Development of history-dependent surrogate models in the context of stochastic multi-scale simulations for elasto-plastic composites

L. Wu, V.-D. Nguyen, M. Mustafa, J. Calleja & L. Noels
University of Liege
Computational & Multiscale Mechanics of Materials
http://www.ltas-cm3.ulg.ac.be

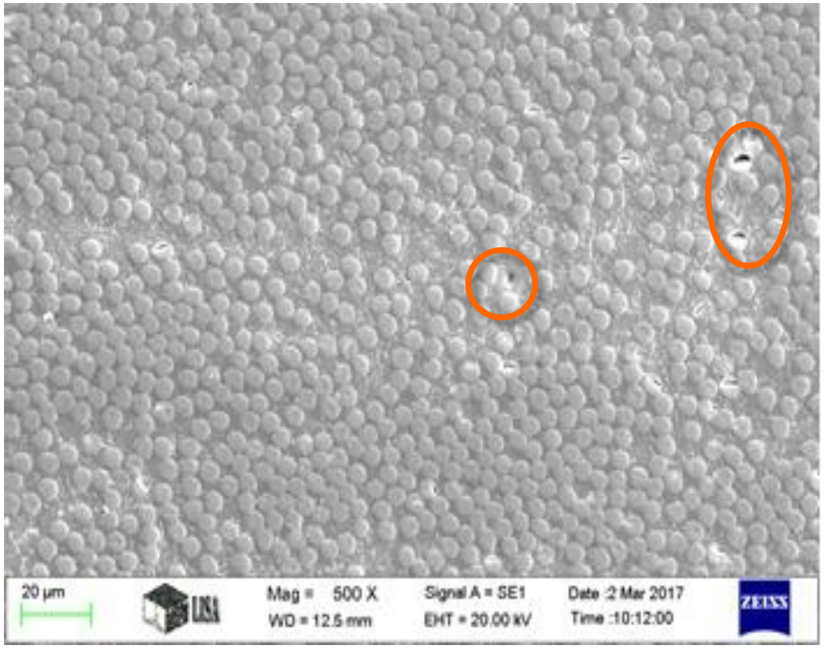
5th International Conference on Uncertainty Quantification in Computational Science and Engineering
12-14 June 2023

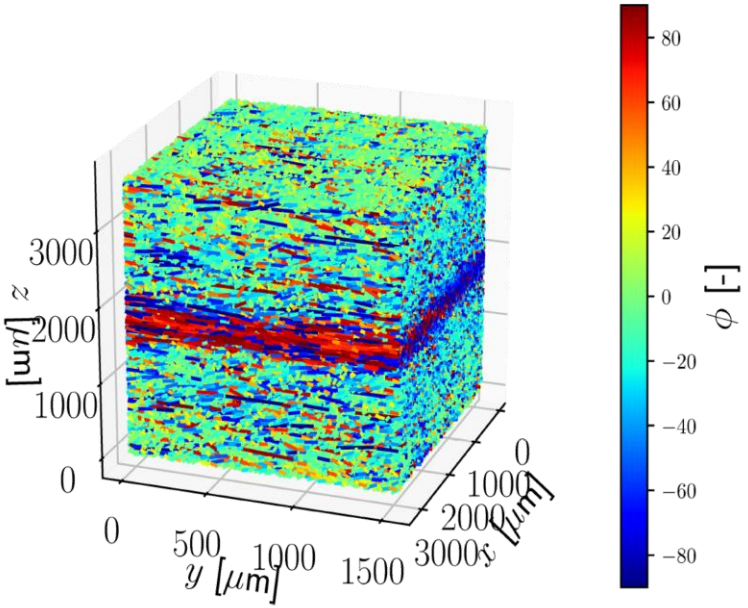
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 862015

MOAMMM
www.moammm.eu

Stochastic multi-scale simulations

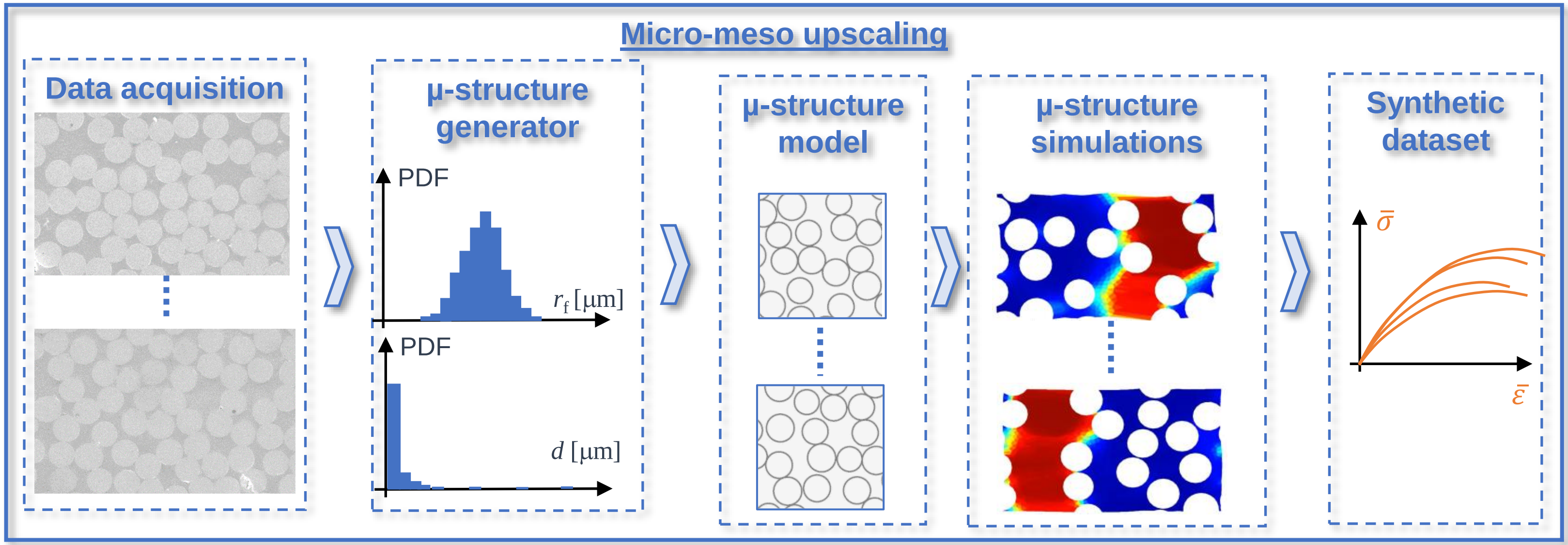
- Motivations
  - Composites (and others) are inhomogeneous/aperiodic materials
  - Inhomogeneities affect structural strength





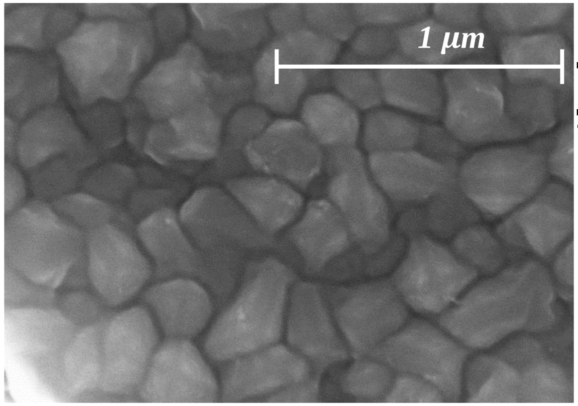
Stochastic multi-scale simulations

- Step 1: Generate a synthetic data base of SVE responses

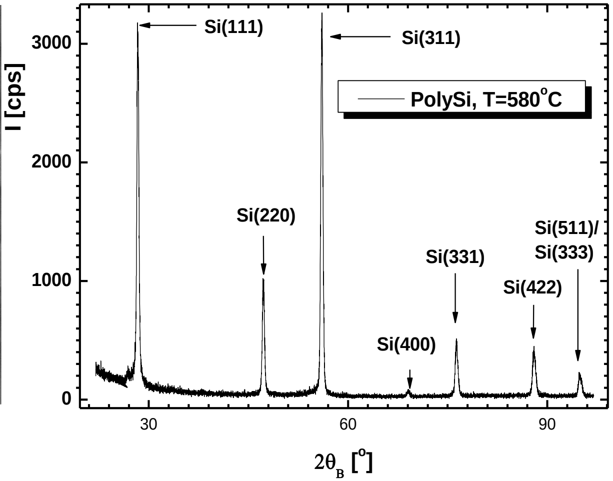


Case of linear elastic material: Polycrystalline Si

- Micro-scale
  - Random grain orientation
    - Can be measured from XRD

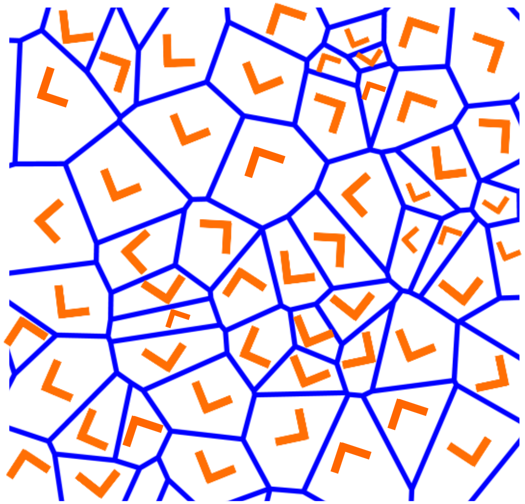


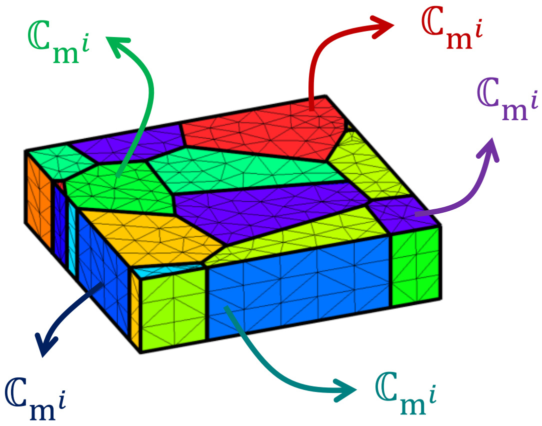
Polycrystalline Si



XRD-measurements

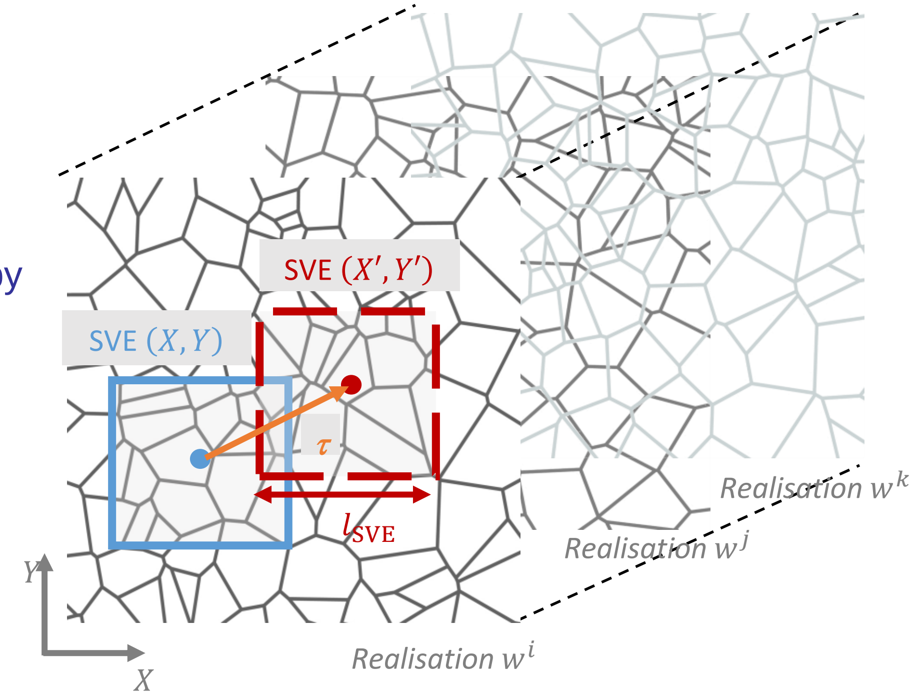
  - Grain Material
    - Anisotropic tensor $\mathbb{C}_{\mathrm{m}^i}$
    - Same but for the orientation in each grain ω_i

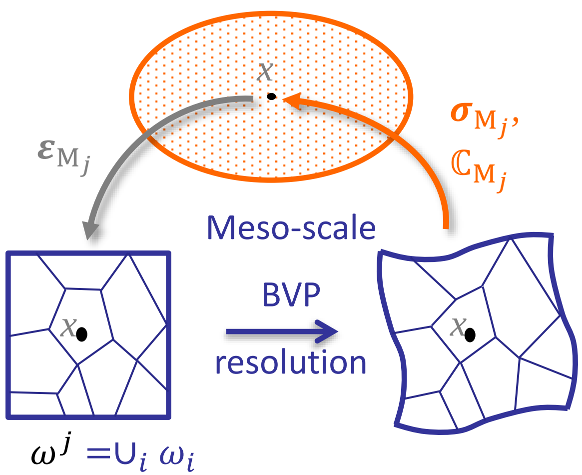


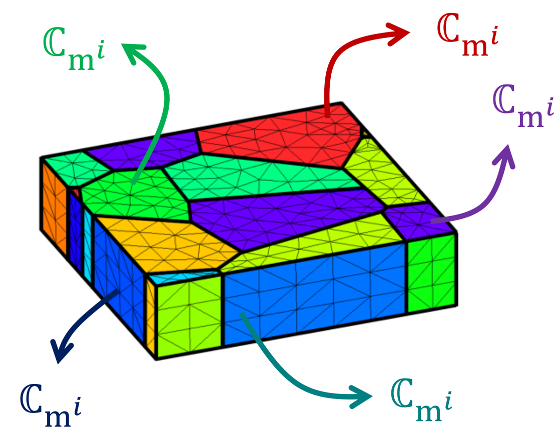


Case of linear elastic material: Polycrystalline Si

- Generation of random Stochastic Volume Elements (SVEs)
  - Extraction of SVEs $\omega^j = \cup_i \omega_i$
    - Large Voronoi tessellations
    - Window technic: SVEs are separated by vector τ
    - Each SVE ω^j has several grains ω_i of different orientations
  - Extraction of homogenised properties



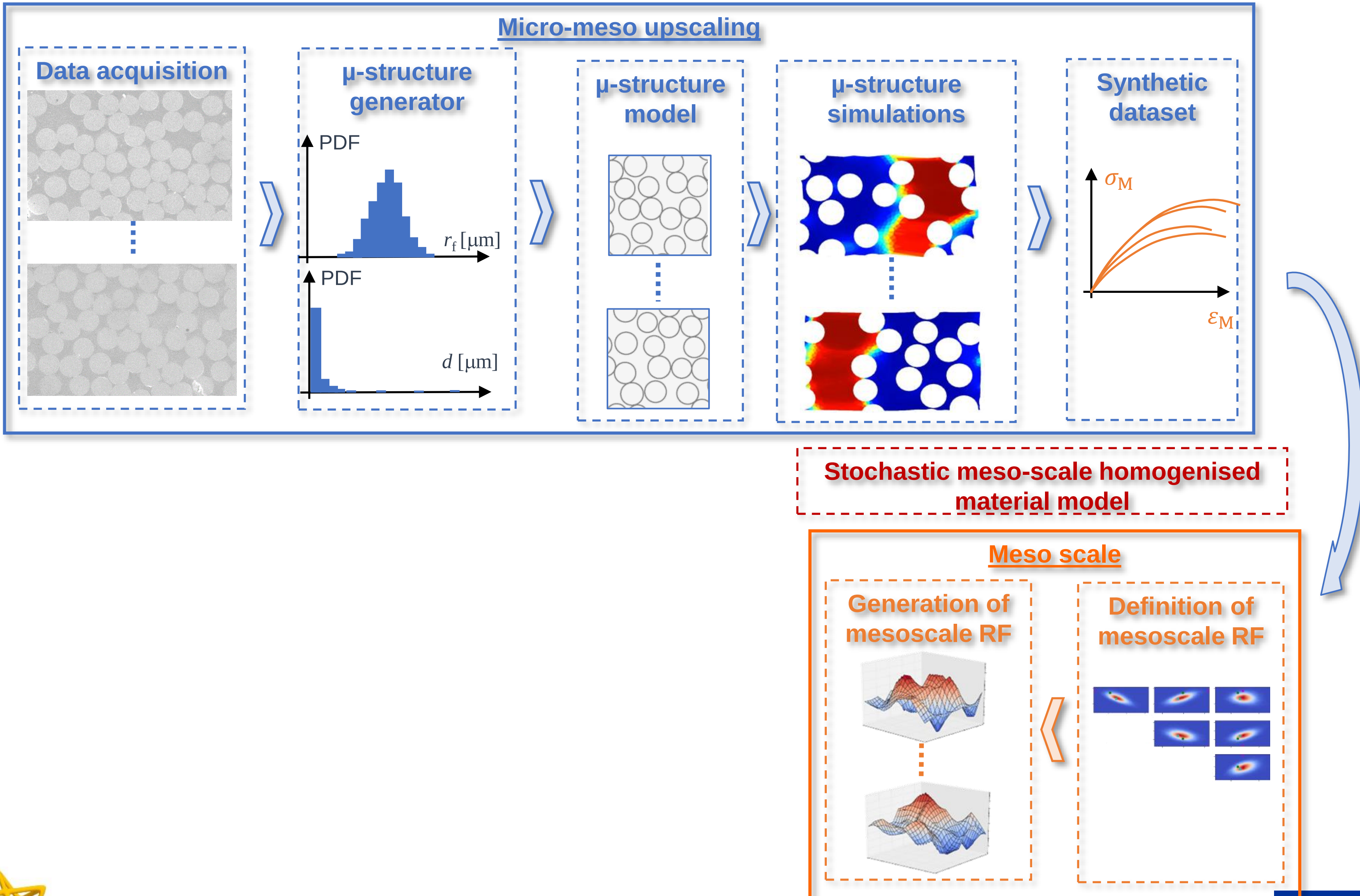




- For each SVE ω^j, we have a homogenised material tensor $\mathbb{C}_M^j$

Stochastic multi-scale simulations

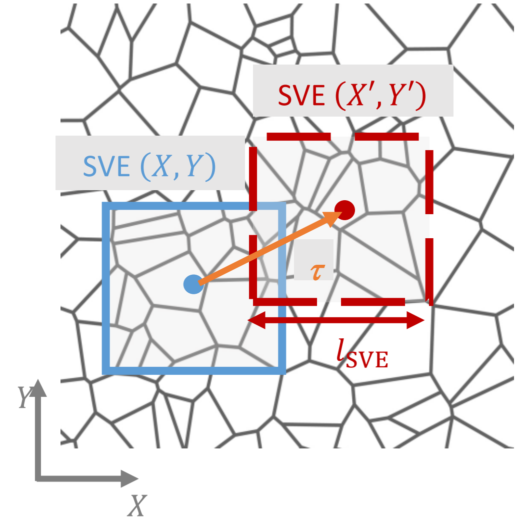
- Step 2: Generate random field of meso-scale properties

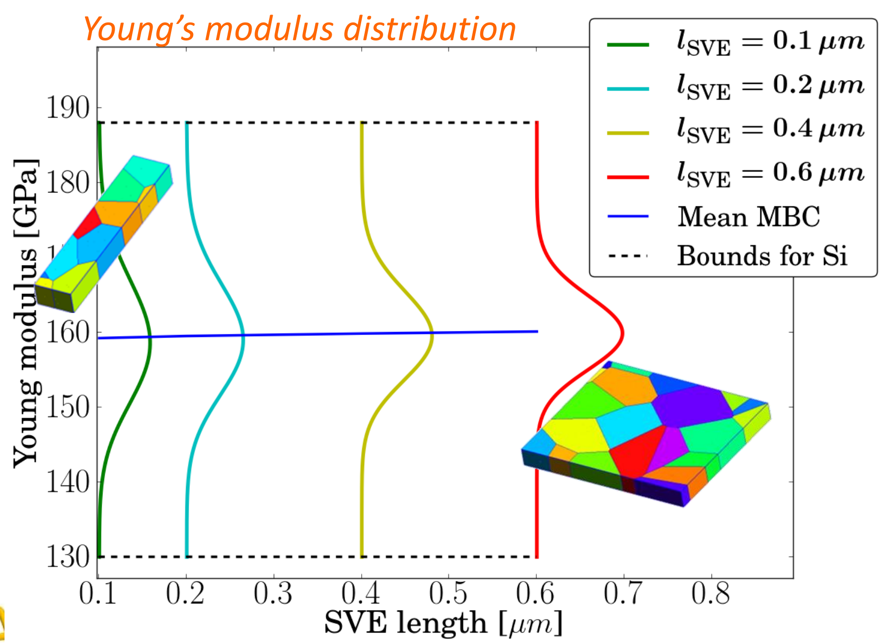


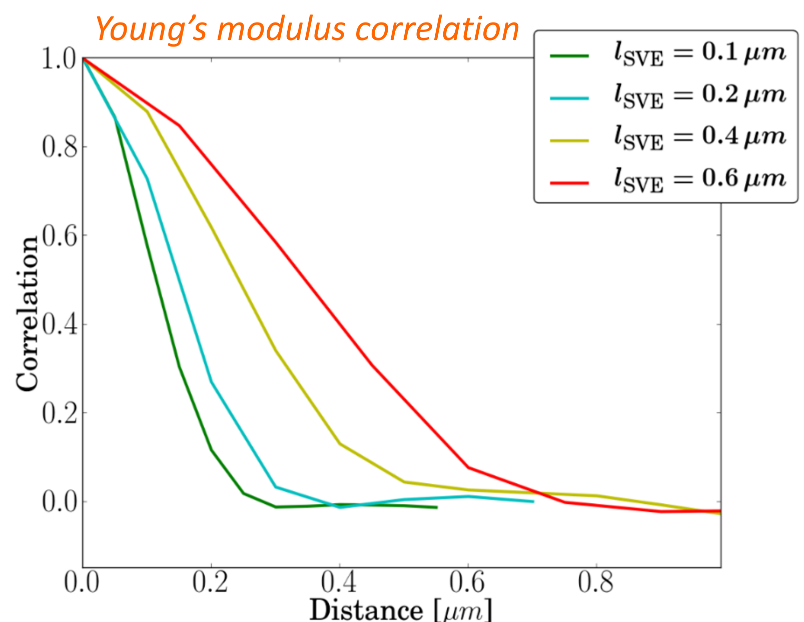
Case of linear elastic material: Polycrystalline Si

- Meso-scale random field
  - Of homogenised material tensor: $\mathbb{C}_M(\Omega)$
    - Extract probability distribution &
    - Spatial correlation

$$R_{E_x}(\boldsymbol{\tau}) = \frac{\mathbb{E}\left[\left(\boldsymbol{E}_x(\boldsymbol{x}) - \mathbb{E}(\boldsymbol{E}_x)\right)\left(\boldsymbol{E}_x(\boldsymbol{x}+\boldsymbol{\tau}) - \mathbb{E}(\boldsymbol{E}_x)\right)\right]}{\mathbb{E}\left[\left(\boldsymbol{E}_x - \mathbb{E}(\boldsymbol{E}_x)\right)^2\right]}$$

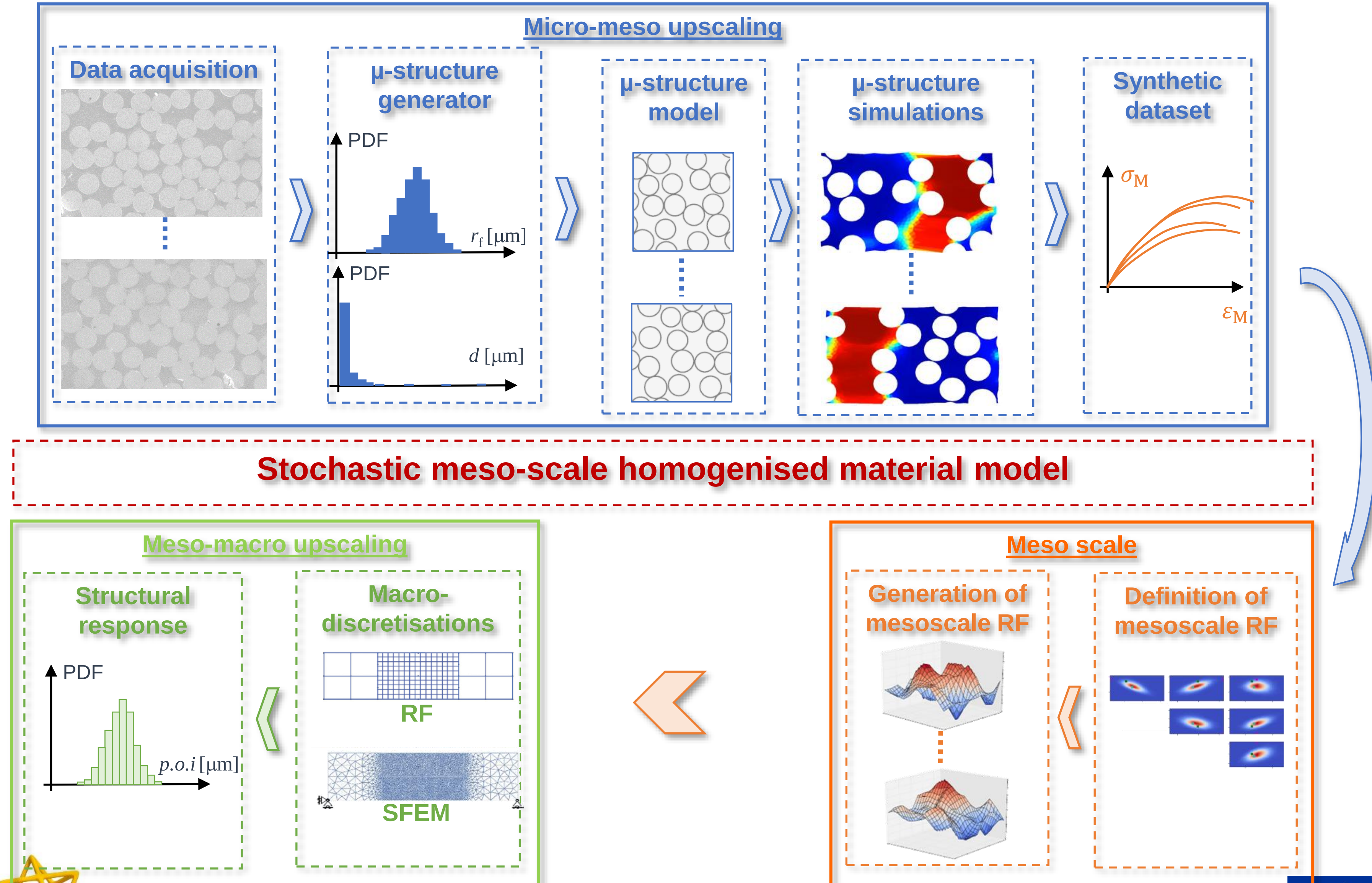






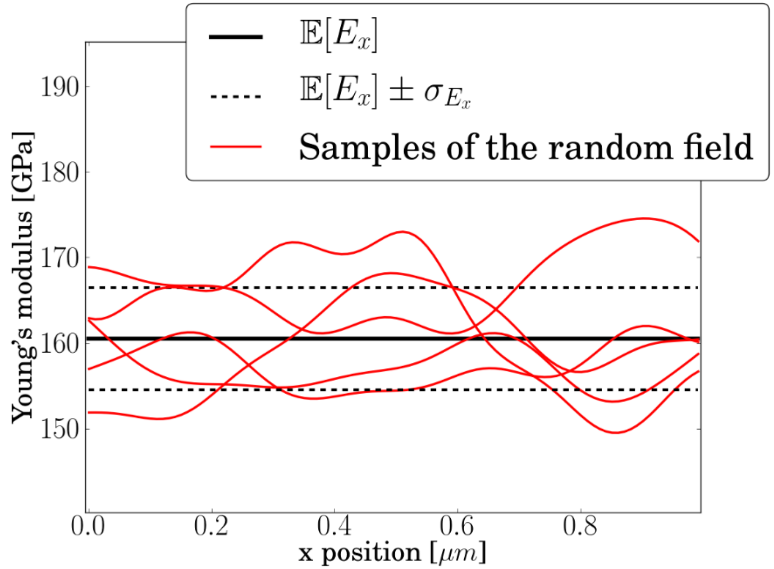
Stochastic multi-scale simulations

- Step 3: Solve macro-scale stochastic finite elements



Case of linear elastic material: Polycrystalline Si

- Meso-Macro upscaling: SFEM
  - Discretisation of random field of material tensor: $\mathbb{C}_{\mathrm{M}}(\Omega)$
    - And generation of realisations

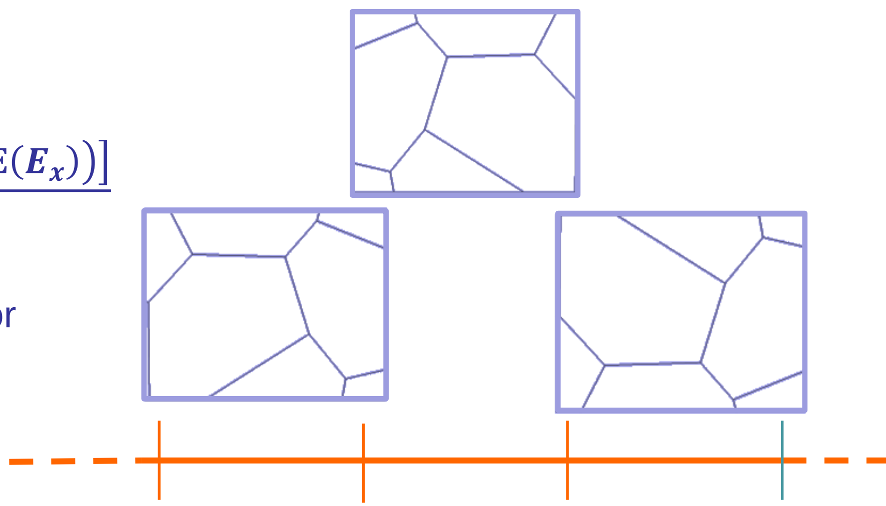


RF discretisation

  - Discretisation into finite-elements
    - Size smaller than correlation length

$$\begin{cases} L_{E_x} = \dfrac{\int_{-\infty}^{\infty} R_{E_x}(\tau)d\tau}{R_{E_x}(0)} \\ R_{E_x}(\boldsymbol{\tau}) = \dfrac{\mathbb{E}\left[\left(\boldsymbol{E}_x(\boldsymbol{x}) - \mathbb{E}(\boldsymbol{E}_x)\right)\left(\boldsymbol{E}_x(\boldsymbol{x}+\boldsymbol{\tau}) - \mathbb{E}(\boldsymbol{E}_x)\right)\right]}{\mathbb{E}\left[\left(\boldsymbol{E}_x - \mathbb{E}(\boldsymbol{E}_x)\right)^2\right]} \end{cases}$$

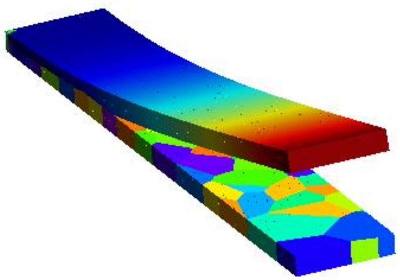
    - Allows spatial correlation to be accounted for



1D finite element discretisation

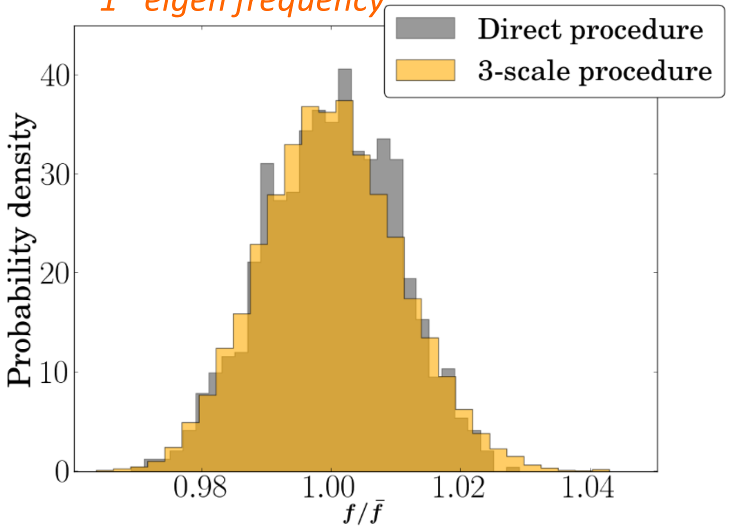
Case of linear elastic material: Polycrystalline Si

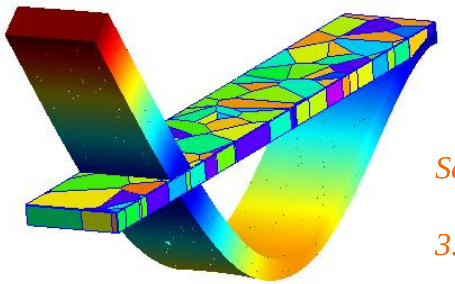
- Meso-Macro upscaling: Property of interest
  - Eigen-mode of MEMS resonator



First bending mode of a 3.2 μm-long beam

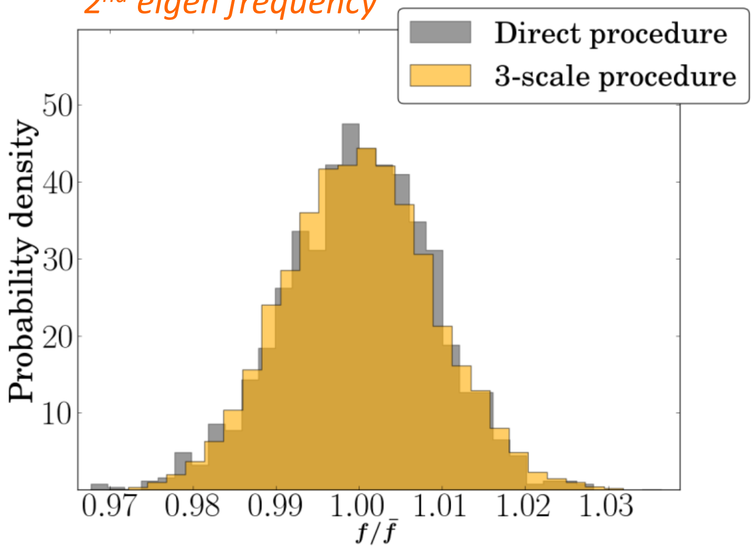
1st eigen frequency





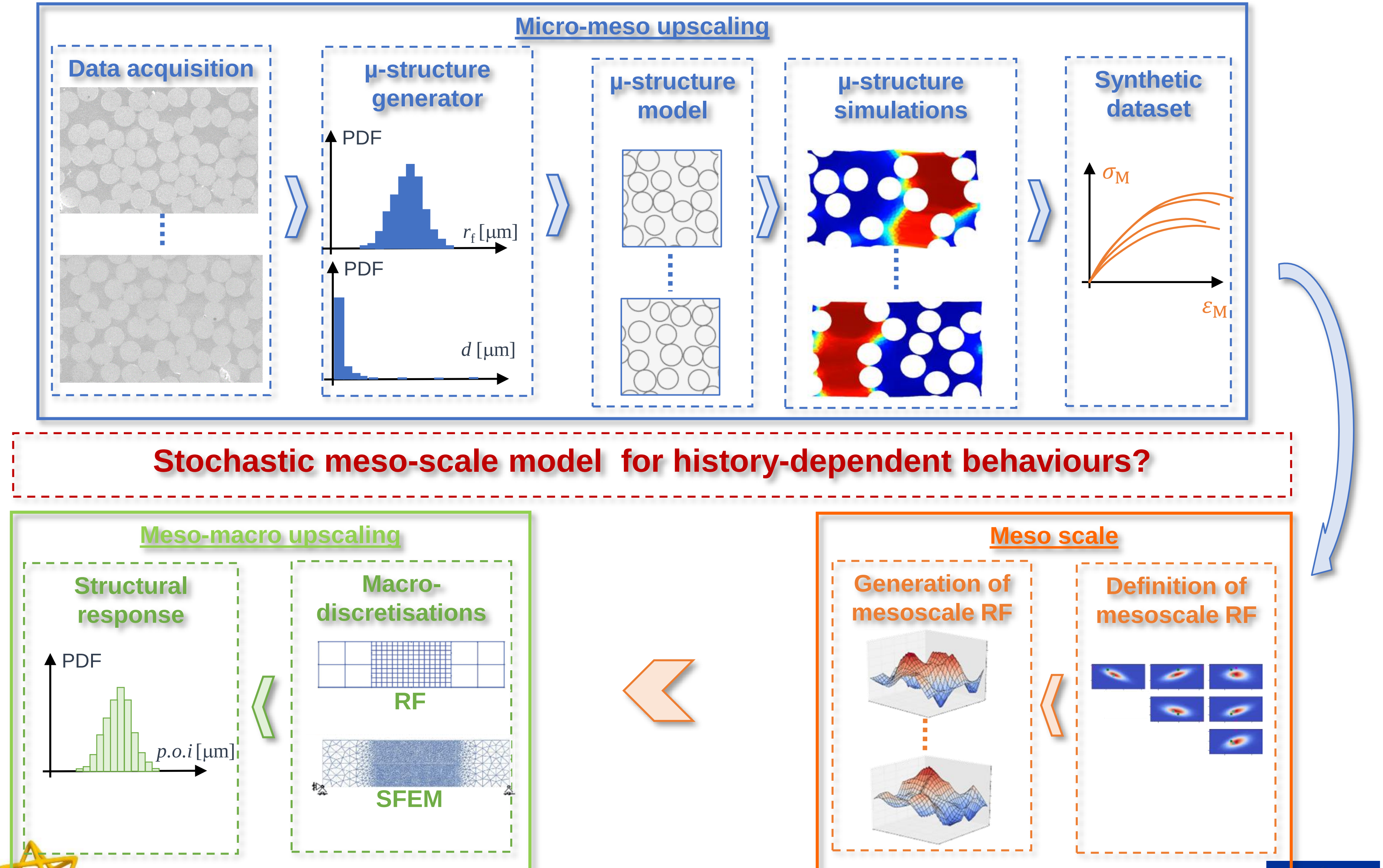
Second bending mode of a 3.2 μm-long beam

2nd eigen frequency

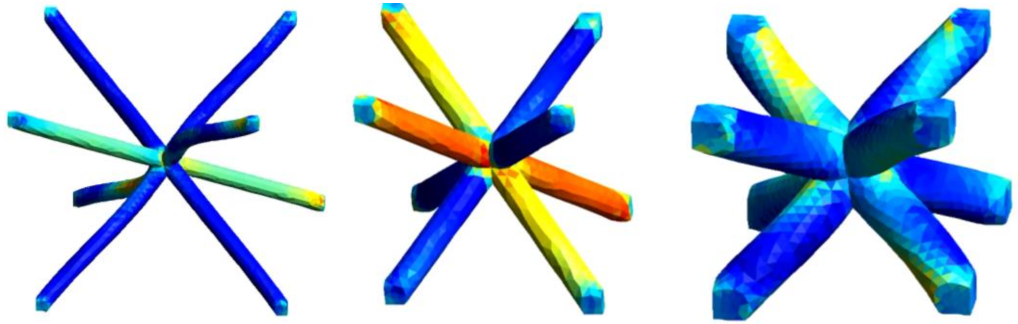


Stochastic multi-scale simulations

- Step 3: Solve macro-scale stochastic finite elements

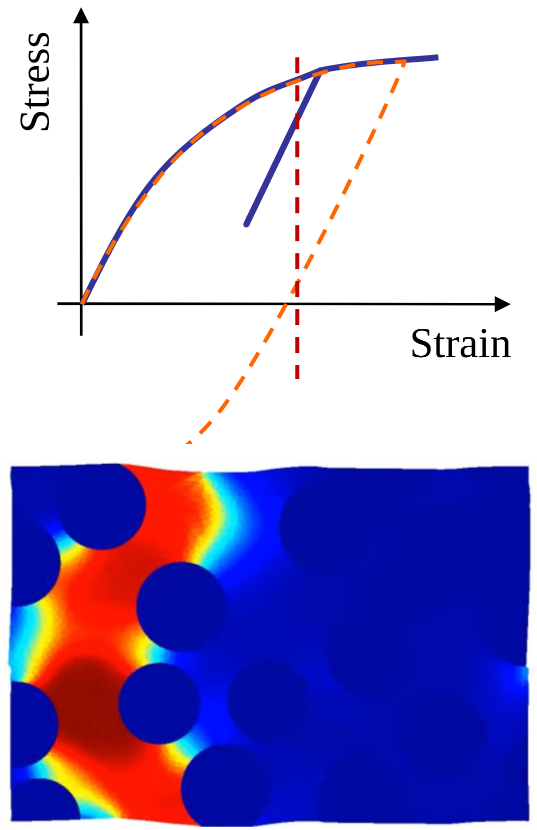


Difficulties in formulating the meso-scale surrogate



- Input / output definition
  - Input:
    - Strain (history): $\mathbf{F}_{\mathrm{M}}$
    - Geometrical parameters: $\boldsymbol{\varphi}_{\mathrm{m}}$
    - Material parameters: $\boldsymbol{\gamma}_{\mathrm{m}}$
  - Output:
    - Stress (history): $\mathbf{P}_{\mathrm{M}}$
- History dependent behaviour
  - $\mathbf{F}_{\mathrm{M}} - \mathbf{P}_{\mathrm{M}}$ is not a bijection
  - History should be tracked
    - Typical material model
    - $\boldsymbol{Z}$ are the internal/state variables

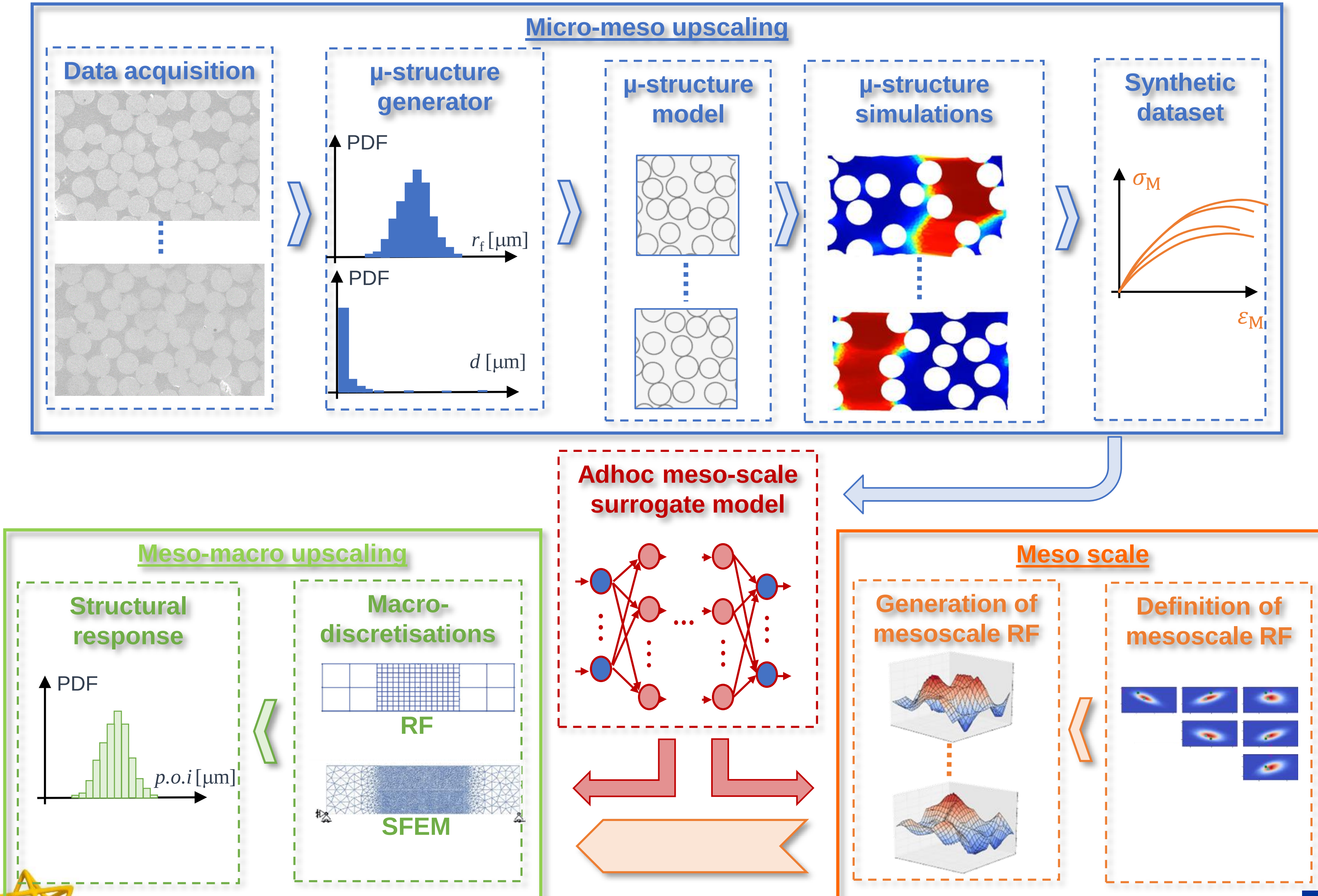
$$\mathbf{P}(\boldsymbol{t}) = \mathbf{P}(\mathbf{F}(t), \boldsymbol{Z}(\tau \leq t))$$



- In case of failure size objectivity is loss
  - $\mathbf{F}_{\mathrm{M}} - \mathbf{P}_{\mathrm{M}}$ relation depends on the SVE size
    - Need for another size objective value

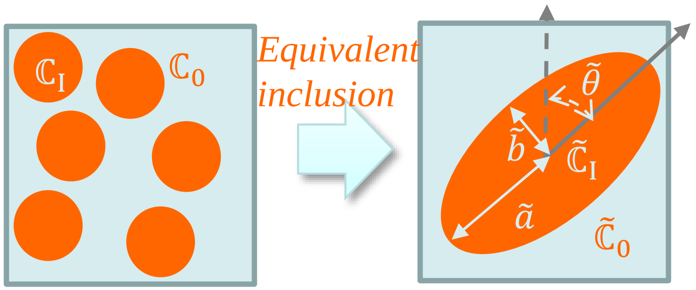
Stochastic multi-scale simulations

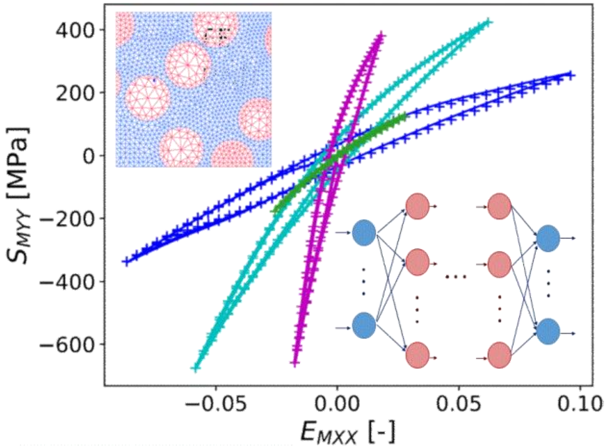
- Challenge: meso-scale surrogate model for complex material systems

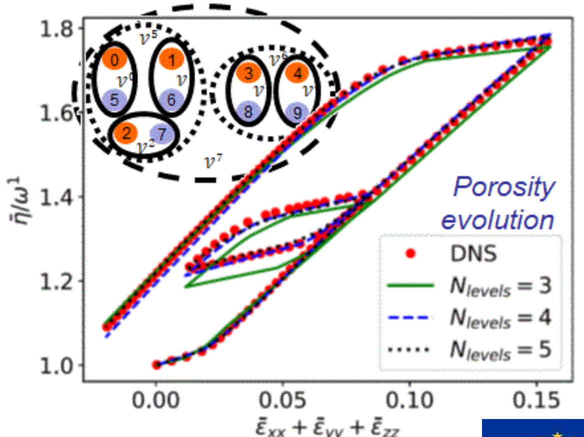


Meso-scale surrogate model for complex material systems

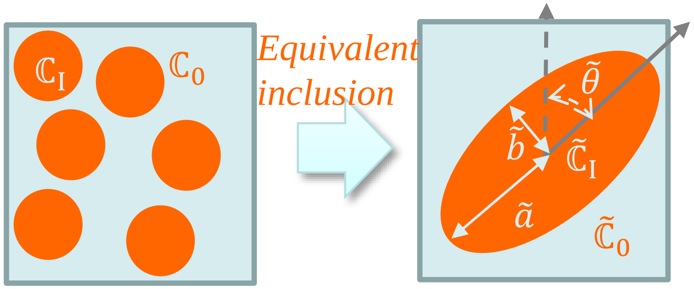
- Micro-mechanical models
  - General for a micro-structure kind
    - Geometrical parameters: $\boldsymbol{\varphi}_{\mathrm{m}}$
    - Material parameters: $\boldsymbol{\gamma}_{\mathrm{m}}$
  - Based on thermodynamic consistency
    - Possesses extrapolation capabilities
  - Delicate identification
- Neural networks
  - Theoretically generic
    - Geometrical parameters: $\boldsymbol{\varphi}_{\mathrm{m}}$
    - Material parameters: $\boldsymbol{\gamma}_{\mathrm{m}}$
  - No extrapolation capabilities
    - Requires extensive data
- Deep material networks
  - Based on thermodynamic consistency
    - Possesses extrapolation capabilities
  - Fixed micro-structure?



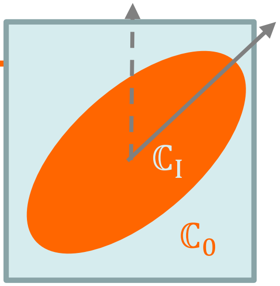




Meso-scale surrogate model for complex material systems

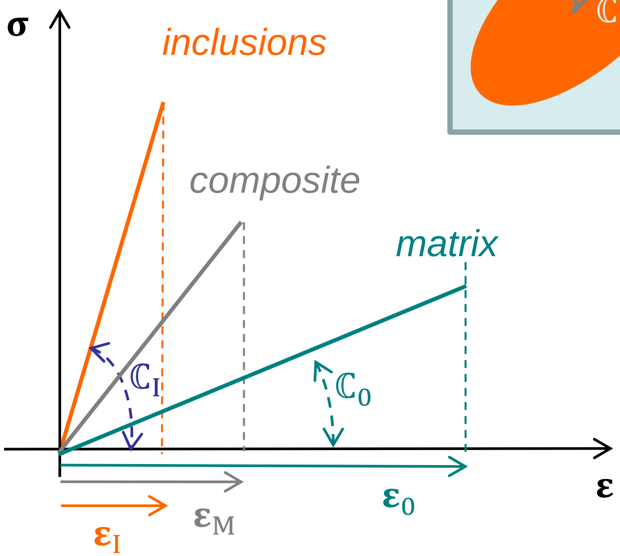


- Micro-mechanical models
  - General for a micro-structure kind
    - Strain (history): $\mathbf{F}_\mathrm{M}$
    - Geometrical parameters: $\boldsymbol{\varphi}_\mathrm{m}$
    - Material parameters: $\boldsymbol{\gamma}_\mathrm{m}$
  - Based on thermodynamic consistency
  - Possesses extrapolation capabilities
- Some works identifying (stochastic) parameters from SVE simulations
  - Based on a macro-scale model (including phase-field)
    - Yi, Chen, To, McVeigh, Liu (2008). Statistical volume element method for predicting micro-structure-constitutive property relations. CMAME
    - Hun, Guilleminot, Yvonnet, Bornert (2019). Stochastic multiscale modeling of crack propagation in random heterogeneous media. IJNME
  - Based on Reduced-Order-Model
    - Fish, Wu (2011). A nonintrusive stochastic multiscale solver. IJNME
  - Based on micro-mechanical Mean-Field Homogenisation (MFH)
    - Wu, Nguyen, Adam, Noels (2019), An inverse micro-mechanical analysis toward the stochastic homogenization of nonlinear random composites. CMAME
    - Calleja, Wu, Nguyen, Noels (Revised) A micromechanical Mean-Field Homogenization surrogate for the stochastic multiscale analysis of composite materials failure. IJNME



- Non-linear Mean-Field-Homogenisation (MFH)
  - Principle
    - Consider an embedded inclusion
    - Apply constitutive laws on the average phase fields
  - Linear composites

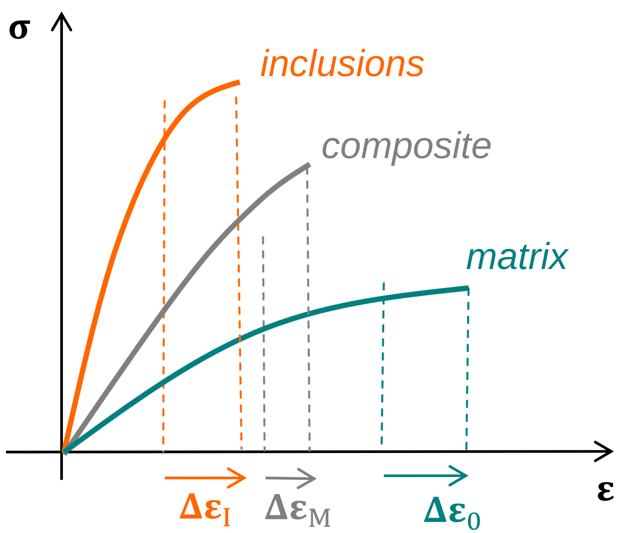
$$\begin{cases} \boldsymbol{\sigma}_{\mathrm{M}} = \bar{\boldsymbol{\sigma}} = v_0 \boldsymbol{\sigma}_0 + v_{\mathrm{I}} \boldsymbol{\sigma}_{\mathrm{I}} \\ \boldsymbol{\varepsilon}_{\mathrm{M}} = \bar{\boldsymbol{\varepsilon}} = v_0 \boldsymbol{\varepsilon}_0 + v_{\mathrm{I}} \boldsymbol{\varepsilon}_{\mathrm{I}} \\ \boldsymbol{\varepsilon}_{\mathrm{I}} = \mathbb{B}^{\varepsilon}(\mathrm{I}, \mathbb{C}_0, \mathbb{C}_{\mathrm{I}}) : \boldsymbol{\varepsilon}_0 \end{cases}$$



  - Non-linear composites

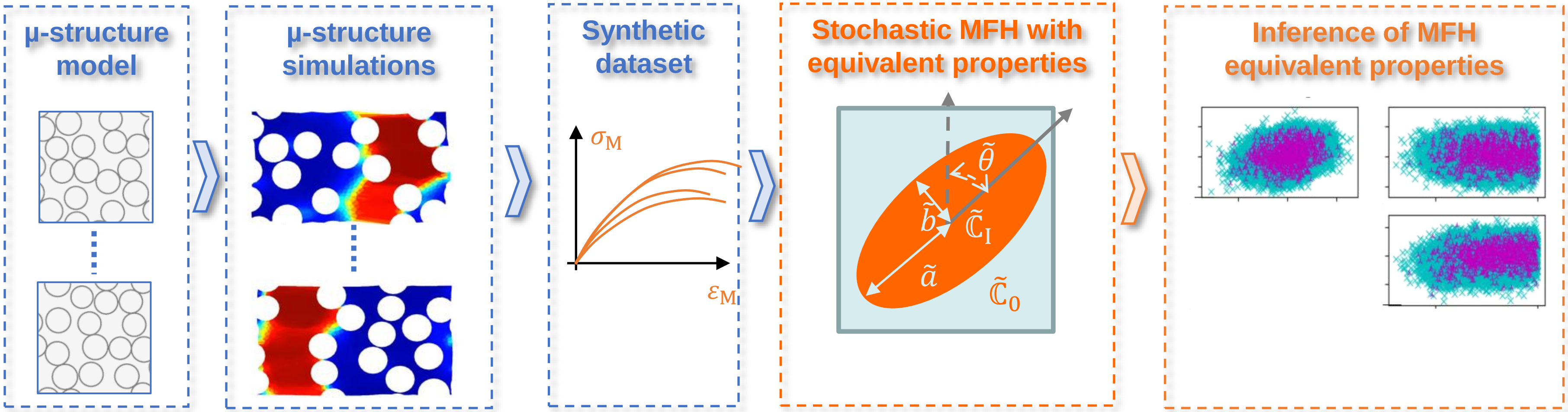
$$\begin{cases} \boldsymbol{\sigma}_{\mathrm{M}} = \bar{\boldsymbol{\sigma}} = v_0 \boldsymbol{\sigma}_0 + v_{\mathrm{I}} \boldsymbol{\sigma}_{\mathrm{I}} \\ \Delta\boldsymbol{\varepsilon}_{\mathrm{M}} = \overline{\Delta\boldsymbol{\varepsilon}} = v_0 \Delta\boldsymbol{\varepsilon}_0 + v_{\mathrm{I}} \Delta\boldsymbol{\varepsilon}_{\mathrm{I}} \\ \Delta\boldsymbol{\varepsilon}_{\mathrm{I}} = \mathbb{B}^{\varepsilon}\left(\mathrm{I}, \mathbb{C}_0^{\mathrm{LCC}}, \mathbb{C}_{\mathrm{I}}^{\mathrm{LCC}}\right) : \Delta\boldsymbol{\varepsilon}_0 \end{cases}$$

Define a linear comparison composite material



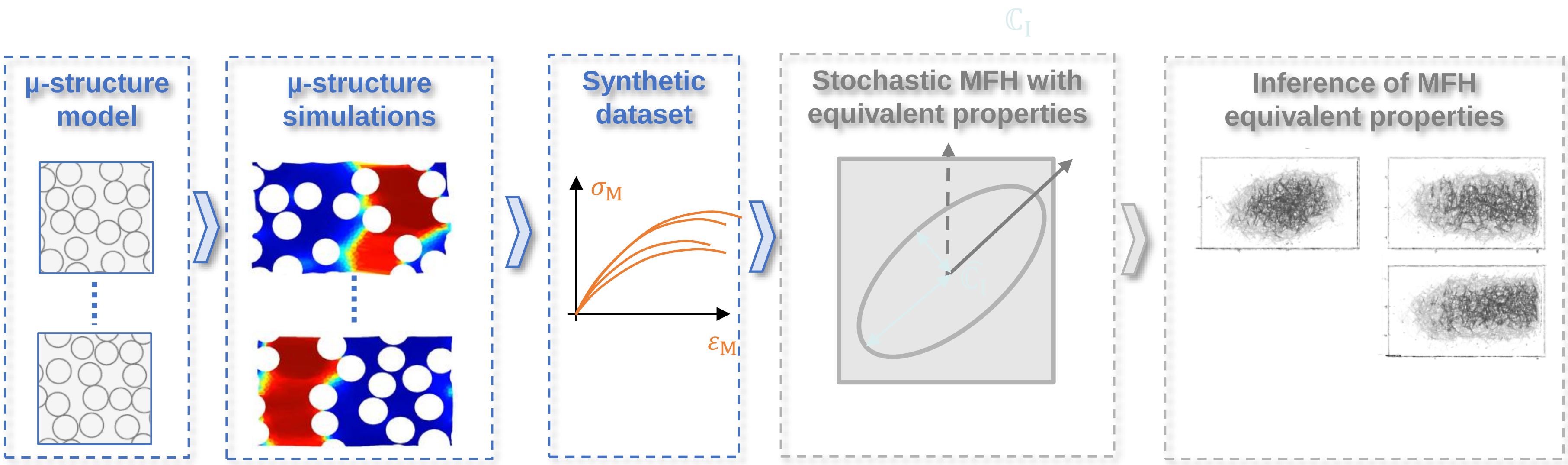
Non-linear stochastic Mean-Field Homogenisation

- MFH
  - Based on an embedded inclusion
  - How to account for stochastic effects?
- Stochastic MFH
  - Infer MFH equivalent properties distribution

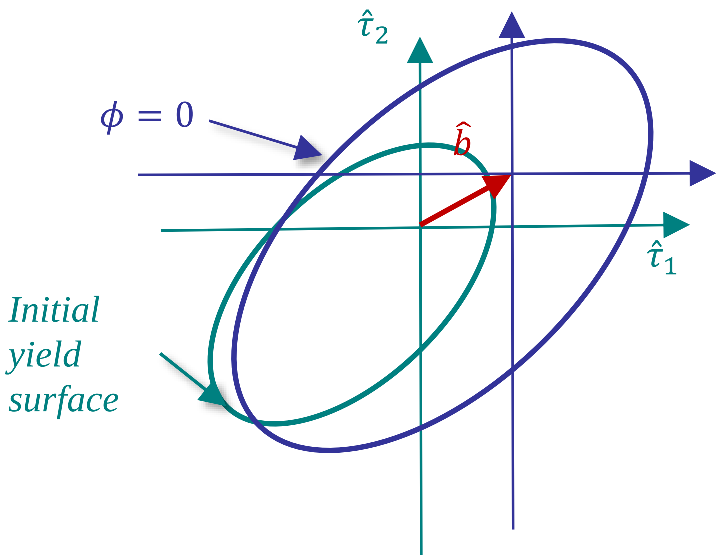


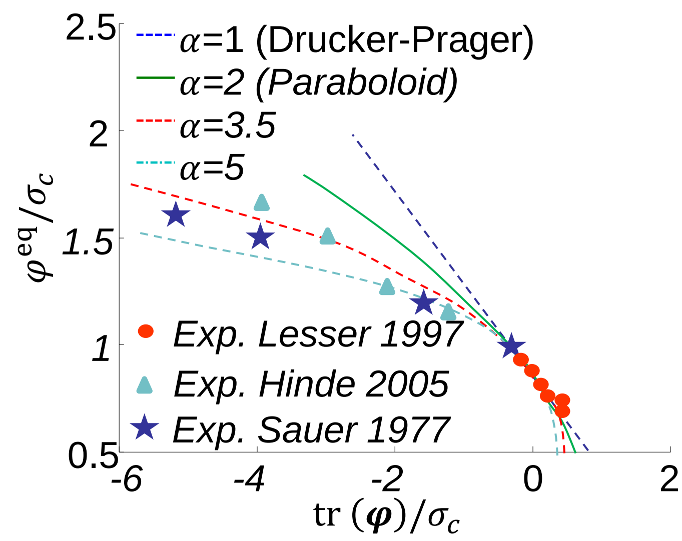
Non-linear stochastic Mean-Field Homogenisation

- MFH
  - Based on an embedded inclusion
  - How to account for stochastic effects?
- Stochastic MFH
  - Infer MFH equivalent properties distribution



- Material model
  - Pressure dependent elastic-plastic finite strain model

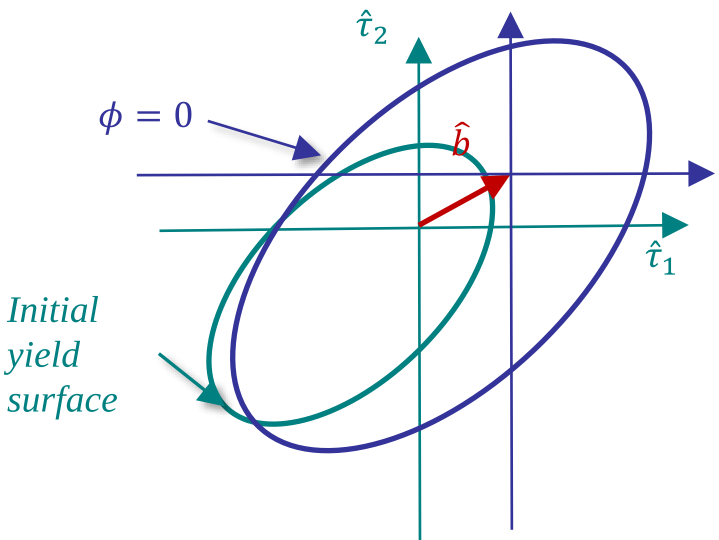


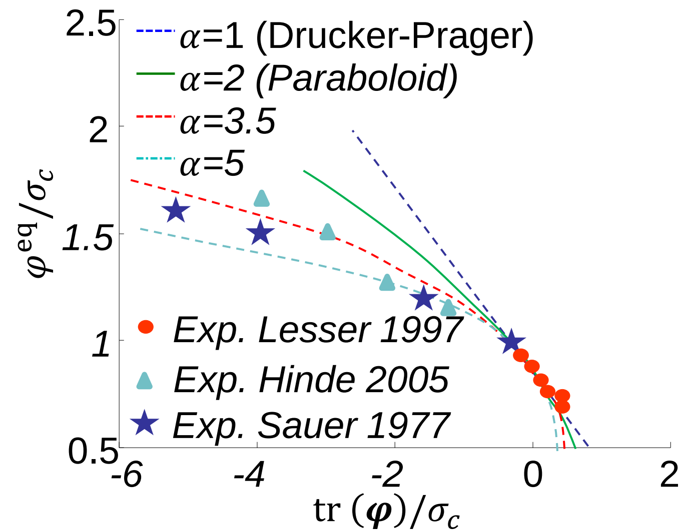


$$
\begin{cases}
\boldsymbol{\varphi} = \hat{\boldsymbol{\tau}} - \hat{\boldsymbol{b}} \\
\phi = \left(\dfrac{\varphi^{\mathrm{eq}}}{\sigma_c}\right)^{\alpha} - \dfrac{m^{\alpha} - 1}{m + 1}\dfrac{\mathrm{tr}\boldsymbol{\varphi}}{\sigma_c} - \dfrac{m^{\alpha} + m}{m + 1} \\
m = \dfrac{\sigma_t}{\sigma_c}
\end{cases}
$$

Generation of SVE responses

- Material model
  - Pressure dependent elastic-plastic finite strain model



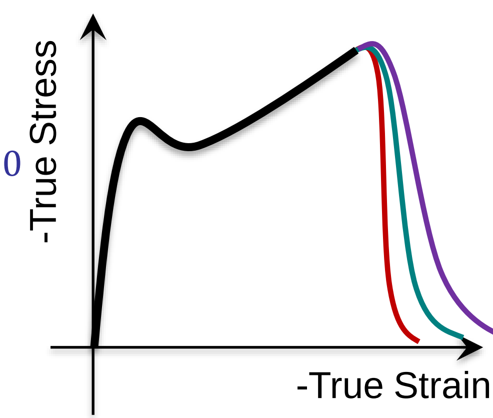


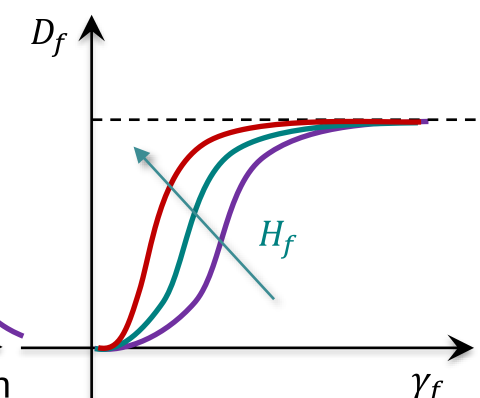
  - (Nonlocal) damaging process
    - Triaxiality-dependent failure surface

$$\begin{cases} \phi_f = \bar{\varepsilon}^{\mathrm{pl}} - a \exp\left(-b\,\dfrac{\mathrm{tr}(\hat{\boldsymbol{\tau}})}{3\hat{\tau}^{eq}}\right) - c \\ \phi_f - \gamma_f \leq 0;\ \dot{\gamma}_f \geq 0; \text{and } \dot{\gamma}_f\left(\phi_f - \gamma_f\right) = 0 \end{cases}$$

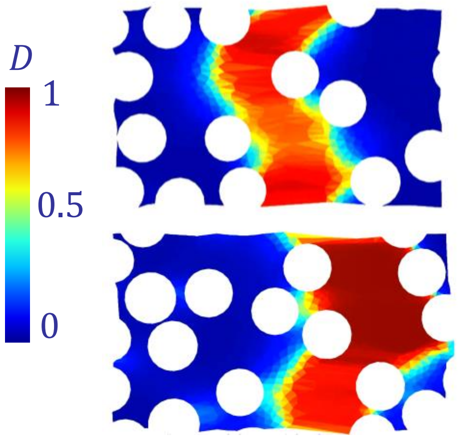
    - Damage evolution

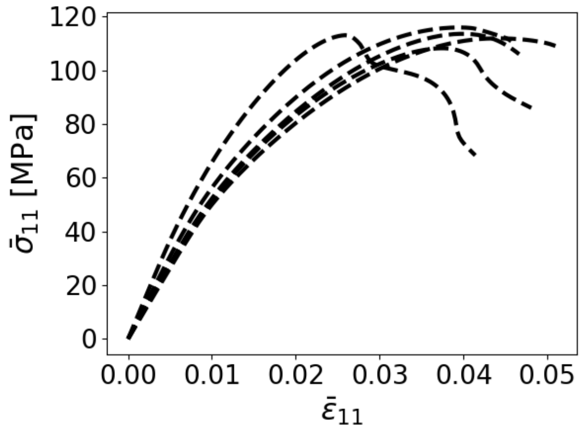
$$\begin{cases} \bar{\gamma}_f - l_f^2\, \Delta\bar{\gamma}_f = \gamma_f \\ \dot{D}_f = H_f\,\left(\bar{\gamma}_f\right)^{\zeta_f}\left(1 - D_f\right)^{-\zeta_d}\,\dot{\bar{\gamma}}_f \end{cases}$$

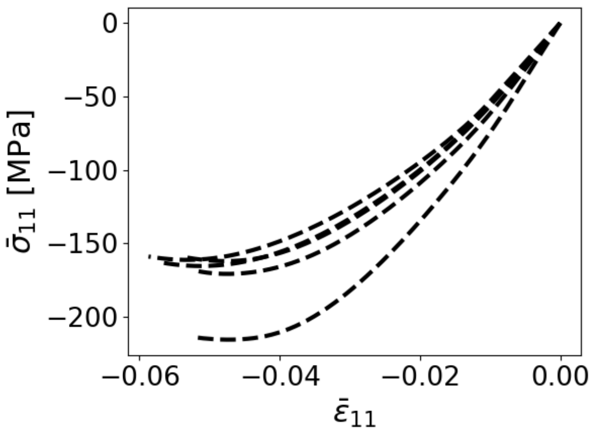




- Responses set
  - Stress-strain responses



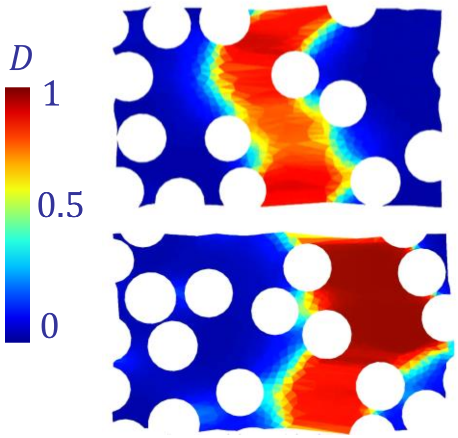


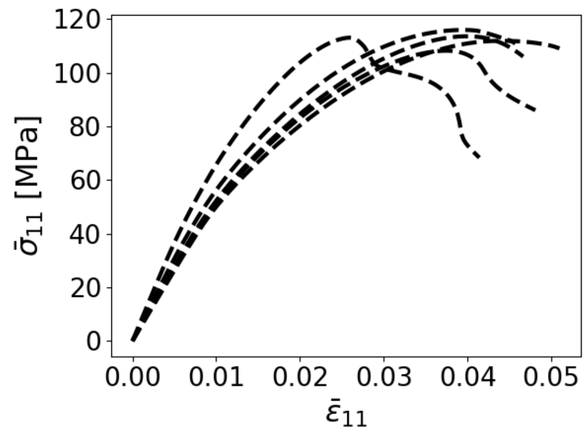


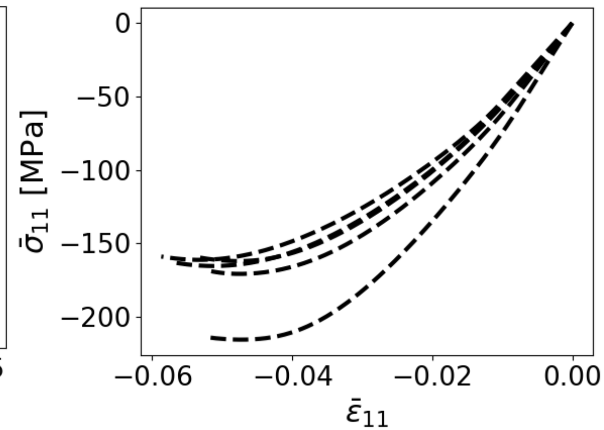
  - Address loss of size objectivity?

Generation of SVE responses

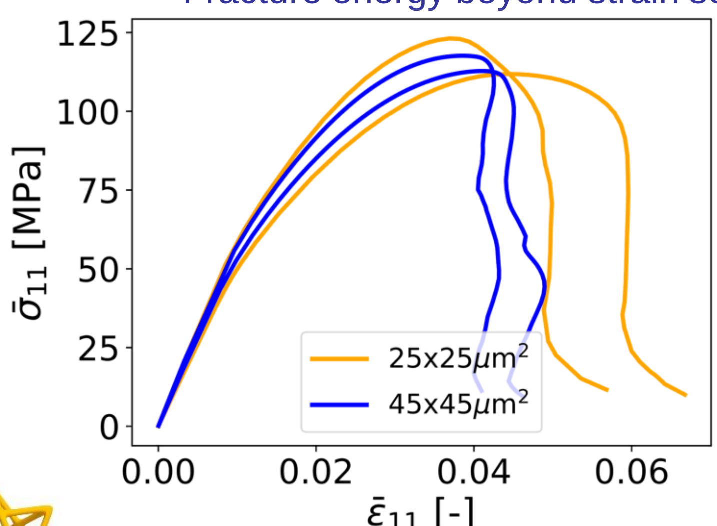
- Responses set
  - Stress-strain responses

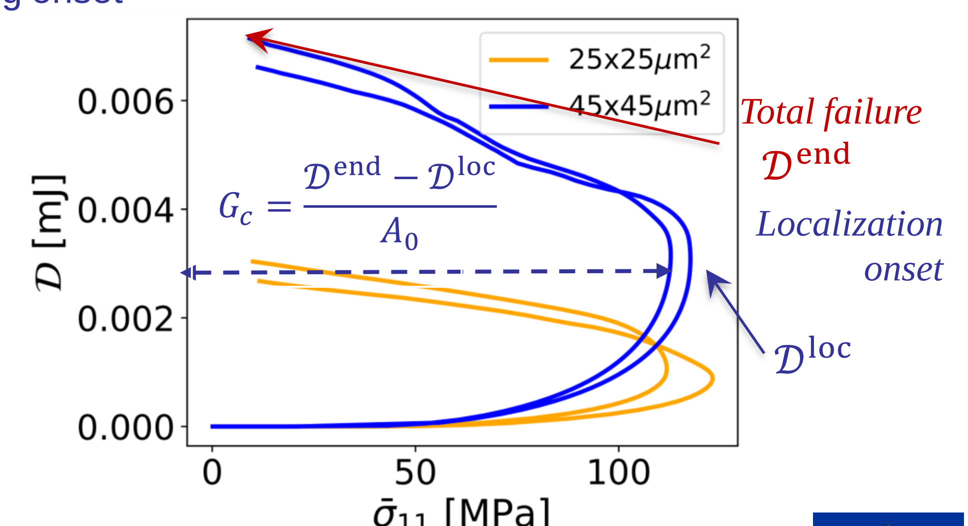






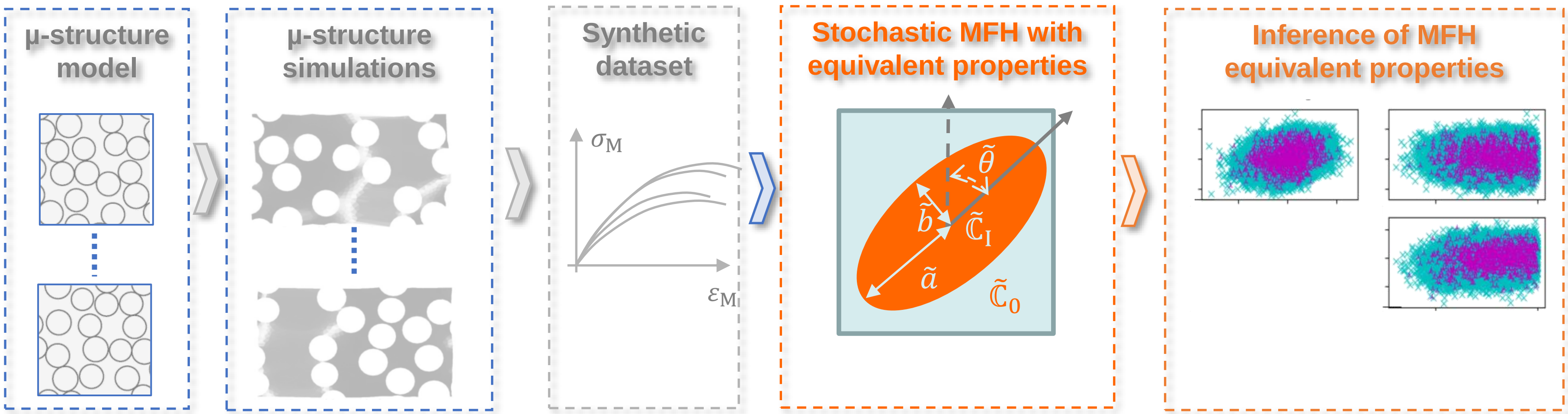
  - Address loss of size objectivity:
    - Fracture energy beyond strain softening onset



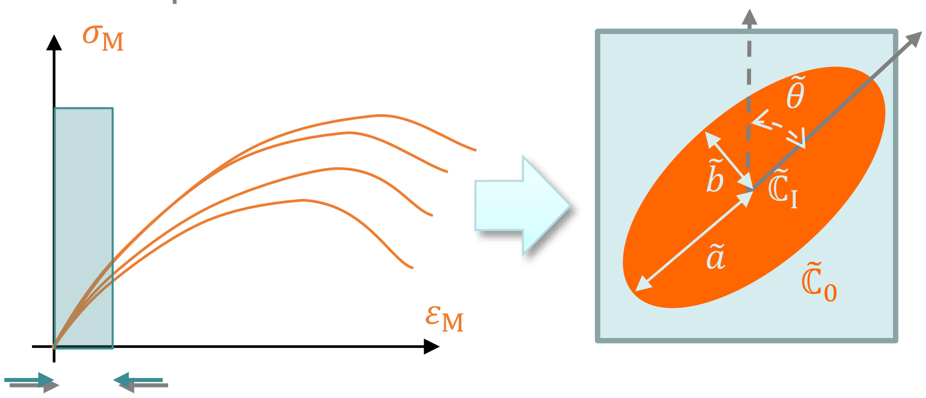


Non-linear stochastic Mean-Field Homogenisation

- MFH
  - Based on an embedded inclusion
  - How to account for stochastic effects?
- Stochastic MFH
  - Infer MFH equivalent properties distribution



- Determination of MFH equivalent properties
  - Linear part

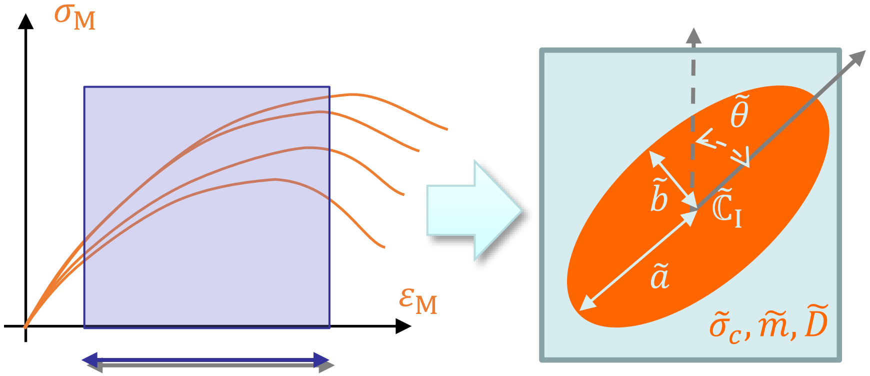


Linear part

Equivalent inclusion: $\left[\tilde{\theta}, \tilde{v}_I, \frac{\tilde{a}}{\tilde{b}}\right]$

Matrix elastic properties: $\left[\tilde{\mathbb{C}}_0\right]$

  - Non-linear part



Non-Linear part

Matrix plastic flow: $\left[\tilde{\sigma}_c(\bar{\varepsilon}^{\mathrm{pl}}), \tilde{m}, \tilde{\alpha}, \tilde{v}_p\right]$

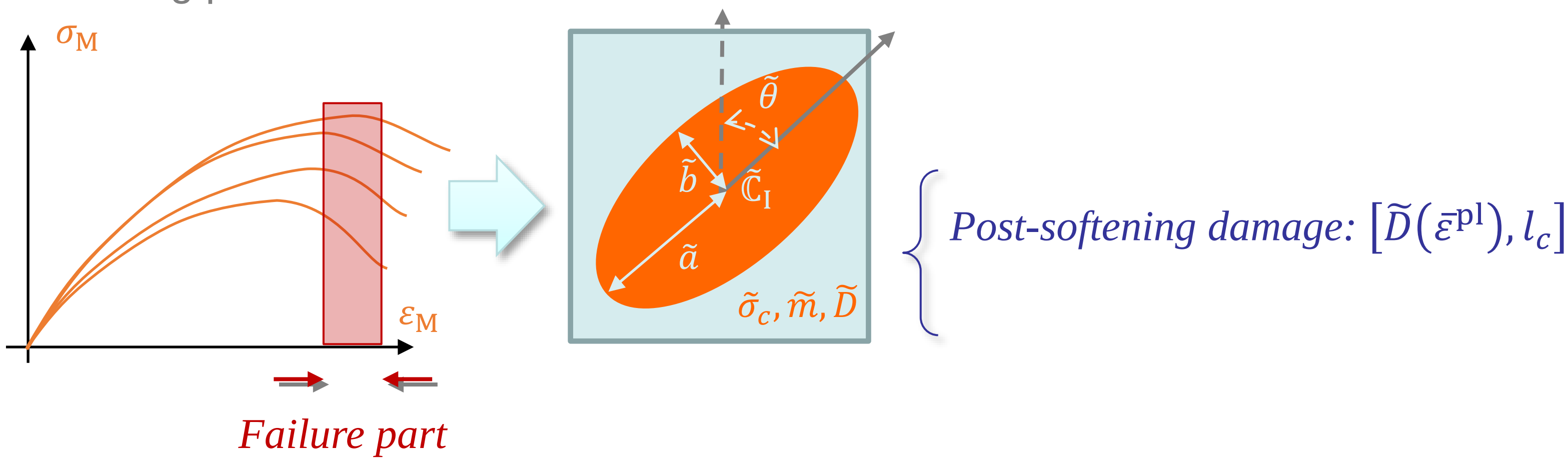
$$\phi = \left(\frac{\varphi^{\mathrm{eq}}}{\tilde{\sigma}_c}\right)^{\tilde{\alpha}} - \frac{\tilde{m}^{\tilde{\alpha}} - 1}{\tilde{m} + 1}\frac{\mathrm{tr}\boldsymbol{\varphi}}{\tilde{\sigma}_c} - \frac{\tilde{m}^{\tilde{\alpha}} + \tilde{m}}{\tilde{m} + 1}$$

$$\tilde{m} = \frac{\tilde{\sigma}_t}{\tilde{\sigma}_c}$$

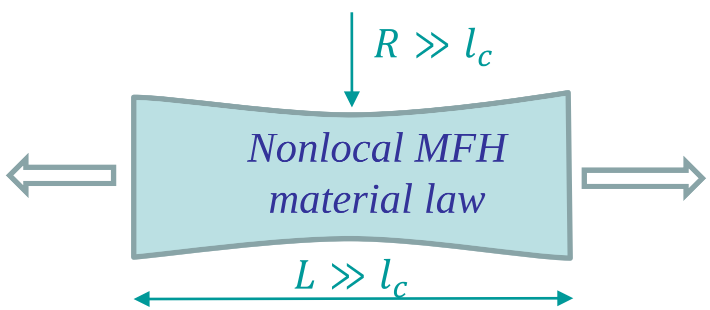
Pre-softening damage: $\left[\tilde{D}(\bar{\varepsilon}^{\mathrm{pl}})\right]$

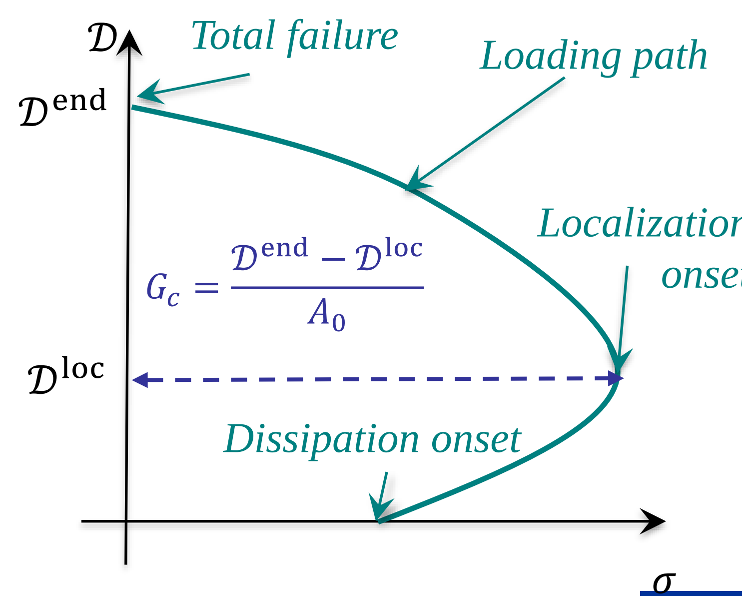
Non-linear stochastic Mean-Field Homogenisation

- Determination of MFH equivalent properties
  - Softening part

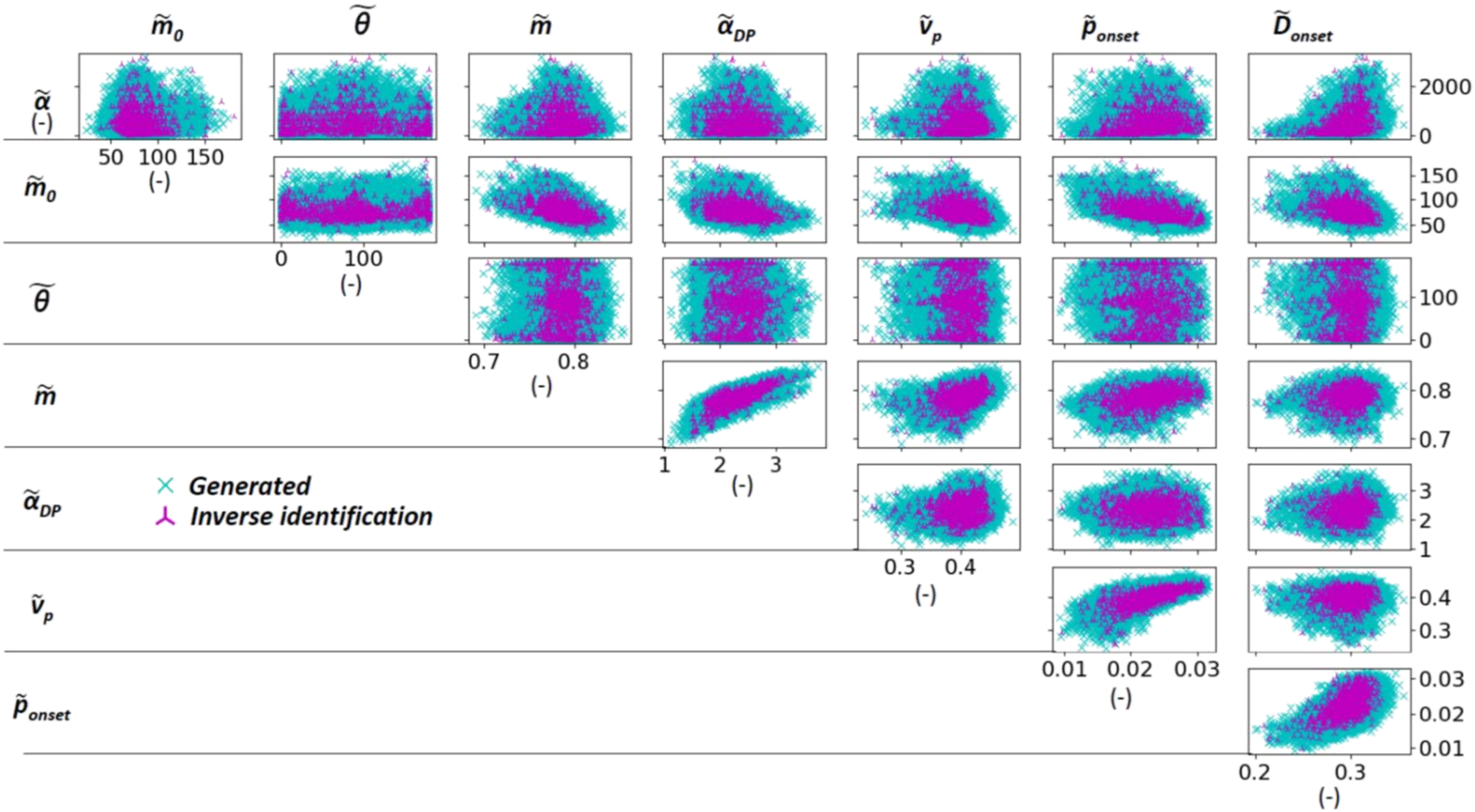


- Identified to recover the right energy release rate
- For a given macro-scale nonlocal length l_c

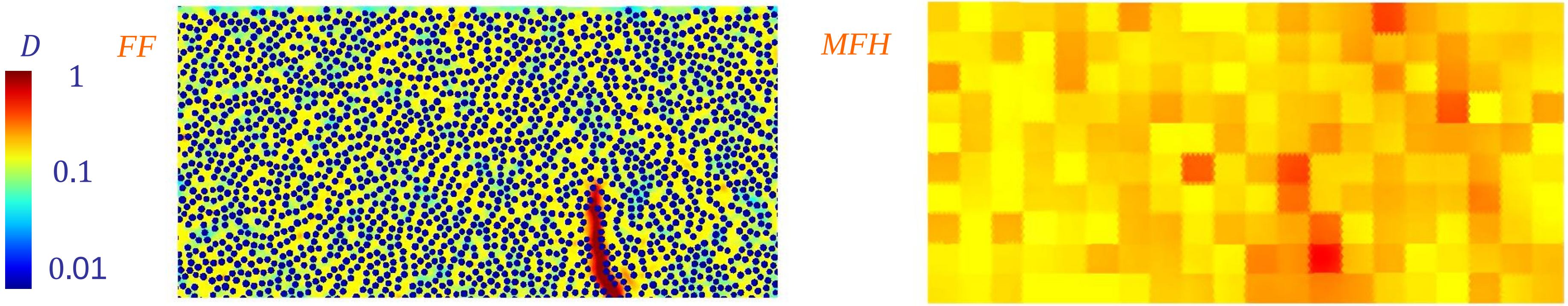


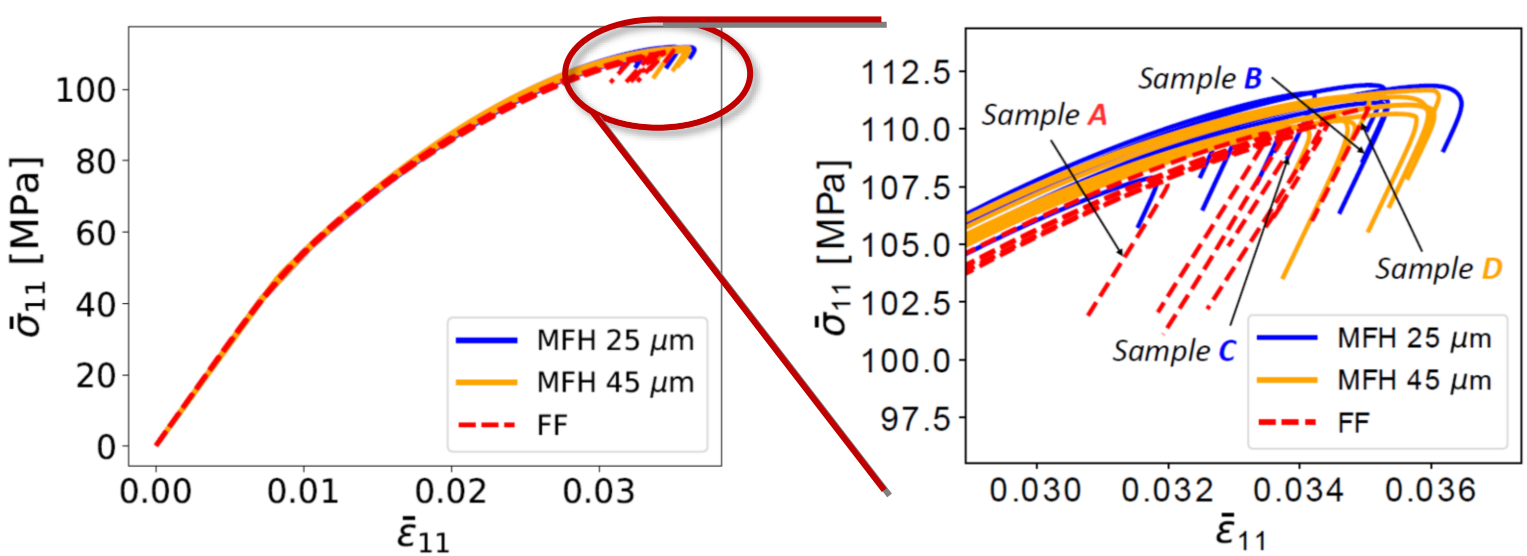


- Generator of MFH parameters
  - Using data-driven sampling method
    - Soize, Ghanem (2016) Data-driven probability concentration and sampling on manifold. JCP

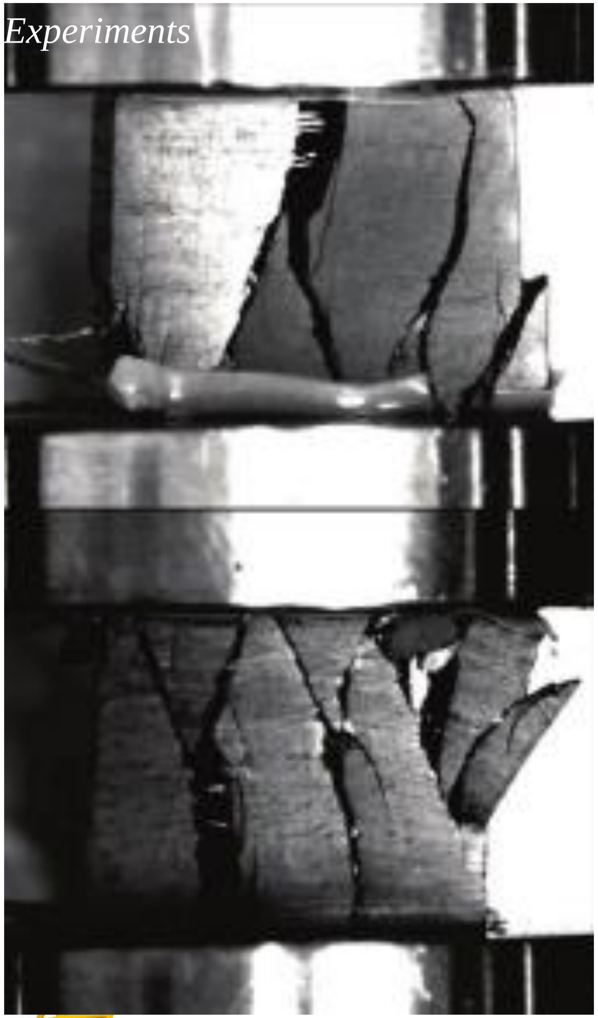


- Verification on ply tensile tests
  - Stochastic Full-field simulations vs. Stochastic MF-ROM multi-scale simulations

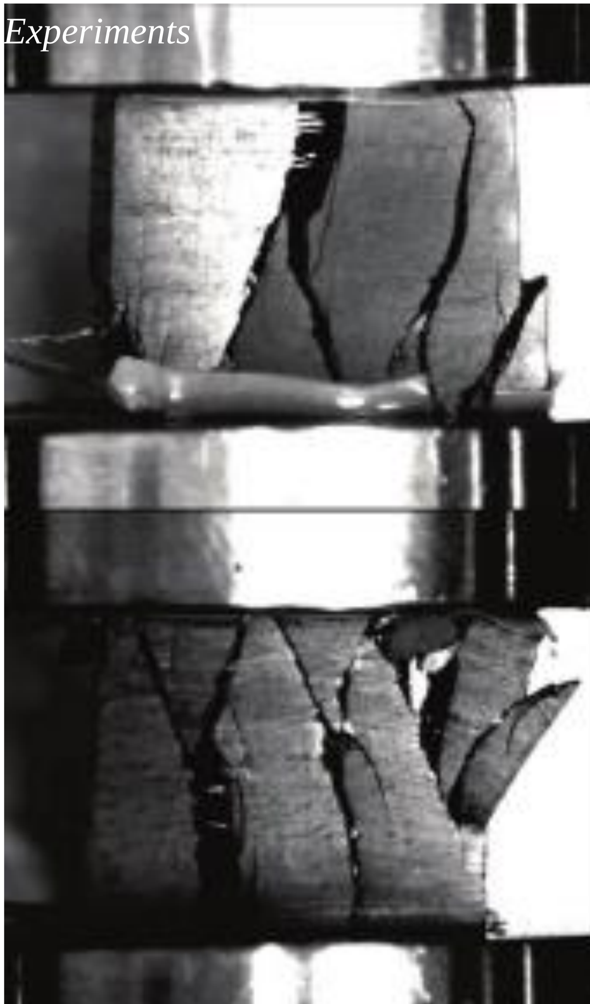


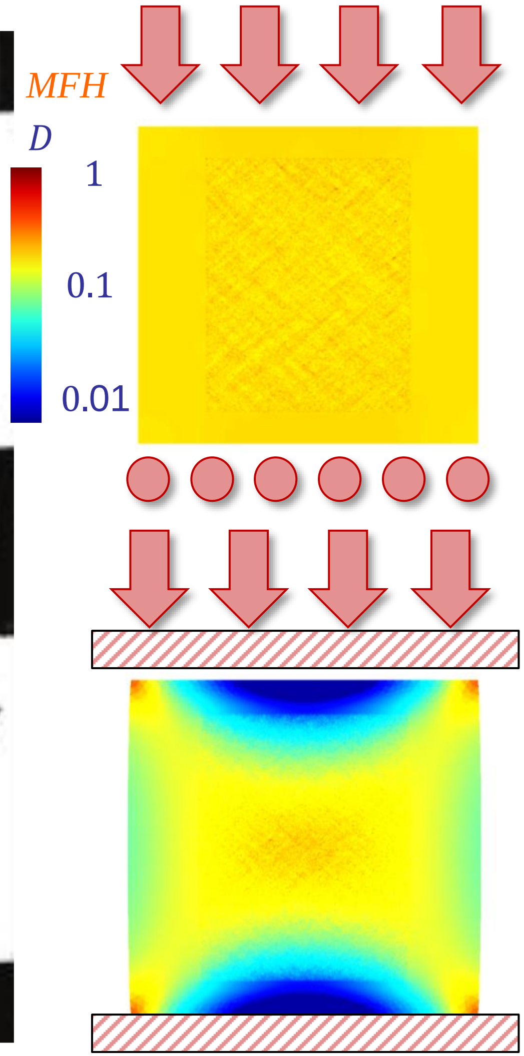


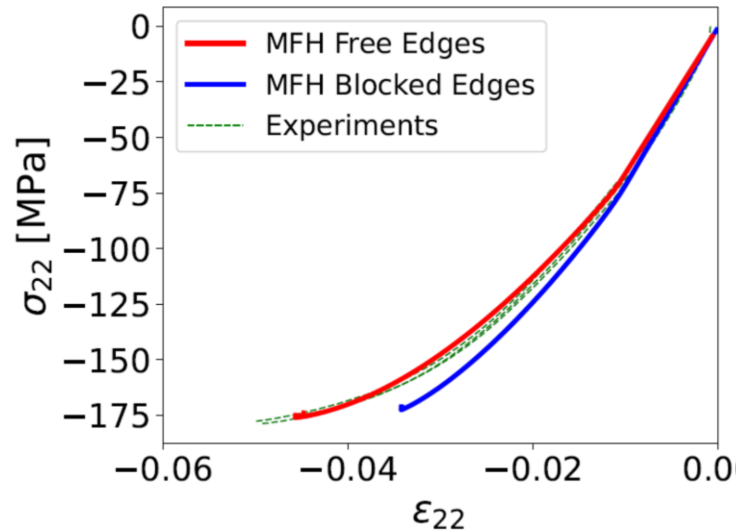
- Comparison with experimental test
  - Transverse compression test [J. Chevalier and P.P. Camanho and F. Lani and T. Pardoen, CS 2019]



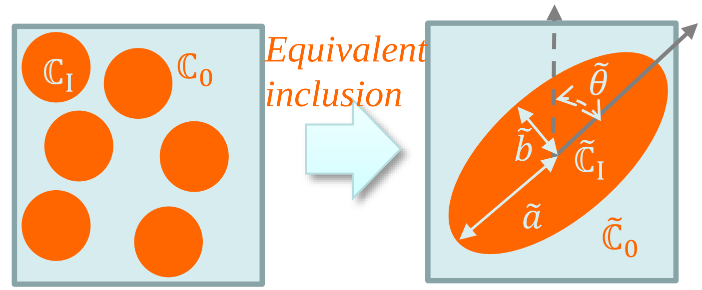
- Comparison with experimental test
  - Transverse compression test [J. Chevalier and P.P. Camanho and F. Lani and T. Pardoen, CS 2019]



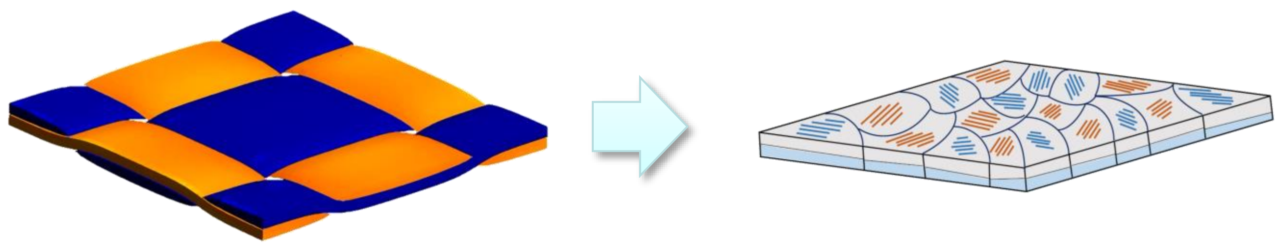




Meso-scale surrogate model for complex material systems

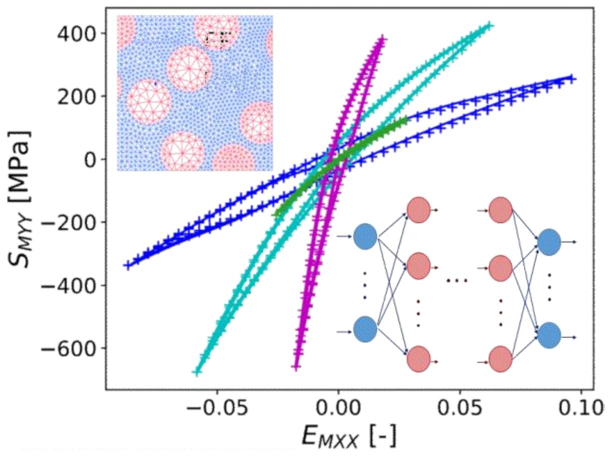


- Micro-mechanical models
  - General for a micro-structure kind
    - Strain (history): $\mathbf{F}_\mathrm{M}$
    - Geometrical parameters: $\boldsymbol{\varphi}_\mathrm{m}$
    - Material parameters: $\boldsymbol{\gamma}_\mathrm{m}$
  - Based on thermodynamic consistency
  - Possesses extrapolation capabilities
- Limitations
  - Composite should be represented by an equivalent inclusion
    - Possibility to extend to other geometries



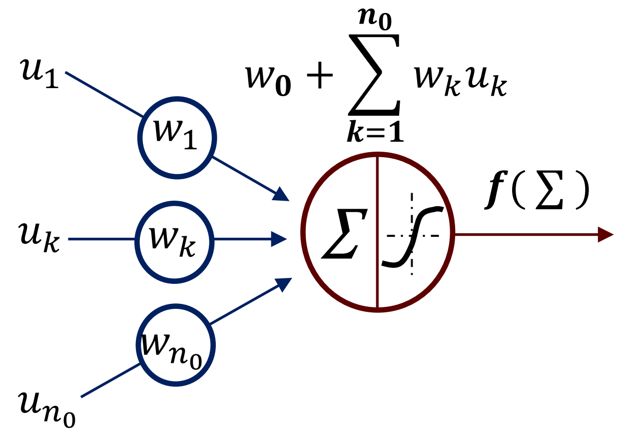
  - Needs to set up an identification process
    - Automatise with Bayesian inference

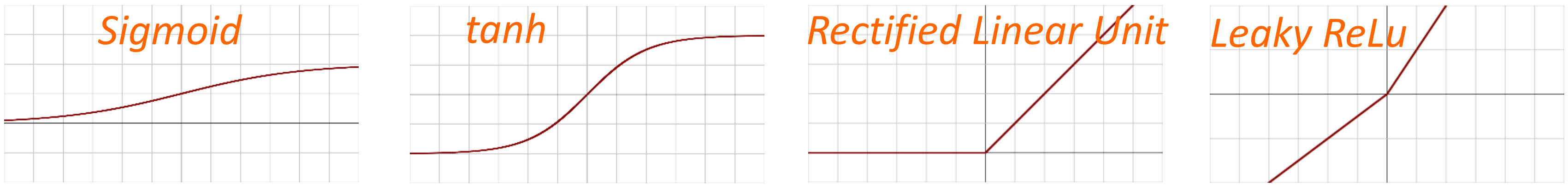
Meso-scale surrogate model for complex material systems



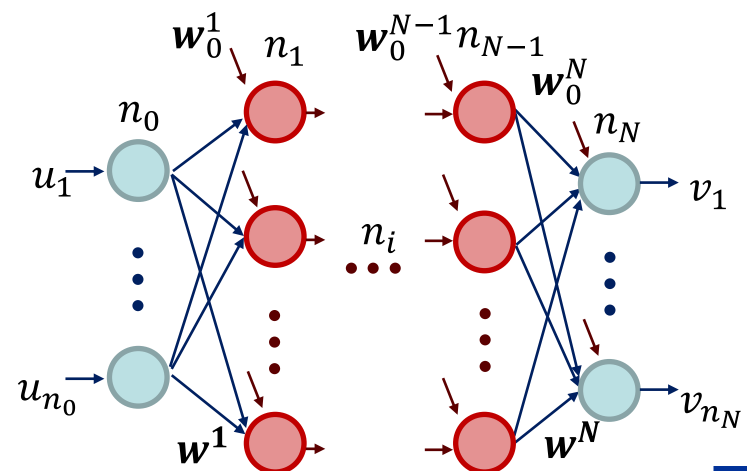
- Neural networks
  - Theoretically generic
    - Geometrical parameters: $\boldsymbol{\varphi}_{\mathrm{m}}$
    - Material parameters: $\boldsymbol{\gamma}_{\mathrm{m}}$
  - No extrapolation capabilities
    - Requires extensive data
- Field of growing interest (non-exhaustive list)
  - History-dependent material behaviours
    - Mozaffar, Bostanabad, Chen, Ehmann, Cao, Bessa (2019). Deep learning predicts path-dependent plasticity. PNAS
    - Ghavamian, Simone (2019). Accelerating multiscale finite element simulations of history-dependent materials using a recurrent neural network. CMAME
    - Bonatti, Mohr (2021) On the importance of self-consistency in recurrent neural network models representing elasto-plastic solids, JMPS
  - Surrogates for multi-scale simulations
    - Wu, Nguyen, Kilingar, Noels (2020). A recurrent neural network accelerated multi-scale model for elasto-plastic heterogeneous materials subjected to random cyclic and non-proportional loading paths. CMAME.
    - Masi, Stefanou (2022) Multiscale modeling of inelastic materials with Thermodynamics-based Artificial Neural Networks (TANN), CMAME
  - Combined with PCA
    - Wu, Noels (2022) Recurrent Neural Networks (RNNs) with dimensionality reduction and break down in computational mechanics; application to multi-scale localization step, CMAME
  - First step to stochastic-multi-scale
    - Lu, Yvonnet, Papadopoulos, Kalogeris, Papadopoulos (2021). A stochastic FE2 data-driven method for nonlinear multiscale modeling. Materials

- 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 $\Re^{n_0} \to \Re^{n_N}: \boldsymbol{v} = \boldsymbol{g}(\boldsymbol{u})$



Artificial Neural Network

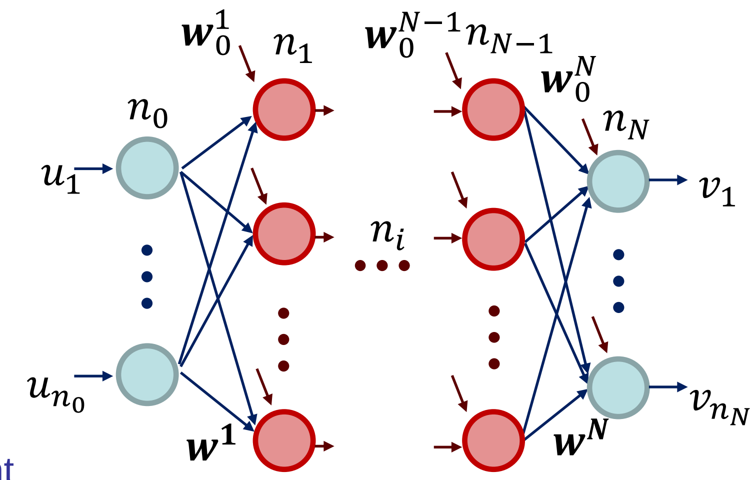
- Training
  - Evaluate
    - The weights w_{kj}^{i}, $k = 1..n_{i-1}, j = 1..n_i$
    - The bias w_0^i
    - Minimise error prediction $\boldsymbol{v}$ vs. real $\boldsymbol{v}^{(p)}$

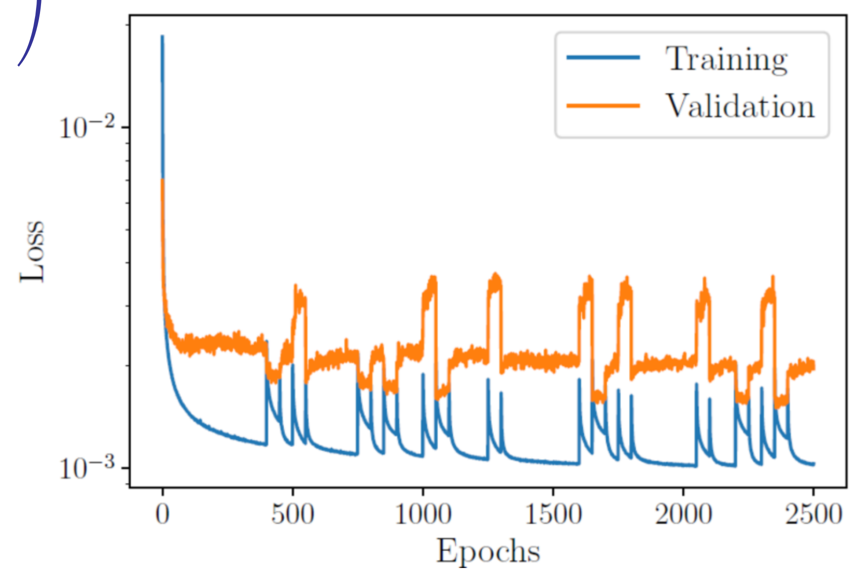
$$L_{\text{MSE}}\,(\mathbf{W}) = \frac{1}{n}\sum_{i}^{n}\left\|\boldsymbol{v}_i(\mathbf{W}) - \boldsymbol{v}_i^{(p)}\right\|^2$$

    - Requires an optimiser: Stochastic Gradient Descent

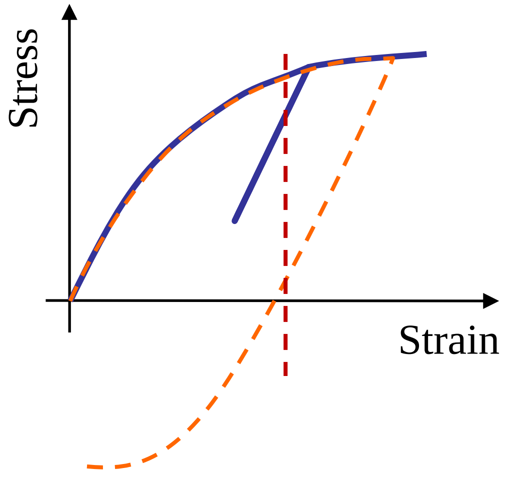
$$\boldsymbol{\Delta}\mathbf{W} = -\mathcal{F}\left(\frac{\partial L_i(\mathbf{W})}{\partial \mathbf{W}}, \quad \left(\frac{\partial L_i(\mathbf{W})}{\partial \mathbf{W}}\right)^2, \text{batch size}, \ldots\right)$$

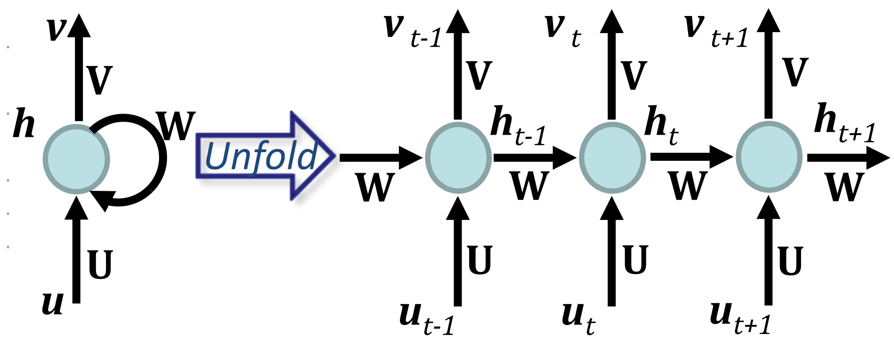
  - Training data
    - Input $\boldsymbol{u}^{(p)}$ & Output $\boldsymbol{v}^{(p)}$
- Testing
  - Use new data
    - Input $\boldsymbol{u}^{(p)}$& Output $\boldsymbol{v}^{(p)}$
    - Verify prediction $\boldsymbol{v}$ vs. real $\boldsymbol{v}^{(p)}$





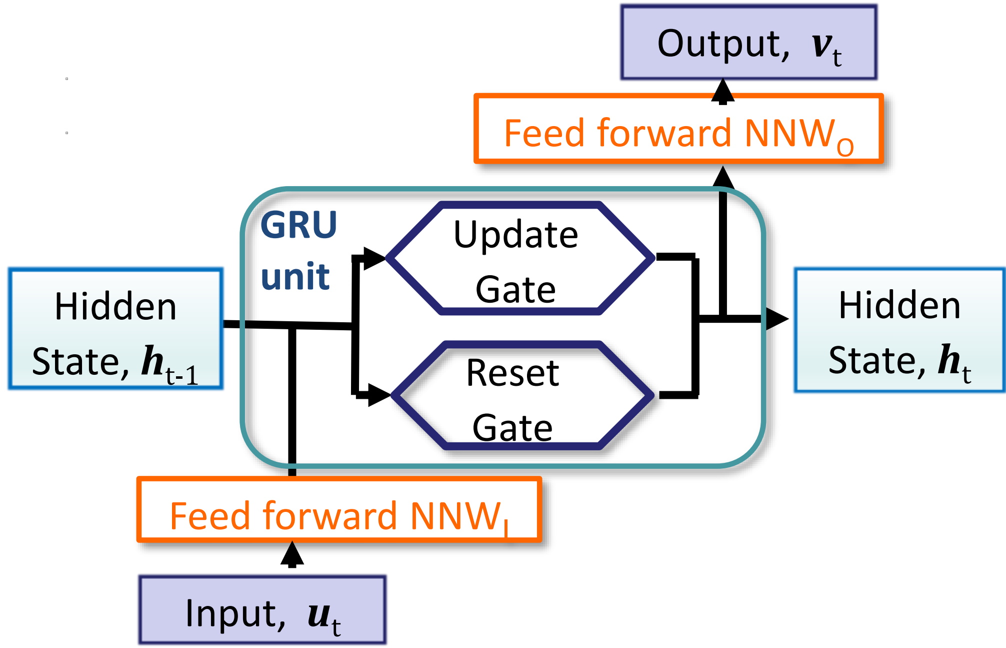
- Elasto-plastic material behaviour
  - No bijective strain-stress relation
    - Feed-forward NNW cannot be used
    - History should be accounted for
- Recurrent neural network
  - Allows a history dependent relation
    - Input $\boldsymbol{u}_t$
    - Output $\boldsymbol{v}_t = \boldsymbol{g}(\boldsymbol{u}_t,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

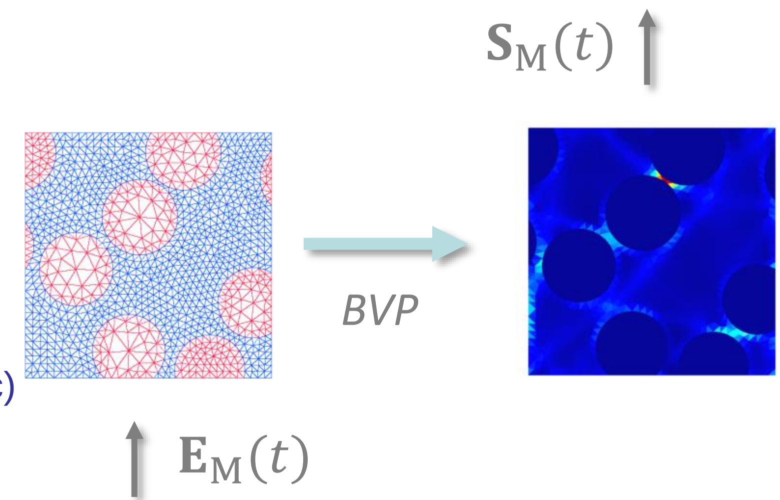




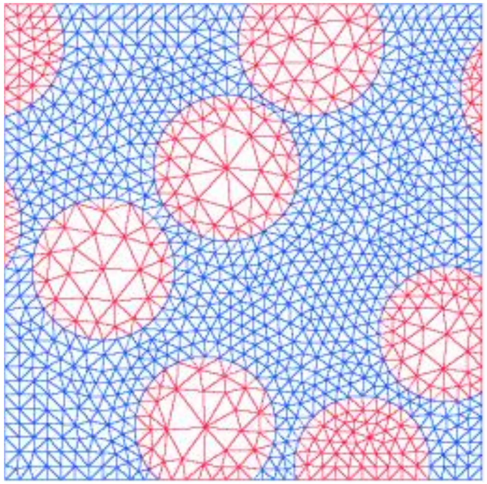
History dependency

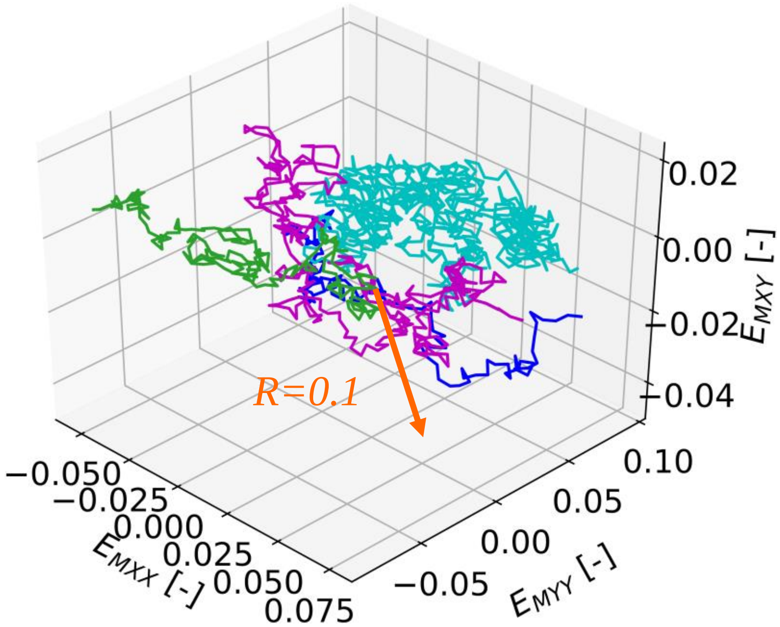
- Recurrent neural network design
  - 1 Gated Recurrent Unit (GRU)
    - Reset gate: select past information to be forgotten
    - Update gate: select past information to be passed along
    - Need to define number of hidden variables $\boldsymbol{h}_t$
  - 2 feed-forward NNWs
    - NNW_I to treat inputs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

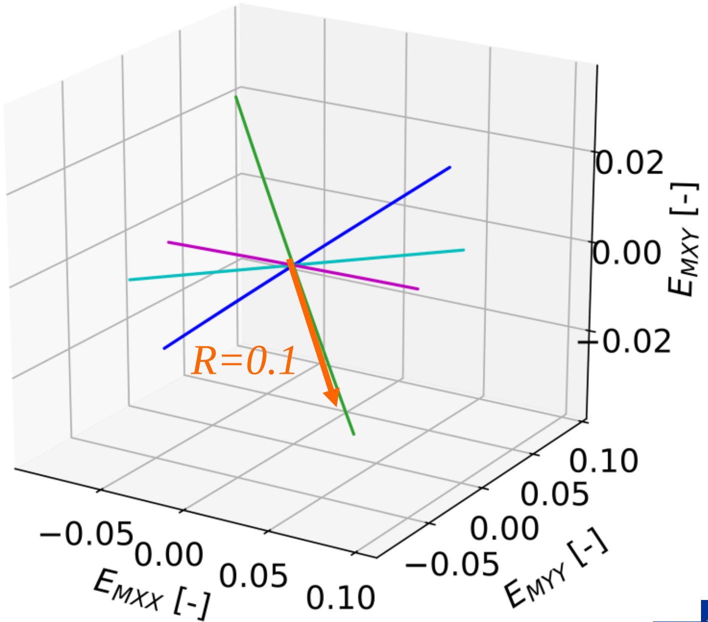




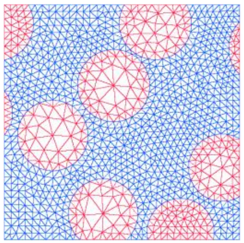
- Data generation
  - Elasto-plastic composite RVE
  - Training stage
    - Should cover full range of possible loading histories
    - Use random walking strategy (thousands)
    - Completed with random cyclic loading (tens)
    - Bounded by a sphere of 10% deformation

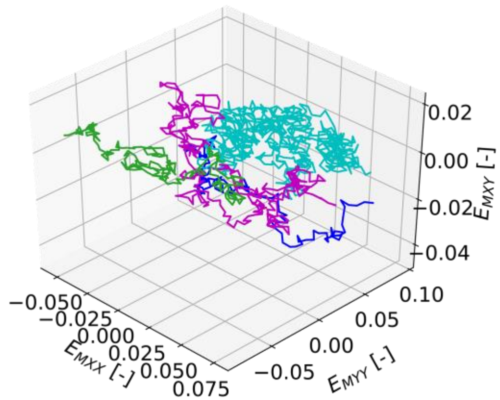


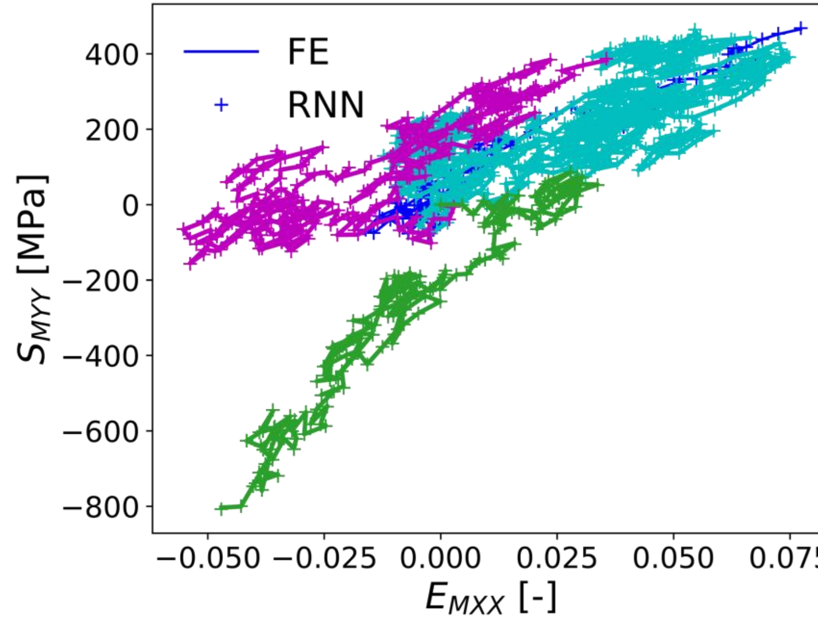


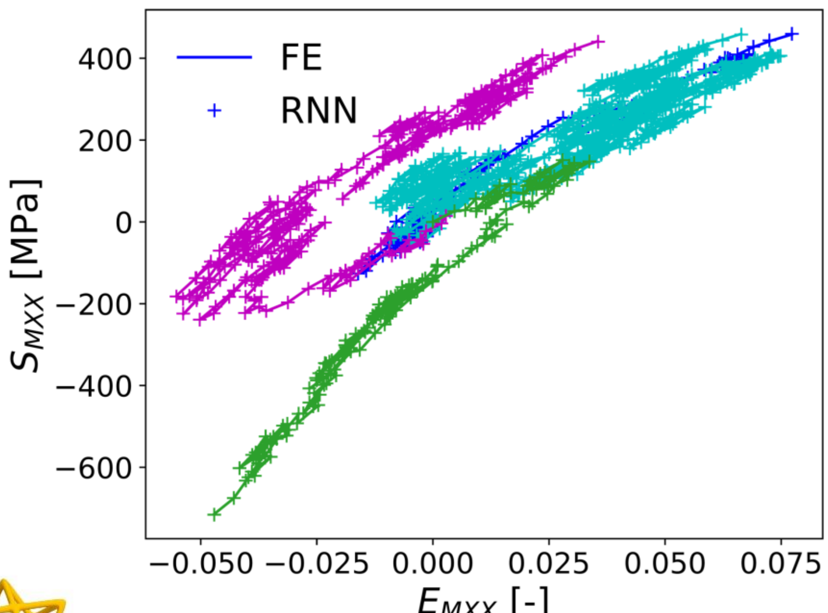


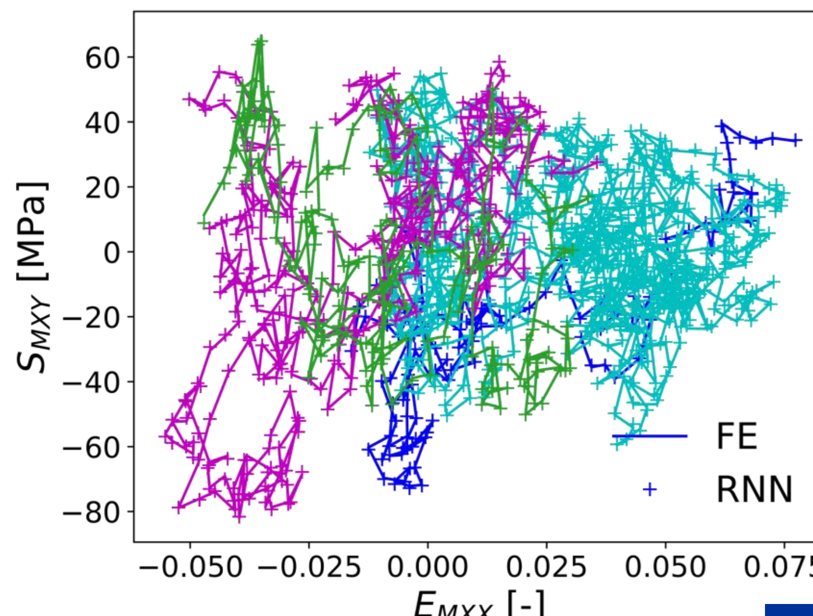
- Testing process (new data)
  - On random walk



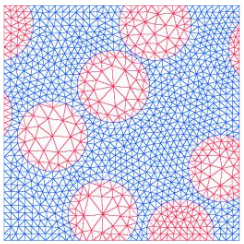


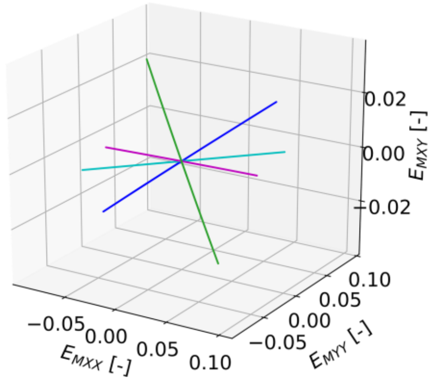


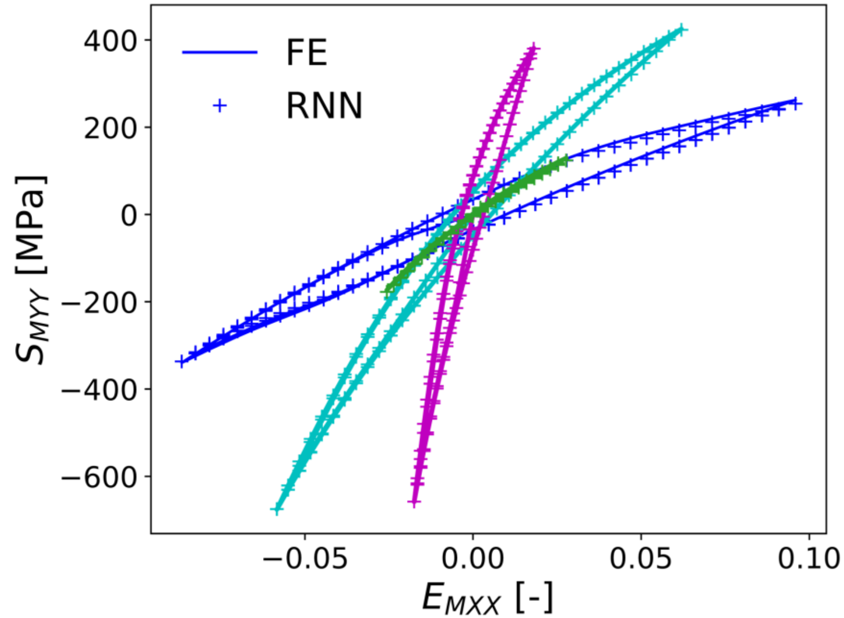


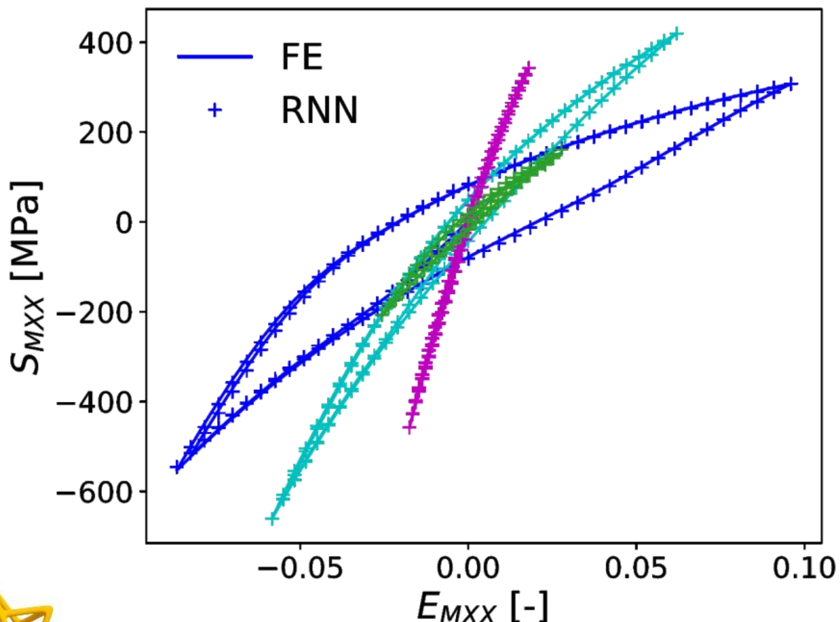


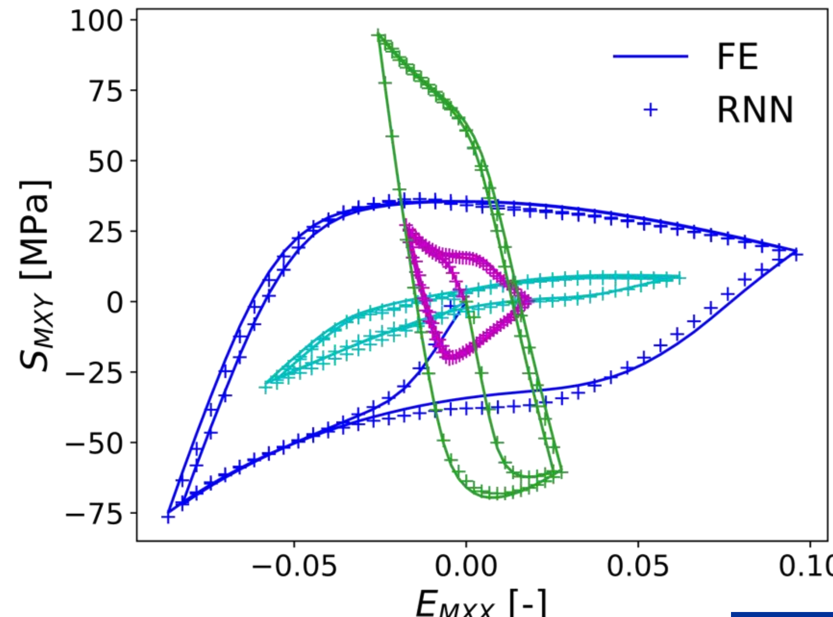
- Testing process (new data)
  - On cyclic loading



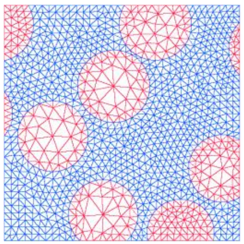


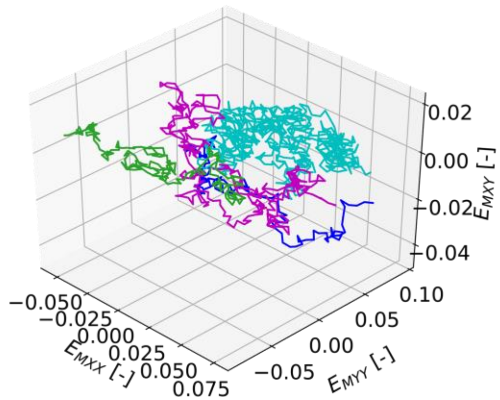


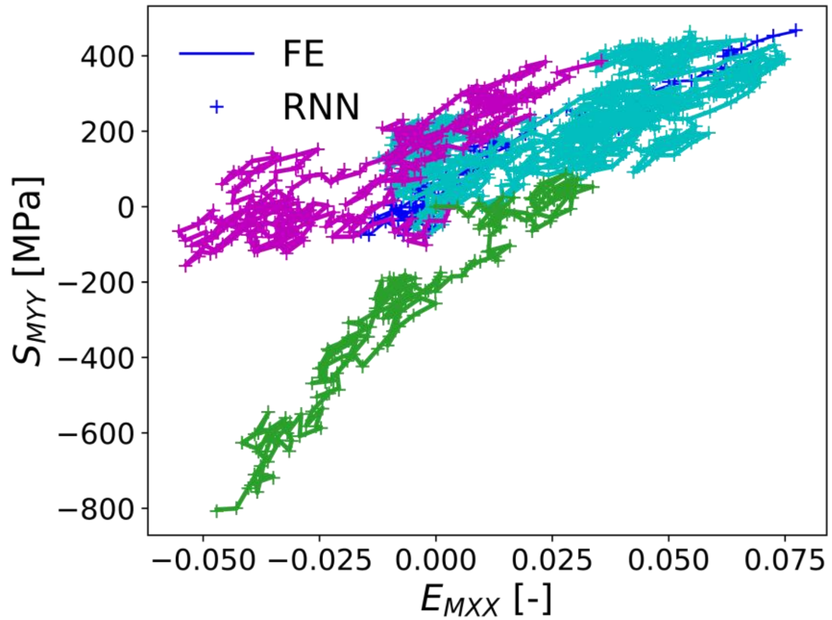




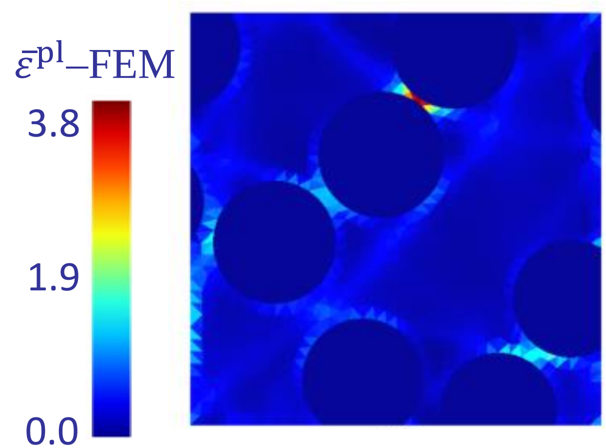
- Only homogenised output is predicted
  - On random walk



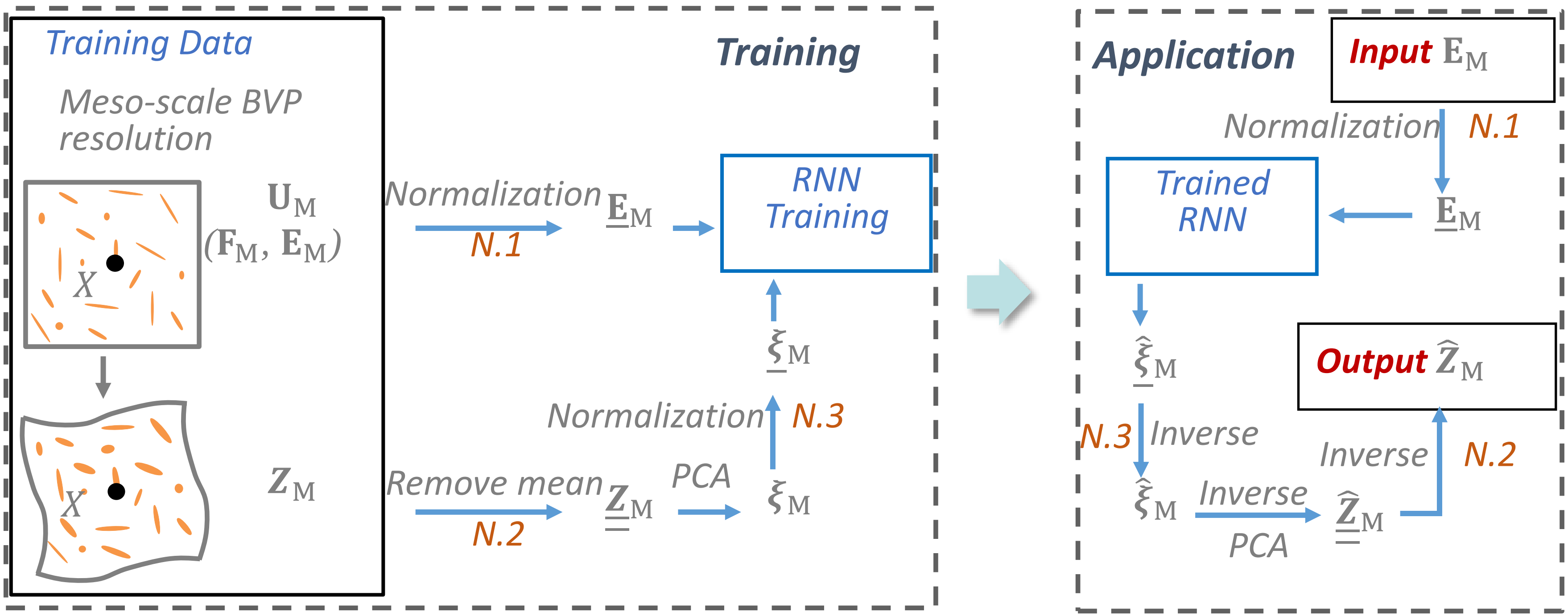




- Quid of local fields?
  - This is an advantage of multiscale methods
  - Useful to predict failure, fatigue etc.
  - Can we get it back at low cost?

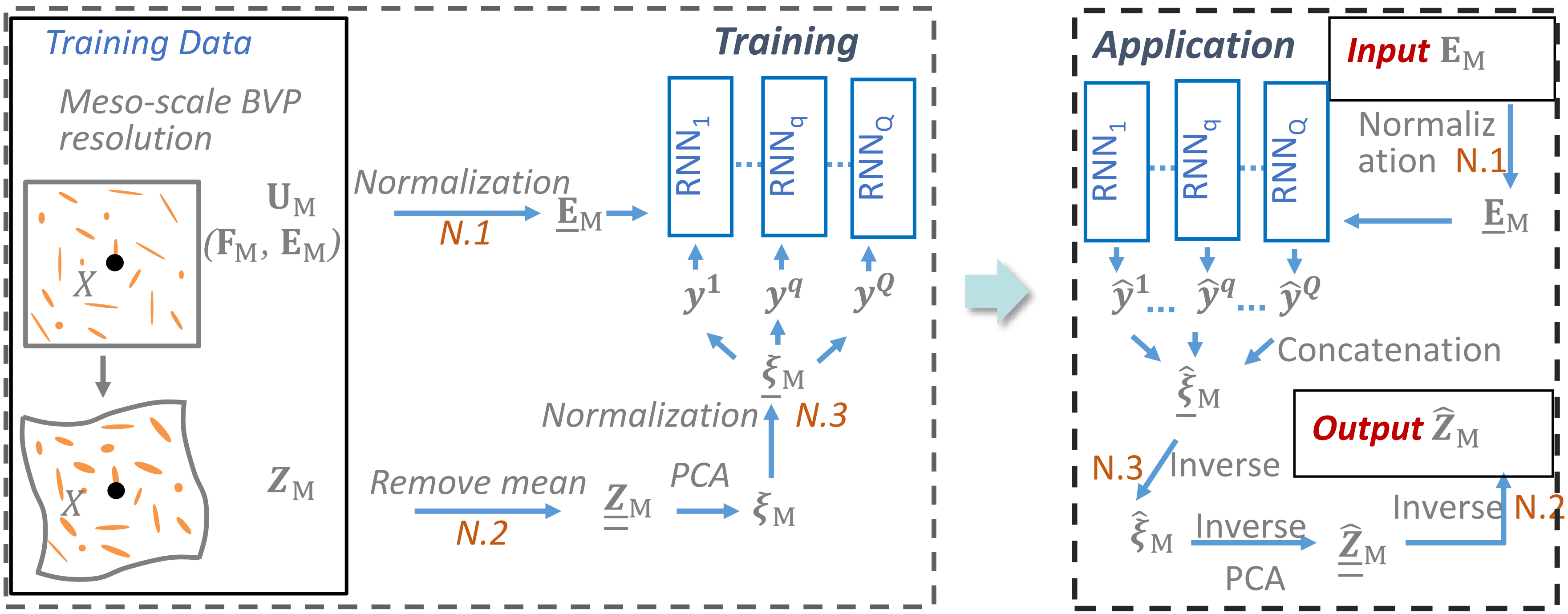


- Optimise the method: reduce the size of the internal variables



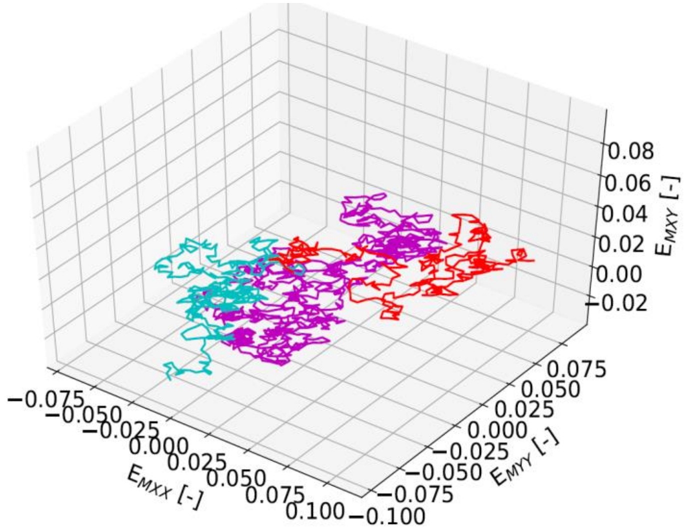
- Principal Component Analysis (PCA) applied on $\underline{Z}_\mathrm{M}$ to reduce the output of RNN
  - Construct matrix $\mathbf{Z_M} = \left[\underline{\underline{Z}}_{\mathrm{M}_1}\ \underline{\underline{Z}}_{\mathrm{M}_2}\ \ldots \underline{\underline{Z}}_{\mathrm{M}_n}\right]_{d\times n}$ from 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 $\mathbf{V} = \left[\ \underline{v}_1\ \underline{v}_2\ \ \ldots \underline{v}_p\ \right]_{d\times p}$ and reduced data $\boldsymbol{\xi}_\mathrm{M} = \mathbf{V}^T\underline{\underline{Z}}_\mathrm{M}$ of size $p < d$
  - Reconstruction $\hat{\underline{\underline{Z}}}_\mathrm{M} = \mathbf{V}\boldsymbol{\xi}_\mathrm{M}$
  - But not enough

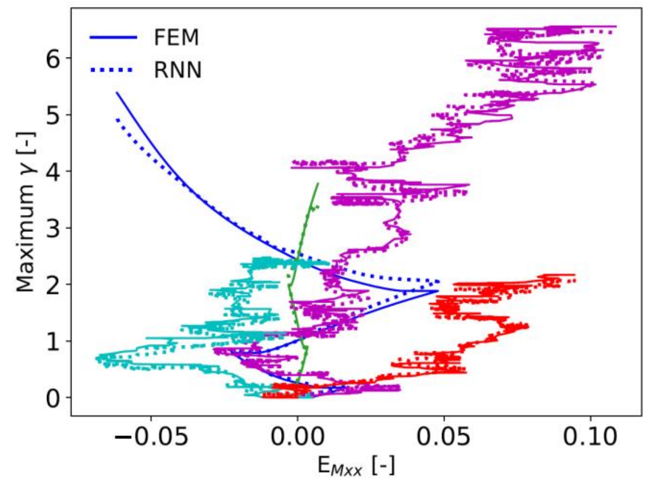
- Dimensionality reduction & break down



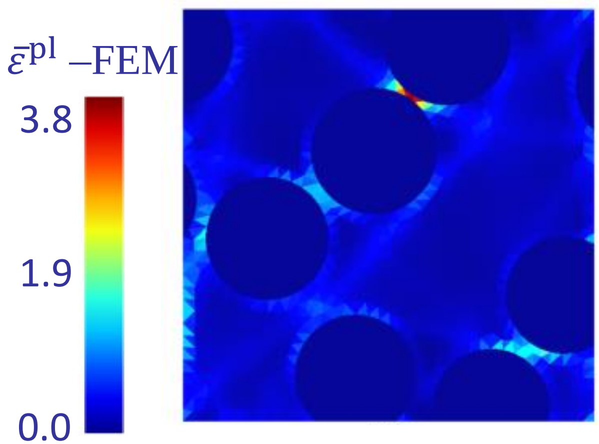
  - To further reduce the output dimension of RNN
    - The surrogate modelling is carried out by a few small RNNs, instead of one big RNN
    - The high dimension output is divided into Q groups, and each RNN is used to reproduce only a part of output
  - PCA reduces Z_M to 180 outputs and we use Q=6

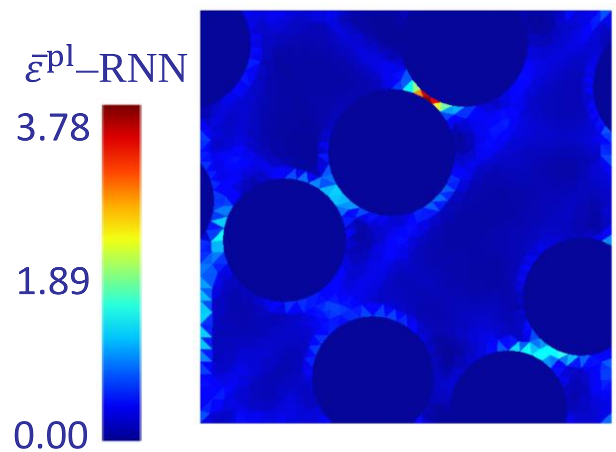
- Evaluation of equivalent plastic strain $\bar{\varepsilon}^{\mathrm{pl}}$: Random loading (testing data)



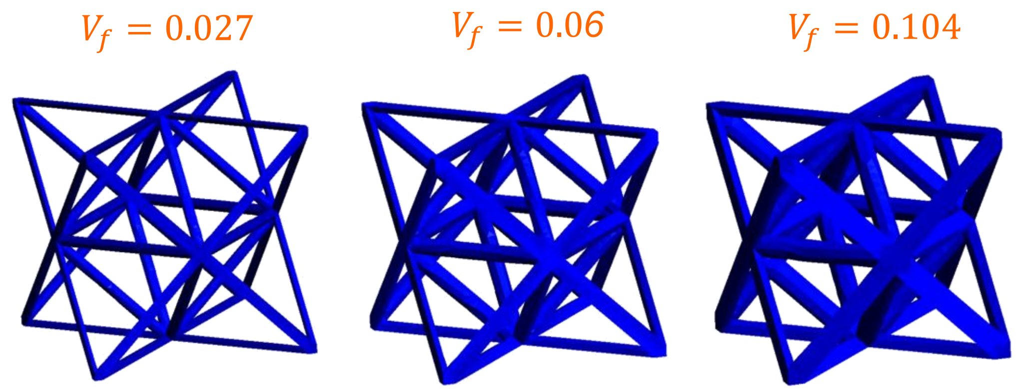


Purple loading – step 500

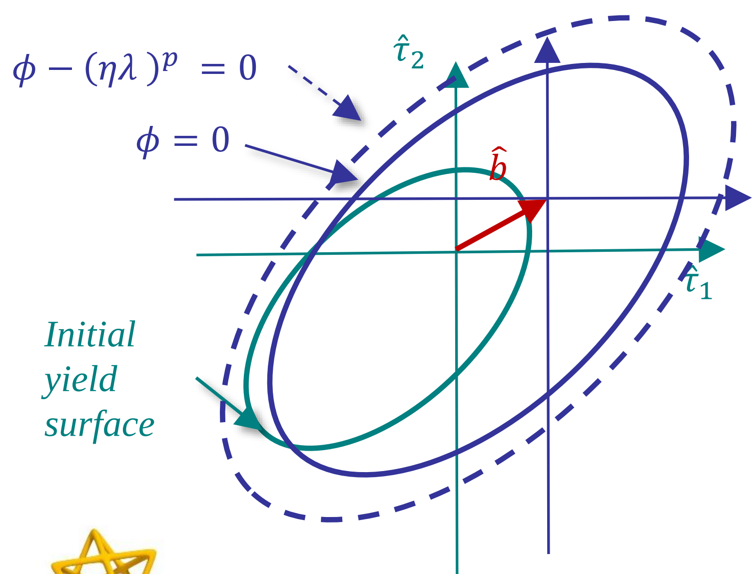


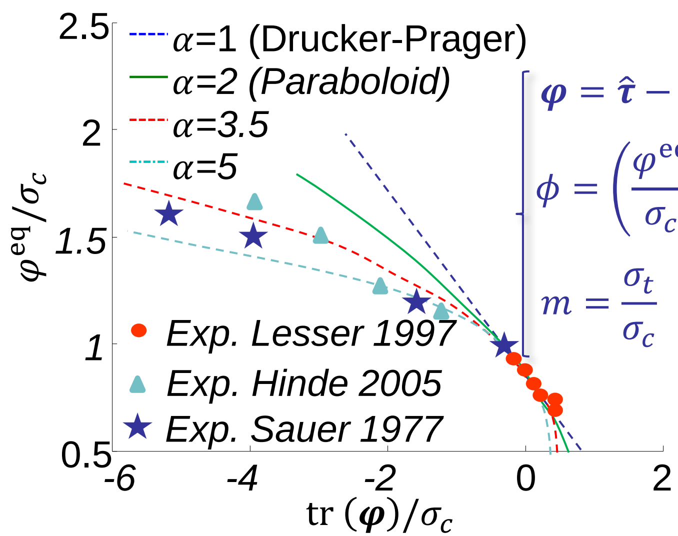


- Study of PA lattices
  - Input:
    - Strain (history): $\mathbf{F}_{\mathrm{M}}$
    - Geometrical parameters: $\boldsymbol{\varphi}_{\mathrm{m}}$
    - Material parameters: $\boldsymbol{\gamma}_{\mathrm{m}}$
  - Output:
    - Stress (history): $\mathbf{P}_{\mathrm{M}}$



- Material model
  - Viscoelastic-viscoplastic finite strain model





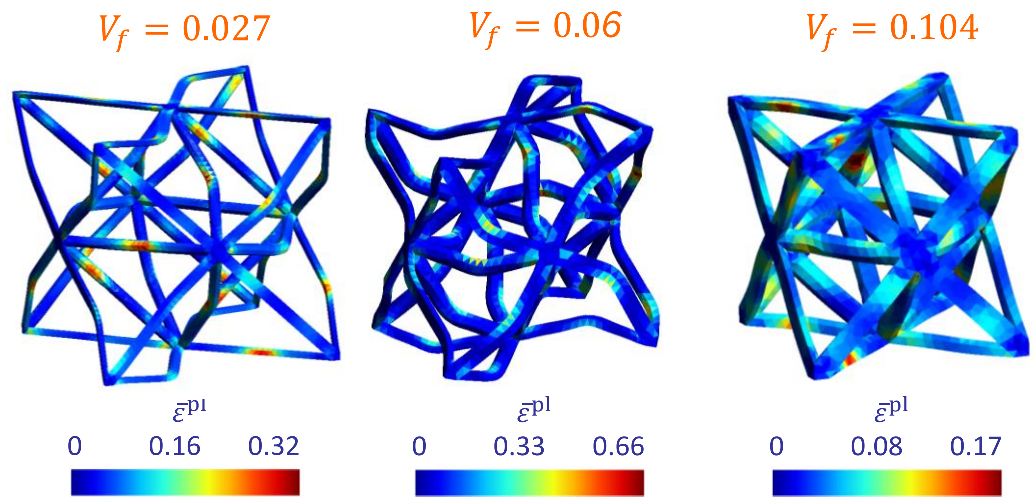
$$\boldsymbol{\varphi} = \hat{\boldsymbol{\tau}} - \hat{\boldsymbol{b}}$$

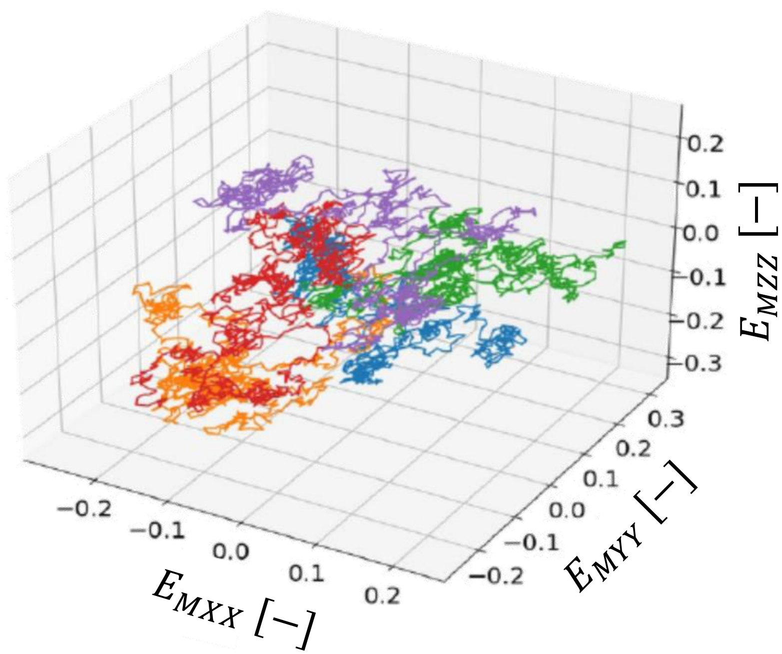
$$\phi = \left(\frac{\varphi^{\mathrm{eq}}}{\sigma_c}\right)^{\alpha} - \frac{m^{\alpha}-1}{m+1}\frac{\mathrm{tr}\boldsymbol{\varphi}}{\sigma_c} - \frac{m^{\alpha}+m}{m+1}$$

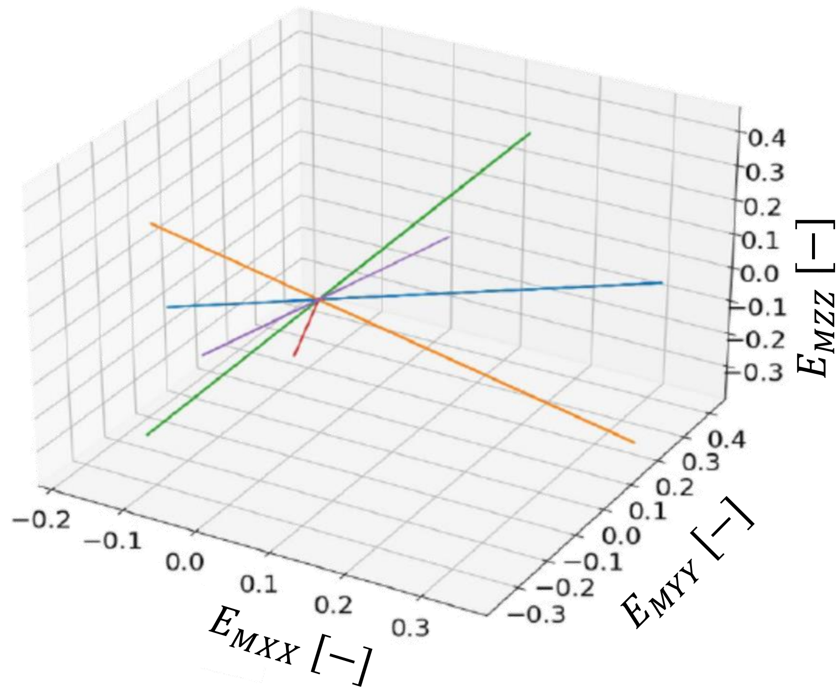
$$m = \frac{\sigma_t}{\sigma_c}$$

Geometrical parameters effect

- Input / output Generation
  - Input:
    - Random strain (history): $\mathbf{F}_{\mathrm{M}}$
    - Random geometrical parameters: $\boldsymbol{\varphi}_{\mathrm{m}}$
  - Output:
    - Stress (history): $\mathbf{P}_{\mathrm{M}}$

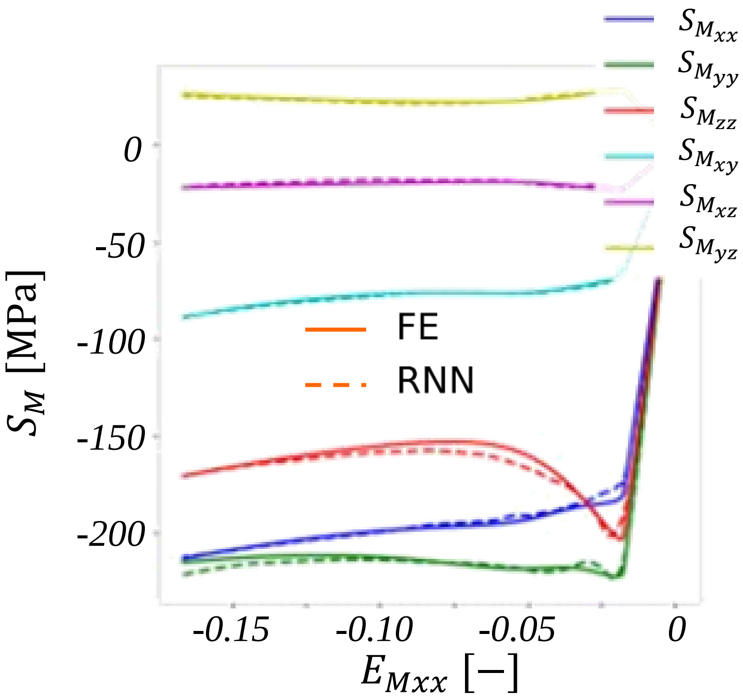


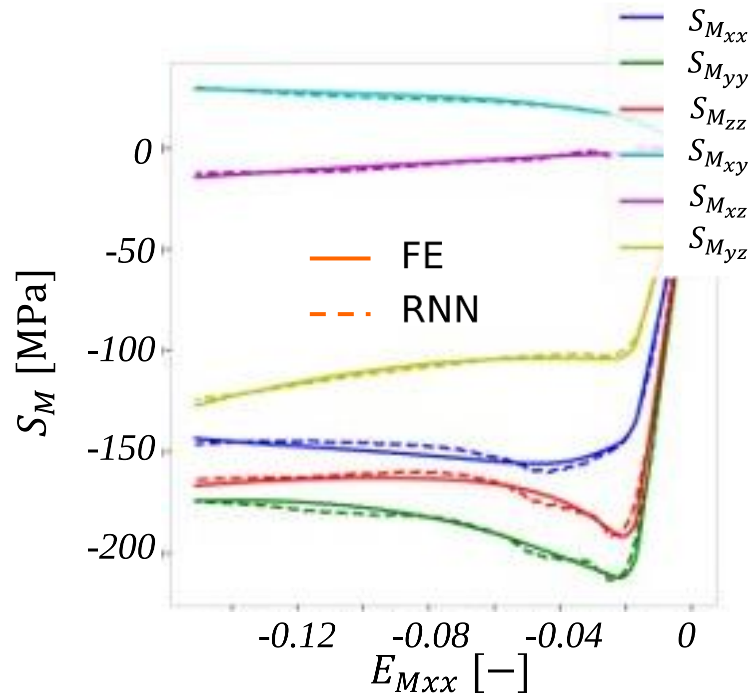




Geometrical parameters effect

- Lattice cell
  - Test on new cells of random volume fraction for new cyclic paths
    (per unit volume of polymer)



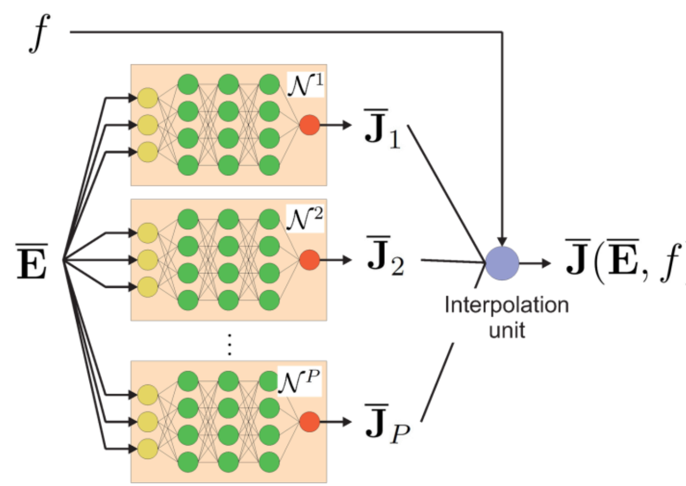


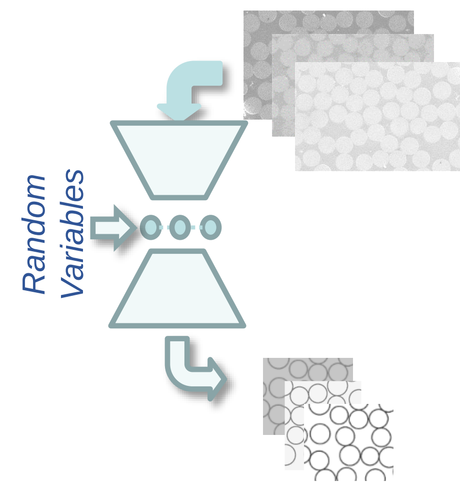
Meso-scale surrogate model for complex material systems

- Neural networks can account for
  - Strain (history): $\mathbf{F}_{\mathrm{M}}$
  - Geometrical parameters: $\boldsymbol{\varphi}_{\mathrm{m}}$
  - Material parameters: $\boldsymbol{\gamma}_{\mathrm{m}}$
- However, this requires
  - Extensive training data
    - Interpolation of neural network trained for different inclusions volume fraction f is considered to reduced the number of training data

    [Lu, Yvonnet, Papadopoulos, Kalogeris, Papadopoulos (2021). A stochastic FE2 data-driven method for nonlinear multiscale modeling. Materials]
  - Identified geometrical features
    - Quid for distribution effect?
    - Possibility is to extract information from image analysis
    - e.g. using CNN

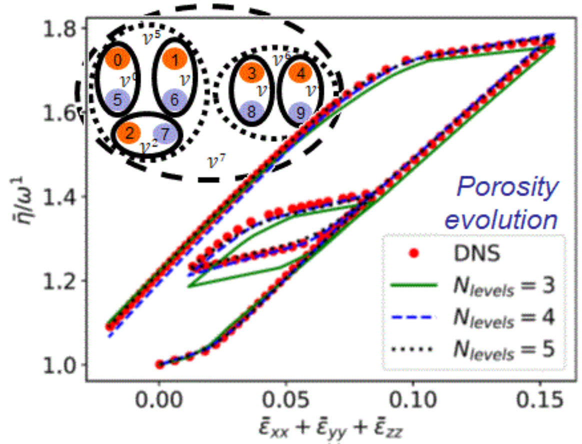
    [Rao, C., & Liu, Y. (2020). Three-dimensional convolutional neural network (3D-CNN) for heterogeneous material homogenization. CMS]



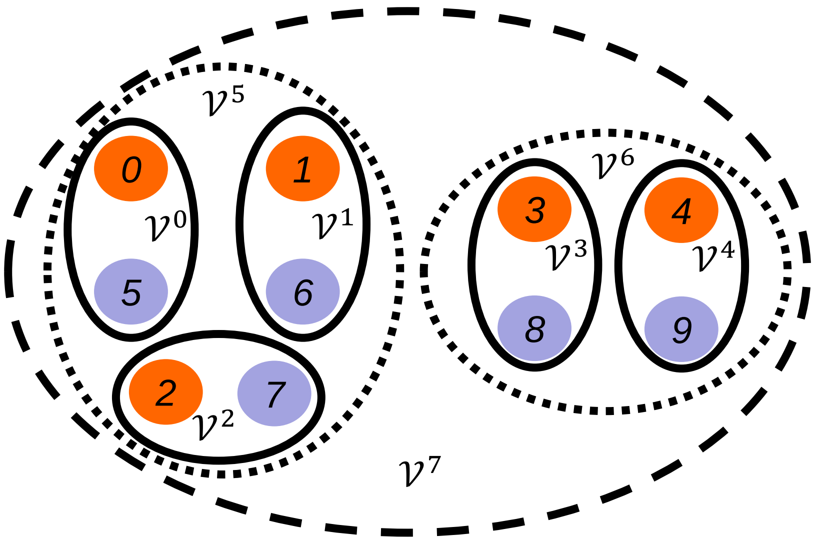


Meso-scale surrogate model for complex material systems

- Deep material networks
  - Based on thermodynamic consistency
  - Possesses extrapolation capabilities in
    - Strain (history): $\mathbf{F}_\mathrm{M}$
    - Material parameters: $\boldsymbol{\gamma}_\mathrm{m}$
- Emerging methodology
  - Seminal work
    - Liu, Wu, Koishi, (2019). A deep material network for multiscale topology learning and accelerated nonlinear modeling of heterogeneous materials. CMAME
  - Reformulation and use as surrogate for arbitrary material law
    - Gajek, Schneider, Böhlke, (2021). An FE–DMN method for the multiscale analysis of short fiber reinforced plastic components. CMAME
    - Nguyen, Noels, L. (2022). Interaction-based material network: A general framework for (porous) microstructured materials. CMAME
  - Interpolate some geometrical features of micro-structure $\boldsymbol{\varphi}_\mathrm{m}$
    - Huang, Liu, Wu, Chen, Wei (2022). Microstructure-guided deep material network for rapid nonlinear material modeling and uncertainty quantification. CMAME



- Architecture of mechanistic building blocks
  - Example for a 2-phase material



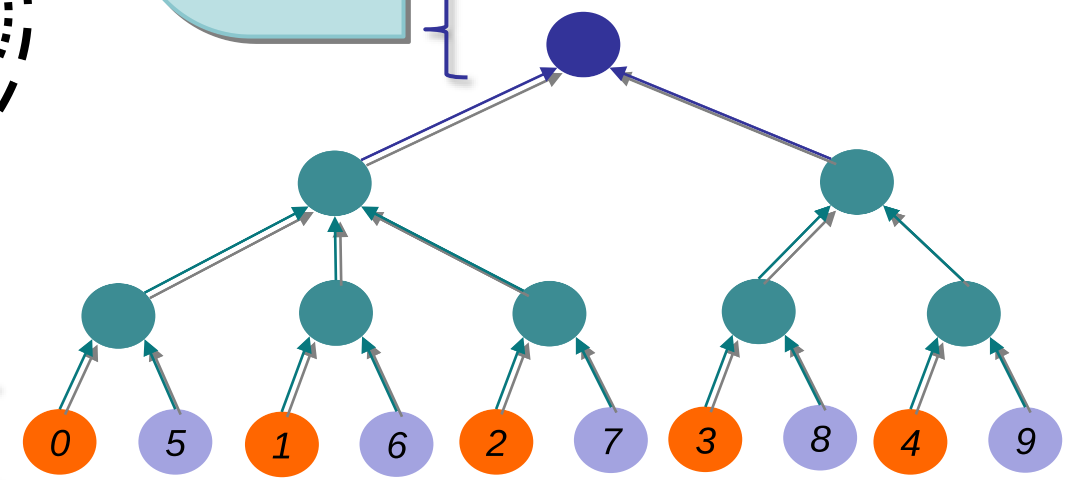
Homogenised behaviour

$$\mathbf{P}_{\mathbf{M}}(t) = \mathbf{P}\,(\mathbf{F}_{\mathrm{M}}(t), \boldsymbol{Z}(\tau \le t))$$

$$\mathbf{P}_{\mathbf{M}}(t) = \sum_{i=0}^{9} W^i\, \mathbf{P}^i(t)$$

$$\mathbf{F}_{\mathrm{M}}(t) = \sum_{i=0}^{9} W^i\, \mathbf{F}^i(t)$$

Weight of node i (parameter)



Material node i =0..9, of weight W^i

Constitutive behaviours: $\mathbf{P}^p(t) = \mathbf{P}^p\left(\mathbf{F}^i(t), \boldsymbol{Z}(\tau \le t)\right)$

if node i ∈ phase p for material p=0 or p=1

Z. Liu, C. Wu, M. Koishi, A deep material network for multiscale topology learning and accelerated nonlinear modeling of heterogeneous materials

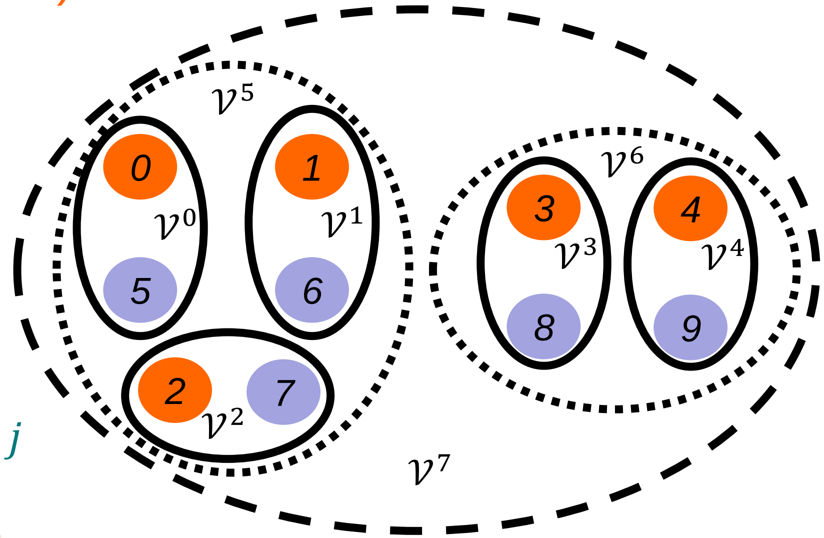
- Alternative to laminate (e.g. for porous material)
- Mechanism $j = 0..M-1$ of interaction $\mathcal{V}^j$
  - Homogenised deformation gradient
    - Construction of a strain fluctuation field

$$\mathbf{F}_\mathrm{M} + \sum_{j:i\in\mathcal{V}^j} \alpha^{i,j}\, \boldsymbol{a}^j \otimes \boldsymbol{N}^j = \boldsymbol{F}^i\,, \quad j = 0..M-1$$

Contribution of node i in mechanism j (parameter?)

Degrees of freedom of mechanism j defining the strain fluctuation

Direction of mechanism j (parameter)



Deep Material Networks from the interactions viewpoint

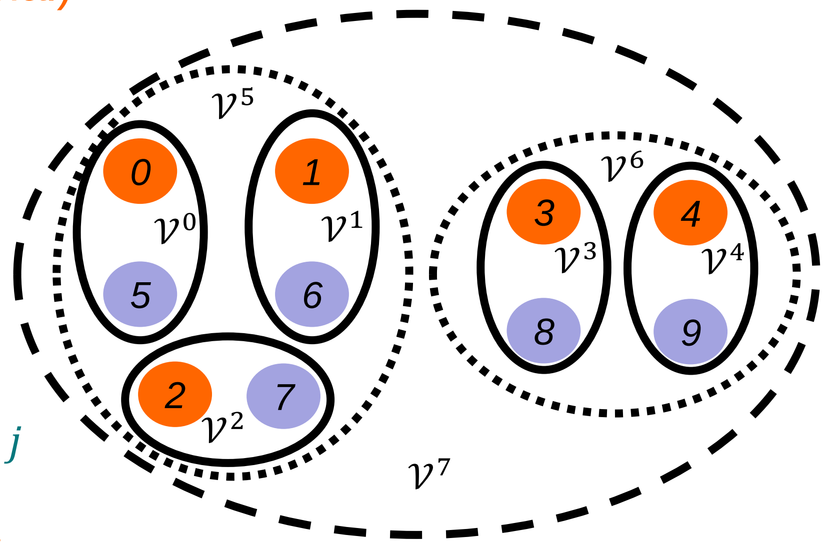
- Alternative to laminate (e.g. for porous material)
- Mechanism $j = 0..M-1$ of interaction $\mathcal{V}^j$
  - Homogenised deformation gradient
    - Construction of a strain fluctuation field

$$\mathbf{F}_\mathrm{M} + \sum_{j:i\in\mathcal{V}^j} \alpha^{i,j}\, \boldsymbol{a}^j \otimes \boldsymbol{N}^j = \boldsymbol{F}^i\,, \quad j = 0..M-1$$

Contribution of node i in mechanism j (parameter?)

Degrees of freedom of mechanism j defining the strain fluctuation

Direction of mechanism j (parameter)

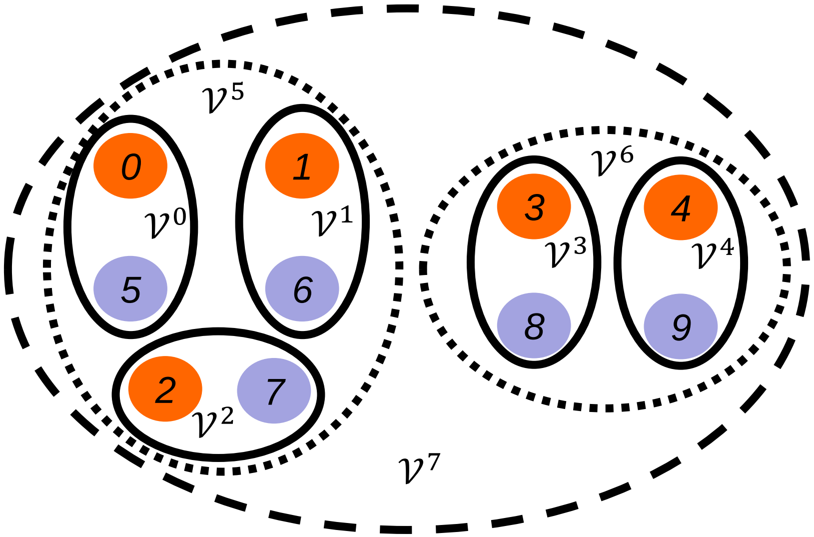


Weight of node i (parameter)

  - Constraints from strain averaging
    - $\mathbf{F}_\mathrm{M} = \sum_i W^i \mathbf{F}^i$ ⇒ $\sum_j \left(\sum_{i\in\mathcal{V}^j} W^i \alpha^{i,j} \right) \boldsymbol{a}^j \otimes \boldsymbol{N}^j = 0$ ⇒ $\sum_{i\in\mathcal{V}^j} W^i \alpha^{i,j} = 0$
  - Weak form from Hill-Mandel
    - $\mathbf{P}_\mathrm{M} : \delta\mathbf{F}_\mathrm{M} = \sum_i W^i\, \mathbf{P}^i : \delta\mathbf{F}^i$ ⇒ $\left[\sum_j \left(\sum_{i\in\mathcal{V}^j} W^i \mathbf{P}^i \alpha^{i,j} \right) \cdot \boldsymbol{N}^j \right] \cdot\, \delta\boldsymbol{a}^j = 0$

- Offline stage on a p-phase RVE
  - Topological parameters $\boldsymbol{\chi}$
    - Nodal weight: $W^i, i = 0..9$
    - Direction of interaction $\mathcal{V}^j$: $\boldsymbol{N}^j, j = 0..7$
    - Interaction weight: $\alpha^{i,j}$

  ⇨ $\boldsymbol{\chi} = [W^0, \dots, W^9, \boldsymbol{N}^0, \dots, \boldsymbol{N}^7, \alpha^{0,0}, \dots \ \alpha^{9,7}]$

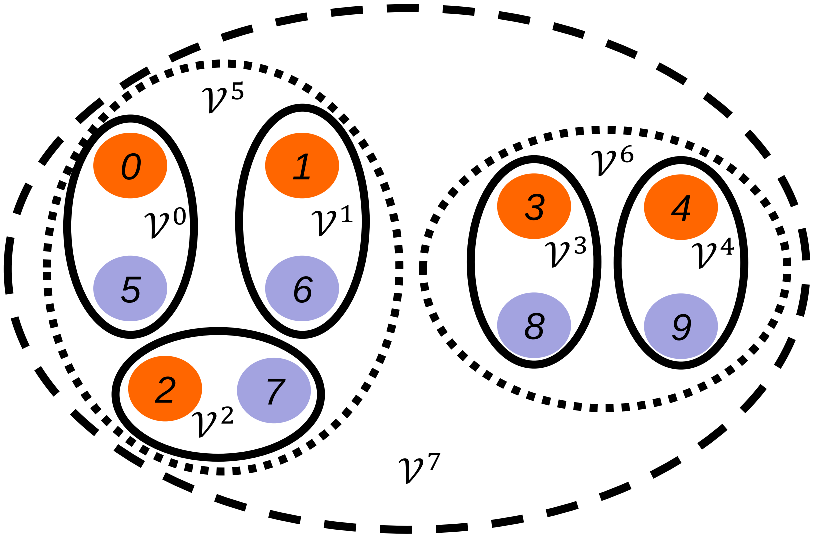


  - Using elastic data
    - Random properties on RVE ⇨ $\hat{\mathbb{C}}_{\mathrm{M}}(\boldsymbol{\gamma}_{\mathrm{m}})$

      $\boldsymbol{\gamma}_{\mathrm{m}} = [E_0, \nu_0, E_1, \nu_1 \dots E_p, \nu_p]$
    - Cost functions to minimise $L(\hat{\mathbb{C}}_{\mathrm{M}}, \mathbb{C}_{\mathrm{M}}(\boldsymbol{\chi})) = \frac{1}{n}\sum_{s=1}^{n} \frac{\|\hat{\mathbb{C}}_{\mathrm{M}}(\boldsymbol{\gamma}_{\mathrm{m}_s}) - \mathbb{C}_{\mathrm{M}}(\boldsymbol{\chi}|\boldsymbol{\gamma}_{\mathrm{m}_s})\|}{\|\hat{\mathbb{C}}_{\mathrm{M}}(\boldsymbol{\gamma}_{\mathrm{m}_s})\|}$
    - By « stochastic gradient descent (SGD) » algorithm

- Offline stage on a p-phase RVE
  - Topological parameters $\boldsymbol{\chi}$
    - Nodal weight: $W^i, i = 0..9$
    - Direction of interaction $\mathcal{V}^j$: $\boldsymbol{N}^j, j = 0..7$
    - Interaction weight: $\alpha^{i,j}$

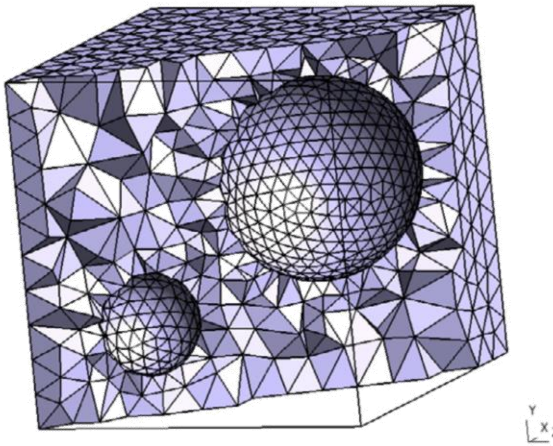
  ⇨ $\boldsymbol{\chi} = [W^0, \dots, W^9, \boldsymbol{N}^0, \dots, \boldsymbol{N}^7, \alpha^{0,0}, \dots \ \alpha^{9,7}]$

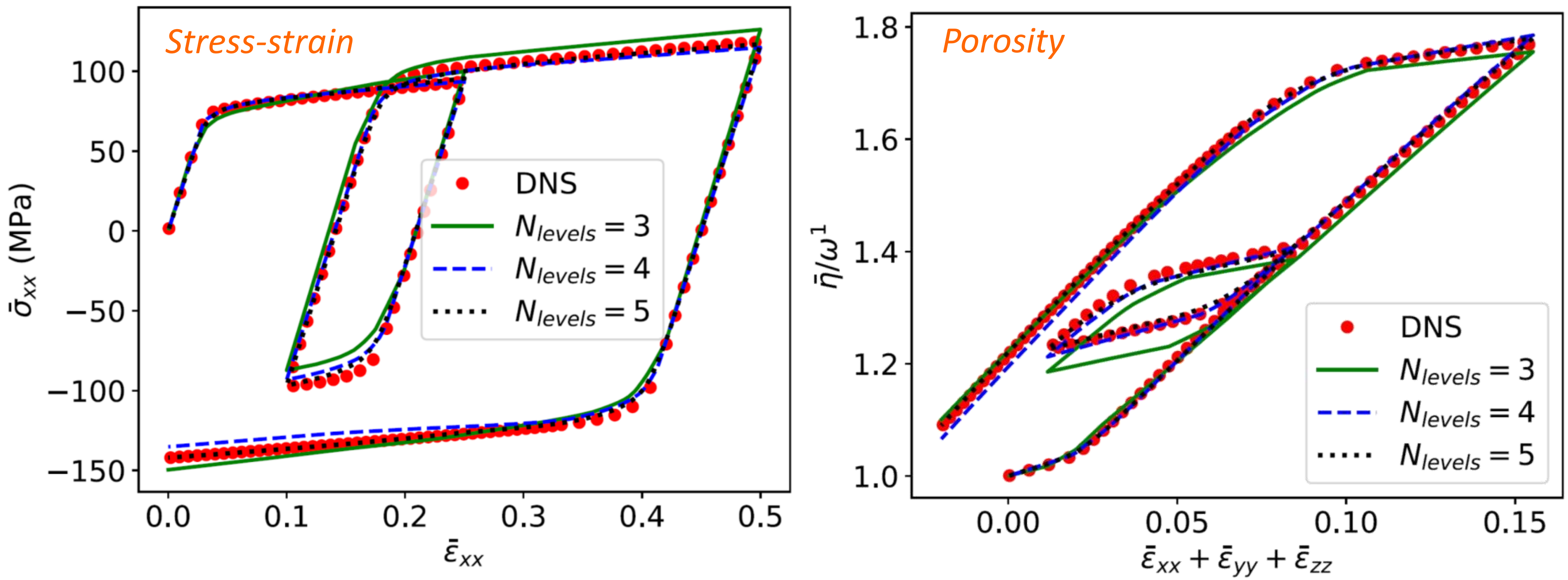


  - Using elastic data
    - Random properties on RVE ⇨ $\hat{\mathbb{C}}_{\mathrm{M}}(\boldsymbol{\gamma}_{\mathrm{m}})$

      $\boldsymbol{\gamma}_{\mathrm{m}} = [E_0, \nu_0, E_1, \nu_1 \dots E_p, \nu_p]$
    - Cost functions to minimise $L(\hat{\mathbb{C}}_{\mathrm{M}}, \mathbb{C}_{\mathrm{M}}(\boldsymbol{\chi})) = \frac{1}{n}\sum_{s=1}^{n} \frac{\|\hat{\mathbb{C}}_{\mathrm{M}}(\boldsymbol{\gamma}_{\mathrm{m}_s}) - \mathbb{C}_{\mathrm{M}}(\boldsymbol{\chi}|\boldsymbol{\gamma}_{\mathrm{m}_s})\|}{\|\hat{\mathbb{C}}_{\mathrm{M}}(\boldsymbol{\gamma}_{\mathrm{m}_s})\|}$
  - Using non-linear response
    - Random loading on RVE (strain sequence $\mathbf{F}_{\mathrm{M}_s}$)
    - Compare stress history $\mathbf{P}_{\mathrm{M}}(\mathbf{F}_{\mathrm{M}_s})$ and quantity of interest $Z(\mathbf{F}_{\mathrm{M}_s})$ (e.g. porosity)
    - Cost function $L\left(\hat{\mathbf{P}}_{\mathrm{M}}, \mathbf{P}_{\mathrm{M}}(\boldsymbol{\chi})\right) = \frac{1}{n}\sum_{s=1}^{n} \frac{\|\hat{\mathbf{P}}_{\mathrm{M}}(\mathbf{F}_{\mathrm{M}_s}) - \mathbf{P}_{\mathrm{M}}(\boldsymbol{\chi}|\mathbf{F}_{\mathrm{M}_s})\|}{\|\hat{\mathbf{P}}_{\mathrm{M}}(\mathbf{F}_{\mathrm{M}_s})\|} + \frac{1}{n}\sum_{s=1}^{n} \frac{\|\hat{Z}(\mathbf{F}_{\mathrm{M}_s}) - \bar{Z}(\boldsymbol{\chi}|\mathbf{F}_{\mathrm{M}_s})\|}{\|\hat{Z}(\mathbf{F}_{\mathrm{M}_s})\|}$
    - By « stochastic gradient descent (SGD) » algorithm

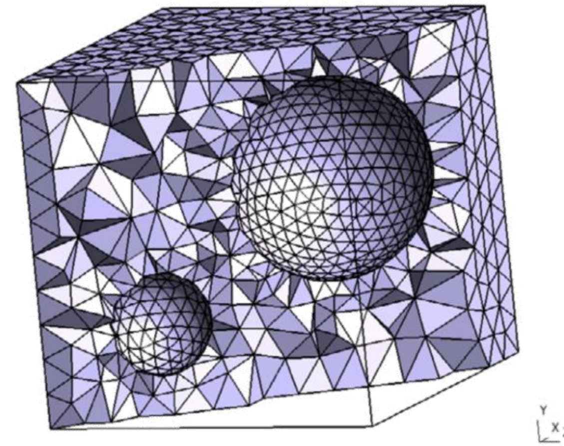
- Online stage on a porous material
  - Properties
    - Elasto-plastic matrix
    - Small strain
  - Non-linear training
  - Uniaxial tension

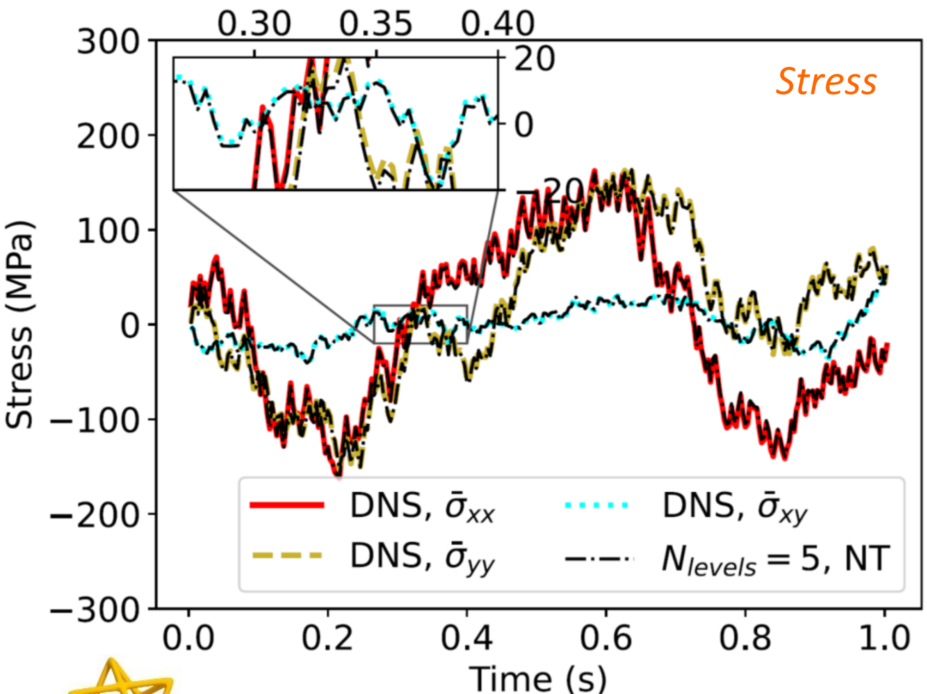


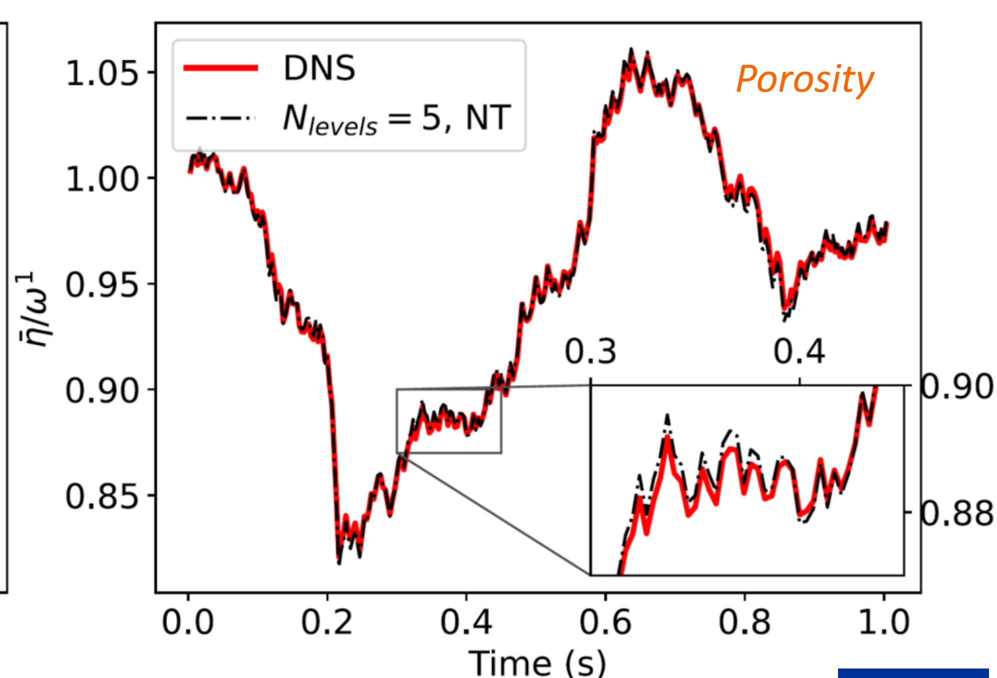


Deep Material Networks from the interactions viewpoint

- Online stage on a porous material
  - Properties
    - Elasto-plastic matrix
    - Small strain
  - Extrapolation capabilities
    - Non-linear training with material parameters γ_{m1}
    - On-line simulation with material parameters γ_{m2}
  - Random loading



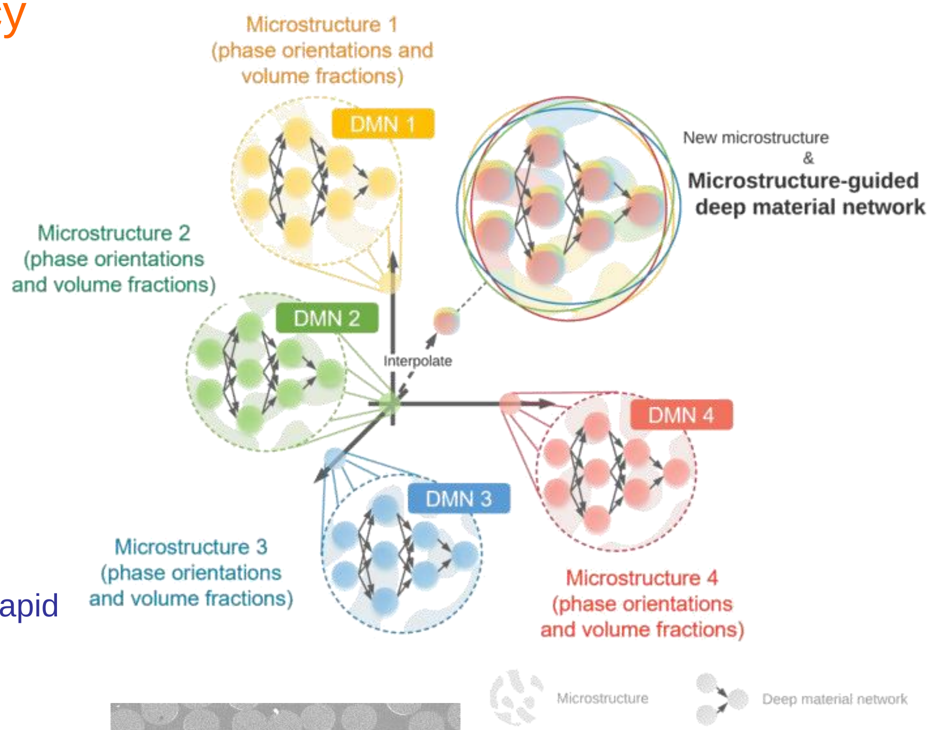


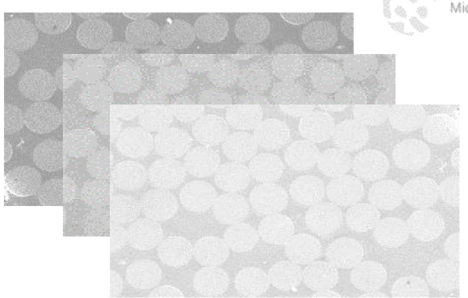


Meso-scale surrogate model for complex material systems

- Deep material networks can account for
  - Strain (history): $\mathbf{F}_\mathrm{M}$
  - Material parameters: $\boldsymbol{\gamma}_\mathrm{m}$
- Because of thermodynamic consistency
  - Possesses extrapolation capabilities
    - ⇨ Reduced training dataset
- However, interactions are defined for
  - Geometrical parameters: $\boldsymbol{\varphi}_\mathrm{m}$
  - For an identified geometrical features
    - Interpolation of DMNs for different inclusions volume fraction f and fibre orientation distribution tensor

    [Huang, T., Liu, A., Wu, C.T., Chen, Wei (2022). Microstructure-guided deep material network for rapid nonlinear material modeling and uncertainty quantification, CMAME]
  - Quid for distribution effect?
    - Possibility is to extract information from image analysis ?





Conclusions

- Micro-mechanical models
  - General for a micro-structure kind
    - Geometrical parameters: $\boldsymbol{\varphi}_{\mathrm{m}}$
    - Material parameters: $\boldsymbol{\gamma}_{\mathrm{m}}$
  - Based on thermodynamic consistency
    - Possesses extrapolation capabilities
  - Delicate identification
- Neural networks
  - Theoretically generic
    - Geometrical parameters: $\boldsymbol{\varphi}_{\mathrm{m}}$
    - Material parameters: $\boldsymbol{\gamma}_{\mathrm{m}}$
  - No extrapolation capabilities
    - Requires extensive data
- Deep material networks
  - Based on thermodynamic consistency
    - Possesses extrapolation capabilities
  - Fixed micro-structure?