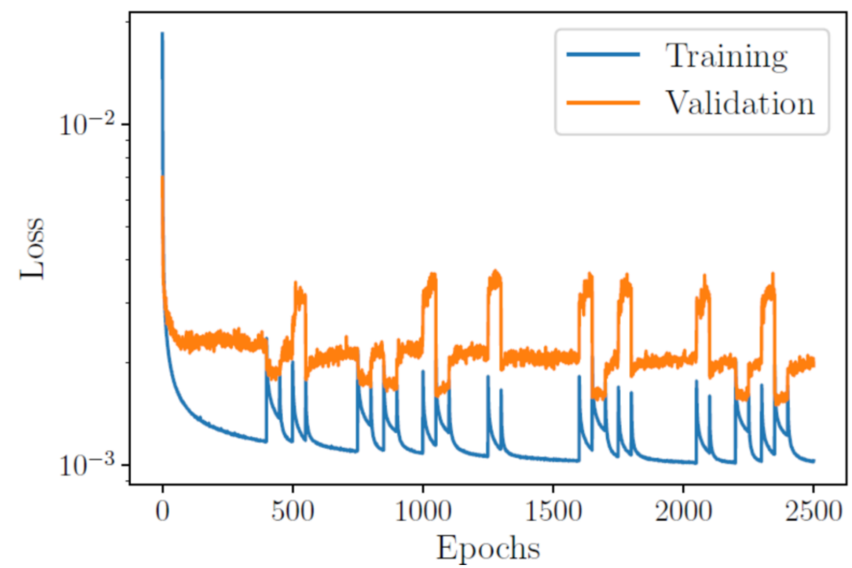
$$L_{\text{MSE}}\left(\mathbf{W}\right) = \frac{1}{n}\sum_{i}^{n}\left\|\boldsymbol{v}_i(\mathbf{W}) - \boldsymbol{v}_i^{(p)}\right\|^2$$

    - Requires an optimizer:
      Stochastic Gradient Descent

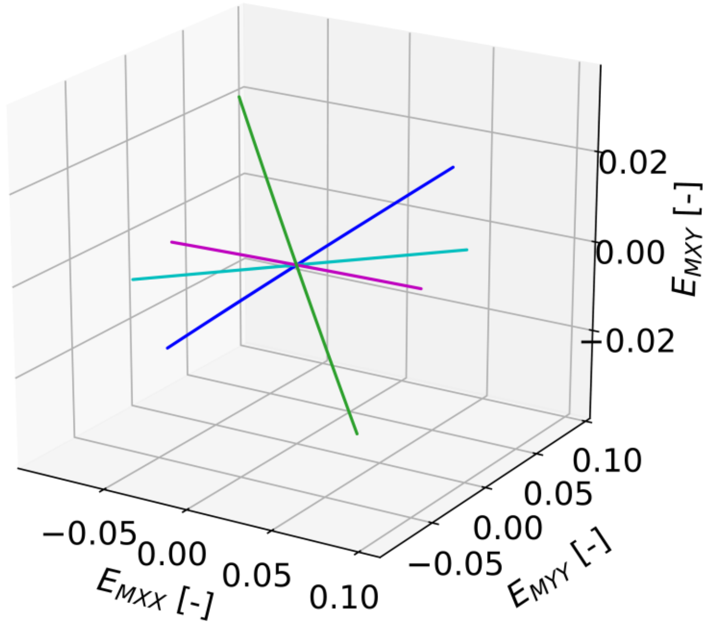
$$\boldsymbol{\Delta}\mathbf{W} = -\mathcal{F}\left(\frac{\partial L_i(\mathbf{W})}{\partial \mathbf{W}}, \quad \left(\frac{\partial L_i(\mathbf{W})}{\partial \mathbf{W}}\right)^2, \text{batch size}, \ldots\right)$$

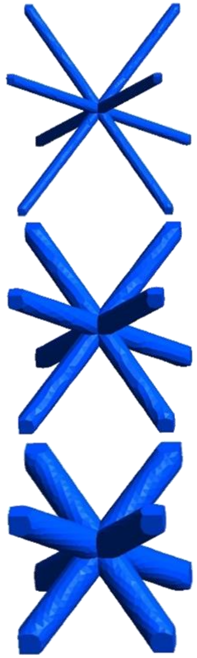
- Testing
  - Use new data
    - Input $\boldsymbol{u}^{(p)}$& Output $\boldsymbol{v}^{(p)}$
    - Verify prediction $\boldsymbol{v}$ vs. real $\boldsymbol{v}^{(p)}$



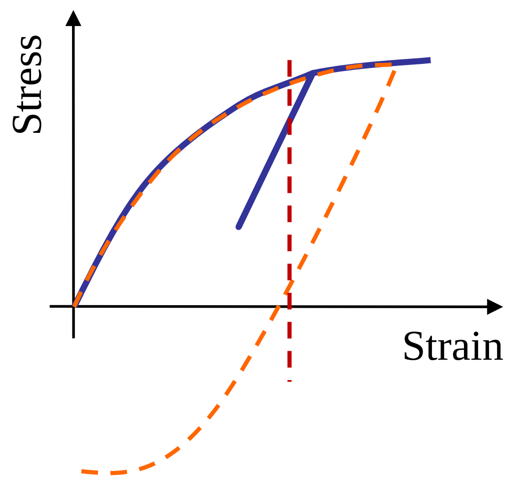


- Input / output definition
  - Input:
    - Strain (history): $\mathbf{F}_{\mathrm{M}}$
    - Geometry/material parameters: $\boldsymbol{\varphi}_{\mathrm{m}}$
  - Output:
    - Stress (history): $\mathbf{P}_{\mathrm{M}}$



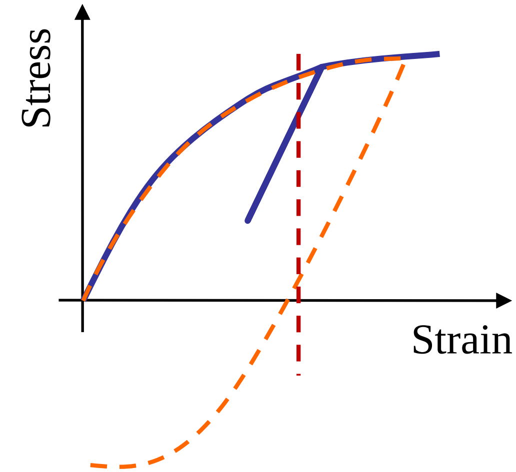


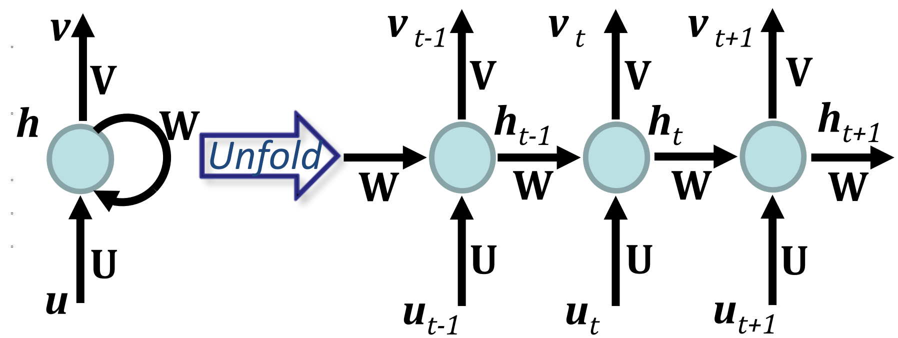
- Methodology
  - Address problem of history dependency
    - RVE without buckling
    - Elasto-plastic composite RVE
  - Address problem of geometry/material effect
    - Octet cells
    - Elastic material at first



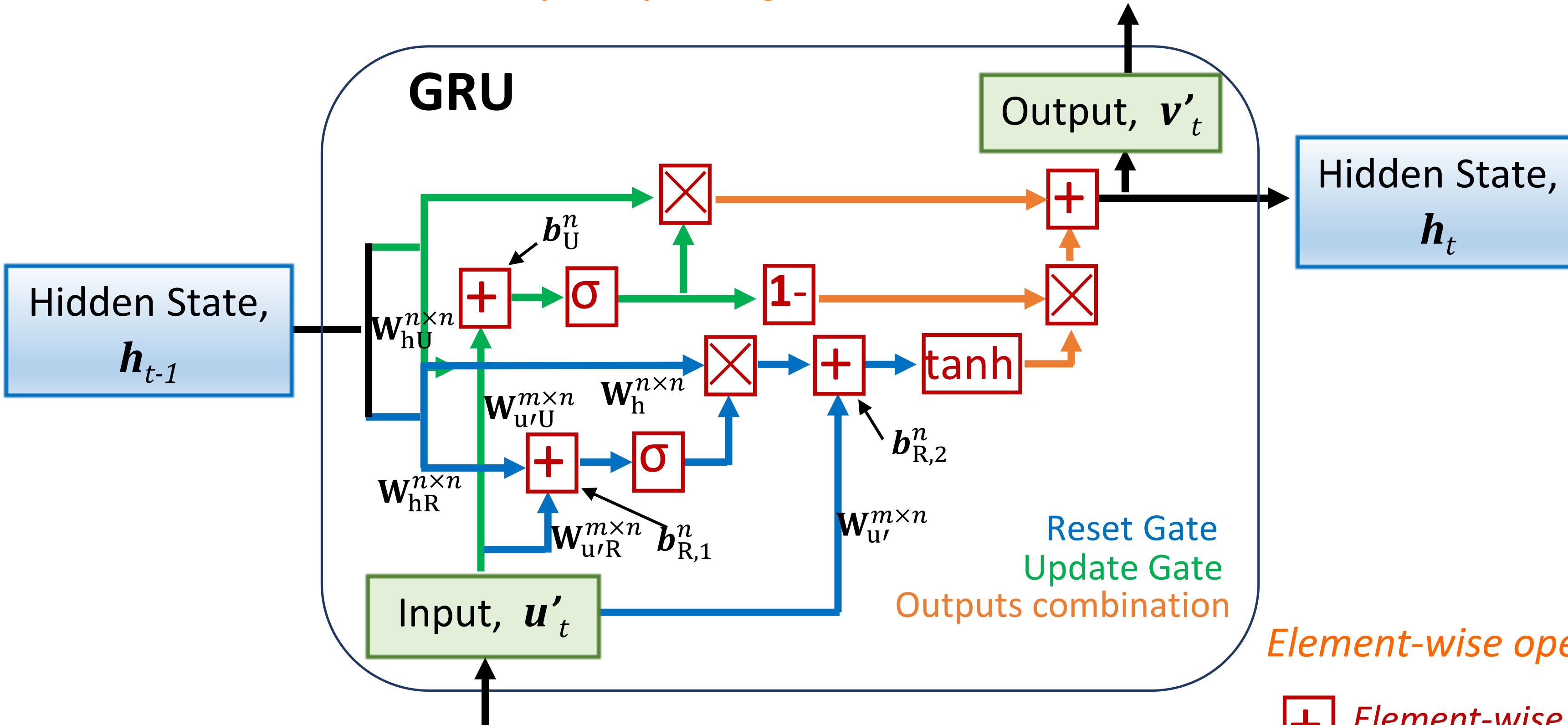
History dependency

- Elasto-plastic material behaviour
  - No bijective strain-stress relation
    - Feed-forward NNW cannot be used
    - History should be accounted for
- Recurrent neural network
  - Allows a history dependent relation
    - Input $\boldsymbol{u_t}$
    - Output $\boldsymbol{v_t} = \boldsymbol{g}(\boldsymbol{u_t}, \boldsymbol{h_{t-1}})$
    - Internal variables $\boldsymbol{h_t} = \boldsymbol{g}(\boldsymbol{u_t}, \boldsymbol{h_{t-1}})$
  - Weights matrices $\mathbf{U}, \mathbf{W}, \mathbf{V}$
    - Trained using sequences
      - Inputs $\boldsymbol{u}_{t-n}^{(p)}, \ldots, \boldsymbol{u}_{t}^{(p)}$
      - Output $\boldsymbol{v}_{t-n}^{(p)}, \ldots, \boldsymbol{v}_{t}^{(p)}$





- Gated Recurrent Unit (GRU) at a glance



Element-wise operations

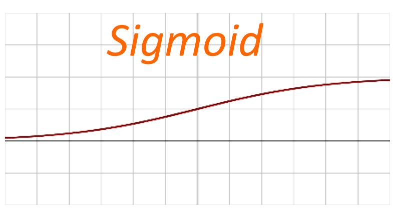
+ *Element-wise sum*

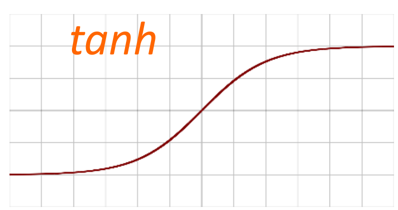
1- *Element-wise 1-*

⊠ *Element-wise product*

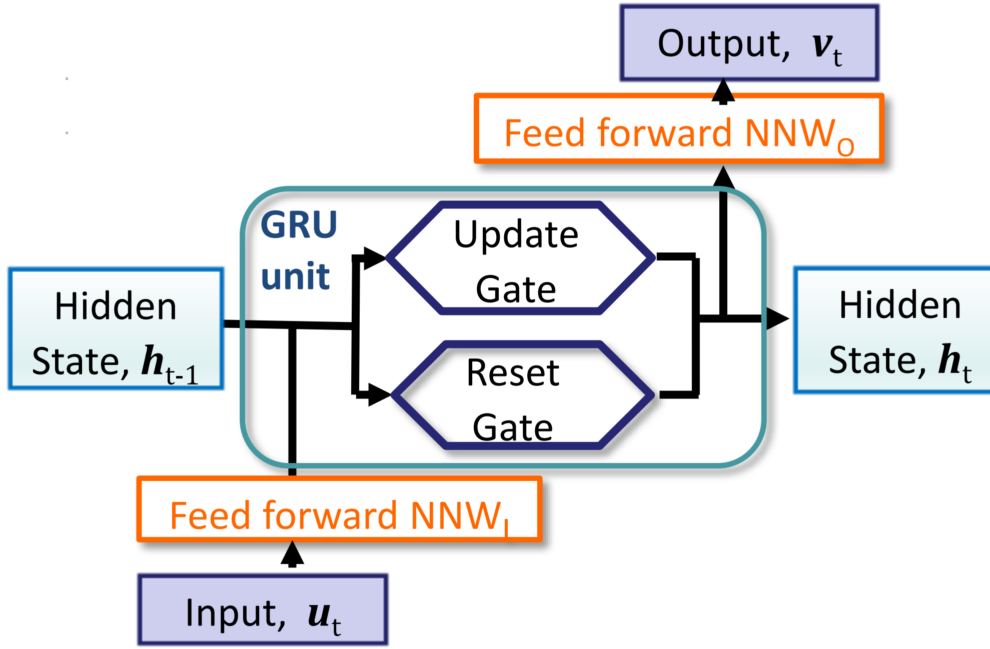
σ *Element-wise sigmoid*

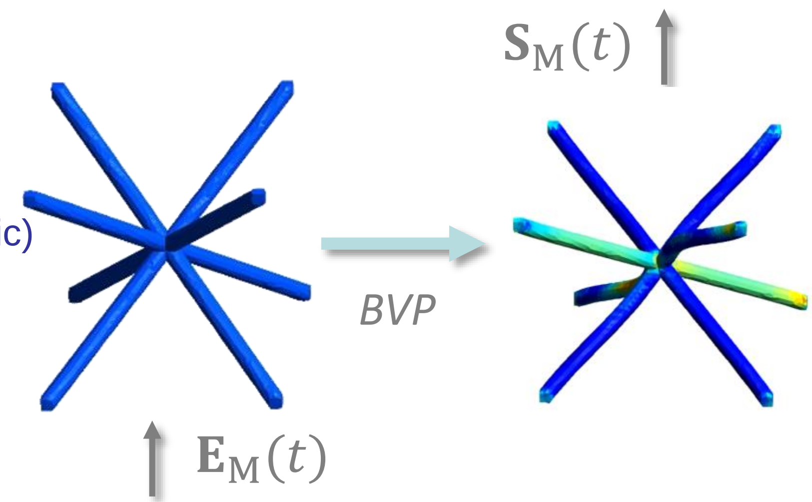
tanh *Element-wise tanh*





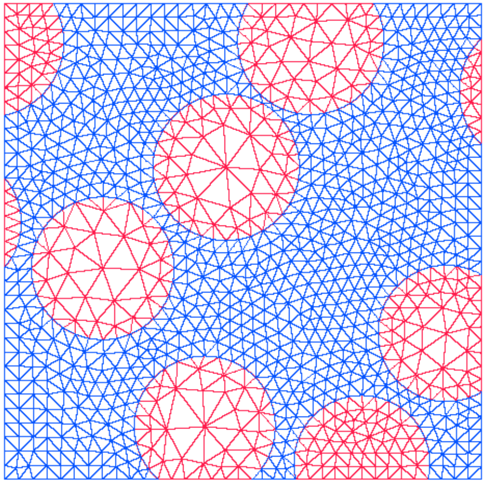
- Recurrent neural network design
  - 1 Gated Recurrent Unit (GRU)
    - Reset gate: select past information to be forgotten
    - Update gate: select past information to be passed along
  - 2 feed-forward NNWs (Leaky ReLU)
    - NNW_I to treat inputs $\boldsymbol{u}_t$
    - NNW_O to produce outputs $\boldsymbol{v}_t$
  - Details
    - $\boldsymbol{u}_t$: homogenised GL strain $\mathbf{E}_{\mathrm{M}}$ (symmetric)
    - $\boldsymbol{v}_t$: homogenised 2nd PK stress $\mathbf{S}_{\mathrm{M}}$ (symmetric)
    - 100 hidden variables $\boldsymbol{h}_t$
    - NNW_I one hidden layer of 60 neurons
    - NNW_O two hidden layers of 100 neurons

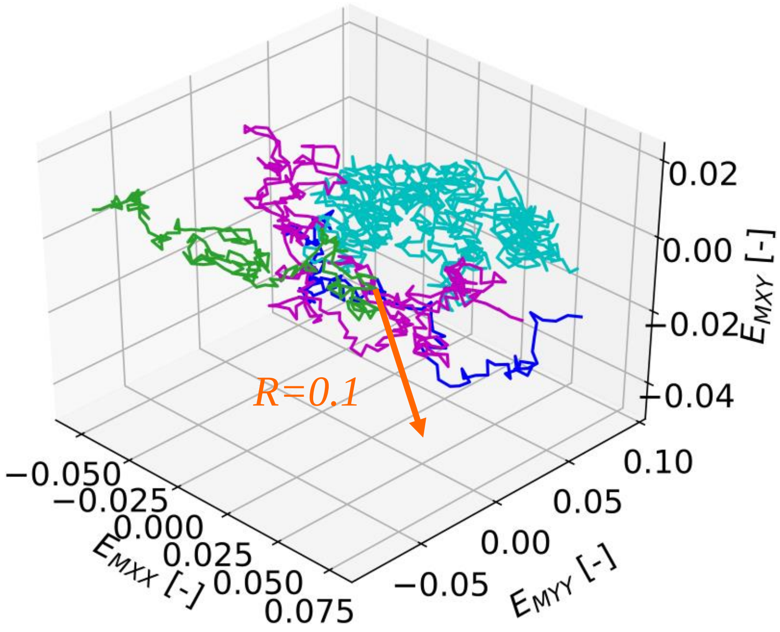


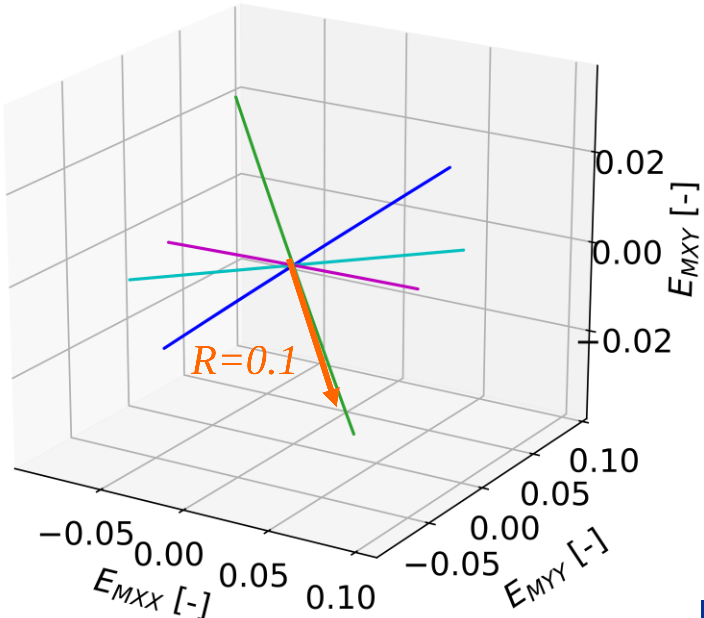


History dependency

- Data generation
  - Elasto-plastic composite RVE
  - Training stage
    - Should cover full range of possible loading histories
    - Use random walking strategy (thousands)
    - Completed with random cyclic loading (tens)
    - Bounded by a sphere of 10% deformation

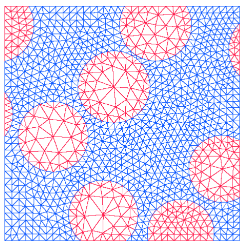


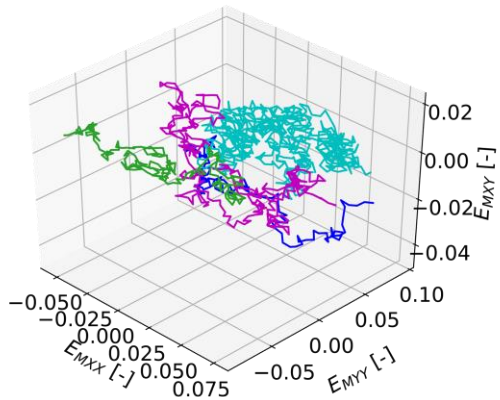


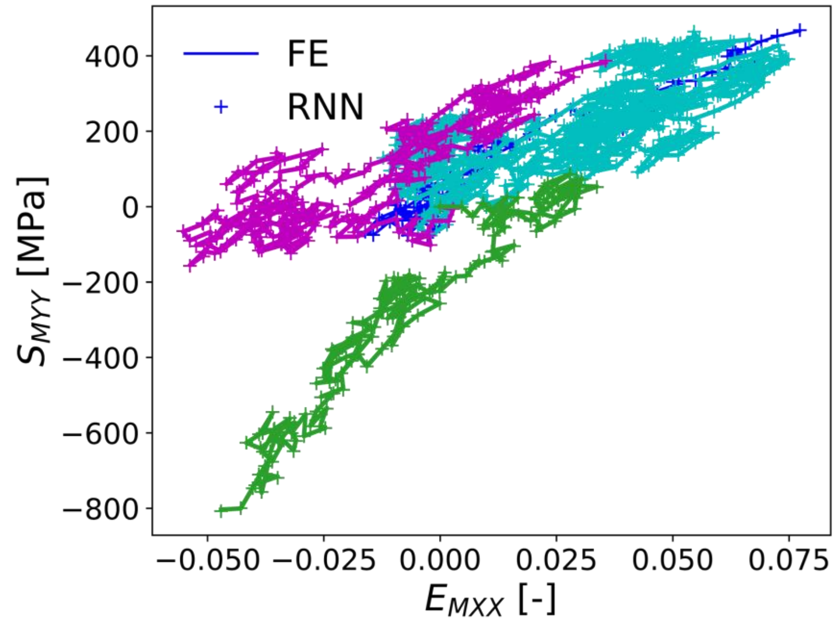


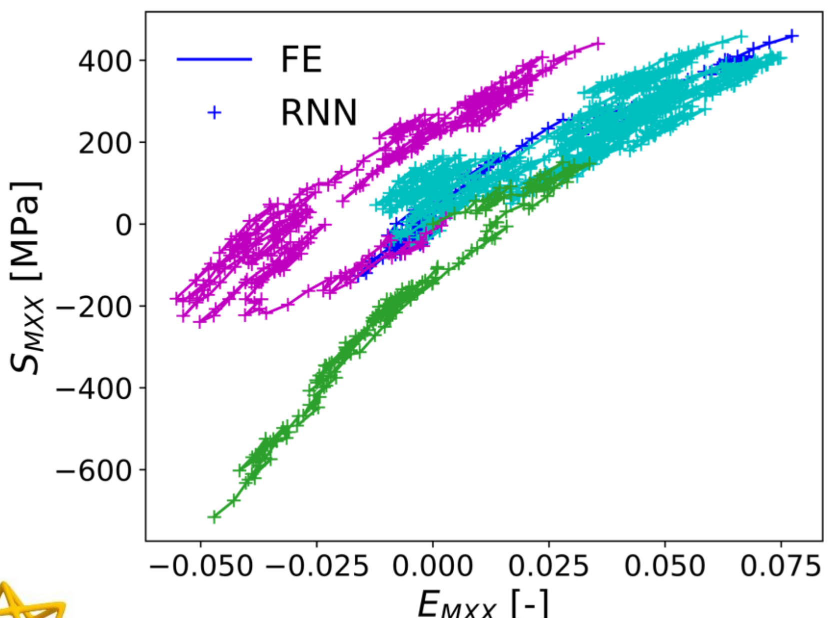
History dependency

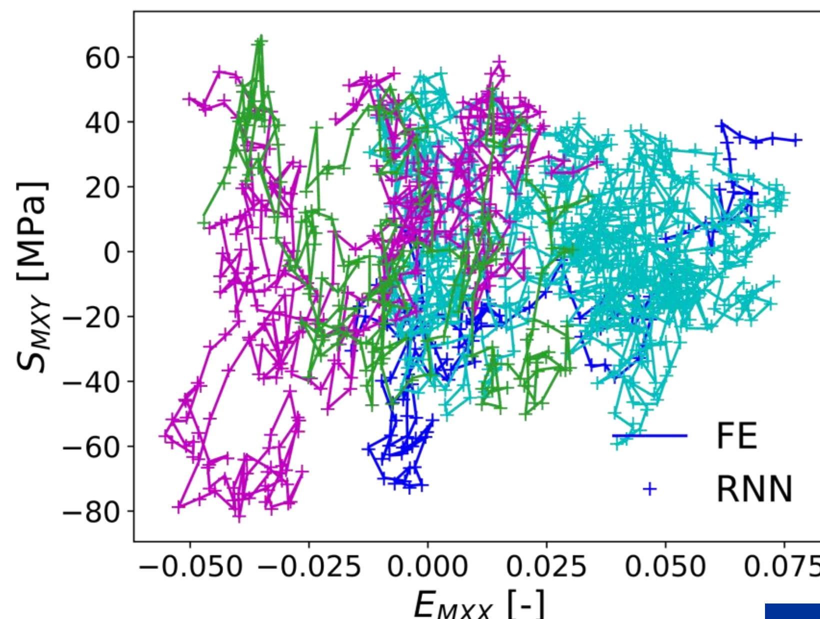
- Testing process (new data)
  - On random walk





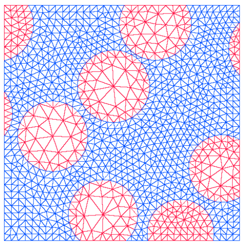


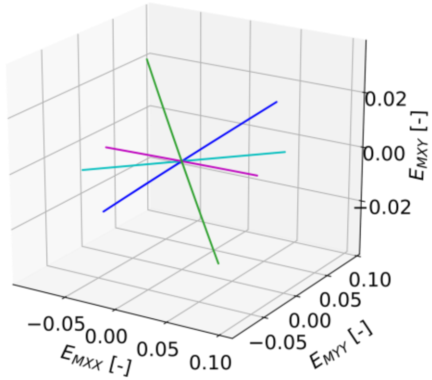


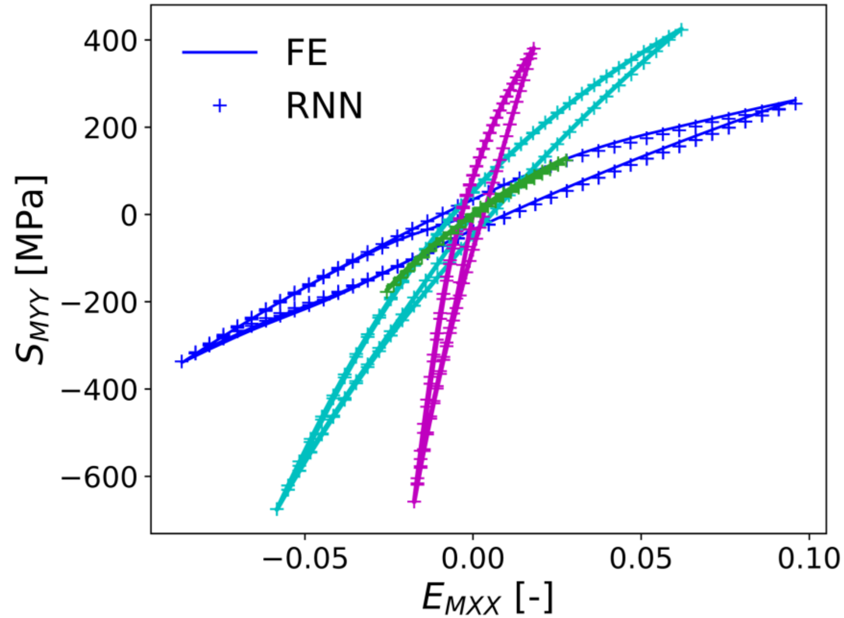


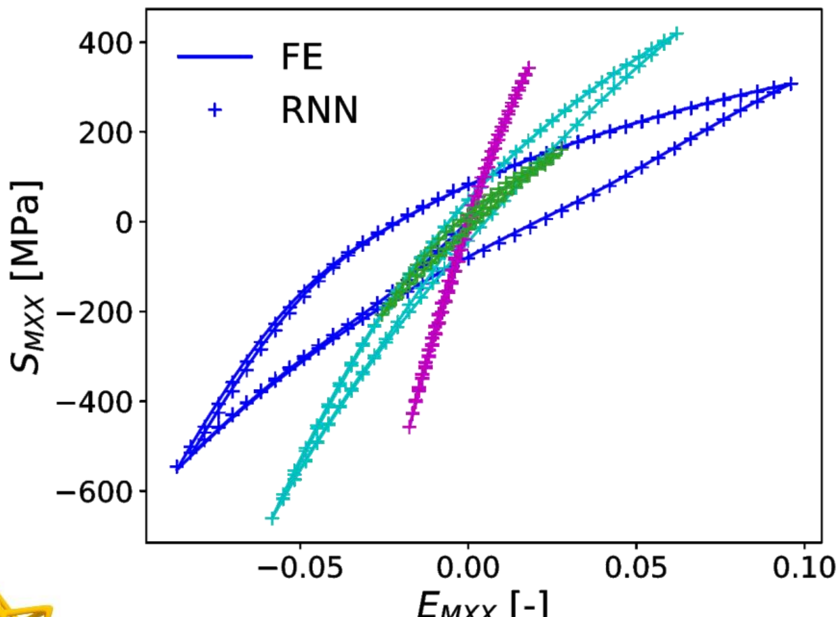
History dependency

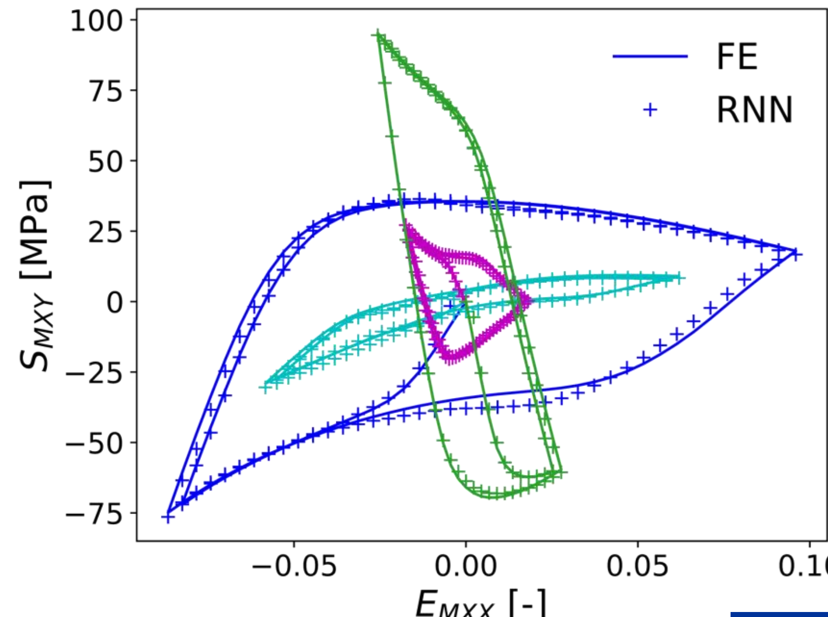
- Testing process (new data)
  - On cyclic loading





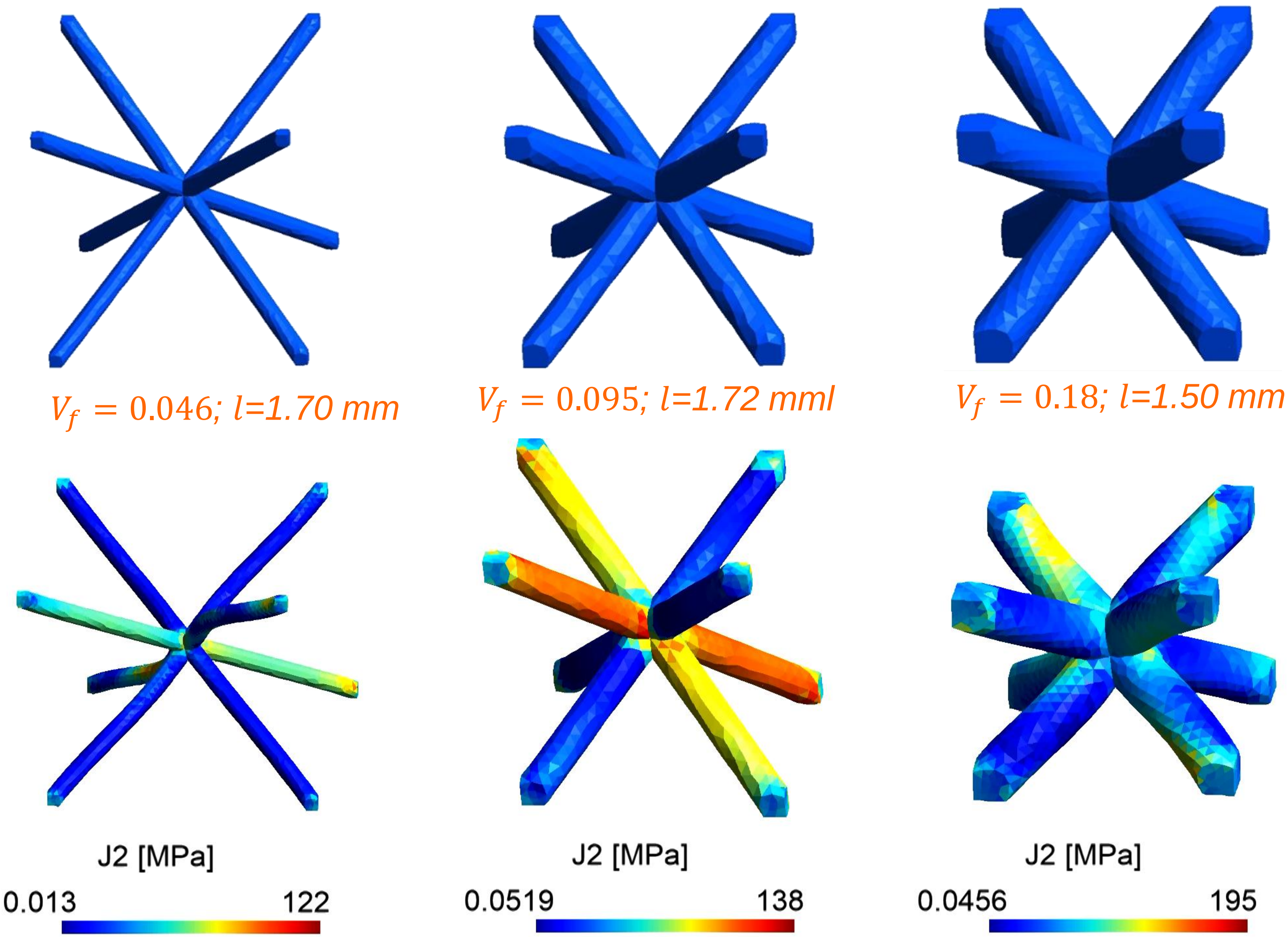




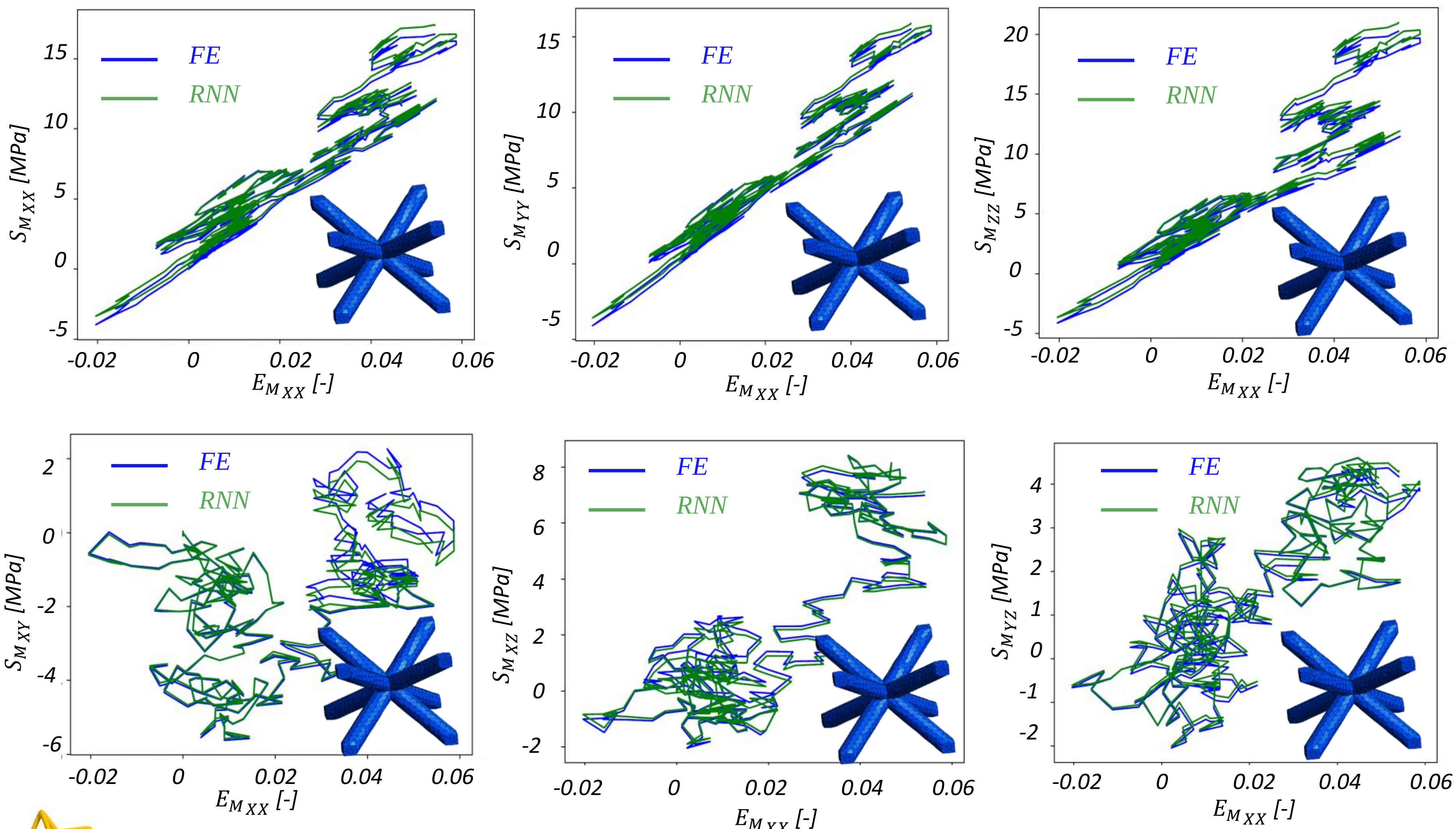


Geometrical parameters effect

- Octet cell
  - Generalised IMDEA script to generate random cells and random loading paths



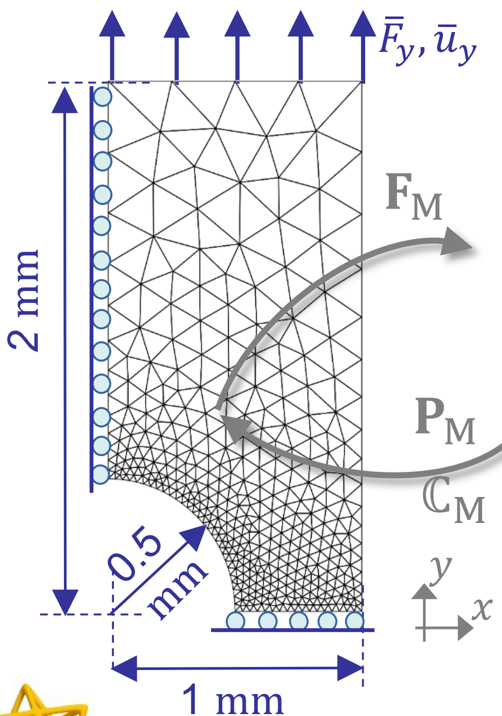
- Octet cell
  - Test on new random cell/path

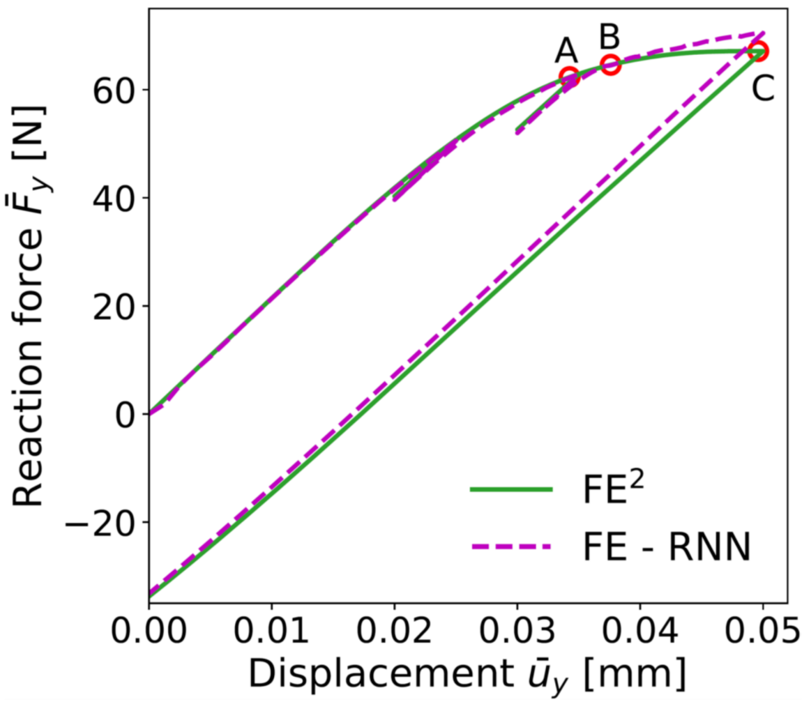


ANN as a mesoscale surrogate model

- Multiscale simulation
  - Elasto-plastic composite RVE
  - Comparison FE^2 vs. RNN-surrogate
  - Training data
    - Bounded at 10% deformation

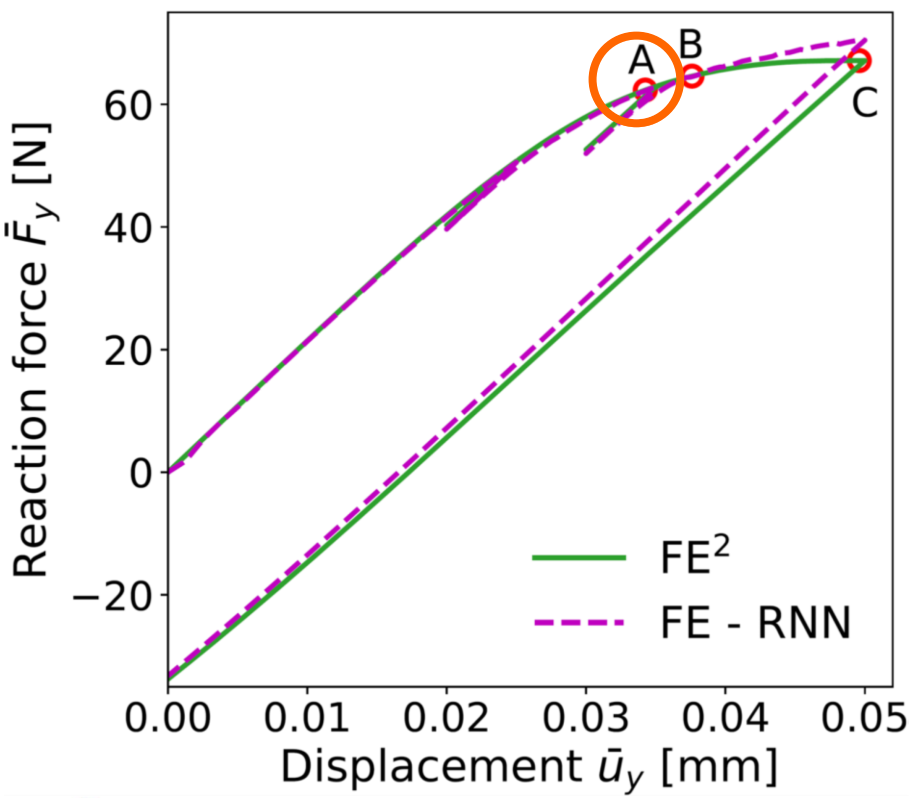
Off-line	FE^2	FE-RNN
Data generation	-	9000 x 2 h-cpu
Training	-	3 day-cpu
On-line	**FE^2**	**FE-RNN**
Simulation	18000 h-cpu	0.5 h-cpu

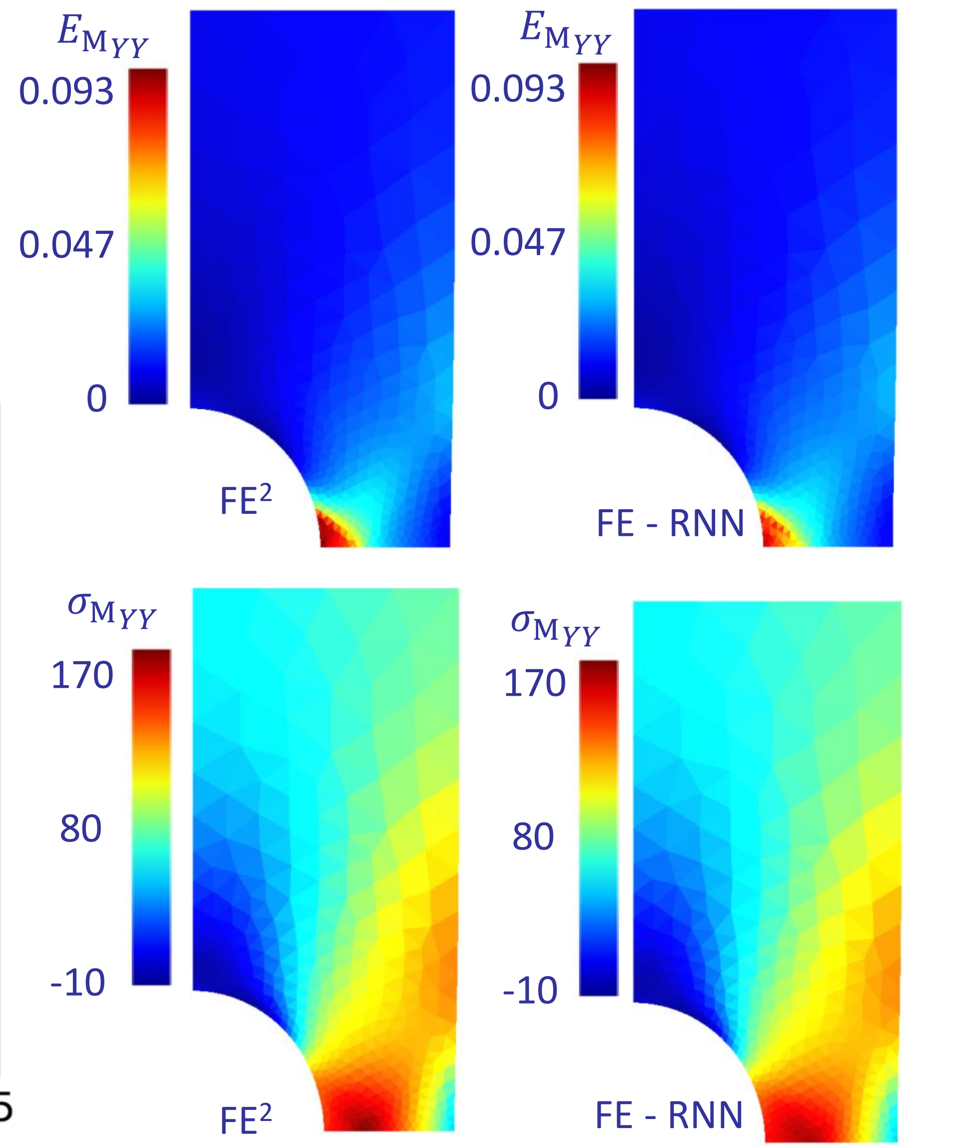




ANN as a mesoscale surrogate model

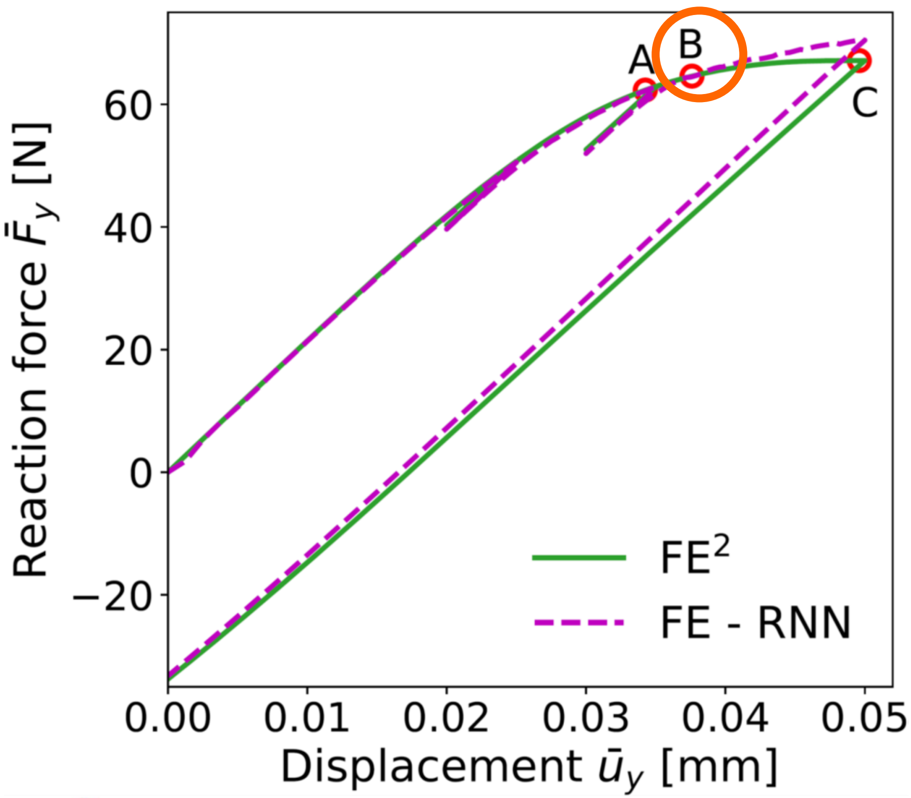
- Multiscale simulation
  - Stress-strain distribution at point A
  - Strain within the 10% training range

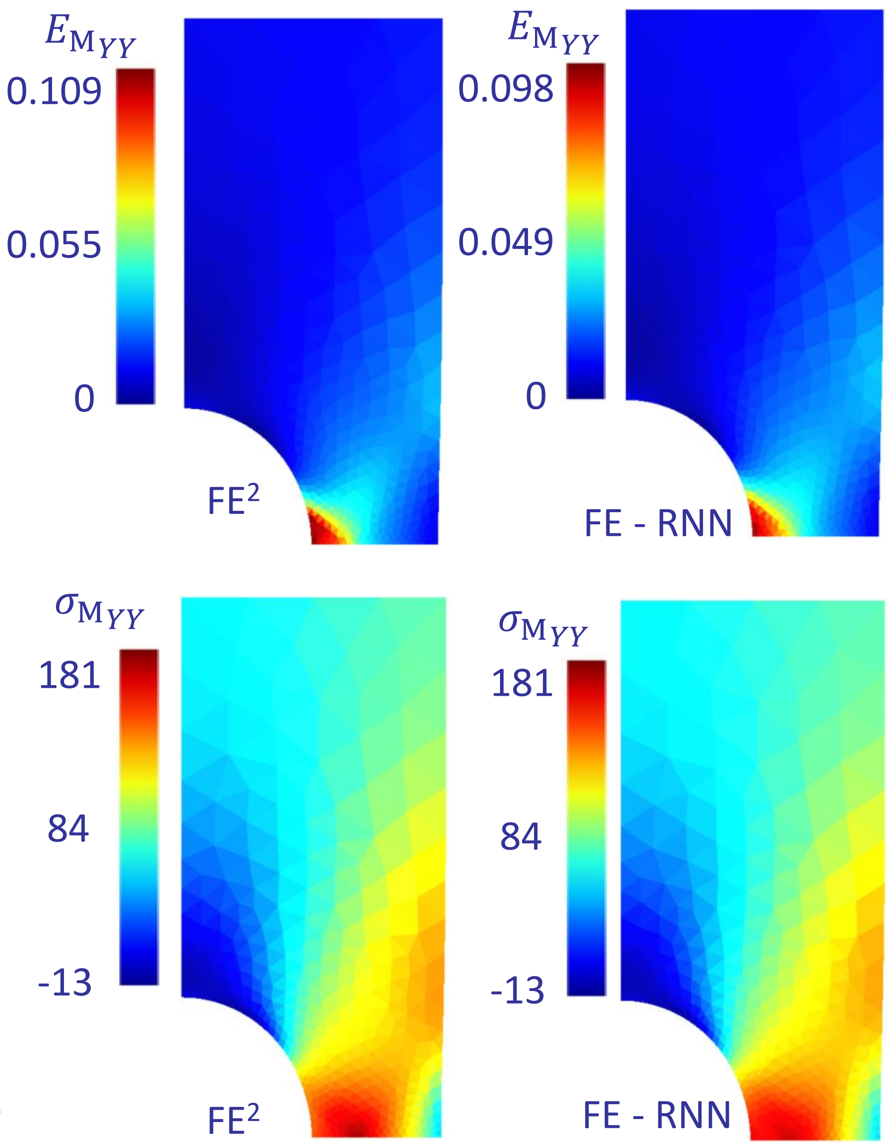




ANN as a mesoscale surrogate model

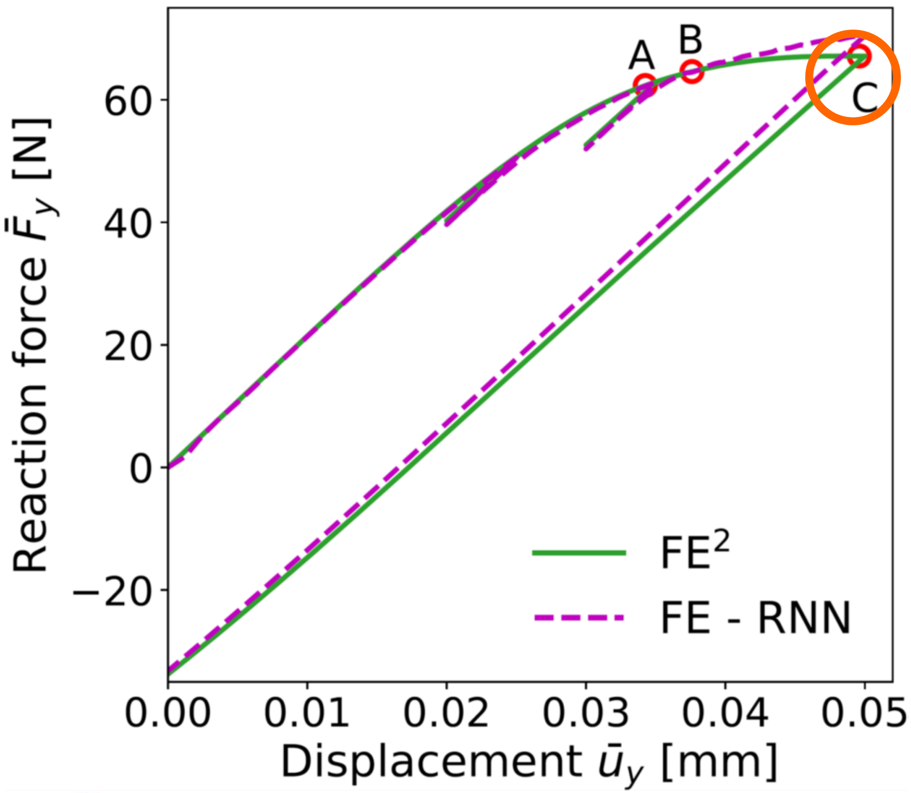
- Multiscale simulation
  - Stress-strain distribution at point B
  - Strain just at 10% training range

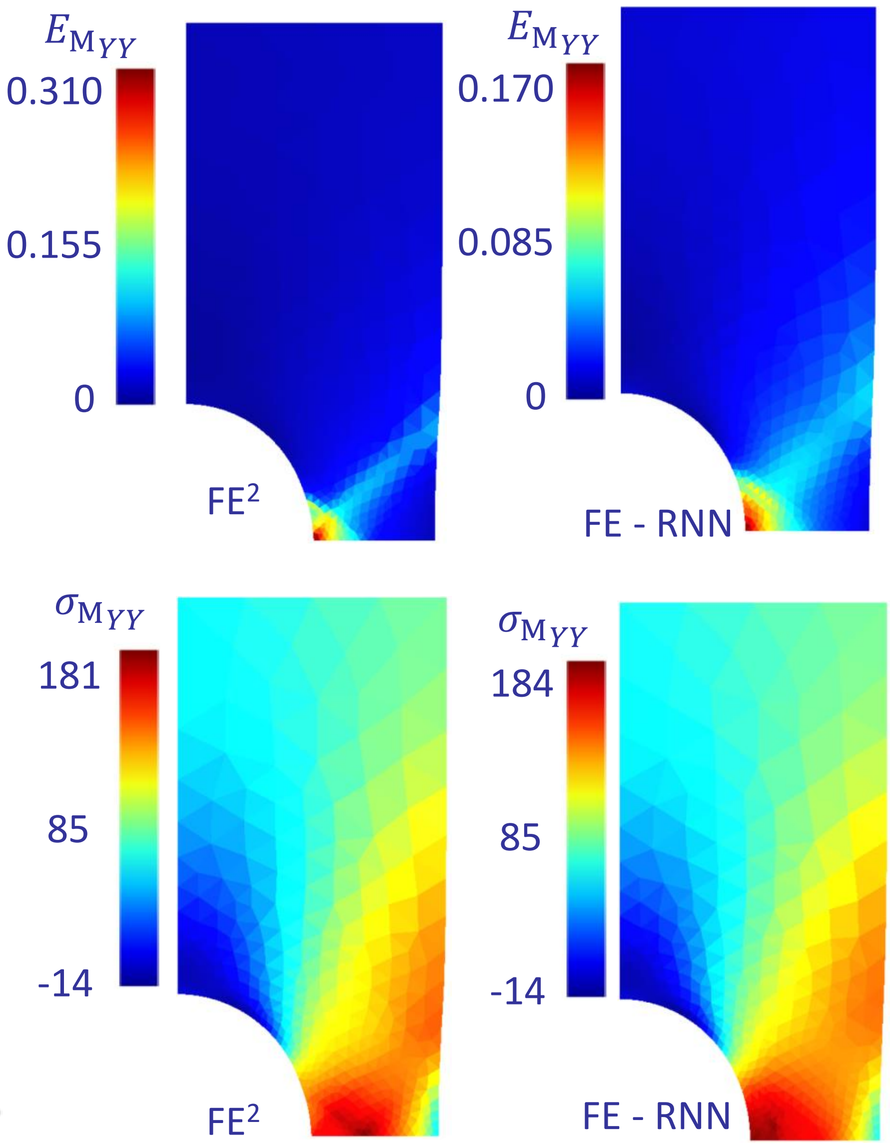




ANN as a mesoscale surrogate model

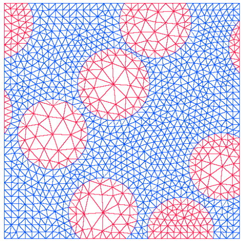
- Multiscale simulation
  - Stress-strain distribution at point C
  - Strain out of 10% training range

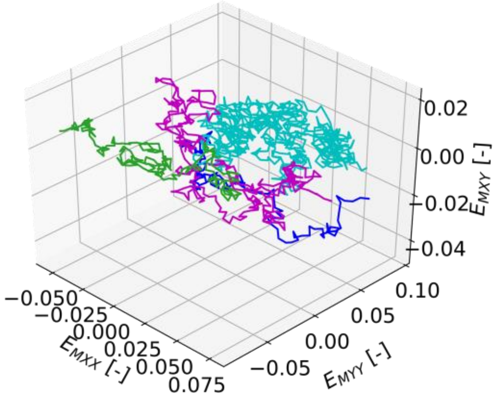


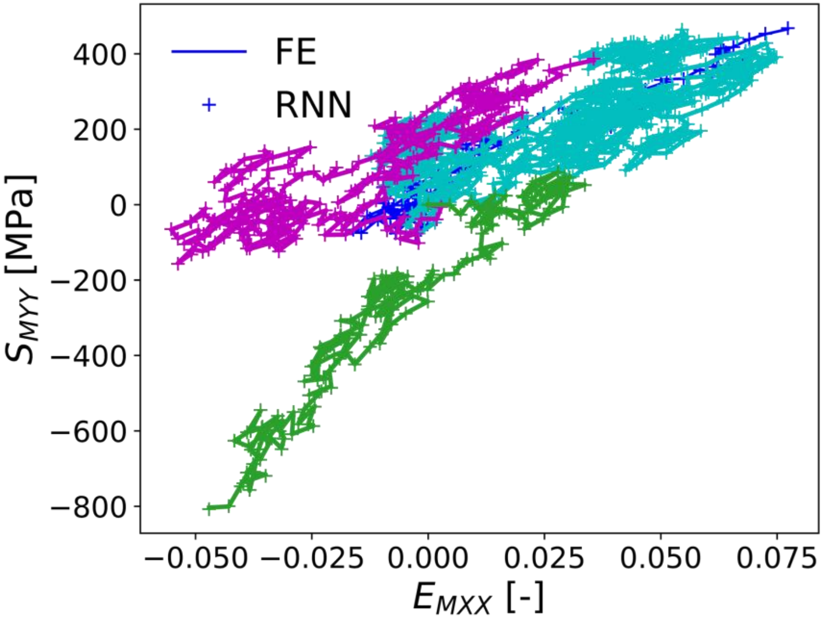


Localisation step

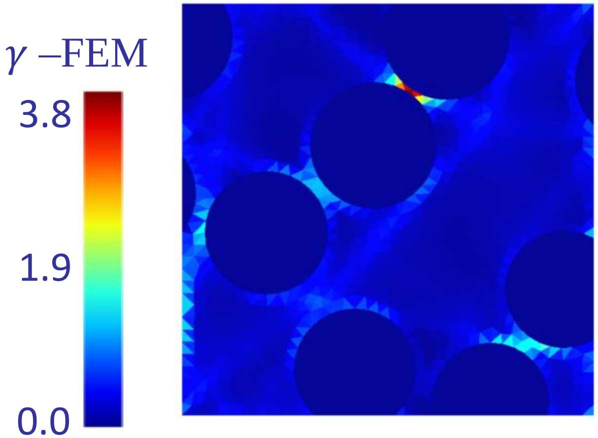
- Only homogenised output is predicted
  - On random walk





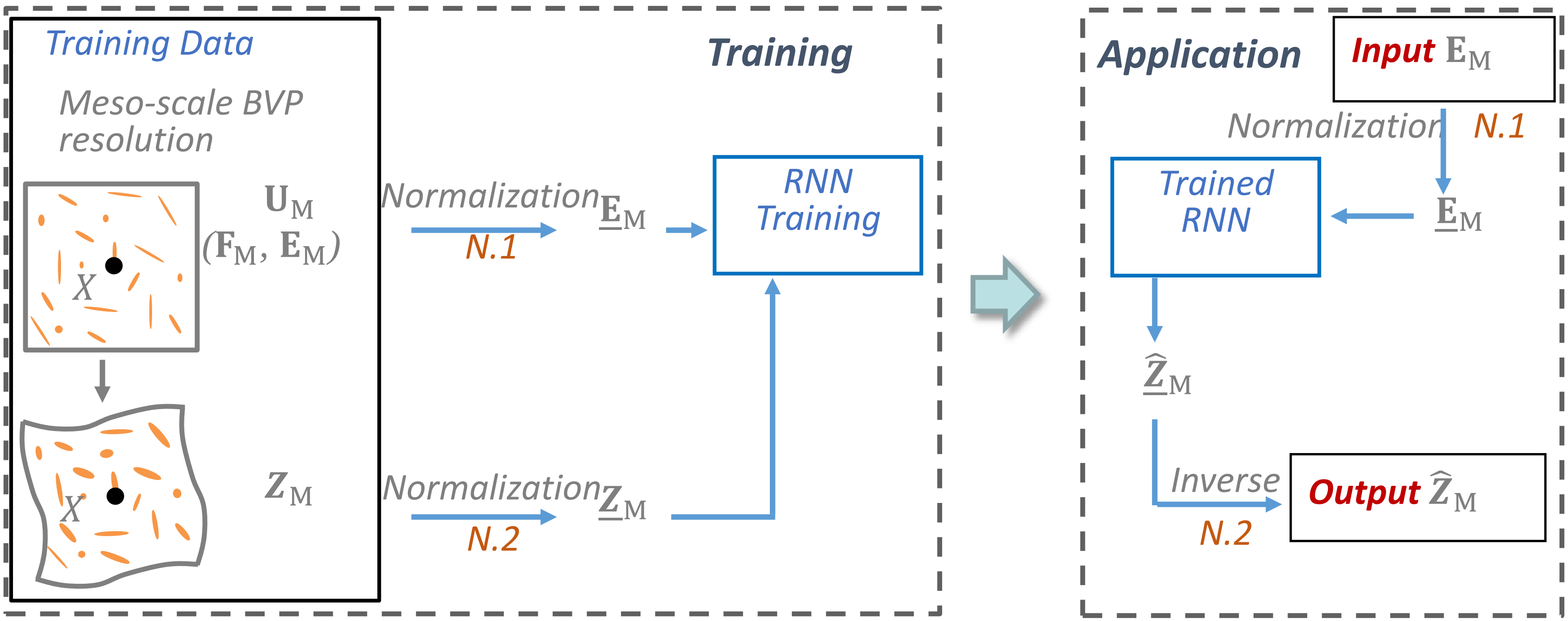


- Quid of local fields?
  - This is an advantage of multiscale methods
  - Useful to predict failure, fatigue etc.
  - Can we get it back at low cost?



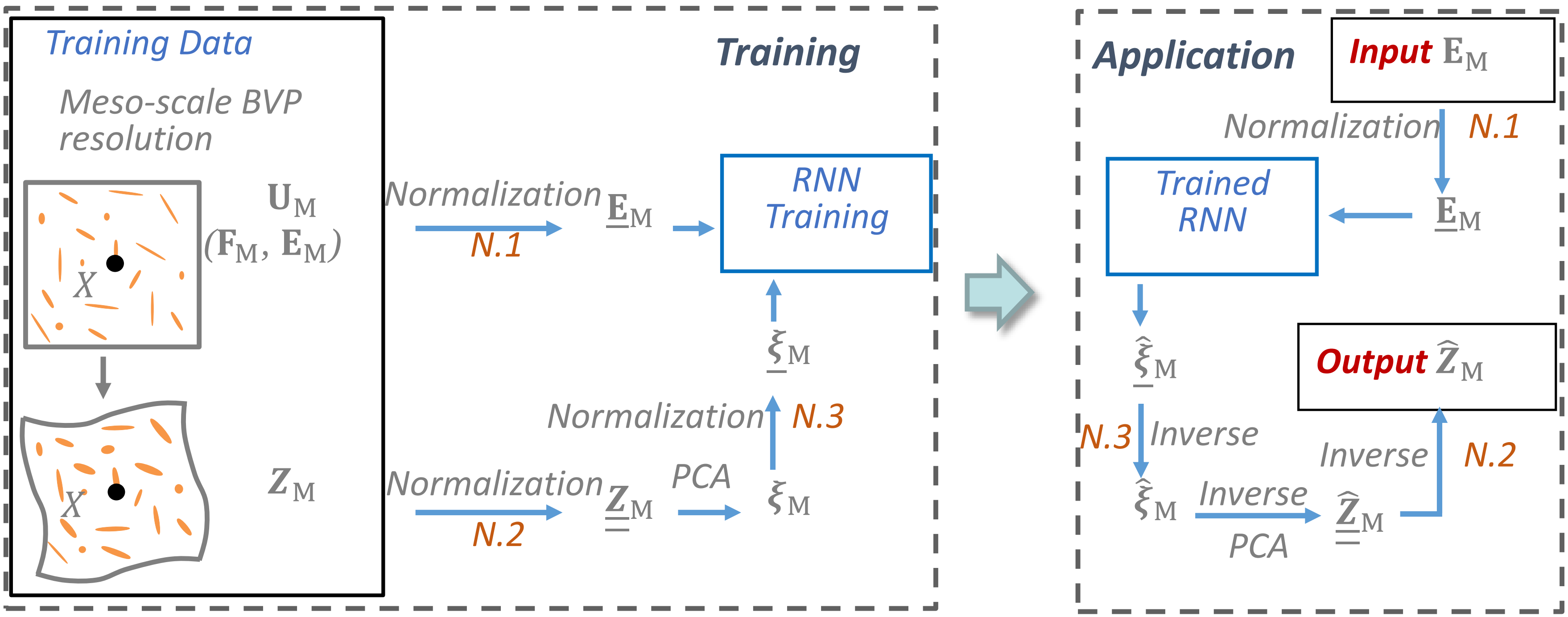
Localisation step

- Also build a surrogate model of the internal variables



  – Problem: The size of $\underline{\mathbf{Z}}_\mathrm{M}$ is large ⇨ overwhelming cost

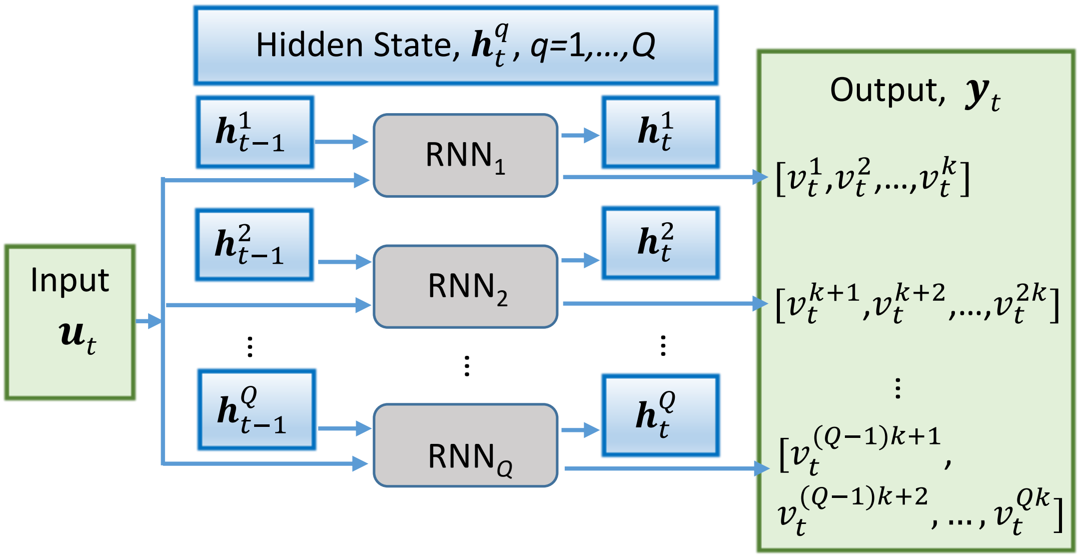
- Optimise the method: reduce the size of the internal variables



  - Principal Component Analysis (PCA) applied on $\underline{\underline{Z}}_M$ to reduce the output of RNN
  - But not enough

Localisation step

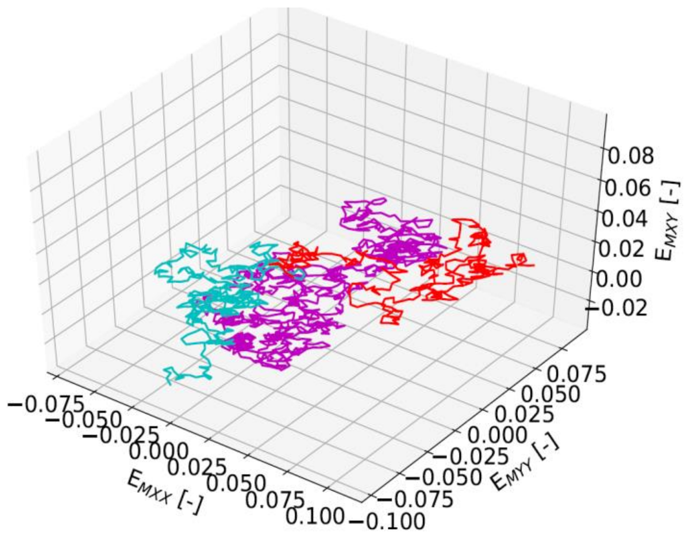
- Dimension breakdown: to further reduce the output dimension of RNN

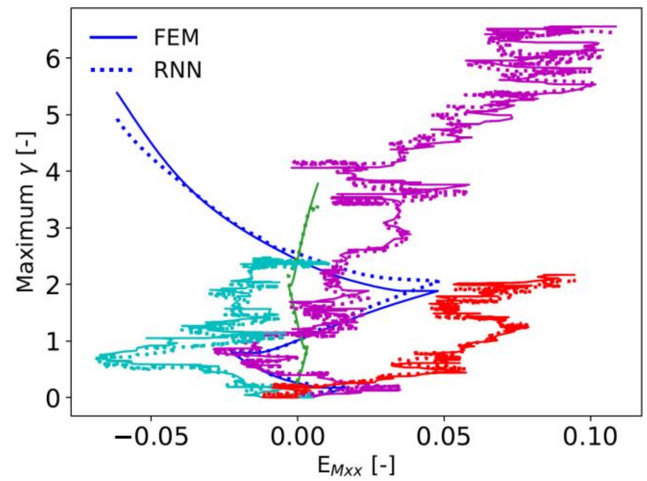


- The surrogate modelling is carried out by a few small RNNs, instead of one big RNN
- The high dimension output is divided into Q groups, and each RNN is used to reproduce only a part of output
- PCA reduces $\underline{\boldsymbol{Z}}_{\mathrm{M}}$ to 180 outputs and we use Q=6

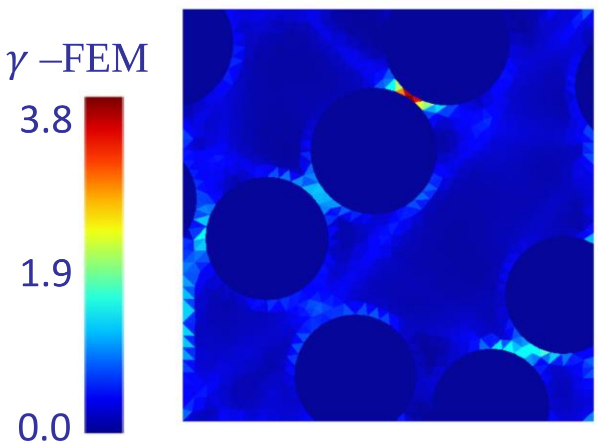
Localisation step

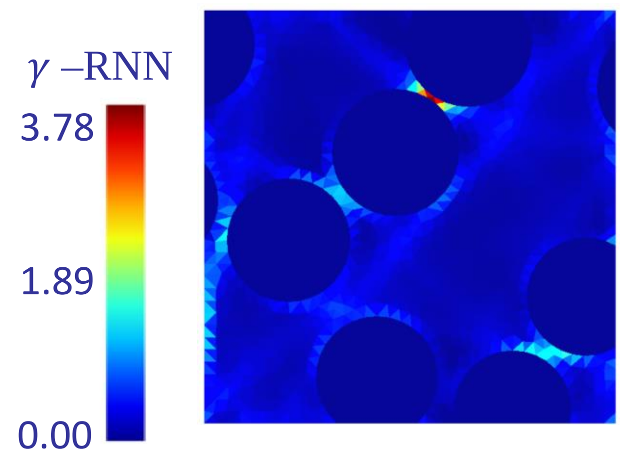
- Evaluation of equivalent plastic strain γ: Random loading (testing data)



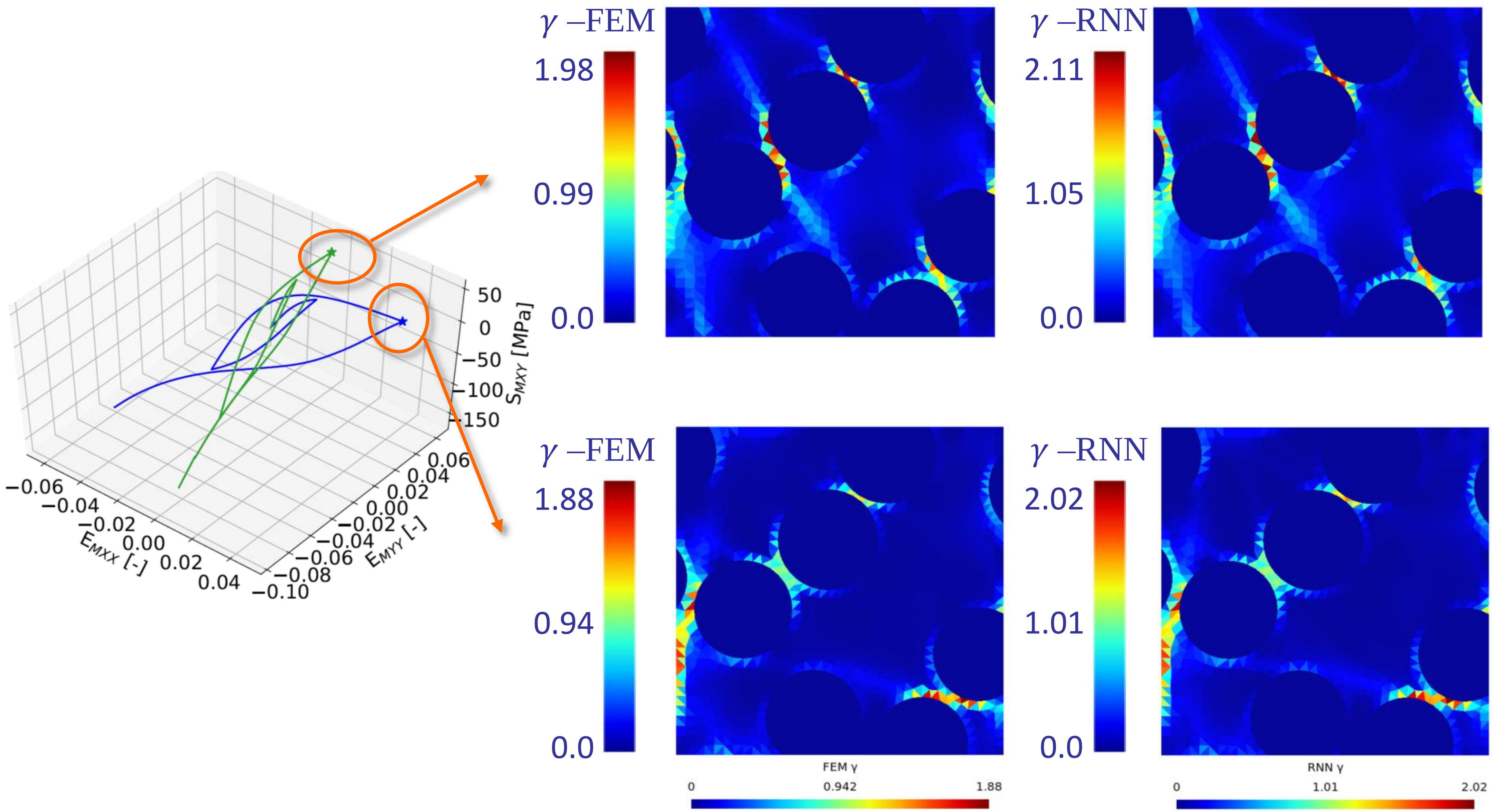


Purple loading – step 500





- Evaluation of equivalent plastic strain γ: Cyclic loading (testing data)



Conclusions

- More on
  - www.moammm.eu
  - L. Wu, V. D. Nguyen, N. G. Kilingar, and L. Noels. "A recurrent neural network-accelerated multi-scale model for elasto-plastic heterogeneous materials subjected to random cyclic and non-proportional loading paths." Computer Methods in Applied Mechanics and Engineering 369 (September 1, 2020): 113234, http://dx.doi.org/10.1016/j.cma.2020.113234