A Recurrent Neural Network-based Surrogate Model for History-Dependent Multi-scale Simulations of Composite Materials

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BRAIA Lecture Series on Technology Frontier

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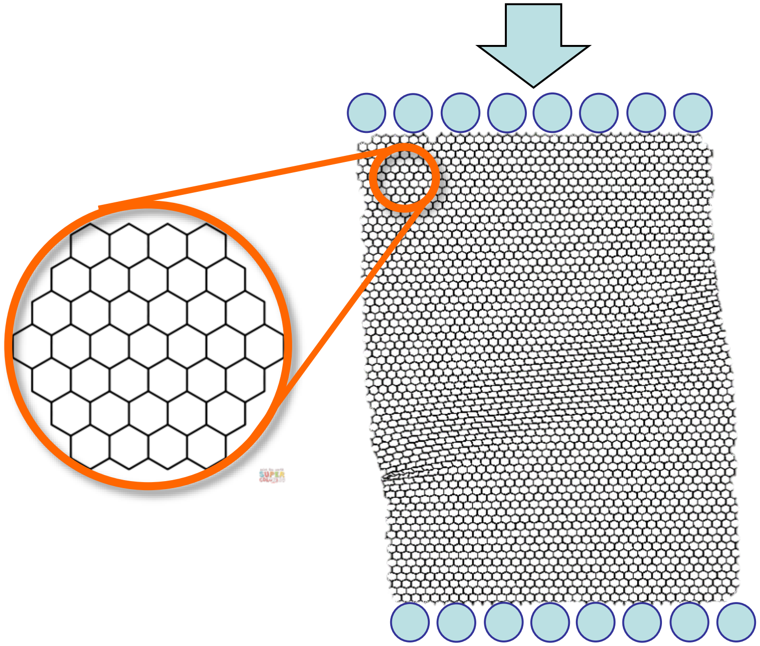
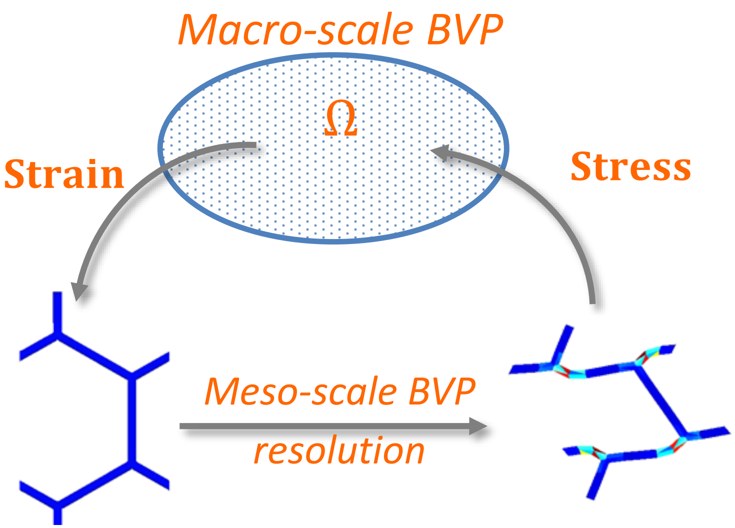
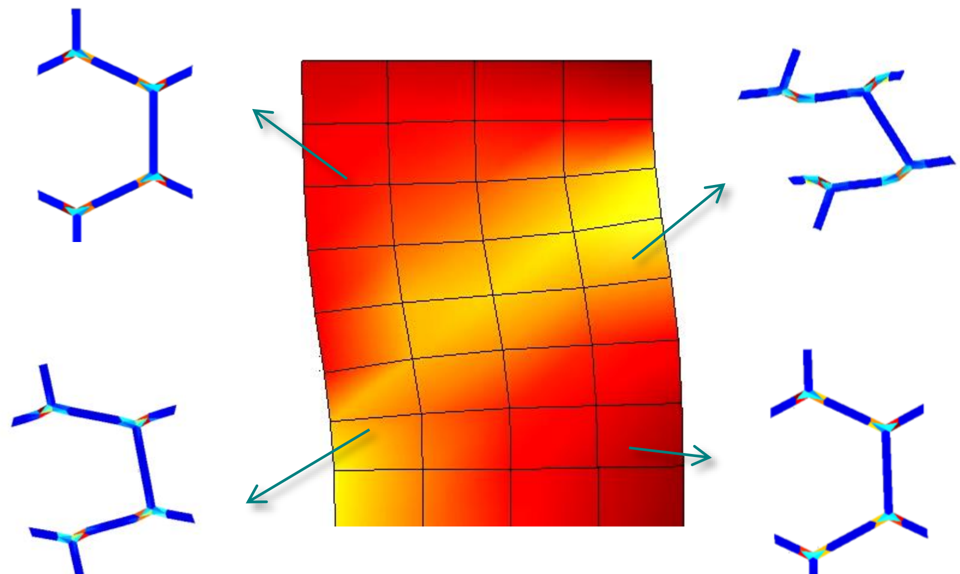
- Computational homogenisation (FE2)
  - Heterogeneous structures
    - Micro-scale: cell, grains, inclusions…
    - Macro-scale: seen as a continuum
  - Direct numerical simulations
    - Time consuming
  - Idea: use multi-scale strategy





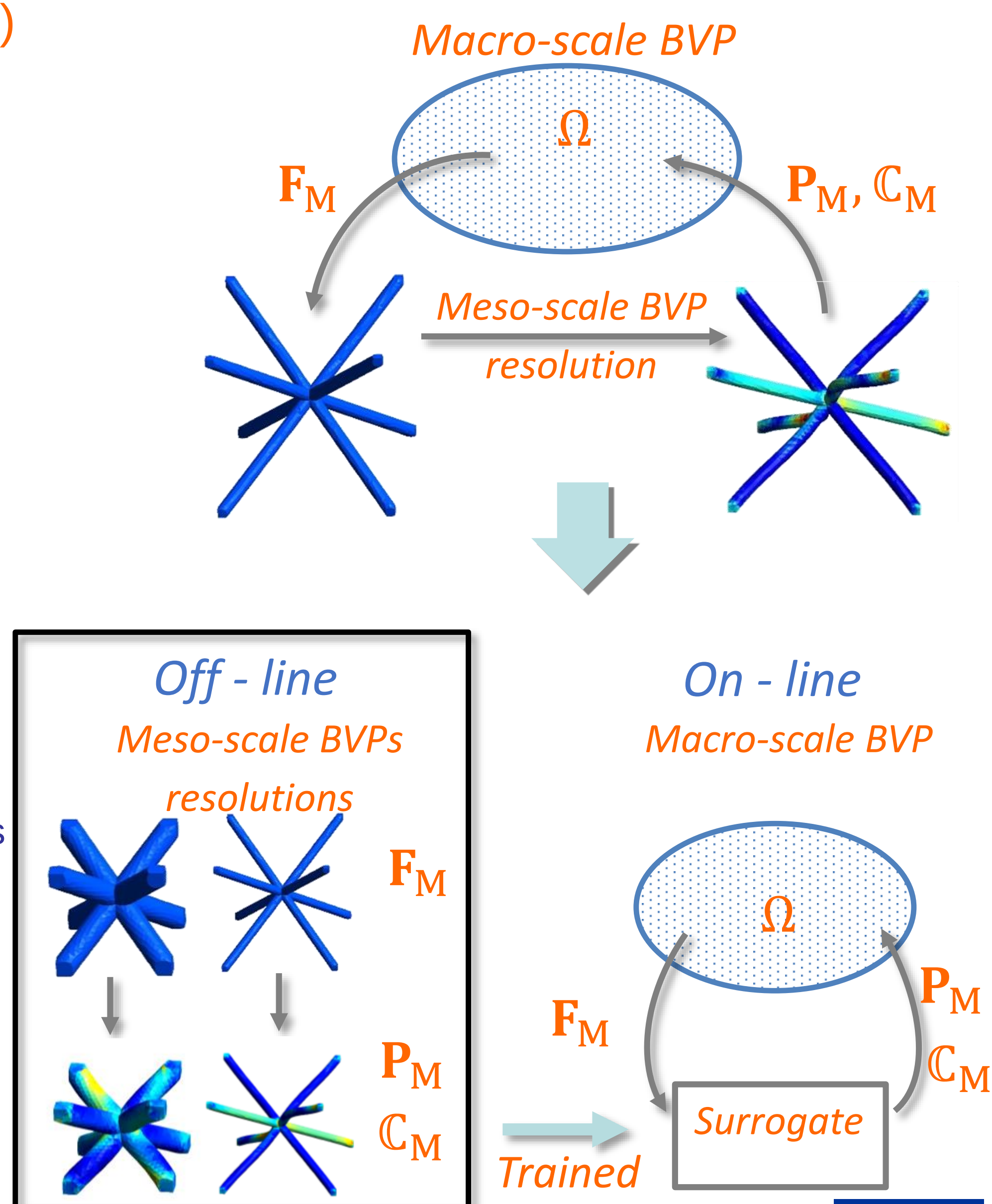


Multi-scale simulations

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

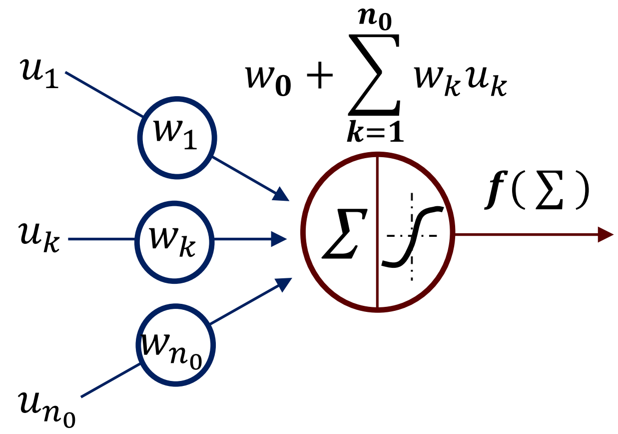
  → *Unaffordable*

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

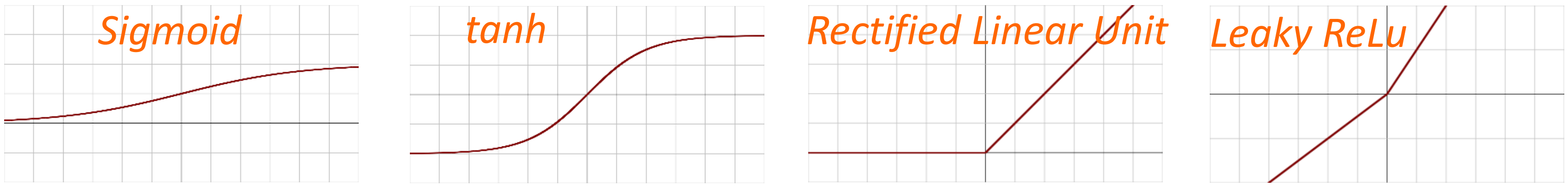


Artificial Neural Network

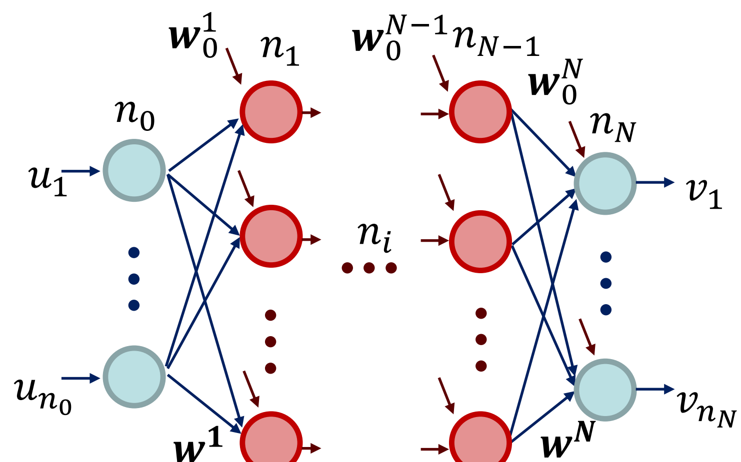
- Definition of the surrogate model
  - Artificial neuron
    - Non-linear function on n_0 inputs u_k
    - Requires evaluation of weights w_k
    - Requires definition of activation function f



  - Activation functions f



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



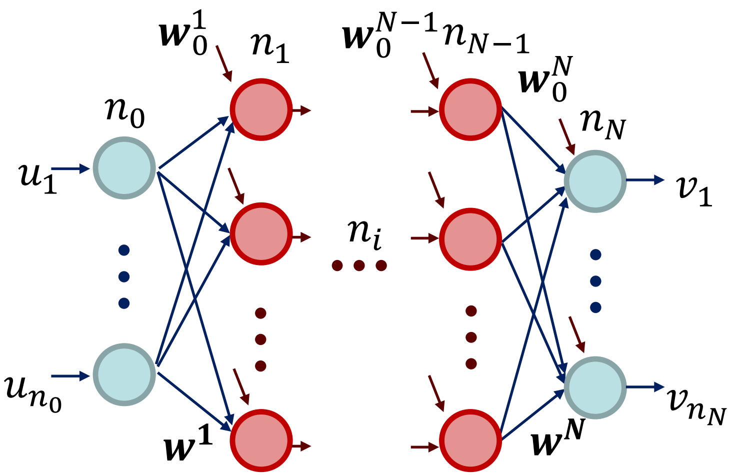
- Training
  - Evaluate
    - The weights w_{kj}^{i}, $k = 1..n_{i-1}, j = 1..n_i$
    - The bias w_0^i
    - Minimise error prediction $\boldsymbol{v}$ vs. real $\boldsymbol{v}^{(p)}$

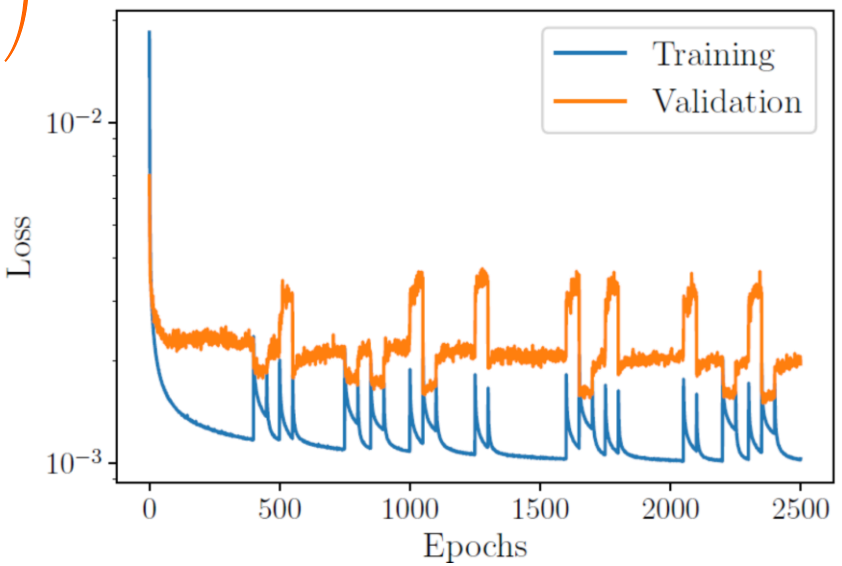
$$L_{\mathrm{MSE}}\,(\mathbf{W}) = \frac{1}{n}\sum_{i}^{n}\left\|\boldsymbol{v}_i(\mathbf{W}) - \boldsymbol{v}_i^{(p)}\right\|^2$$

    - Requires an optimizer: Stochastic Gradient Descent

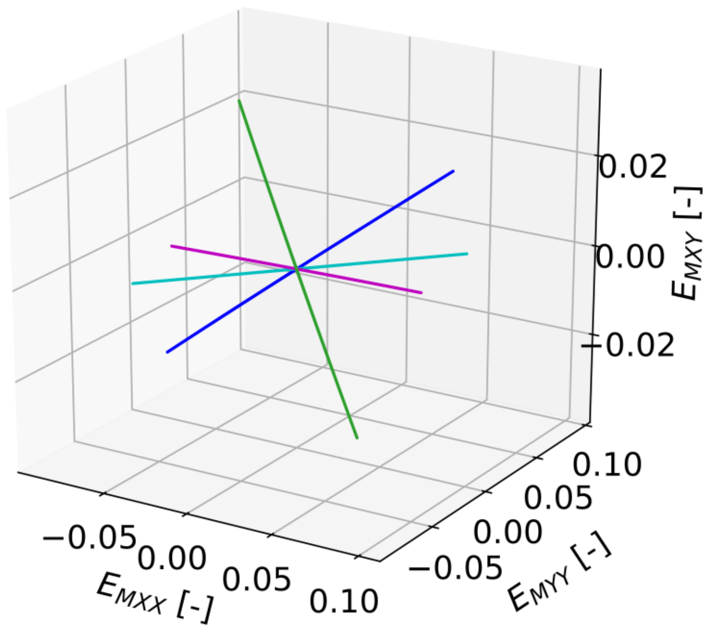
$$\boldsymbol{\Delta}\mathbf{W} = -\mathcal{F}\left(\frac{\partial L_i(\mathbf{W})}{\partial \mathbf{W}},\quad \left(\frac{\partial L_i(\mathbf{W})}{\partial \mathbf{W}}\right)^2,\ \text{batch size}, \ldots\right)$$

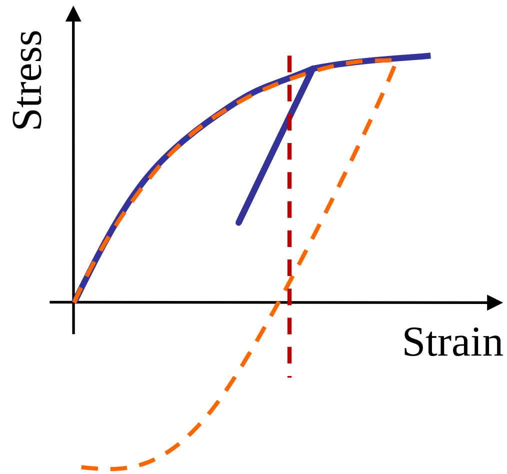
  - Training data
    - Input $\boldsymbol{u}^{(p)}$ & Output $\boldsymbol{v}^{(p)}$
- Testing
  - Use new data
    - Input $\boldsymbol{u}^{(p)}$ & Output $\boldsymbol{v}^{(p)}$
    - Verify prediction $\boldsymbol{v}$ vs. real $\boldsymbol{v}^{(p)}$



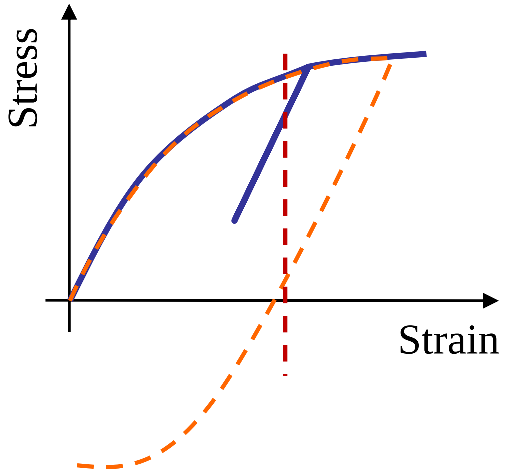


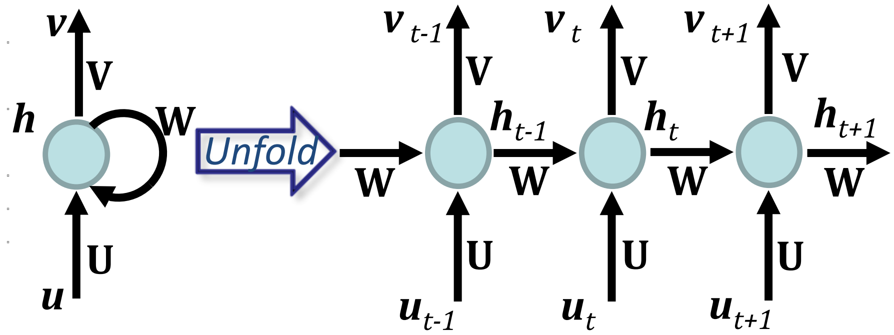
- Input / output definition
  - Input:
    - Strain (history): $\mathbf{F}_M$
  - Output:
    - Stress (history): $\mathbf{P}_M$
- Methodology
  - Address problem of history dependency
    - RVE without buckling
    - Elasto-plastic composite RVE



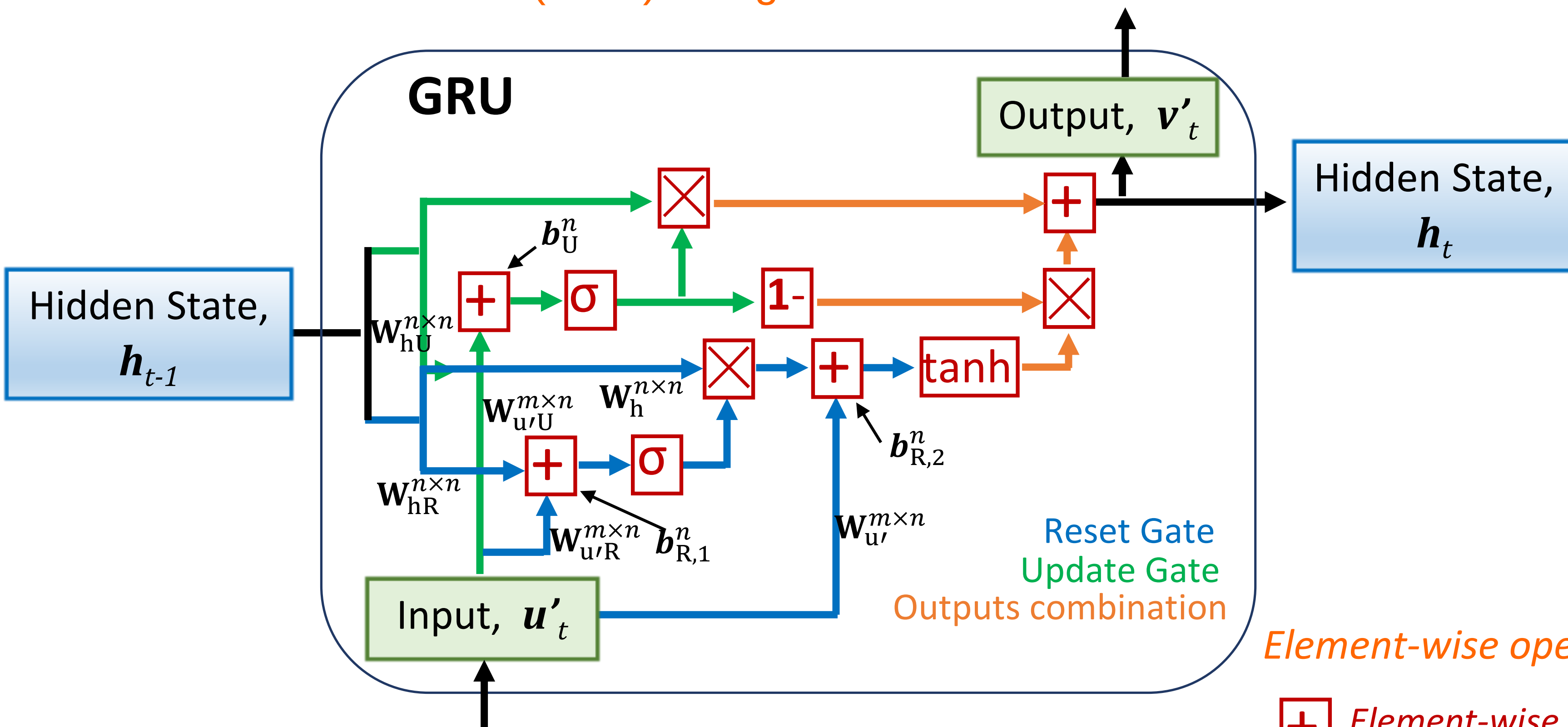


- Elasto-plastic material behaviour
  - No bijective strain-stress relation
    - Feed-forward NNW cannot be used
    - History should be accounted for
- Recurrent neural network
  - Allows a history dependent relation
    - Input $\boldsymbol{u}_t$
    - Output $\boldsymbol{v}_t = \boldsymbol{g}(\boldsymbol{u}_t, \boldsymbol{h}_{t-1})$
    - 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

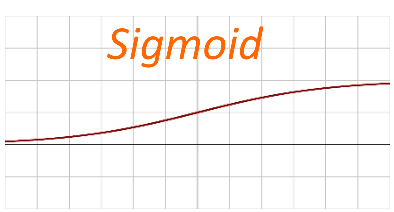
+ *Element-wise sum*

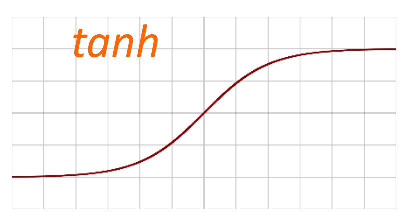
1- *Element-wise 1-*

⊠ *Element-wise product*

σ *Element-wise sigmoid*

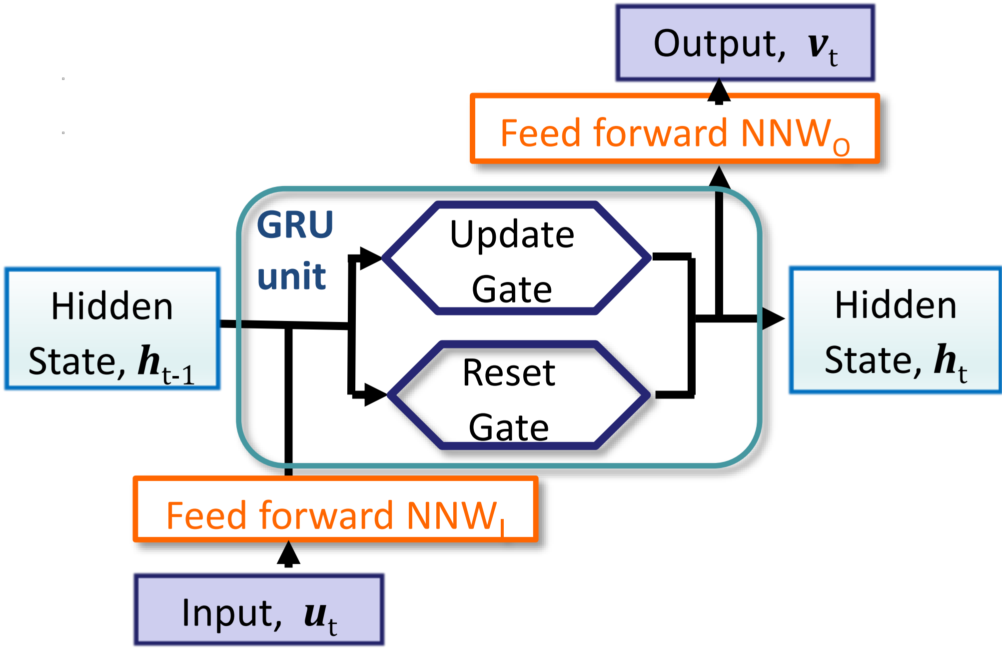
tanh *Element-wise tanh*

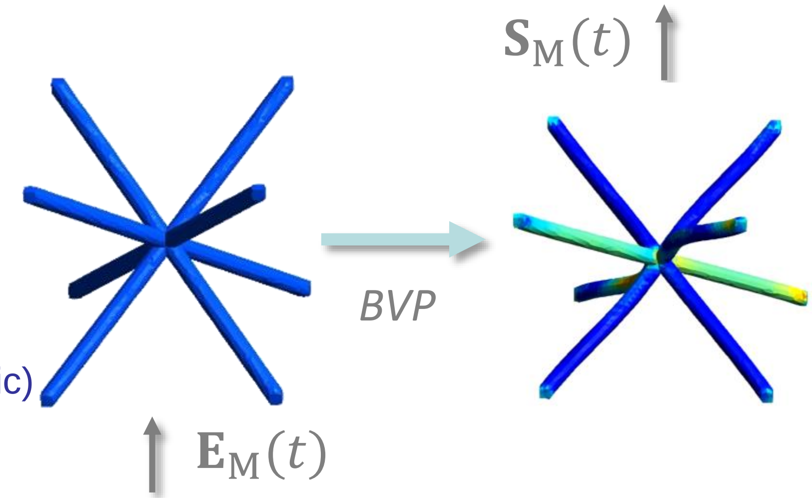




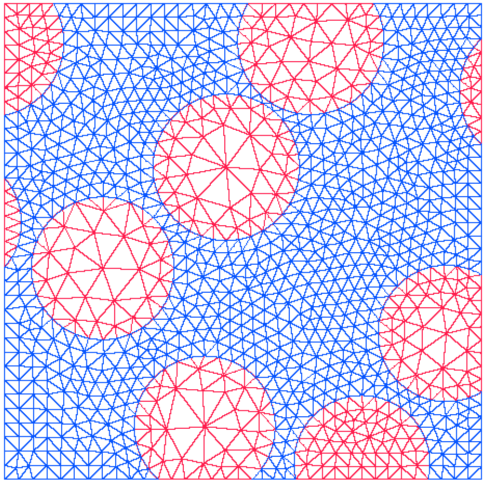
History dependency

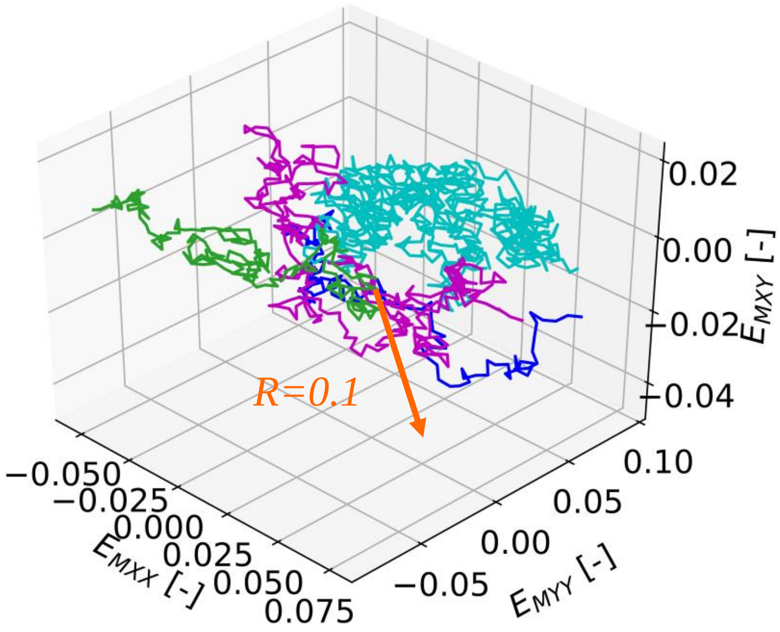
- Recurrent neural network design
  - 1 Gated Recurrent Unit (GRU)
    - Reset gate: select past information to be forgotten
    - Update gate: select past information to be passed along
    - Need to define number of hidden variables $\boldsymbol{h}_t$
  - 2 feed-forward NNWs
    - NNW_I to treat inputs $\boldsymbol{u}_t$
    - NNW_O to produce outputs $\boldsymbol{v}_t$
  - Input and Output
    - $\boldsymbol{u}_t$: homogenised GL strain $\mathbf{E}_\text{M}$ (symmetric)
    - $\boldsymbol{v}_t$: homogenised 2nd PK stress $\mathbf{S}_\text{M}$ (symmetric)

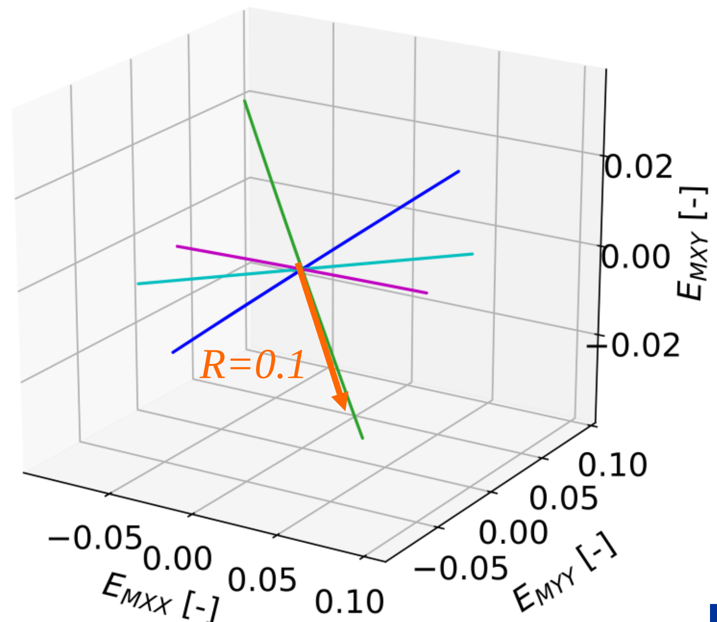




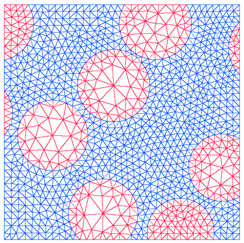
- Data generation
  - Elasto-plastic composite RVE
  - Training stage
    - Should cover full range of possible loading histories
    - Use random walking strategy (thousands)
    - Completed with random cyclic loading (tens)
    - Bounded by a sphere of 10% deformation

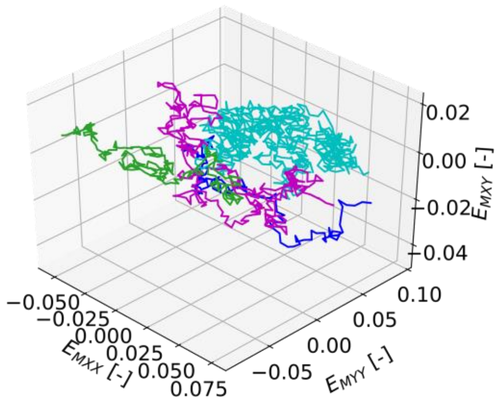


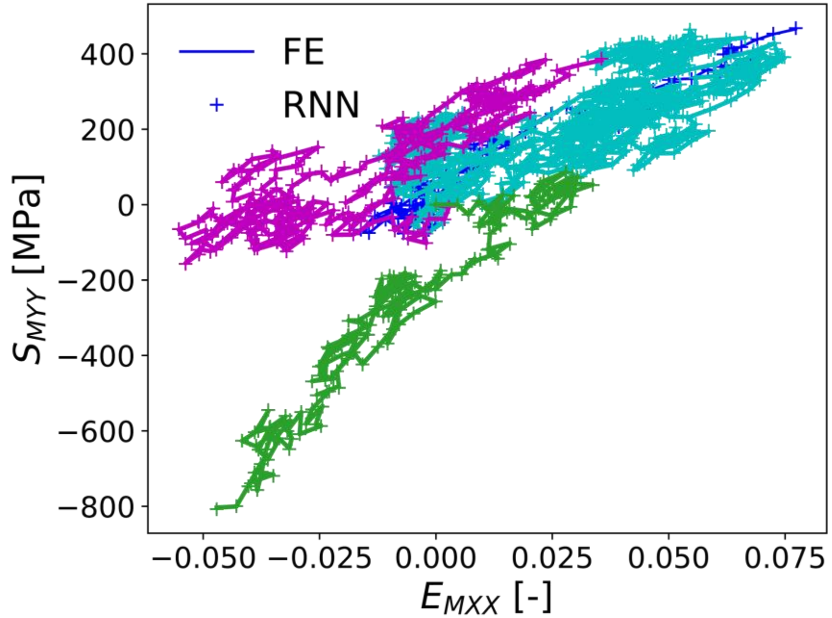


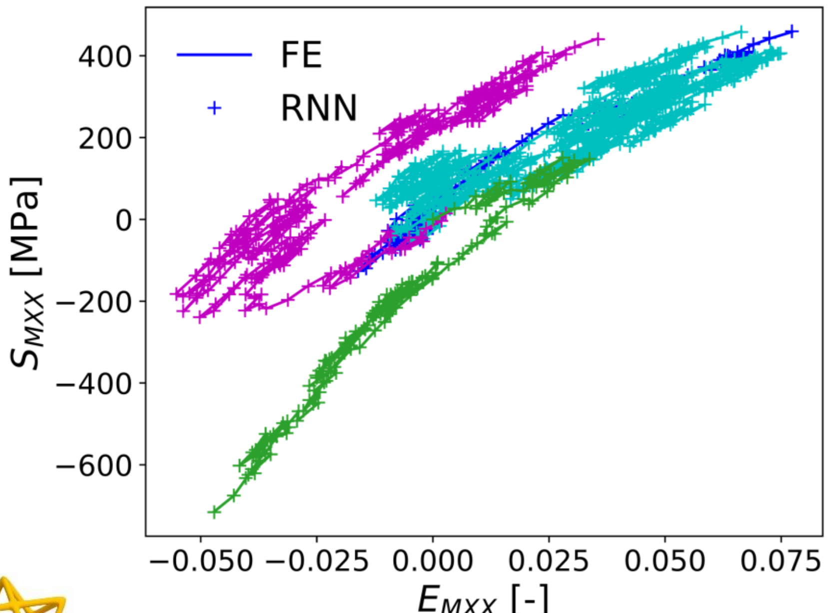


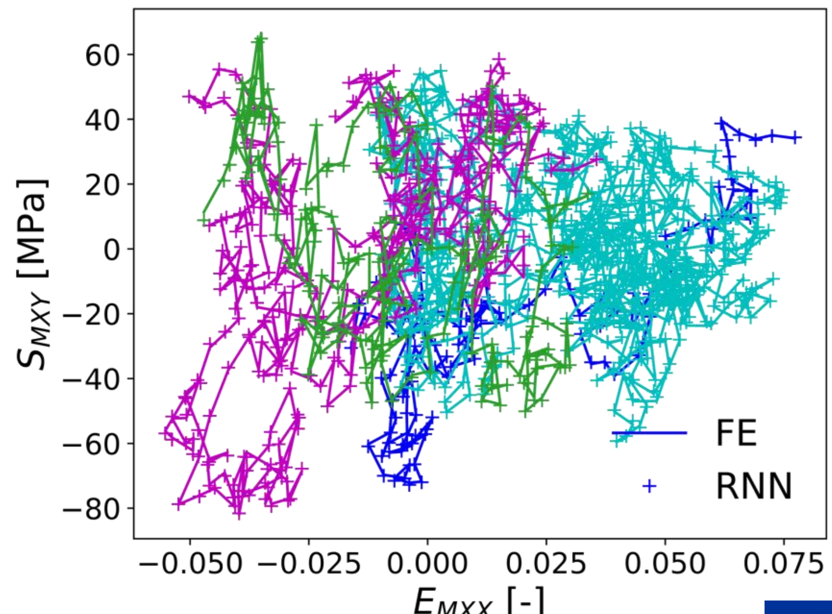
- Testing process (new data)
  - On random walk



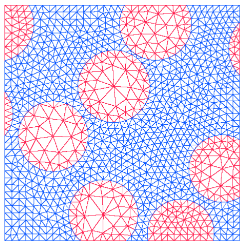


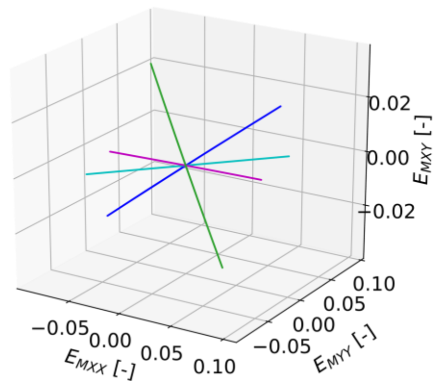


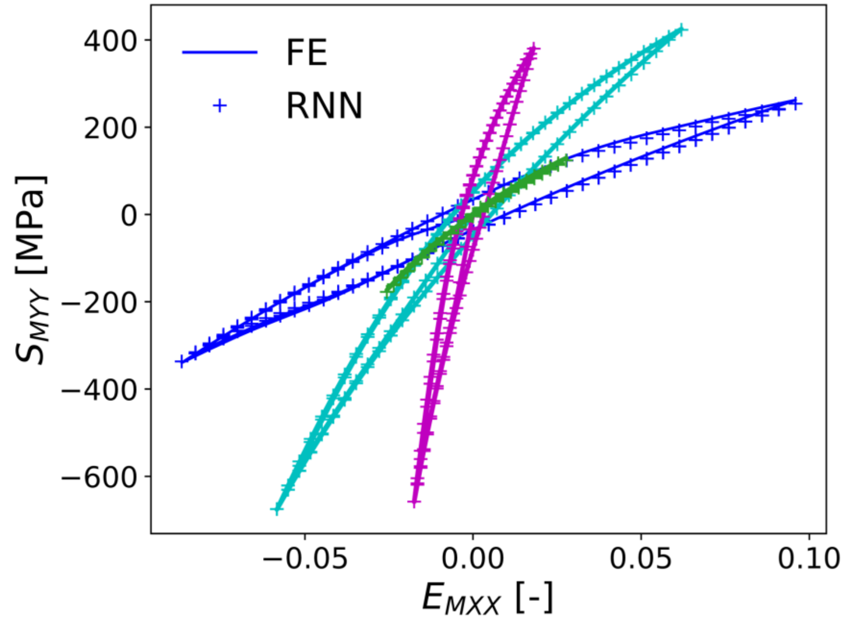


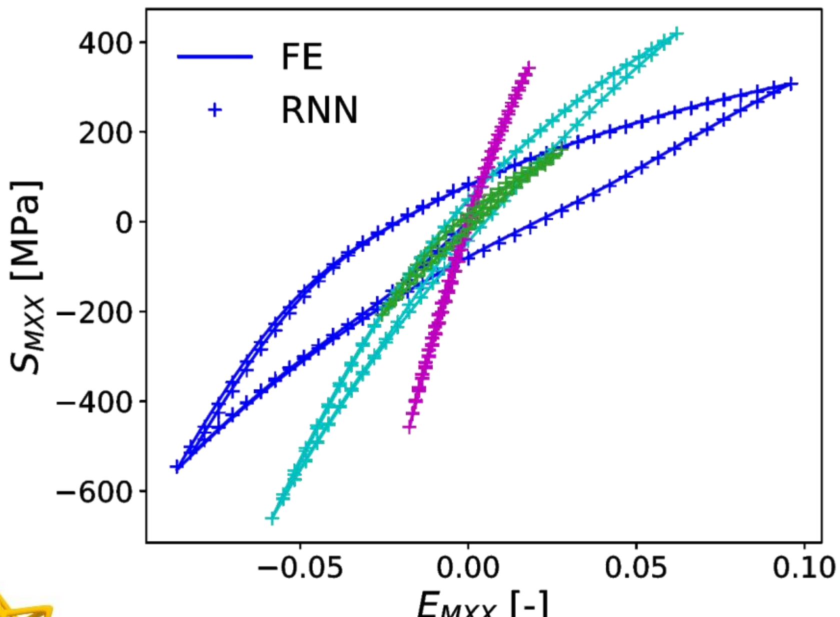


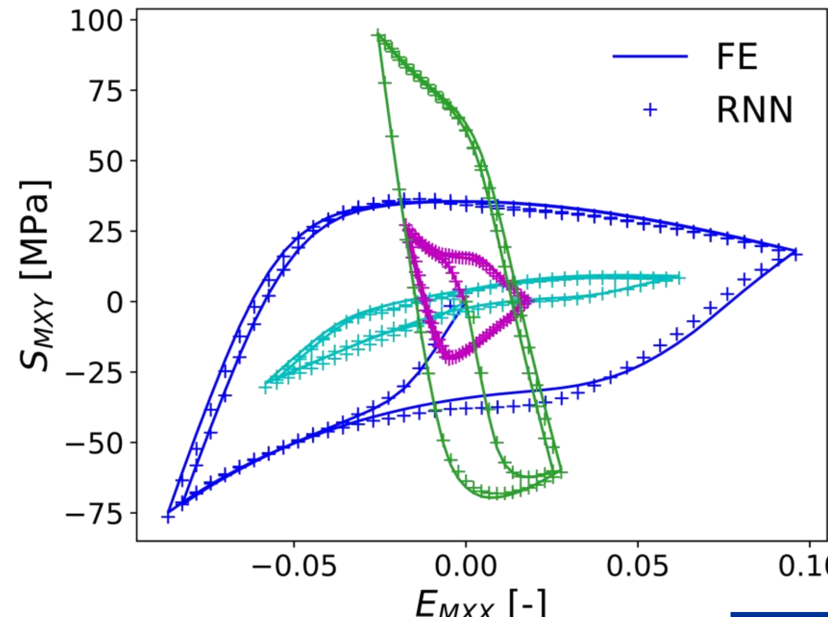
- Testing process (new data)
  - On cyclic loading







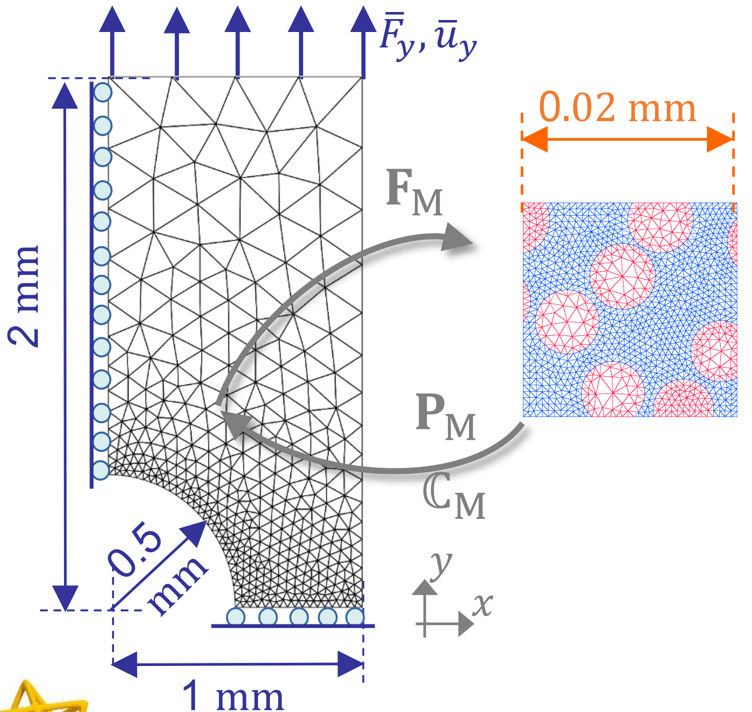


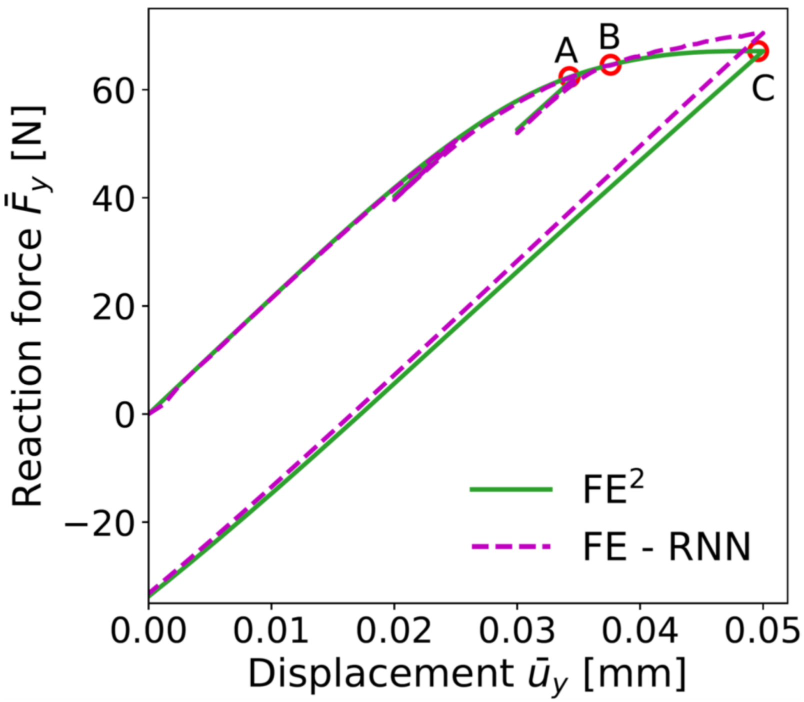


ANN as a mesoscale surrogate model

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

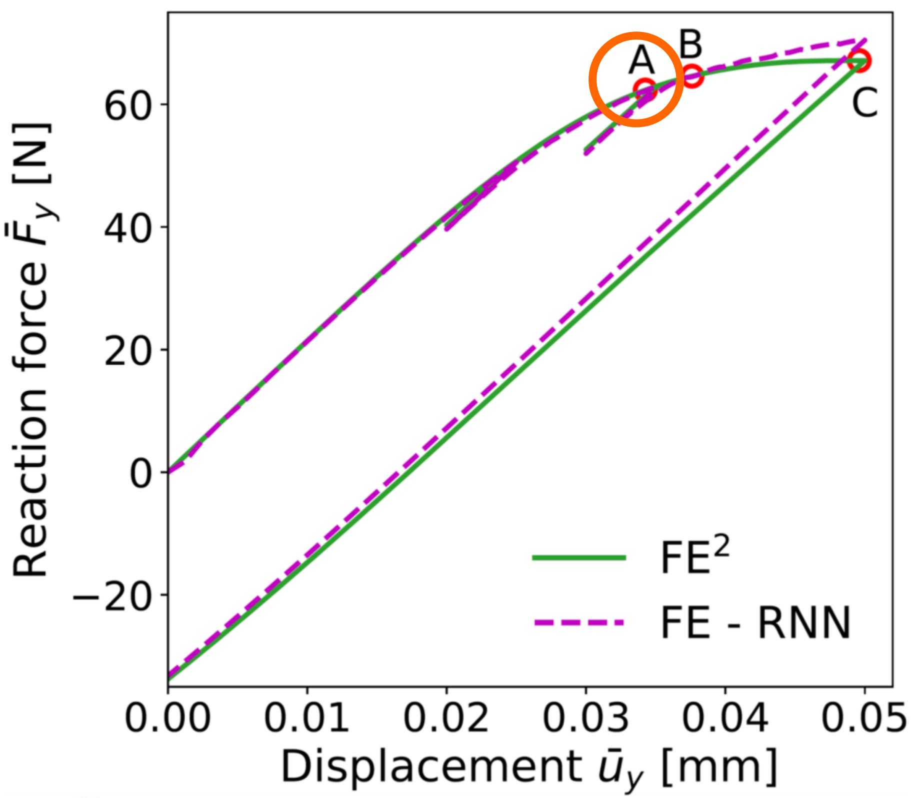
Off-line	FE^2	FE-RNN
Data generation	-	9000 x 2 h-cpu
Training	-	3 day-cpu
On-line	**FE^2**	**FE-RNN**
Simulation	18000 h-cpu	0.5 h-cpu

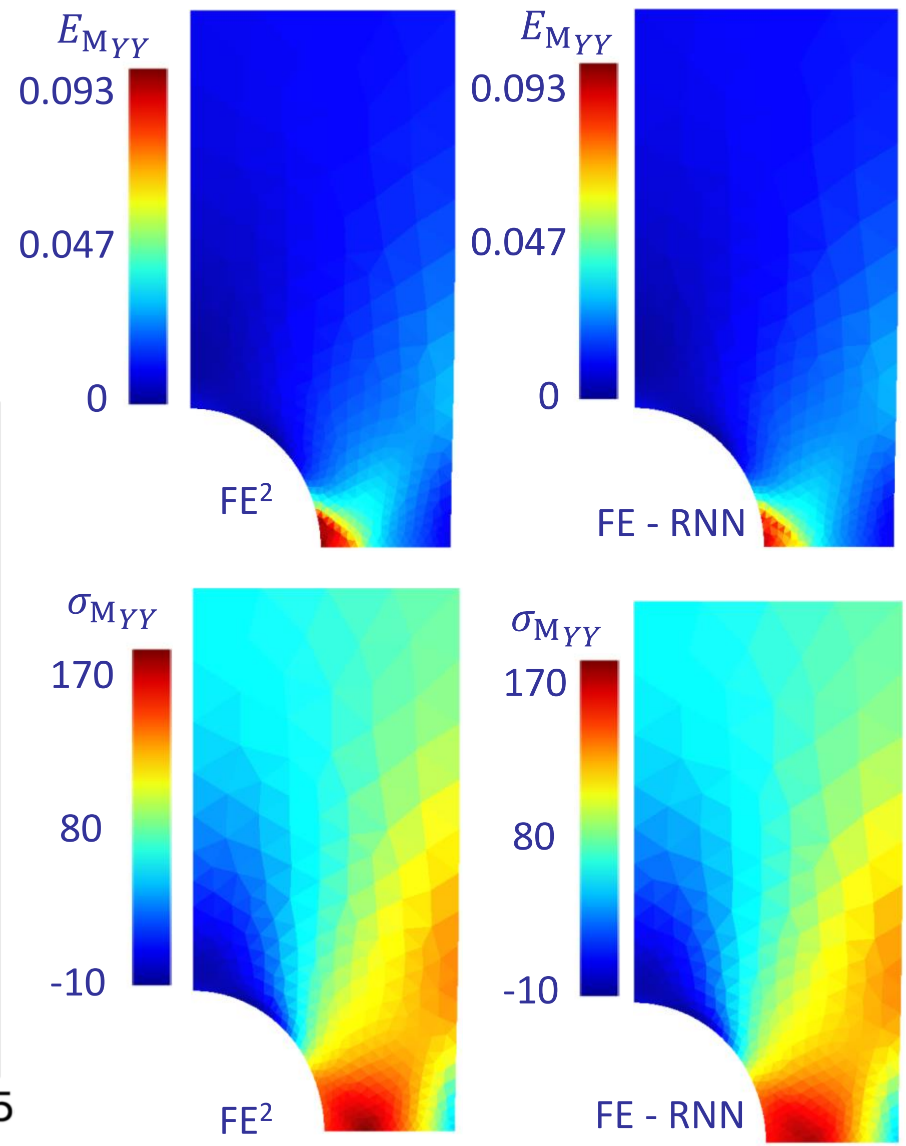




ANN as a mesoscale surrogate model

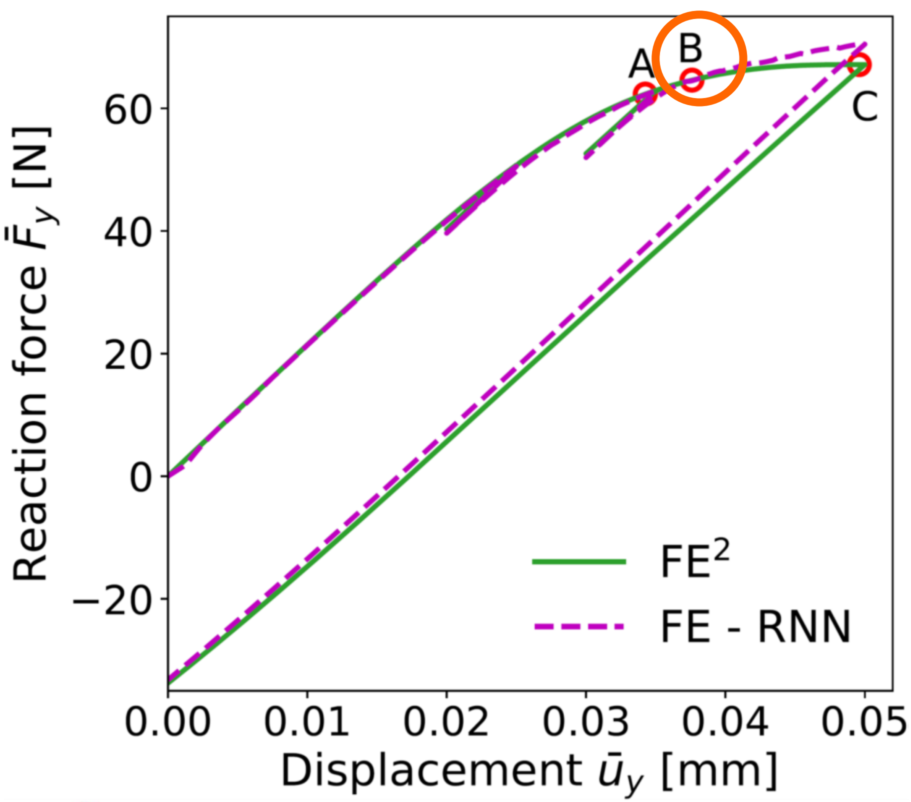
- Multiscale simulation
  - Stress-strain distribution at point A
  - Strain within the 10% training range

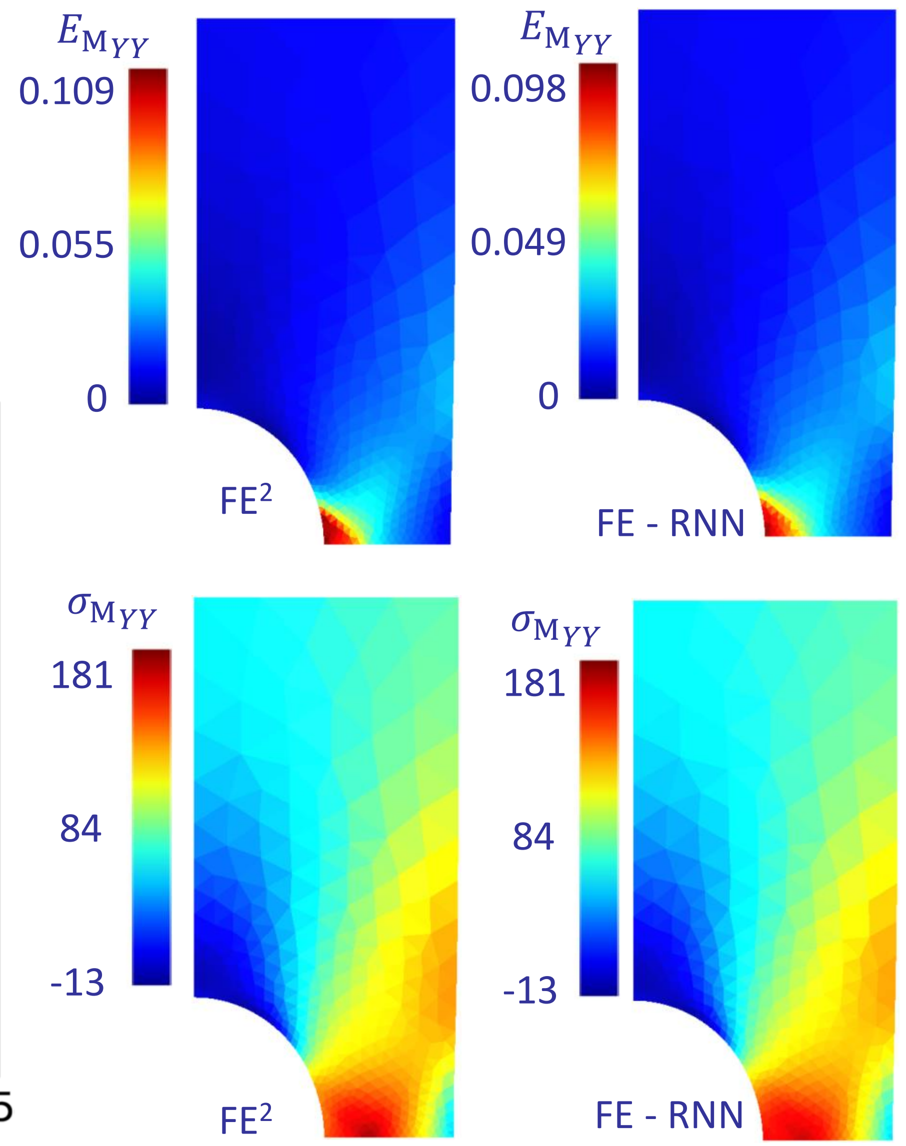




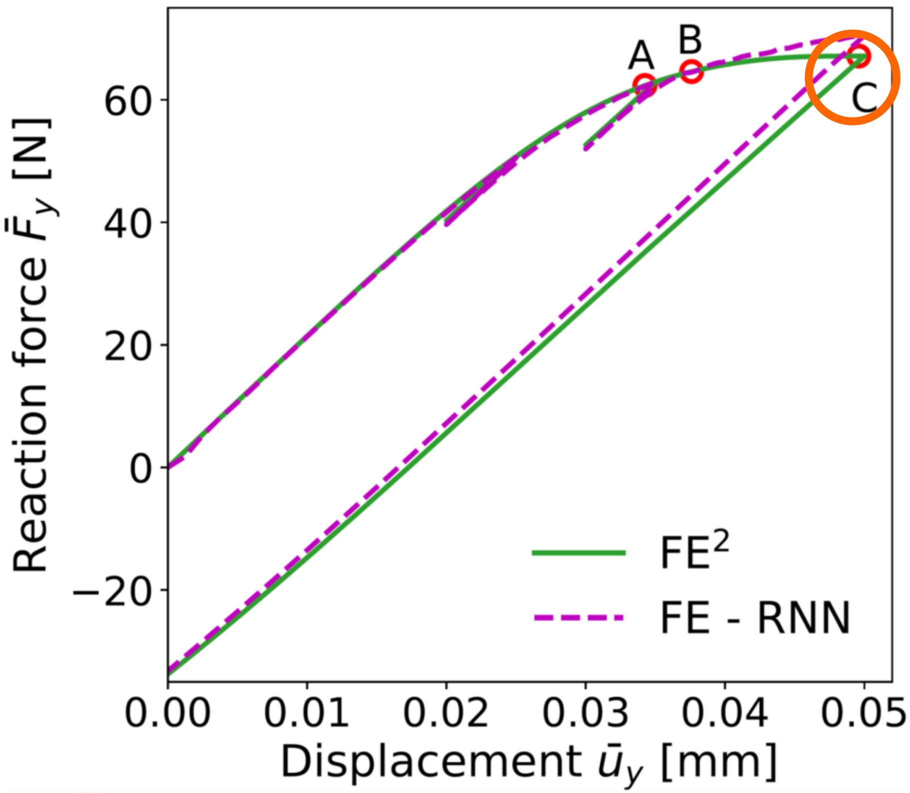
ANN as a mesoscale surrogate model

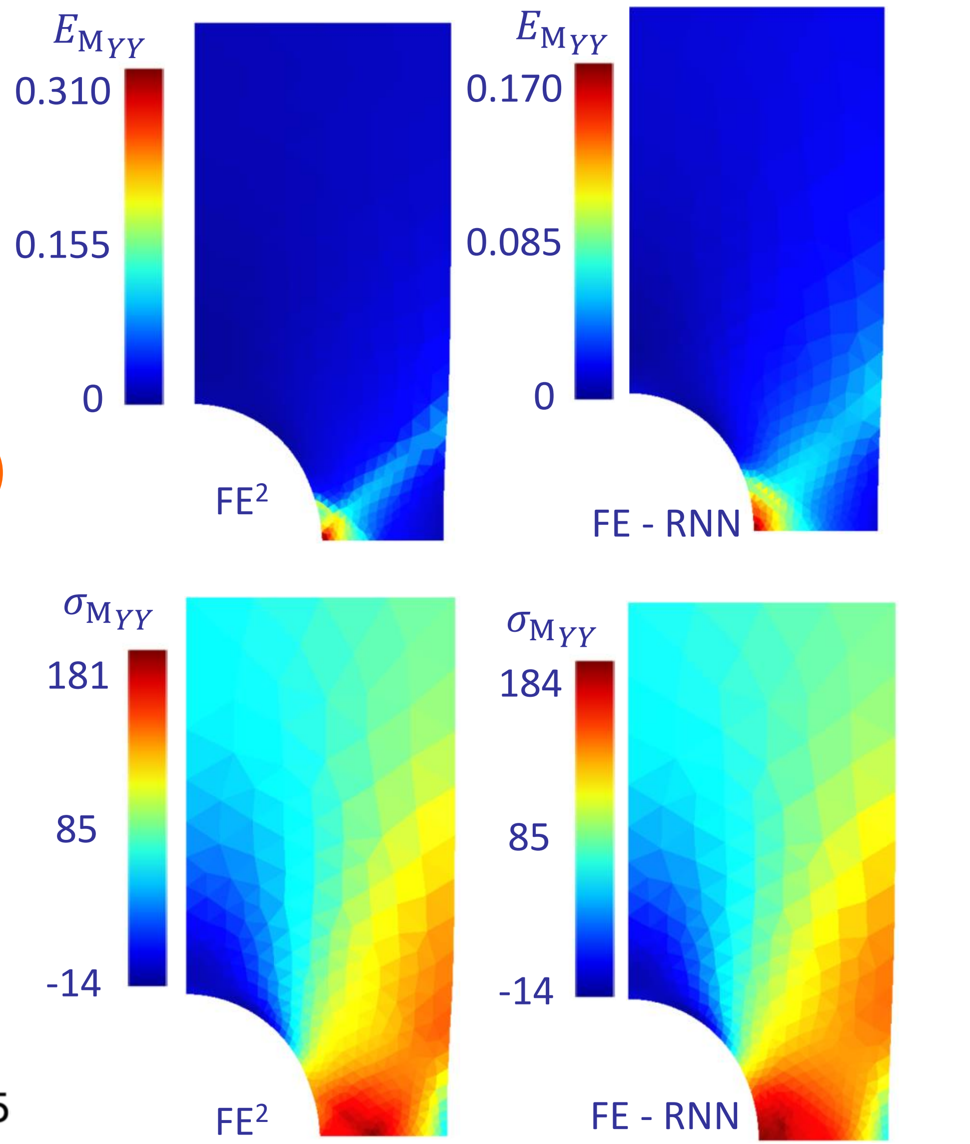
- Multiscale simulation
  - Stress-strain distribution at point B
  - Strain just at 10% training range





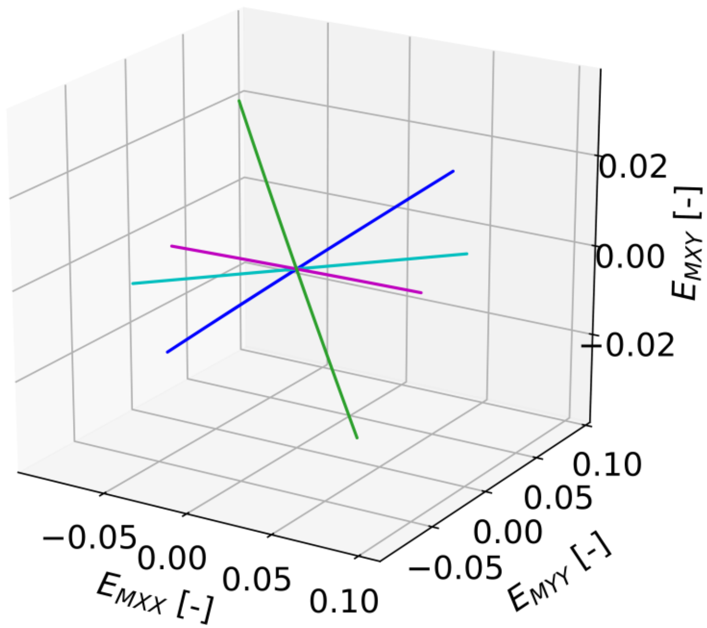
- Multiscale simulation
  - Stress-strain distribution at point C
  - Strain out of 10% training range

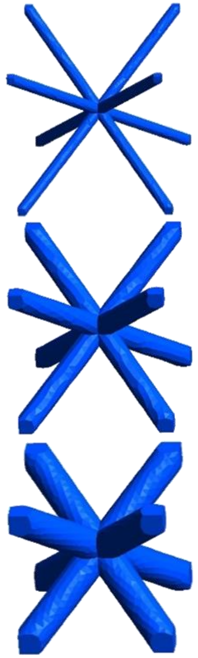




Complex micro-structures

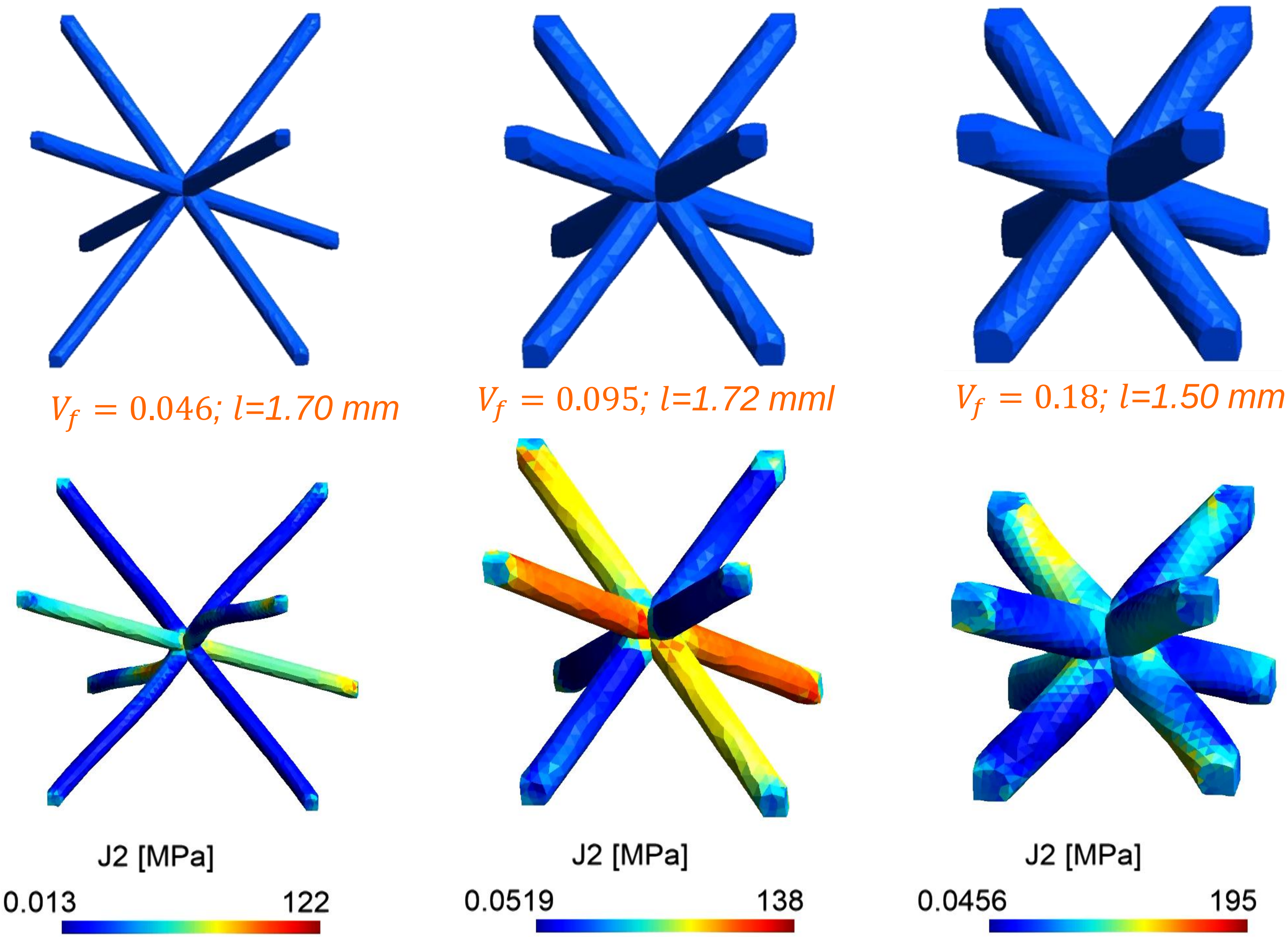
- Input / output definition
  - Input:
    - Strain (history): $\mathbf{F}_\mathrm{M}$
    - Geometry/material parameters: $\boldsymbol{\varphi}_\mathrm{m}$
  - Output:
    - Stress (history): $\mathbf{P}_\mathrm{M}$





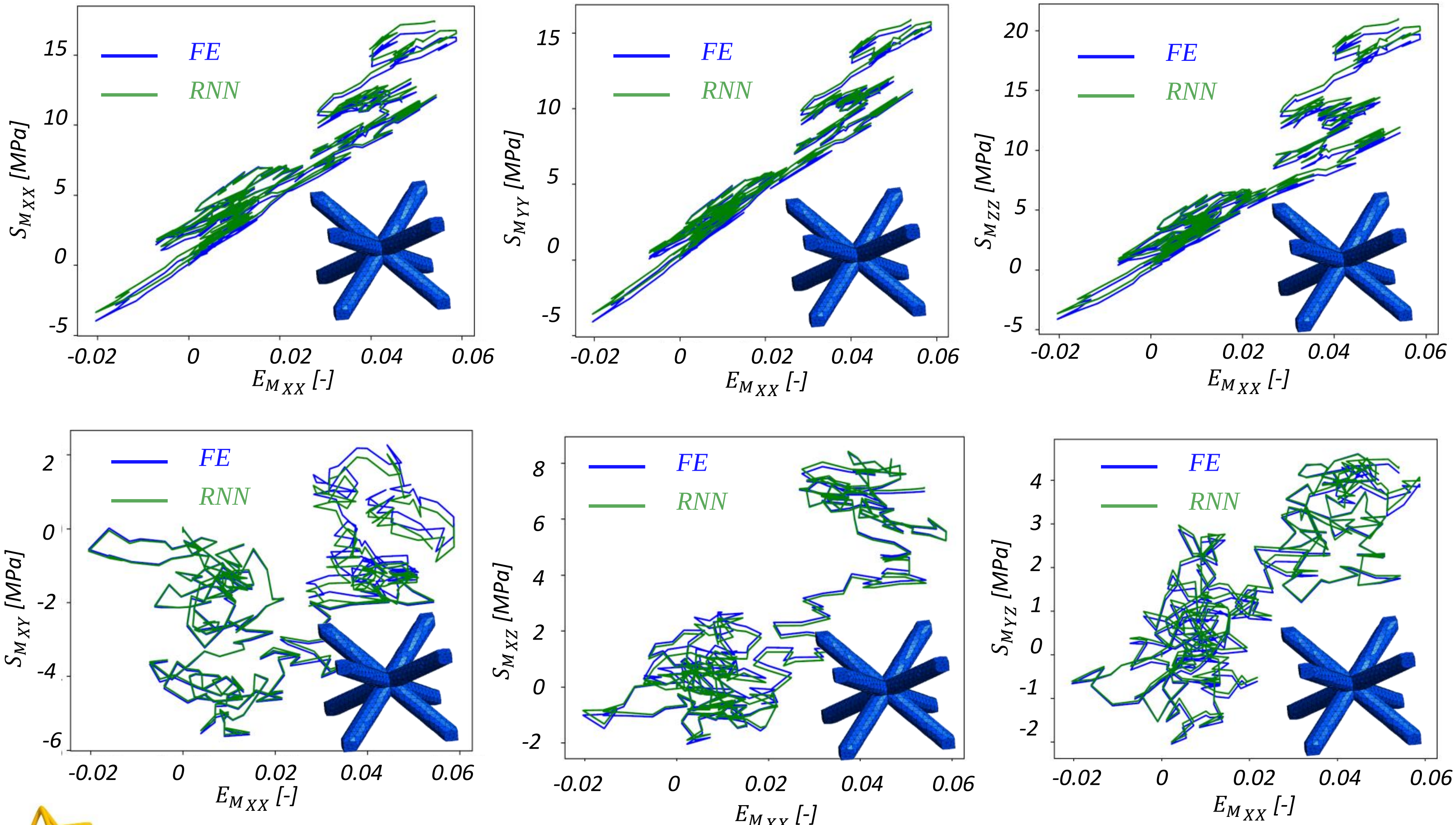
- Methodology
  - Address problem of geometry/material effect
    - Octet cells
    - Elastic material at first

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



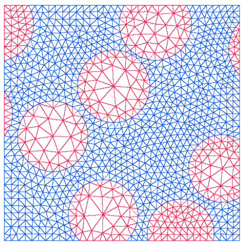
Geometrical parameters effect

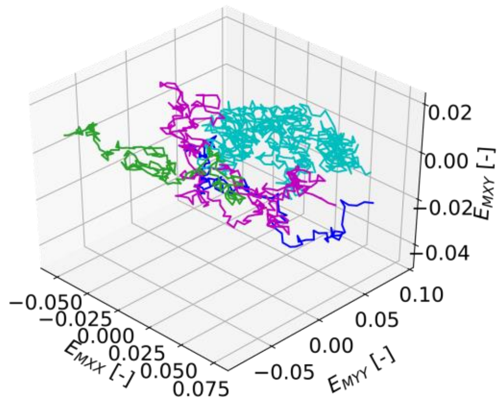
- Octet cell
  - Test on new random cell/path

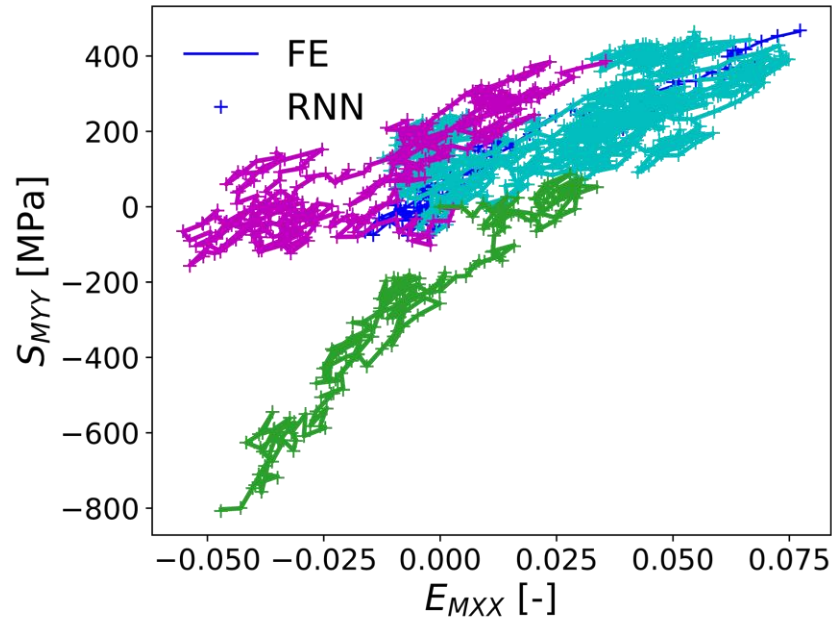


Localisation step

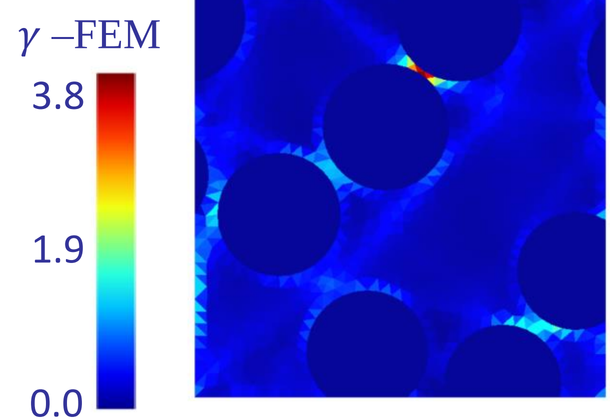
- Only homogenised output is predicted
  - On random walk





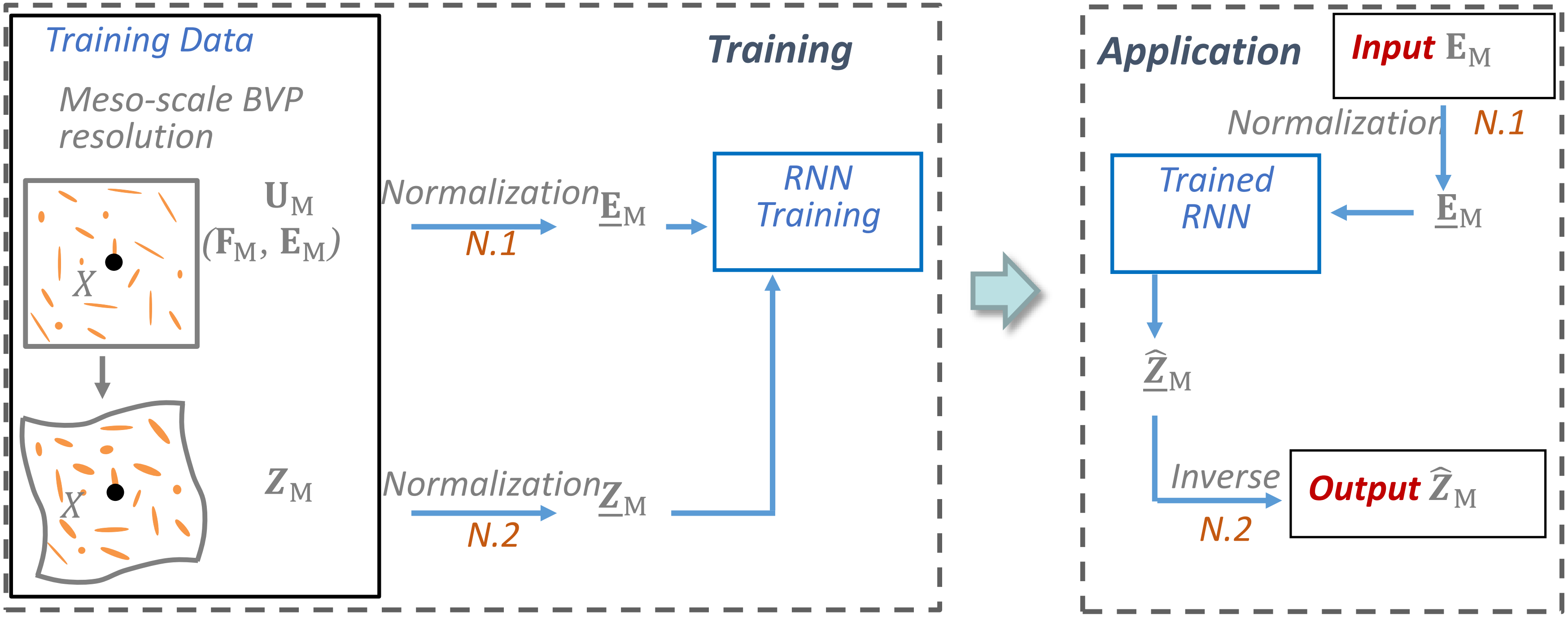


- Quid of local fields?
  - This is an advantage of multiscale methods
  - Useful to predict failure, fatigue etc.
  - Can we get it back at low cost?



Localisation step

- Also build a surrogate model of the internal variables



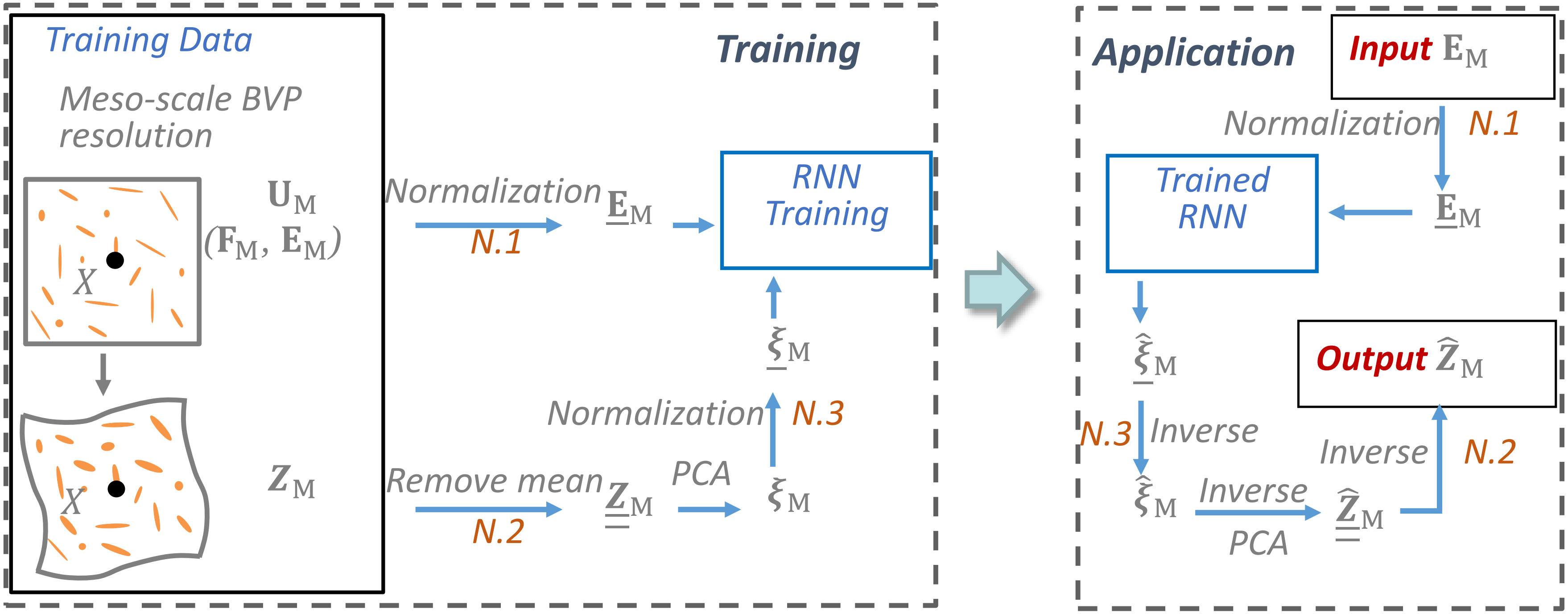
– Problem: The size of $\underline{Z}_M$ is large

- $\underline{Z}_M$ of size d the number of Gauss points of the RVE × internal variables by Gauss point

 overwhelming cost

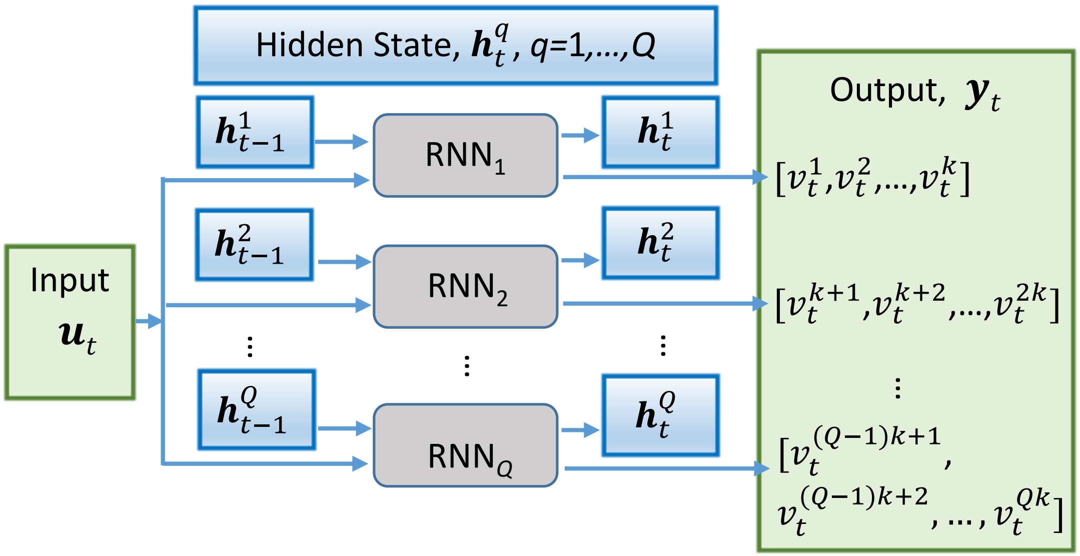
Localisation step

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



  – Principal Component Analysis (PCA) applied on $\mathbf{Z}_\mathrm{M}$ to reduce the output of RNN
    - Construct matrix $\mathbf{Z}_\mathbf{M} = \left[\underline{\mathbf{Z}}_{\mathrm{M}_1}\ \underline{\mathbf{Z}}_{\mathrm{M}_2}\ \dots \underline{\mathbf{Z}}_{\mathrm{M}_n}\right]_{d\times n}$ from n observations (1% from all data)
    - Extract n ordered eigenvalues Λ_i and eigen vector $\underline{v}_i$ of $\mathbf{Z}_\mathrm{M}^T\mathbf{Z}_\mathrm{M}$
    - Build reduced basis $\mathbf{V} = \left[\ \underline{v}_1\ \underline{v}_2\ \dots \underline{v}_p\ \right]_{d\times p}$ and reduced data $\boldsymbol{\xi}_\mathrm{M} = \mathbf{V}^T\underline{\mathbf{Z}}_\mathrm{M}$ of size $p < d$
    - Reconstruction $\hat{\underline{\mathbf{Z}}}_\mathrm{M} = \mathbf{V}\boldsymbol{\xi}_\mathrm{M}$
    - But not enough

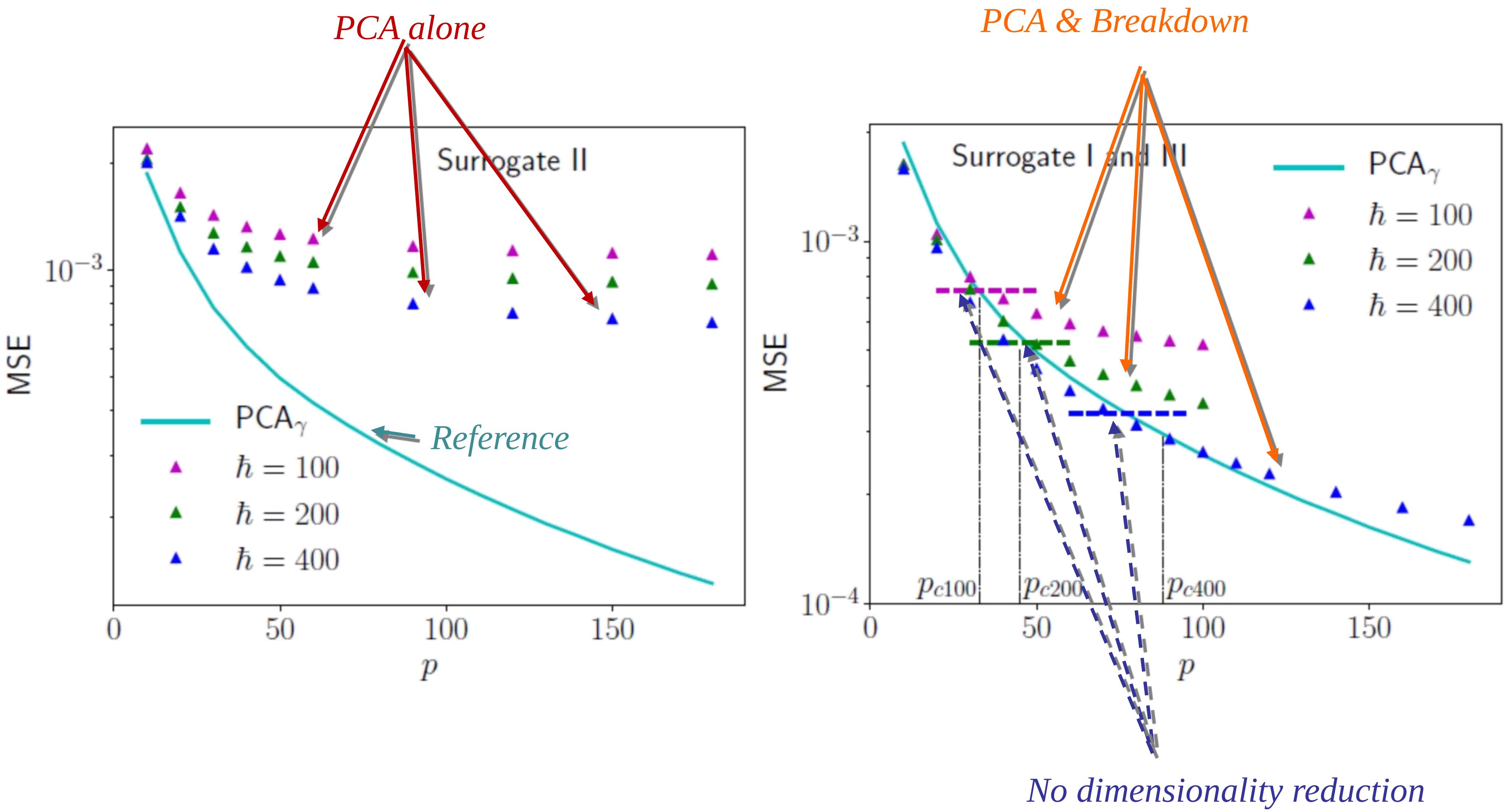
- Dimensionality reduction & break down



- 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 $\boldsymbol{Z}_{\mathrm{M}}$ to 180 outputs and we use Q=6

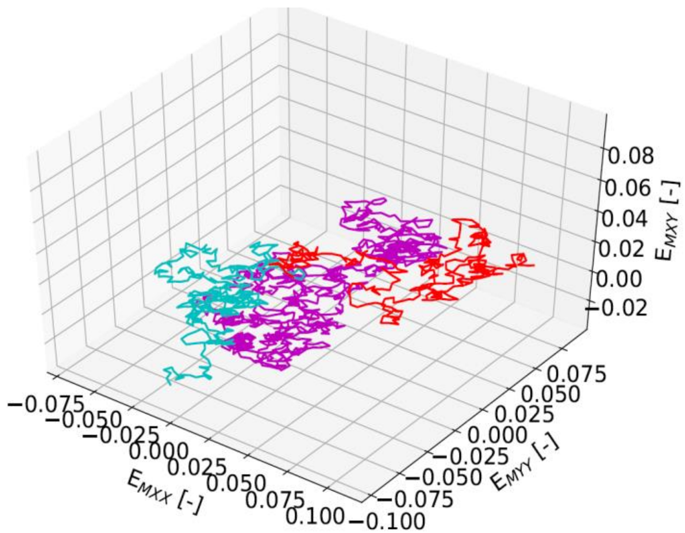
Localisation step

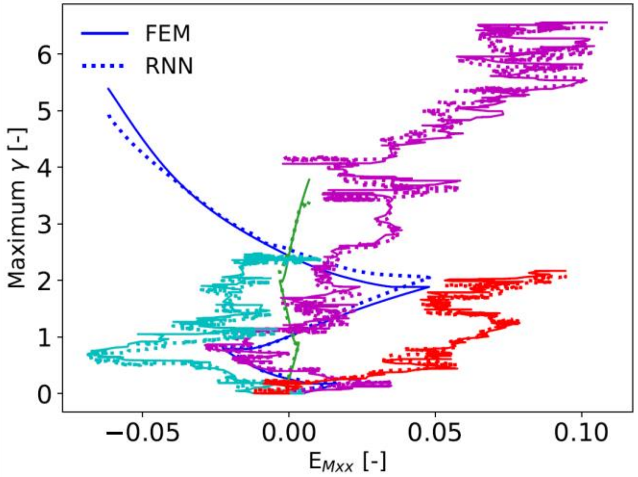
- Effect of dimensionality reduction and number of hidden variables



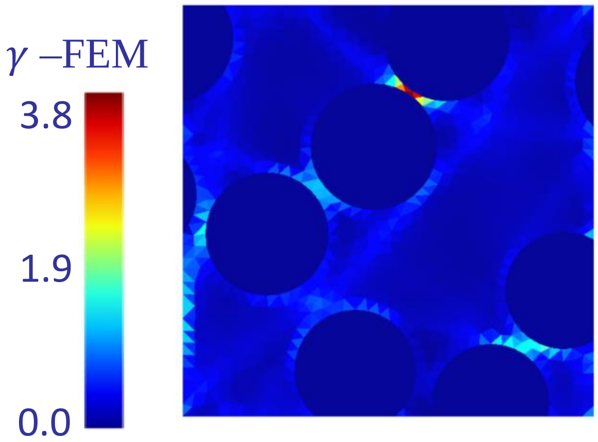
Localisation step

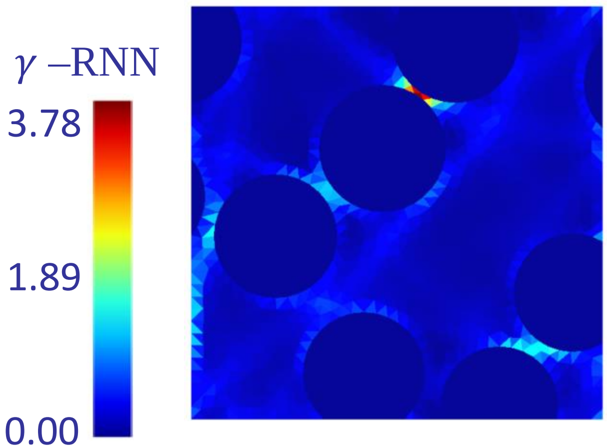
- Evaluation of equivalent plastic strain γ: Random loading (testing data)





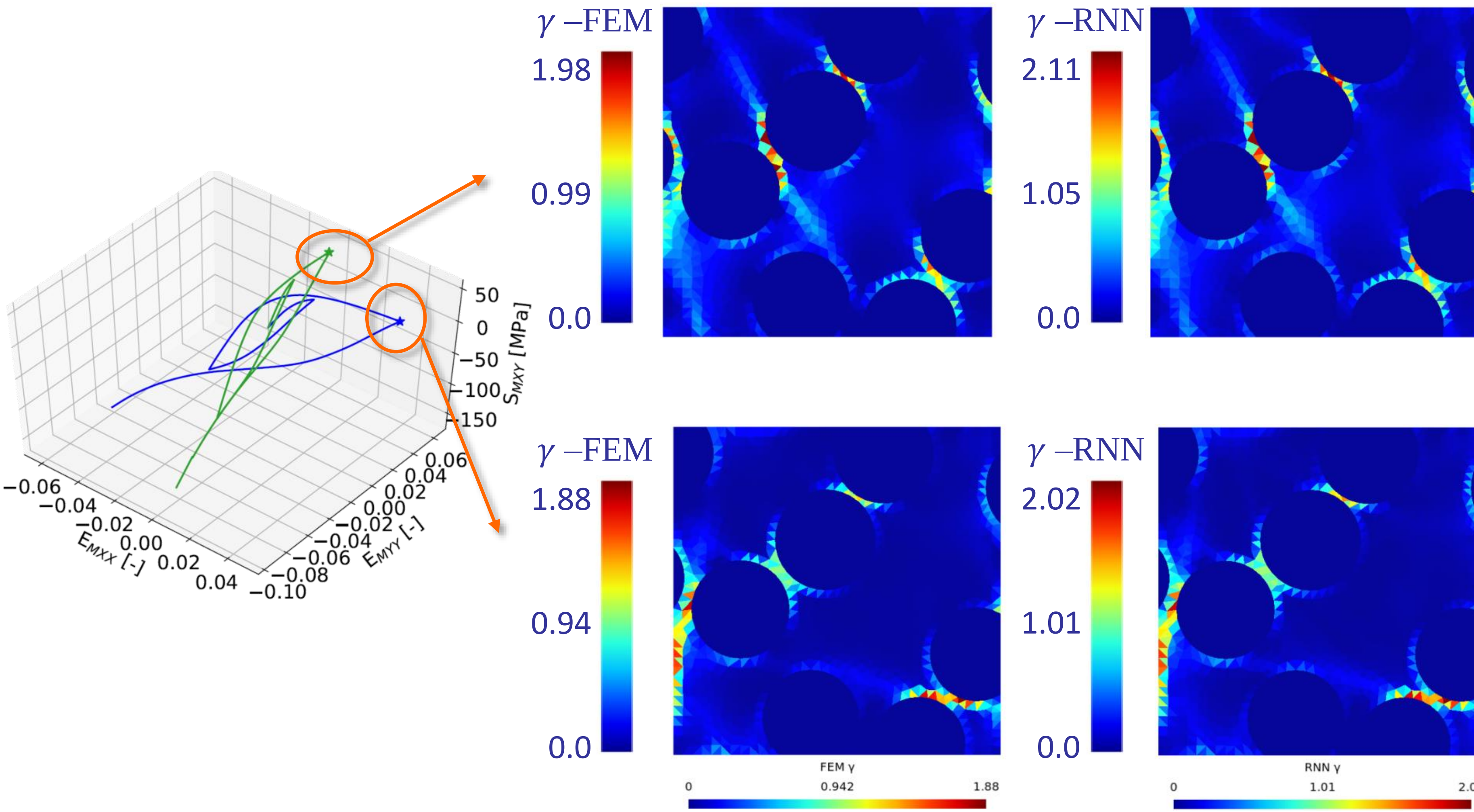
Purple loading – step 500





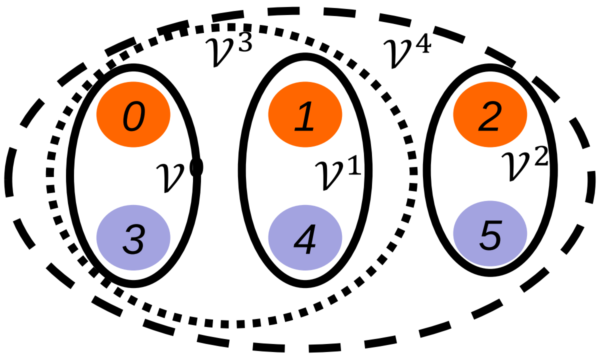
Localisation step

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



Perspective

- Promising methodology
  - For 3D problems, complex behaviours etc. requires more random loading paths
    - Order reduction might become mandatory to generate the synthetic database
  - New interesting approach: Deep Material Network
    - Original paper by Z. Liu, C. Wu, M. Koishi, Comp. Meth. in Appl. Mech. and Engng. 2019
    - Formalism rewritten by V.D Nguyen & L. Noels, Comp. Meth. in Appl. Mech. Engng. 2022



Strain averaging: $\bar{\boldsymbol{\varepsilon}} + \sum_j \alpha^{i,j}\, \boldsymbol{a}^j \otimes \boldsymbol{n}^j = \boldsymbol{\varepsilon}^i$ *for node i*

Hill-Mandel condition: $\left(\sum_{i\in\mathcal{V}^j} W^i \boldsymbol{\sigma}^i \alpha^{i,j}\right)\cdot \boldsymbol{n}^j = 0$ *for interaction j*

Boundary conditions: $\sum_{i\in\mathcal{V}^j} W^i \alpha^{i,j} = 0$ *for interaction j*

Constitutive behaviours: $\boldsymbol{\sigma}^p(t) = \boldsymbol{\sigma}^p\left(\boldsymbol{\varepsilon}^i(t), z(\tau \leq t)\right)$ *for material p*

Offline stage: system parameters $\alpha^{i,j}, W^i, \boldsymbol{n}^j$, *evaluated by data-driven approaches*

Online stage: system unknowns $\boldsymbol{a}^j$ *evaluated by Newton-Raphson iterations*

References

- 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
  - Data on https://dx.doi.org/10.5281/zenodo.3902663
  - L. Wu, L. Noels. "Recurrent Neural Networks (RNNs) with dimensionality reduction and break down in computational mechanics; application to multi-scale localization step" Computer Methods in Applied Mechanics and Engineering (under revision)