University of Liège
Aerospace & Mechanical Engineering

AI and data-driven methods for composite multi-scale analyses

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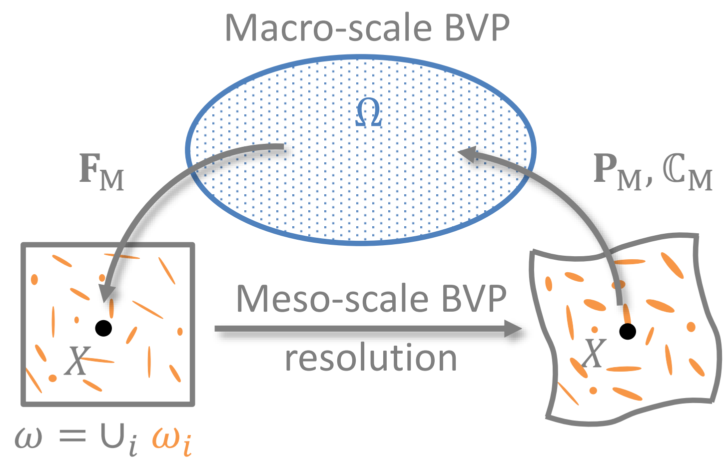
Multi-scale formalism

- 2-Scale problem
  - Idea:
    - Substitute the explicit constitutive model

      $\boldsymbol{\sigma}_{\mathrm{M}}(\boldsymbol{X}, t) = \boldsymbol{\sigma}_{\mathrm{M}}\big(\boldsymbol{\varepsilon}_{\mathrm{M}}(\boldsymbol{X}, t); \boldsymbol{z}_{\mathrm{M}}(\boldsymbol{X}, \tau), \tau \in [0, t]\big)$
    - By an implicit relation resulting from the lower-scale BVP resolution
    - Macro-scale state variables correspond to the set of RVE state variables

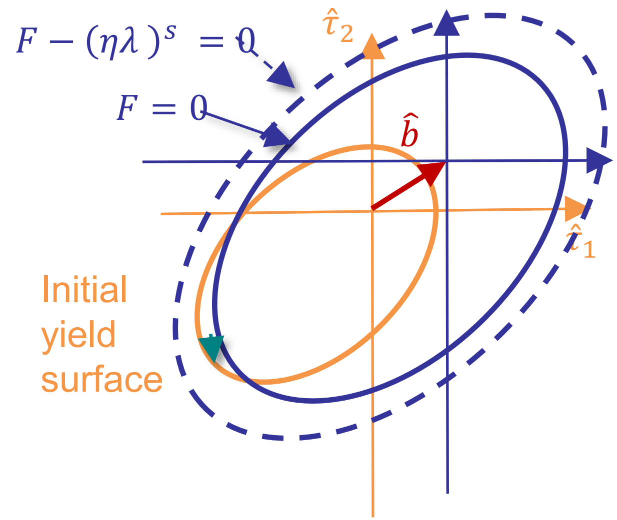
      $\boldsymbol{z}_{\mathrm{M}}(\boldsymbol{X}, t) = \{\boldsymbol{z}_{\mathrm{m}}(\mathbf{x}, t)\ \forall \boldsymbol{x} \in \boldsymbol{\omega}(\boldsymbol{X})\}$
  - Basic assumption: separation of scale

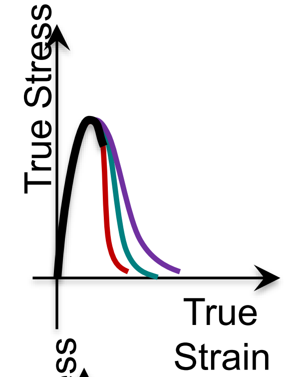
    $l_{\mathrm{M}} >> l_{\mathrm{RVE}} >> l_{\mathrm{m}}$
  - Opportunities
    - Complex simulations (accounting for complex failure modes
    - Stochastic analyses
    - …

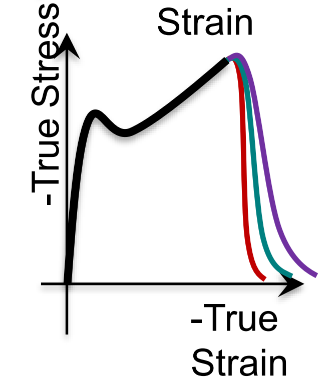


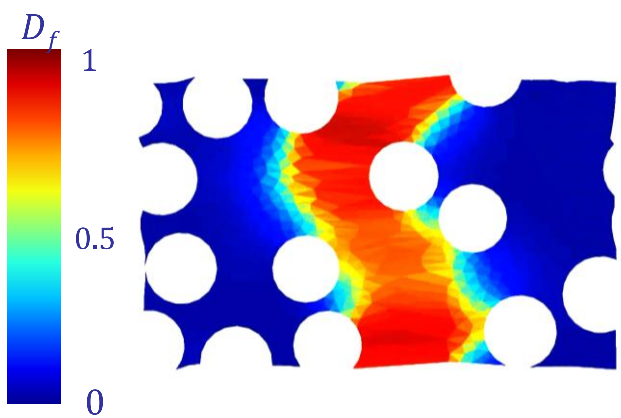
Multi-scale formalism

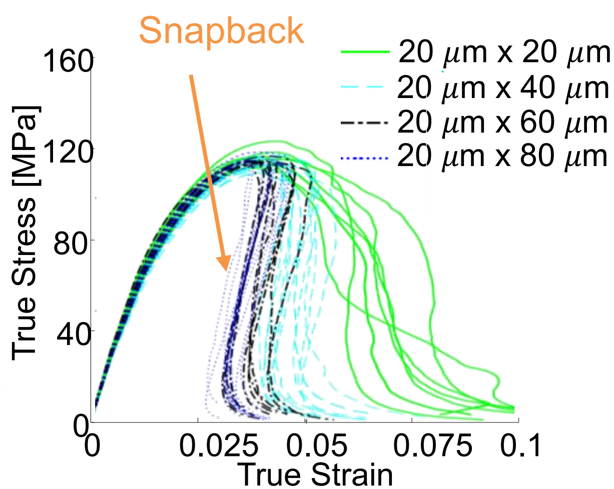
- RVE simulations:
  - Complex material model for resin
    - (Visco-Elasticity-)Visco-plasticity with pressure dependency
    - Triaxiality-dependent damage models
    - Non-local damage models
  - Transverse anisotropy for fibre
    - Failure with phase-field
  - Experimentally validated

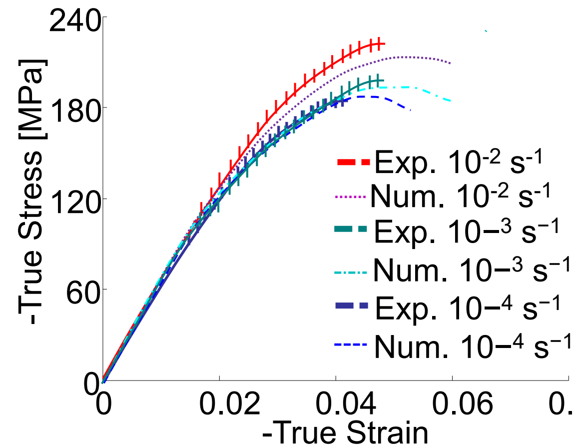








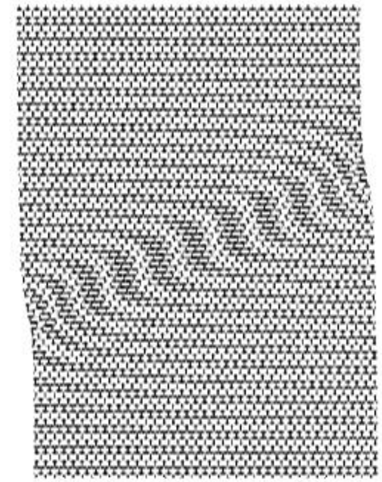


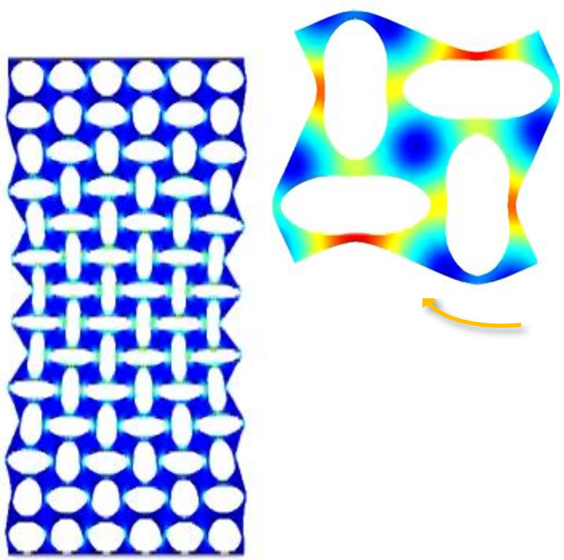


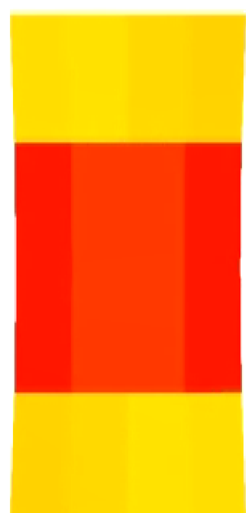
Multi-scale formalism

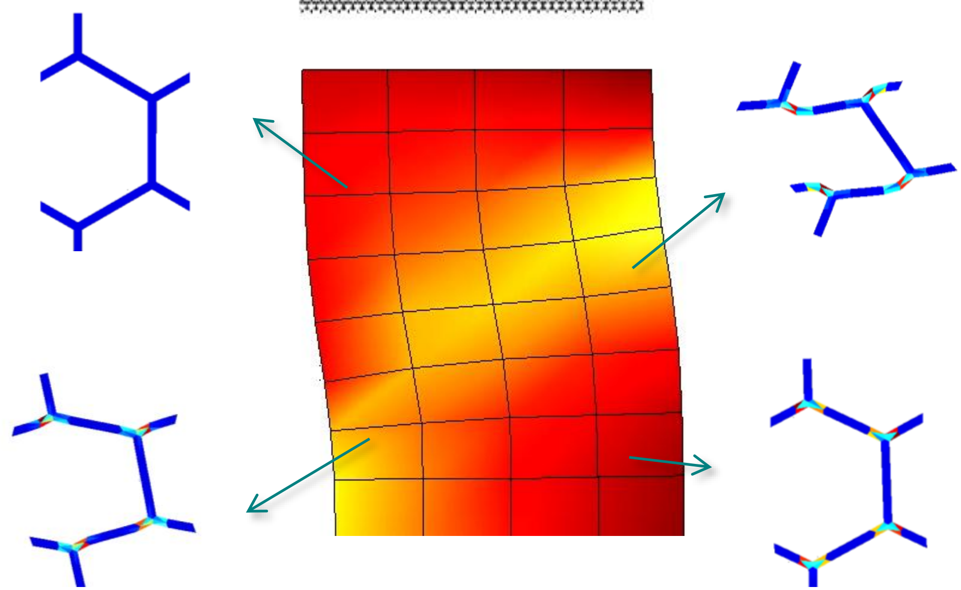
- Multi-Scale FE^2 resolution
  - Method has been applied to a wide variety of problems
  - Several drawbacks
    - Overwhelming computation time
    - Fixed micro-structure

Not manageable for real applications



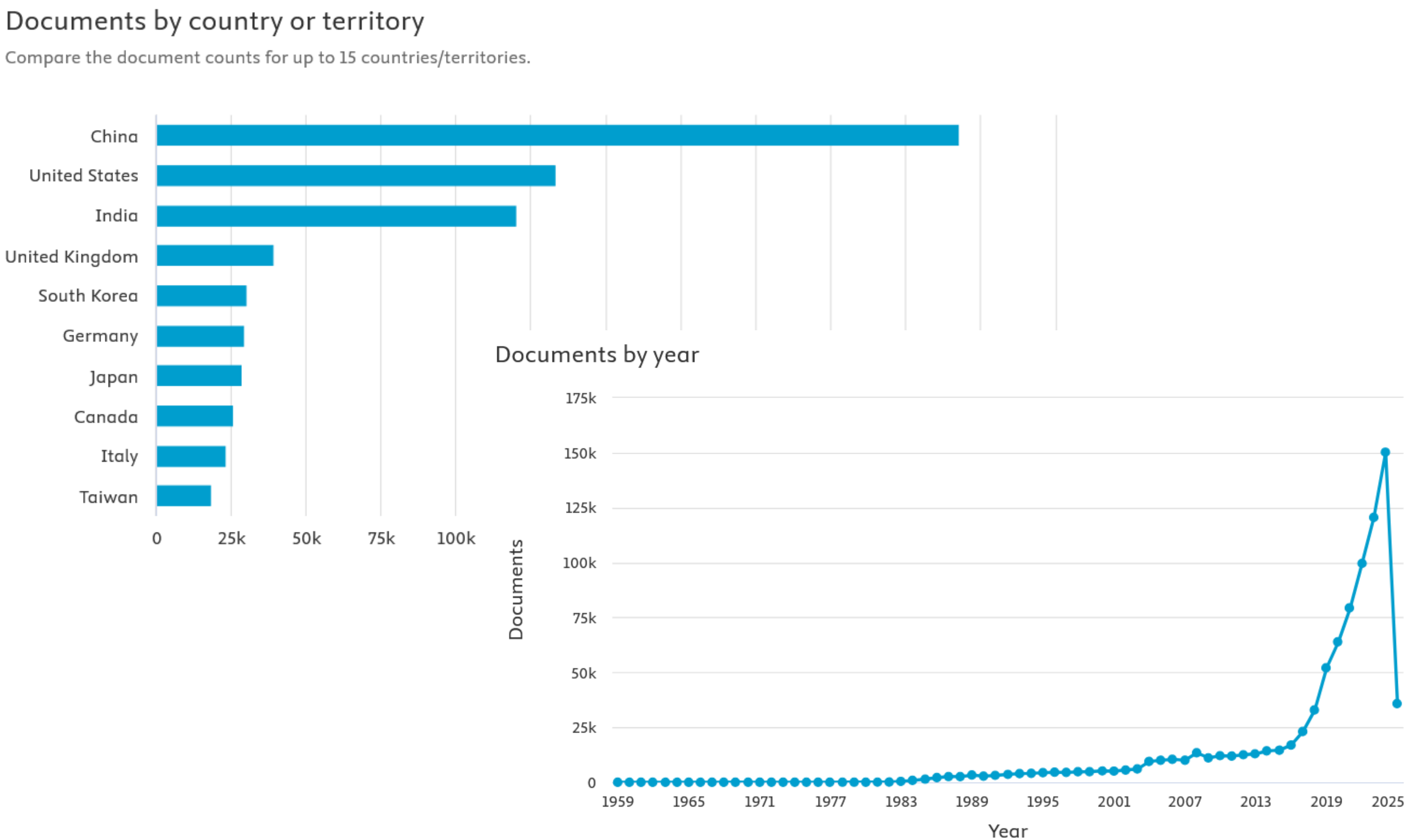






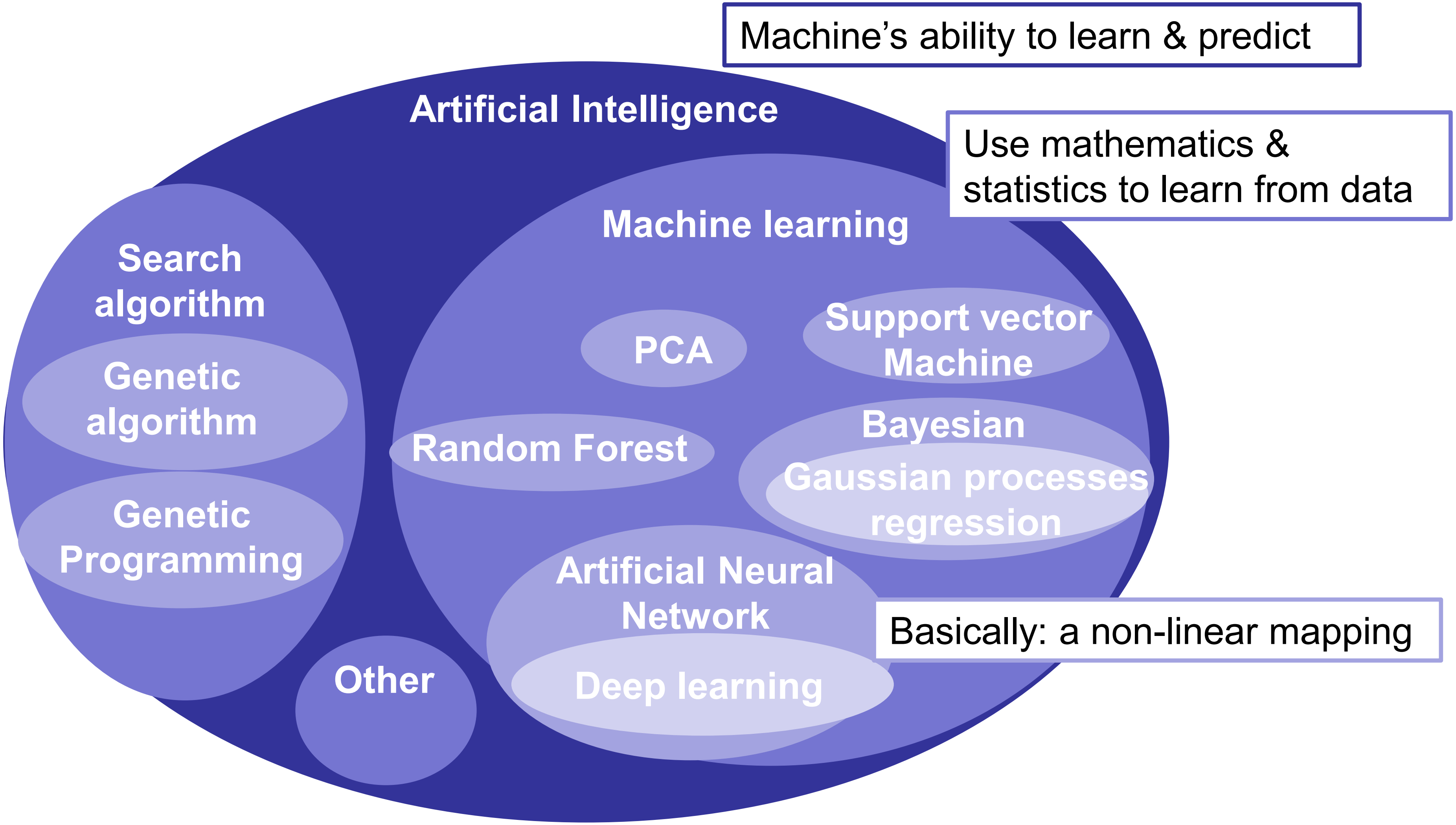
Can AI help?

- Artificial intelligence / machine learning / neural network in engineering



Can AI help?

- What is Artificial Intelligence?



Can AI help?

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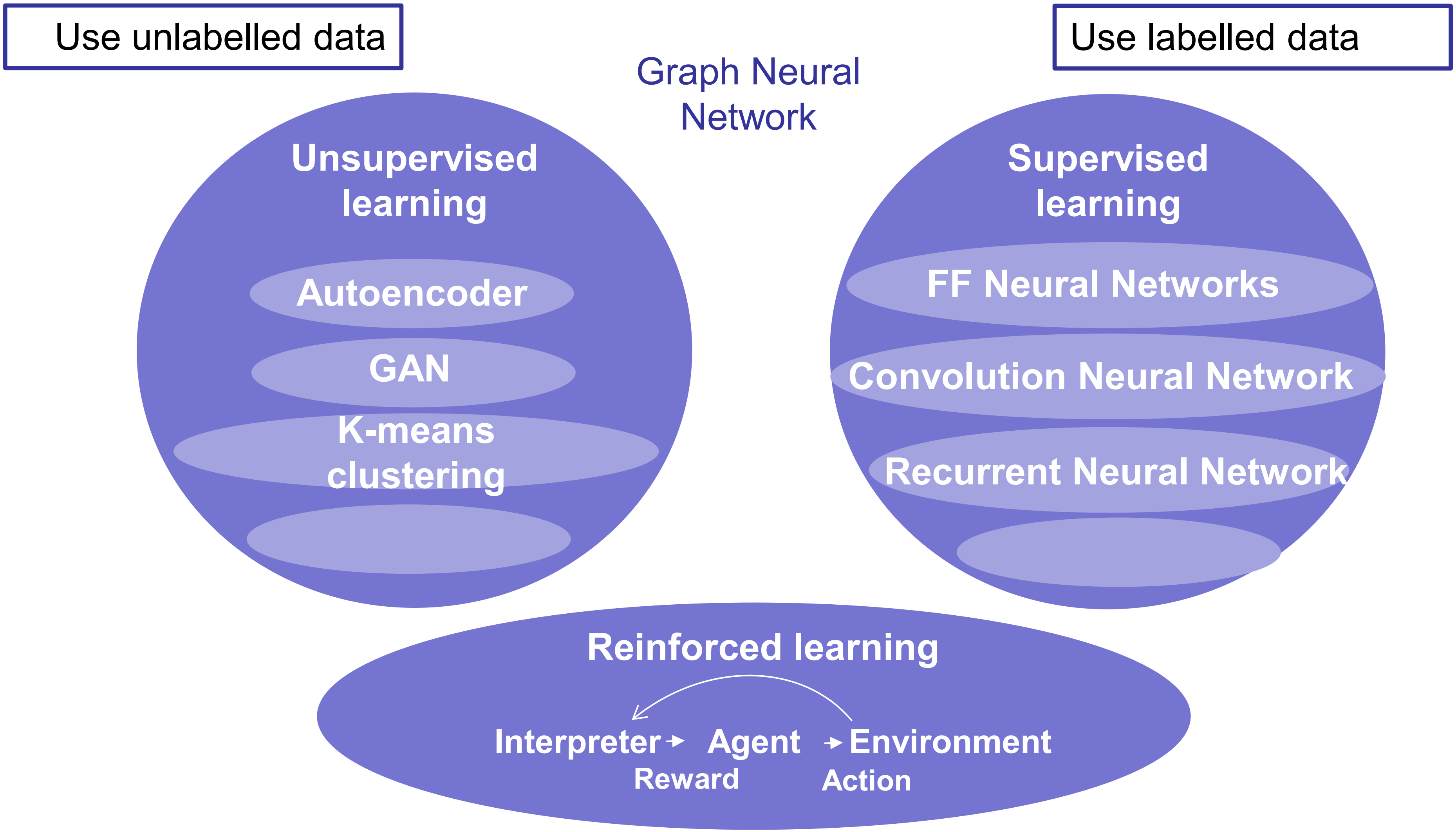
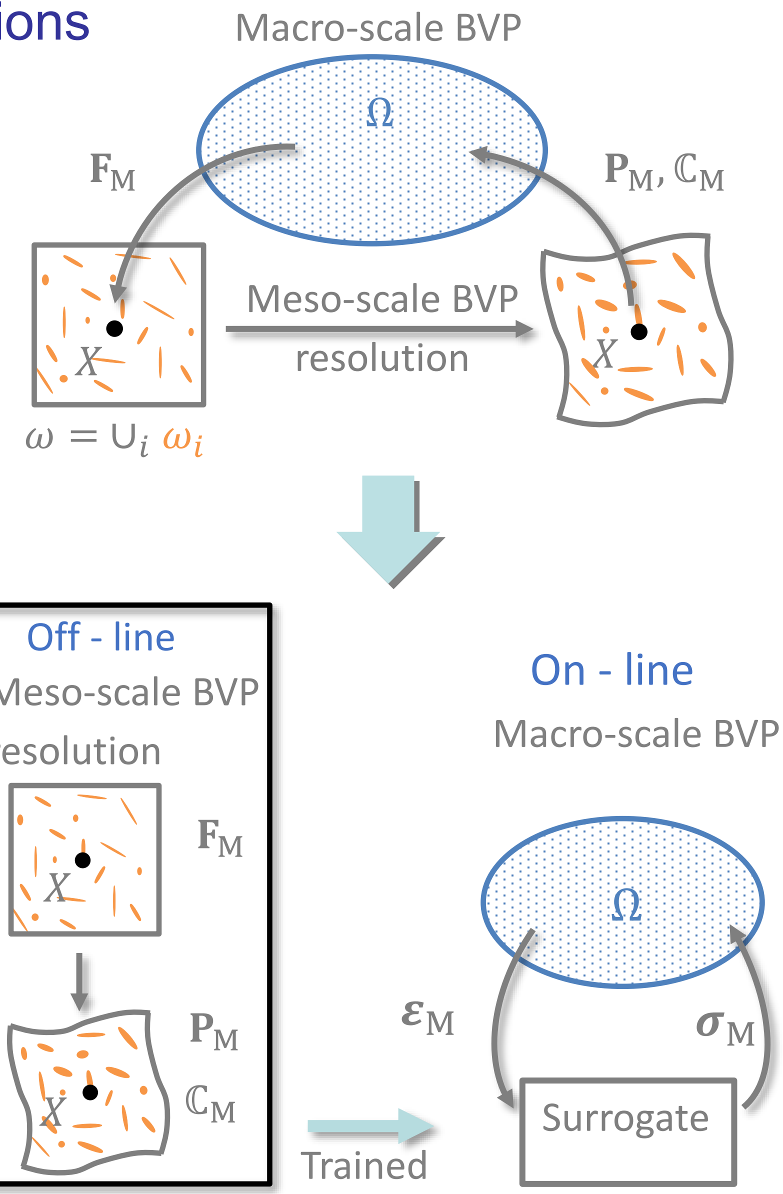
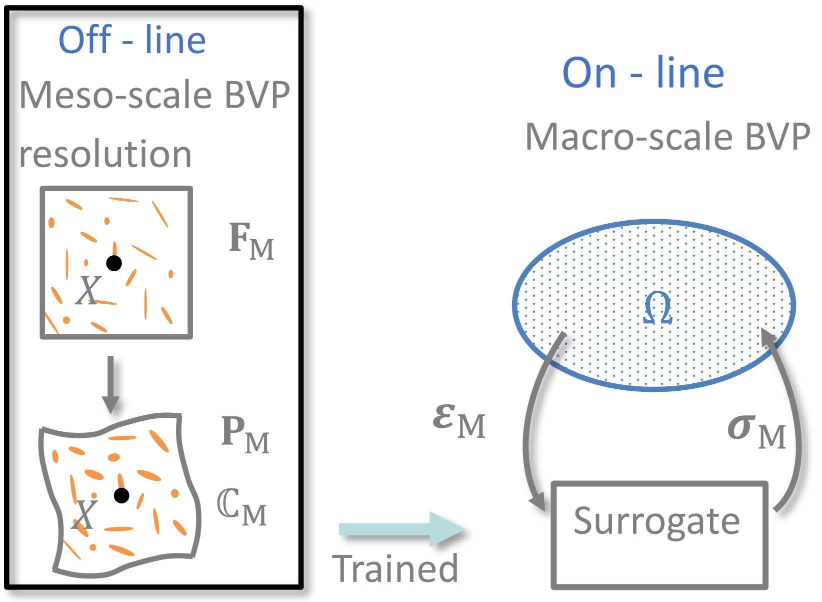


- Surrogated non-linear multi-scale simulations
  - FE multi-scale simulations
    - Problems to be solved at two scales
    - Require Newton-Raphson iterations at both scales
  - Use of surrogate models
    - Train a meso-scale surrogate model
      - Off-line
      - Requires data from RVE simulations
      - Supervised learning
    - Use the trained surrogate
      - On-line analyses
      - Surrogate acts as a homogenised constitutive law
      - Speed-up of 4-5 orders



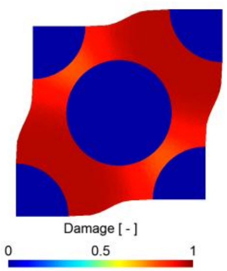
AI-accelerated multi-scale formalism

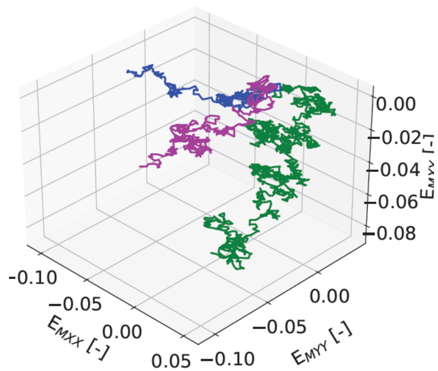
- Opportunities
  - Account for micro-structural effects on macro-scale responses
    - Failure origin
    - Micro-structural variation
  - Accelerate simulations
    - Makes virtual testing possible
- Challenges
  - Which surrogate/ML tool?
  - How to get a relevant database?
  - Quid extrapolating capabilities?

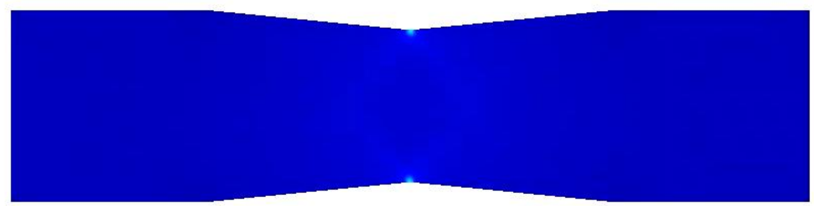


AI-accelerated multi-scale formalism

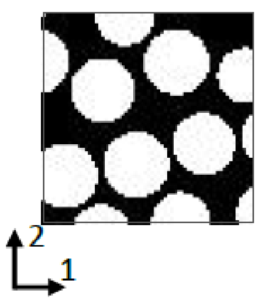
- 2 developments
  - Recurrent neural networks for composite failure analyses

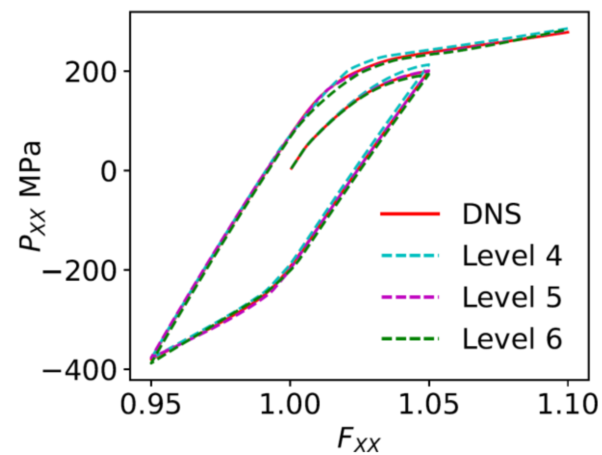




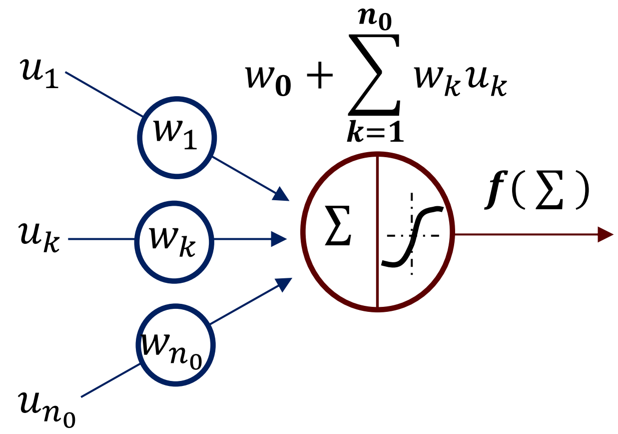


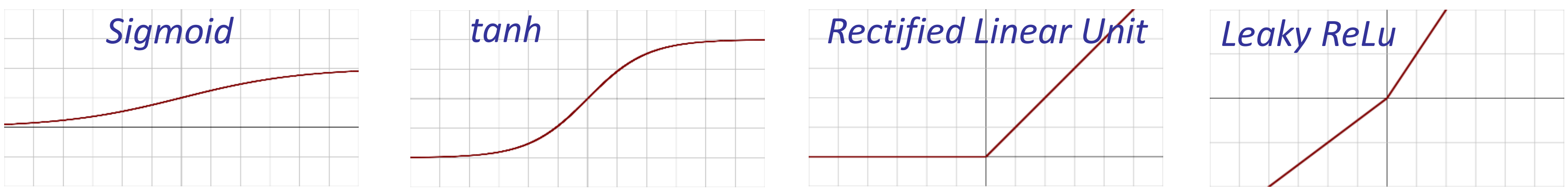
  - Stochastic deep material network





- 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





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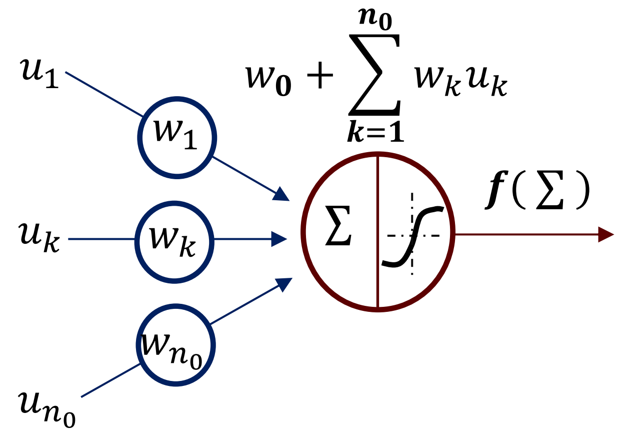

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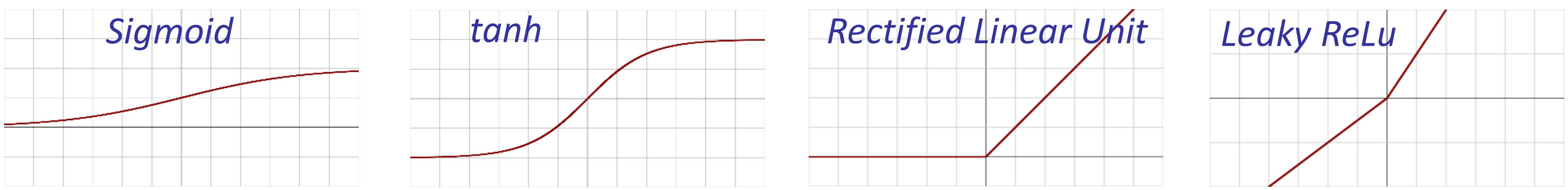
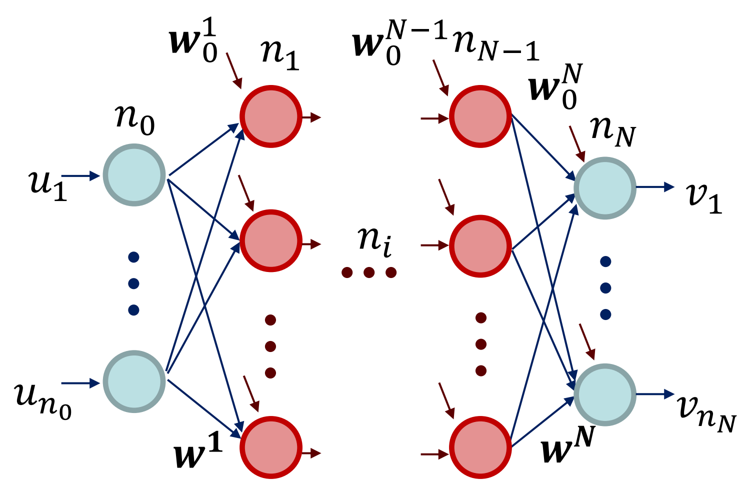


  - Feed-Forward Neuron Network
    - Simplest architecture
    - Layers of neurons
      - Input layer
      - $N-1$ hidden layers
      - Output layers
    - Mapping $\mathfrak{R}^{n_0} \rightarrow \mathfrak{R}^{n_N}$: $\boldsymbol{v} = \boldsymbol{g}(\boldsymbol{u})$



AI-accelerated multi-scale formalism

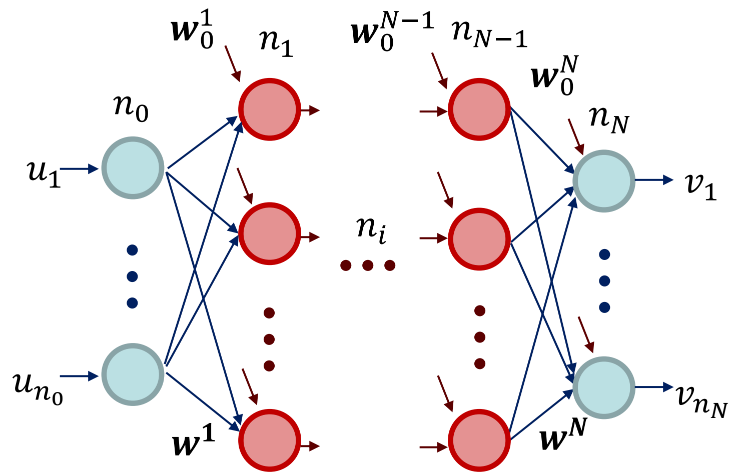
- Training
  - Evaluate
    - The weights w_{kj}^{i}, $k = 1..n_{i-1}, j = 1..n_i$
    - The bias w_0^i
    - Minimise error on prediction $\boldsymbol{v}$ vs. n observations (real) $\boldsymbol{v}^{(p)}$

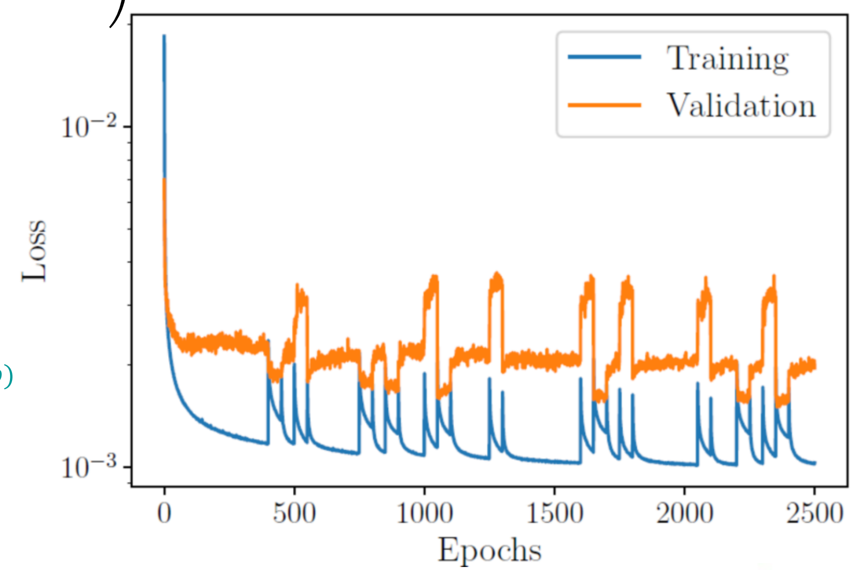
$$L_{\text{MSE}}\left(\mathbf{W}\right) = \frac{1}{n}\sum_{i}^{n}\left\|\boldsymbol{v}_i(\mathbf{W}) - \boldsymbol{v}_i^{(p)}\right\|^2$$

    - Requires an optimiser:

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

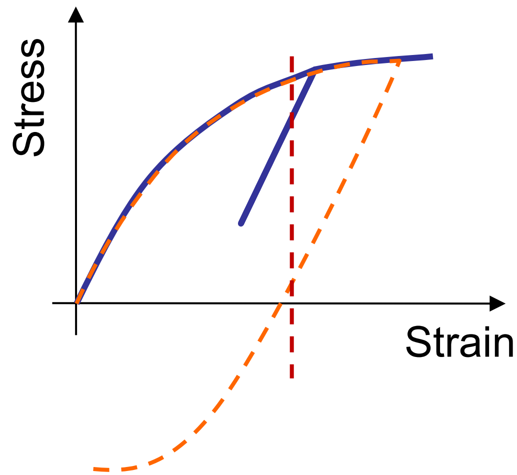
  - Training data
    - Input $\boldsymbol{u}^{(p)}$ & Output $\boldsymbol{v}^{(p)}$
- Testing
  - Use new data
    - Input $\boldsymbol{u}^{(p)}$ & Output $\boldsymbol{v}^{(p)}$
    - Verify prediction $\boldsymbol{v}$ vs. observations (real) $\boldsymbol{v}^{(p)}$





Recurrent Neural Network for multi-scale simulations

- Input / output definition
  - Input: Strain (history): $\mathbf{F}_{\mathrm{M}}$
  - Output: Stress (history): $\mathbf{P}_{\mathrm{M}}$
- Elasto-plastic material behaviour
  - No bijective strain-stress relation
    - Feed-forward NNW cannot be used
    - History should be accounted for



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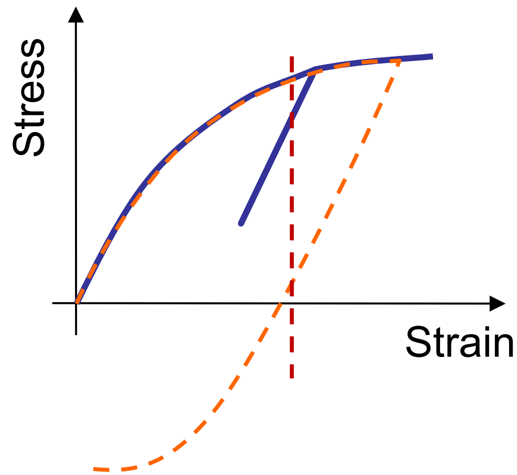

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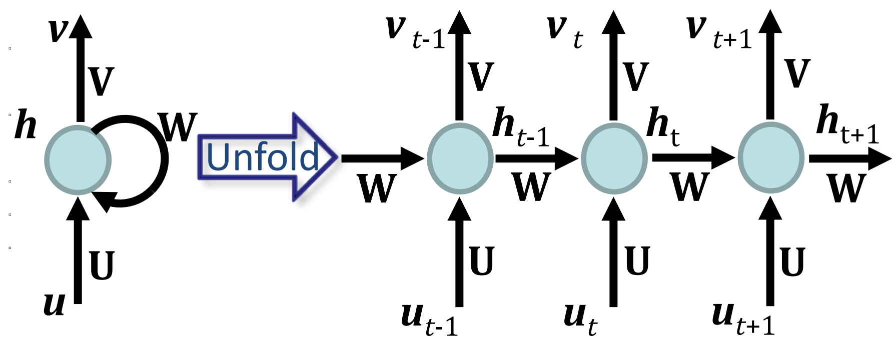
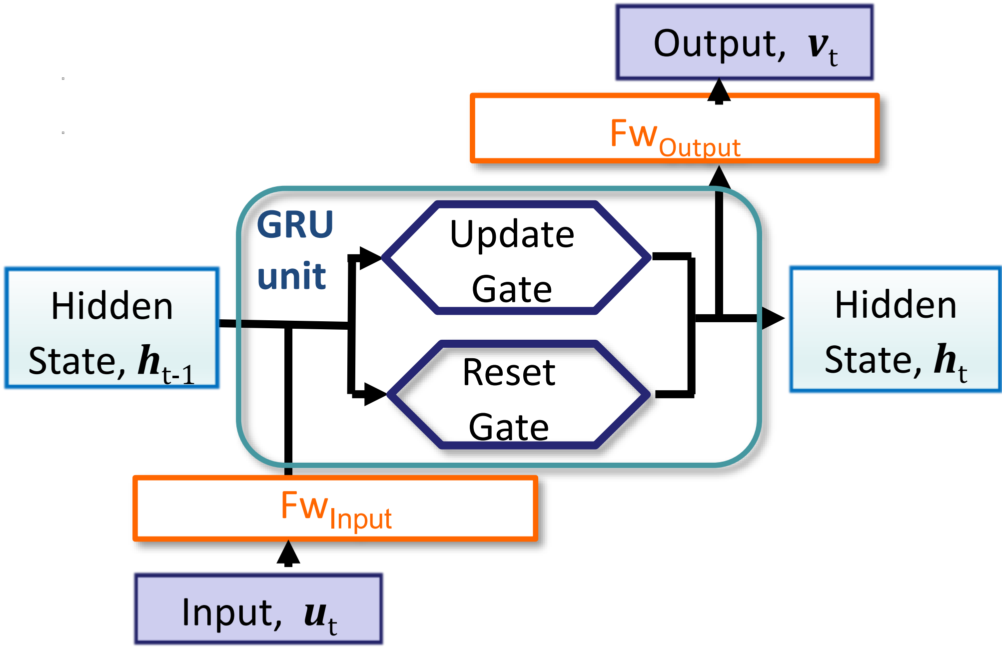


- Recurrent neural network
  - Allows a history dependent relation
    - Input: sequence $\boldsymbol{u}_t$
    - Output: sequence $\boldsymbol{v}_t = \boldsymbol{g}(\boldsymbol{u}_t, \boldsymbol{h}_{t-1})$
    - Internal variable $\boldsymbol{h}_t = \boldsymbol{g}(\boldsymbol{u}_t, \boldsymbol{h}_{t-1})$
  - Existing recurrent units
    - GRU, LSTM
    - Both developed for Nature Language Processing
    - …

Recurrent Neural Network-accelerated multi-scale simulations

- 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
  - FW_{Input} to treat inputs $\boldsymbol{u}_t$
  - FW_{Output} to produce outputs $\boldsymbol{v}_t$



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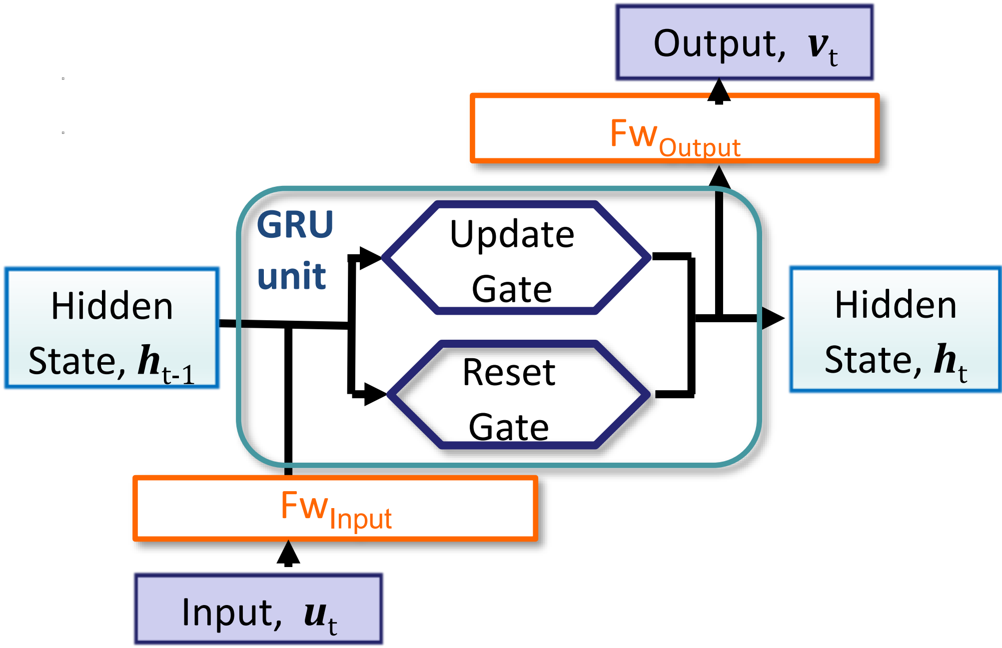
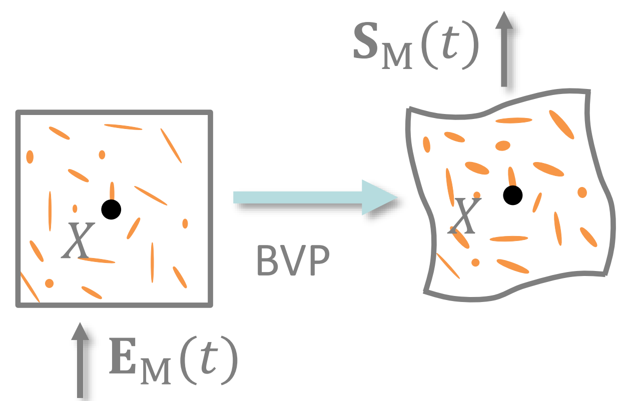
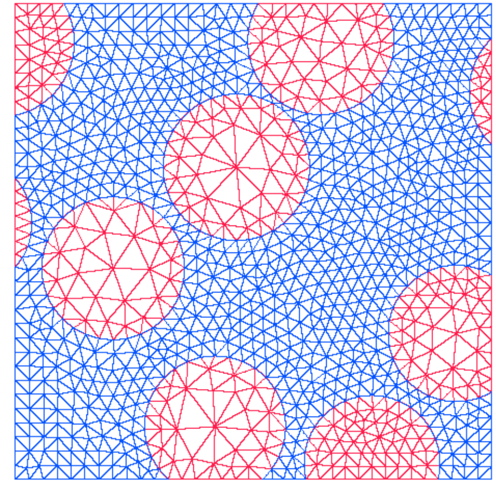
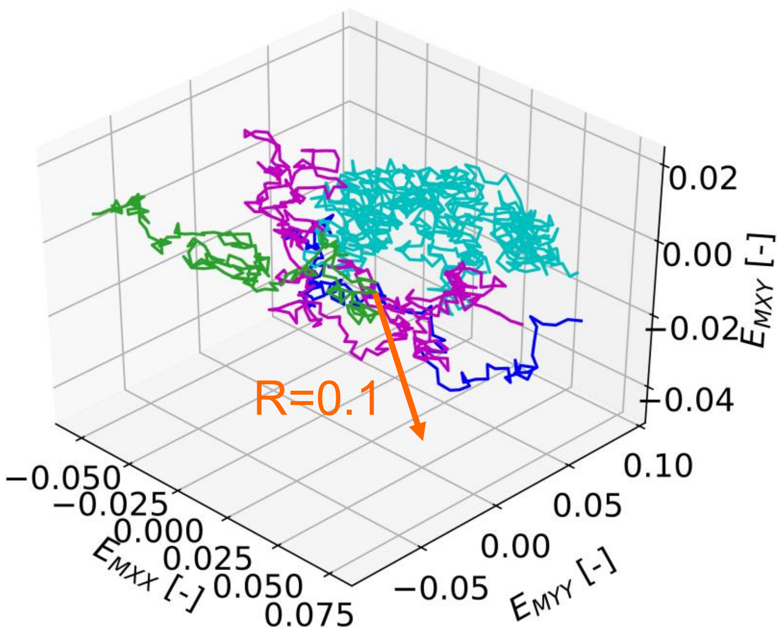


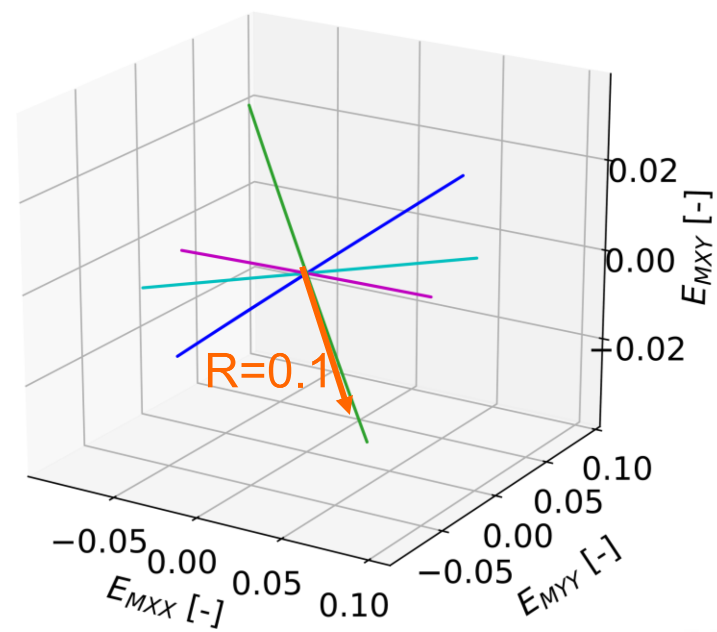
- Details
  - $\boldsymbol{u}_t$: homogenised GL strain $\mathbf{E}_\text{M}$ (symmetric)
  - $\boldsymbol{v}_t$: homogenised 2nd PK stress $\mathbf{S}_\text{M}$ (symmetric)
  - 100 hidden variables $\boldsymbol{h}_t$



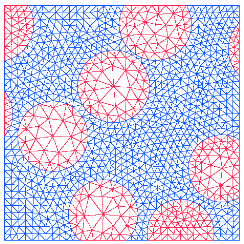
- Data generation
  - Elasto-plastic composite RVE
  - Training stage
    - Should cover full range of possible loading histories
    - Use random walking strategy (thousands)
    - Completed with random cyclic loading (tens)
    - Bounded by a sphere of 10% deformation

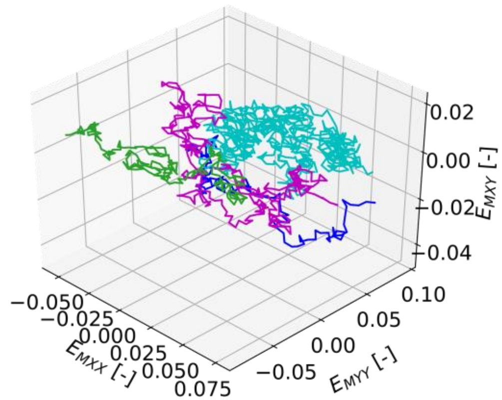


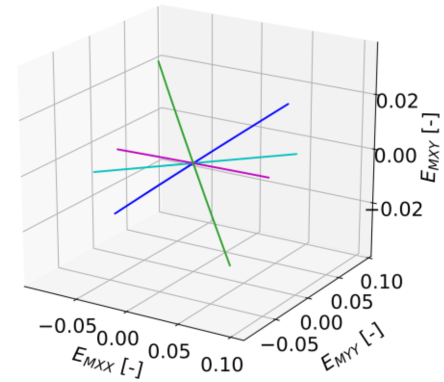


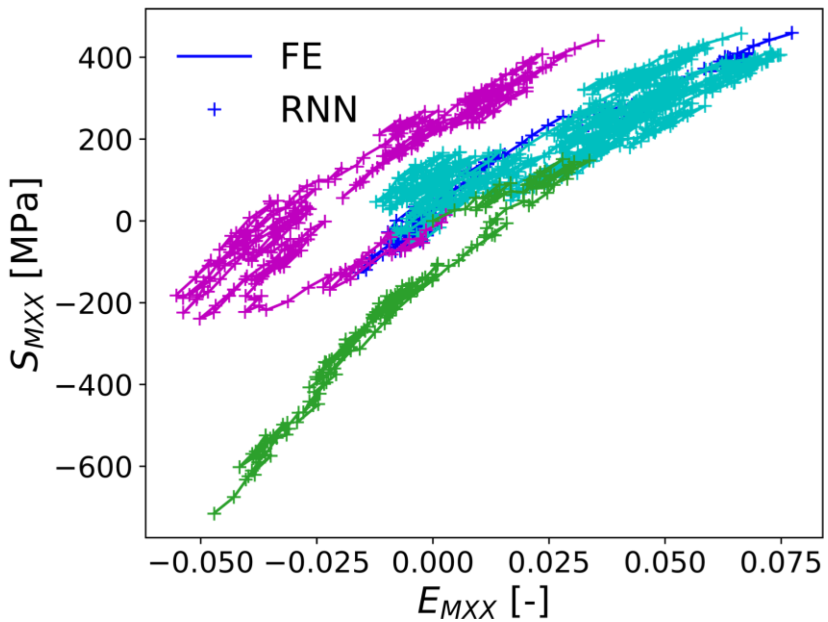


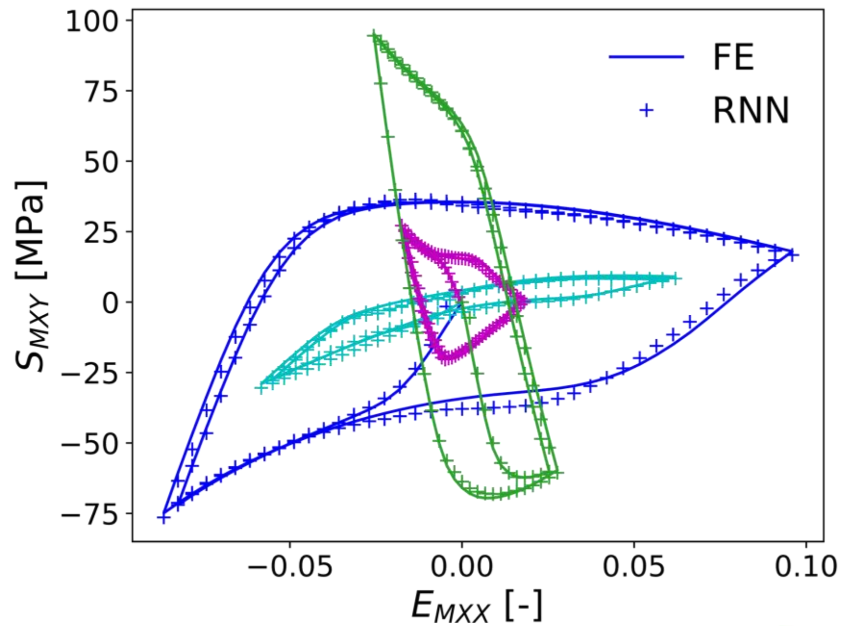
- Testing process (new data)
  - On random walk & cyclic loading







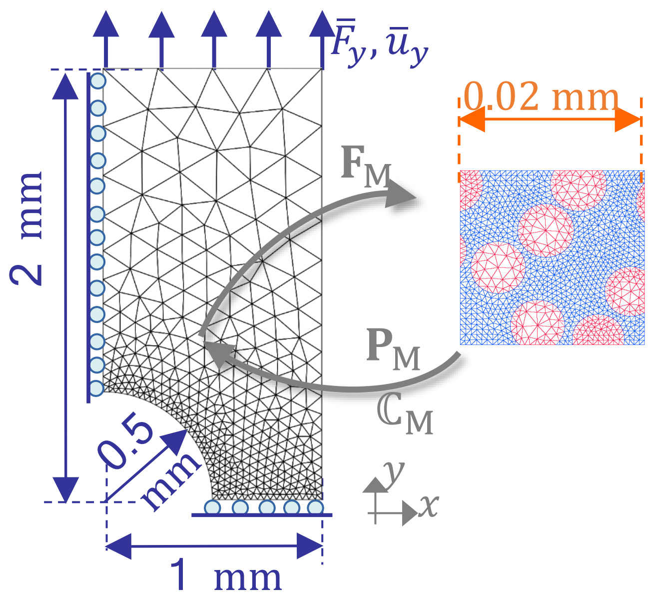


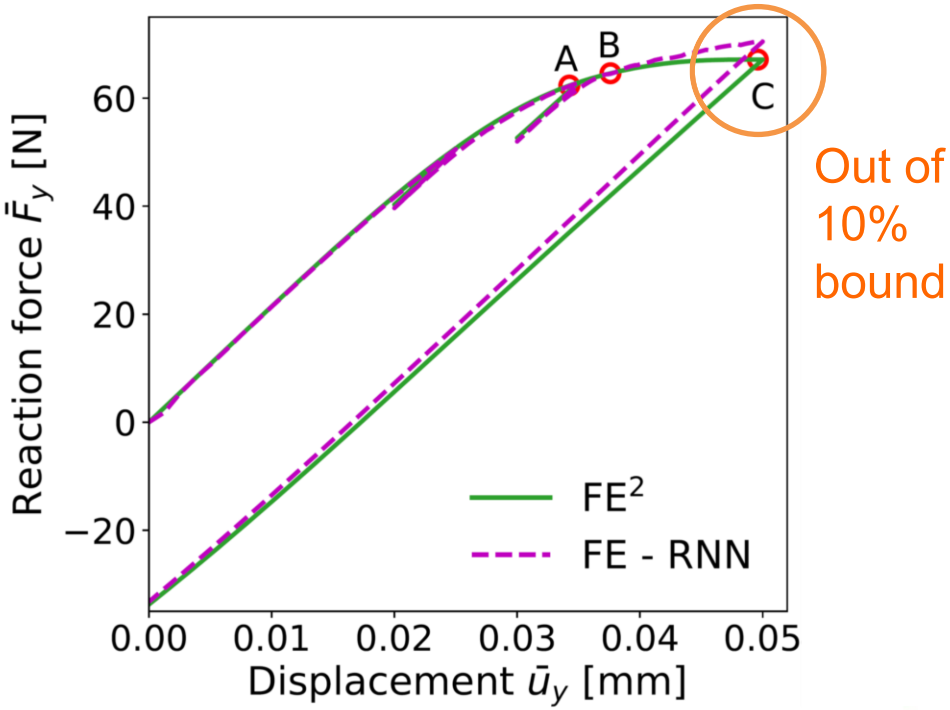


Recurrent Neural Network-accelerated multi-scale simulations

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

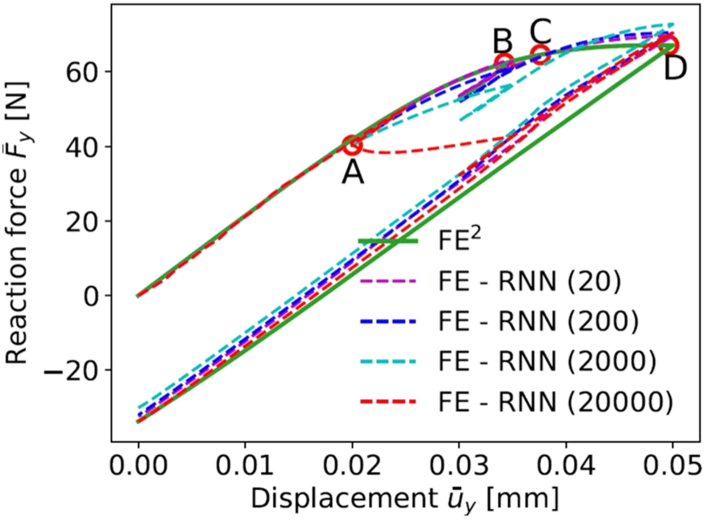
Off-line	FE^2	FE-RNN
Data generation	-	9000 x 2 h-cpu
Training	-	3 day-cpu
On-line	**FE^2**	**FE-RNN**
Simulation	18000 h-cpu	0.5 h-cpu





- What if online simulations use smaller increments?
  - Oscillations / loss of accuracy can appear with GRU, LSTM*
    - Both developed for Nature Language Processing
  - One needs to enforce self-consistency*
  - Need to replace the GRU/LSTM unit

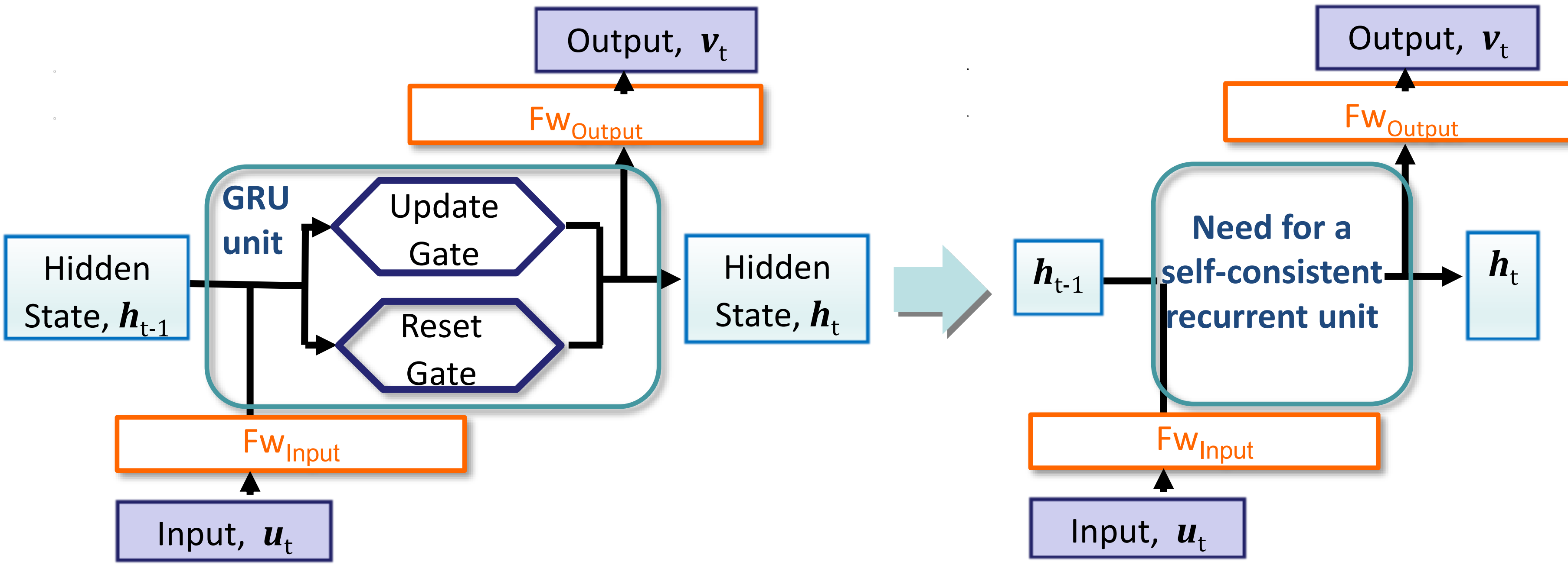
Simplified minimal recurrent unit



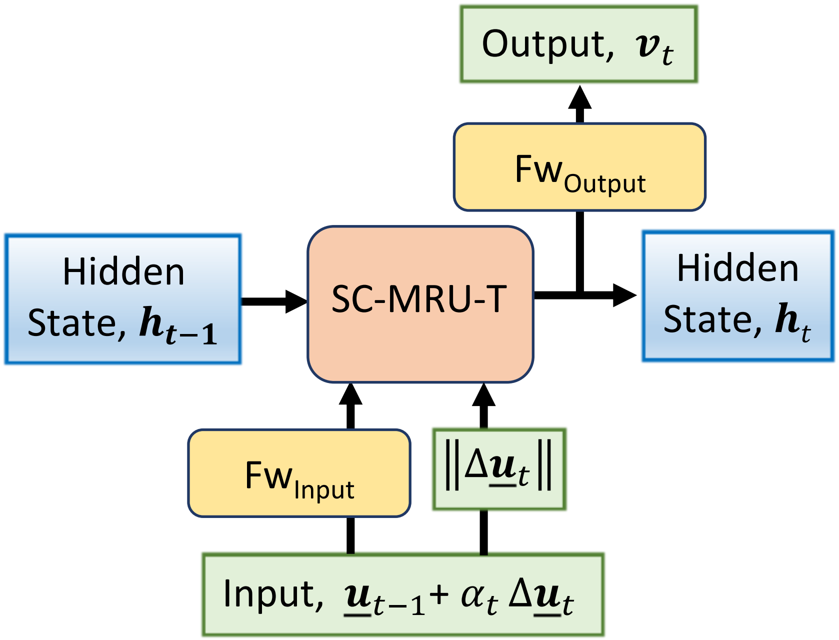
*Colin Bonatti, Dirk Mohr, On the importance of self-consistency in recurrent neural network models representing elasto-plastic solids, Journal of the Mechanics and Physics of Solids, 158, 2022, 104697, https://doi.org/10.1016/j.jmps.2021.104697.

Self-Consistent Recurrent Neural Network for multi-scale simulations

- Self-Consistency reinforcement through ad hoc recurrent unit/cell
  - SC-cell originally to surrogate a constitutive model
  - Can we develop easy and fast to train surrogate for RVE responses?

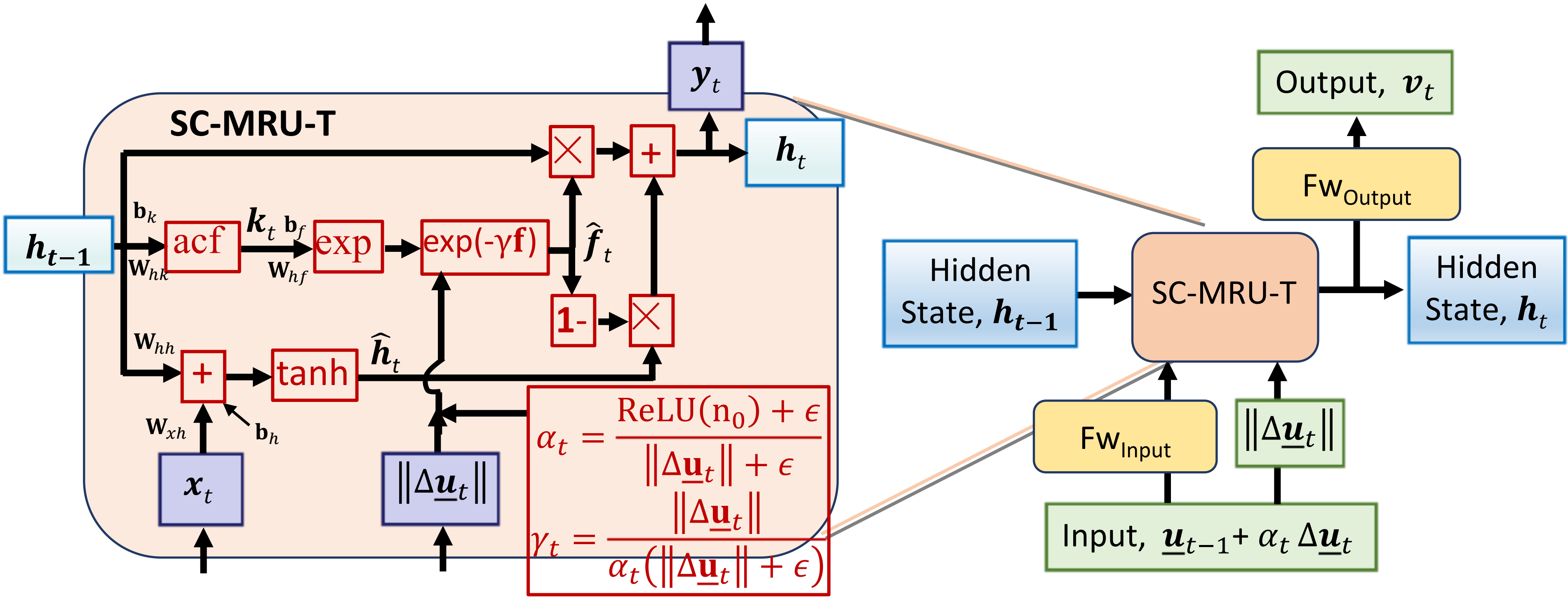


- The Self-Consistent Recurrent Neural Network based on a SC unit



- The **total form of the input variable**
  - Use as input $\underline{\boldsymbol{u}}_{t-1} + \alpha_t \Delta \underline{\boldsymbol{u}}_t$
  - Lift the size of the input to the one of the hidden state with $\mathrm{Fw}_{\mathrm{input}}$
- & **increment norm** $\|\Delta \boldsymbol{u}_t\|$
  - For $\|\Delta \boldsymbol{u}_t\| \rightarrow 0$ the hidden state should not be updated
  - For larger $\|\Delta \boldsymbol{u}_t\|$, the hidden state should be updated

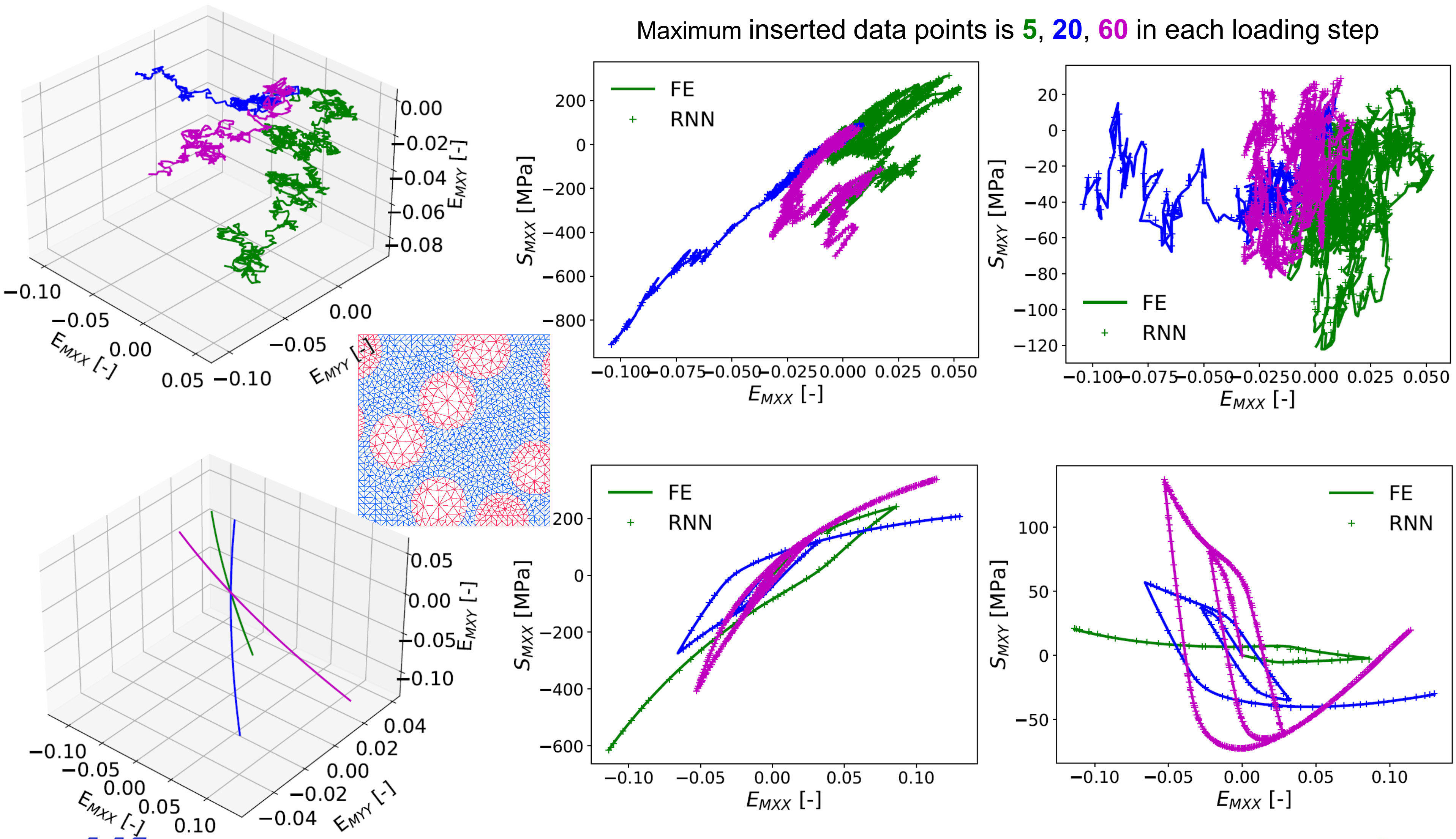
- The Self-Consistent Minimal Recurrent Unit



- **Self-consistency enforced**
  - Double exponential function $f_t = \exp[W_f k_t + b_f] > 0$ & $\hat{f}_t = \exp[-\gamma(\|\Delta u_t\|)\, f_t] \in [0, 1]$
  - h_t is an element-wise interpolation (ratio $\hat{f}_t$ dependent on $\|\Delta u_t\|$) between
    - previous value h_{t-1}
    - & update hidden variables $\hat{h}_t$
  - n_0 is a learnable parameter

- SC-MRU-T: Testing data with inserted extra-points

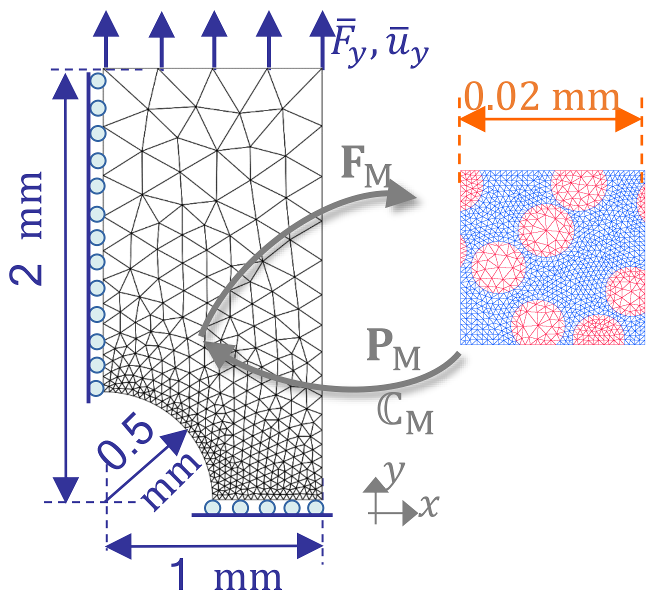
Maximum inserted data points is **5**, **20**, **60** in each loading step

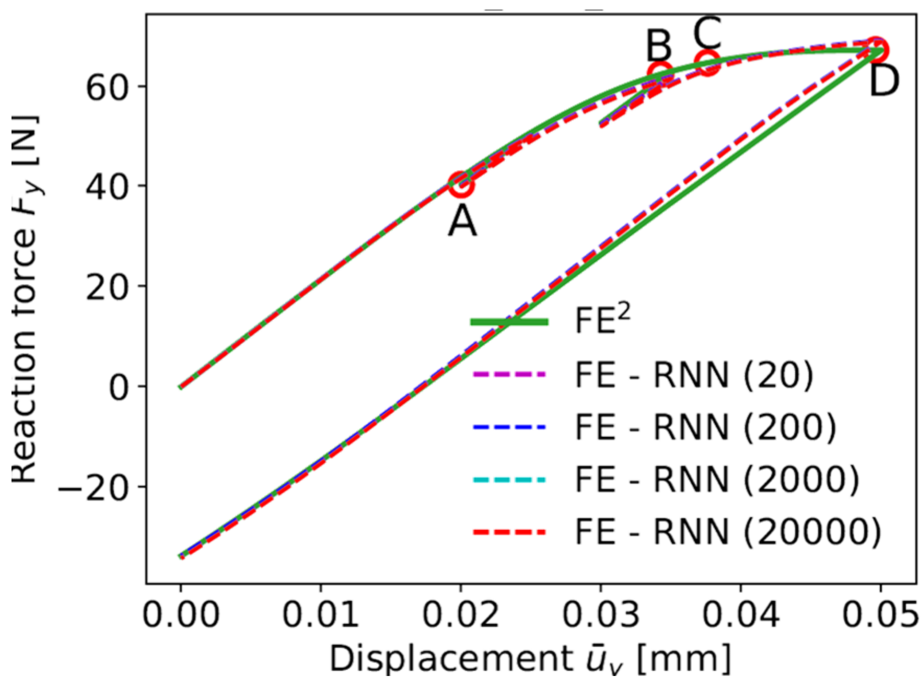


Self-Consistent Recurrent Neural Network for multi-scale simulations

- FE2 vs. FE-RNN:
  - Change in the increment size between points A&B
  - Training is much faster with the SC-MRU cell

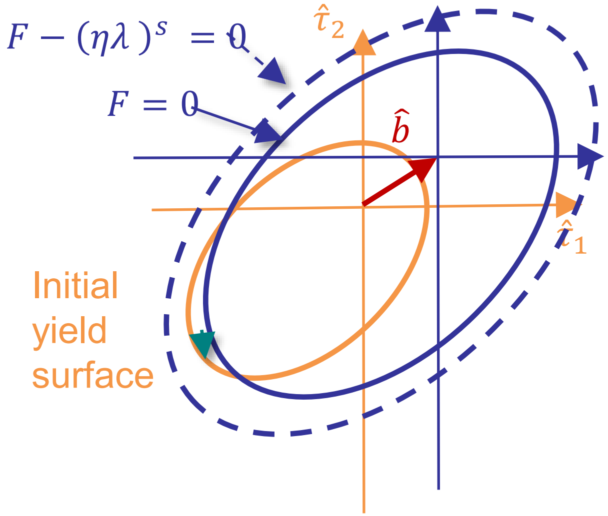
Off-line	FE^2	FE-GRU	FE-SC
Data generation	-	9000 x 2 h-cpu	23 500 h-cpu
Training	-	3 day-cpu	<10 h-cpu
On-line	**FE^2**	**FE-GRU**	**FE-SC**
Simulation	18000 h-cpu	0.5 h-cpu	0.4 h-cpu

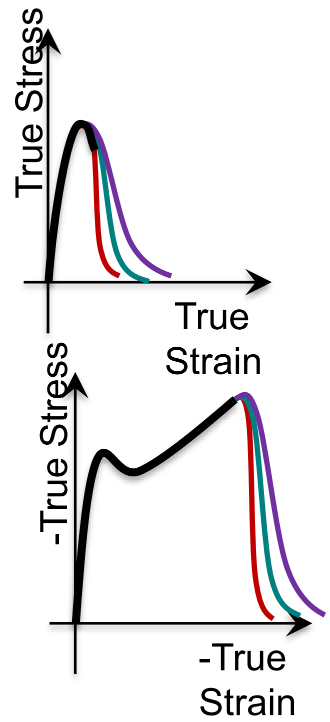


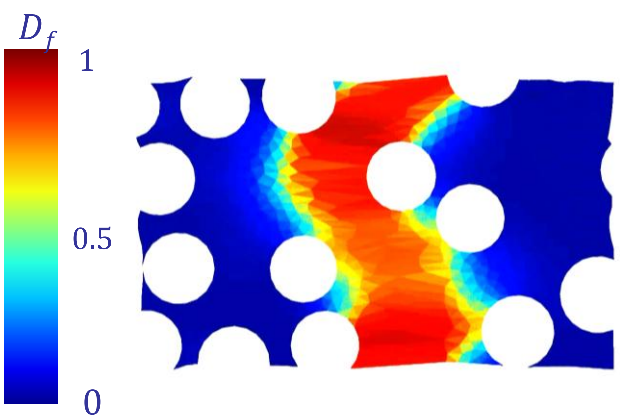


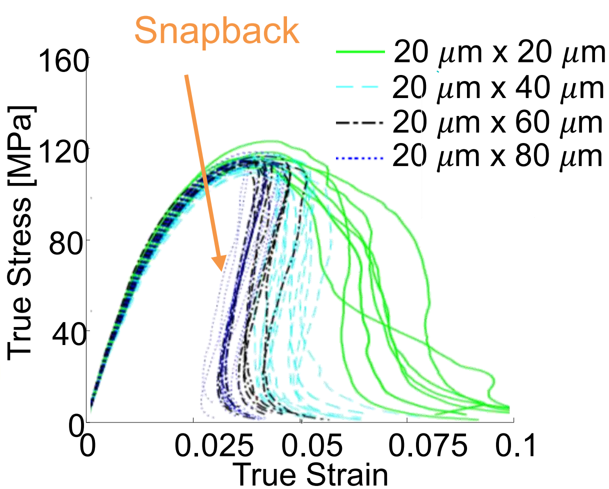
AI-accelerated multi-scale analysis of composite failure

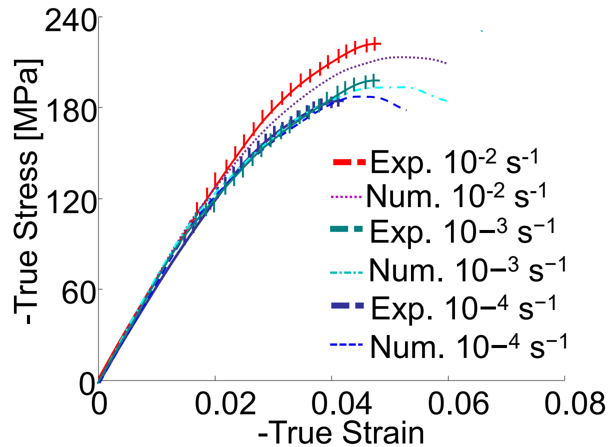
- RVE simulations:
  - Complex material model for resin
    - (Visco-Elasticity-)Visco-plasticity with pressure dependency
    - Triaxiality-dependent damage models
    - Non-local damage models
  - Transverse anisotropy for fibre
    - Failure with phase-field
  - Experimentally validated







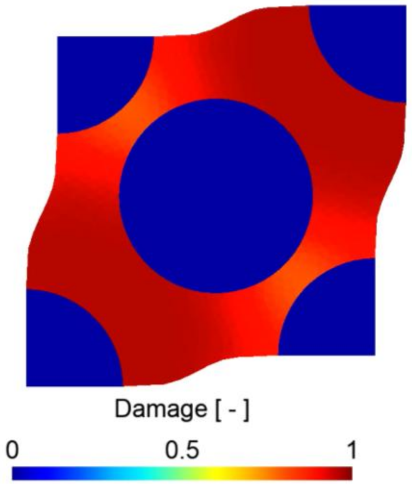


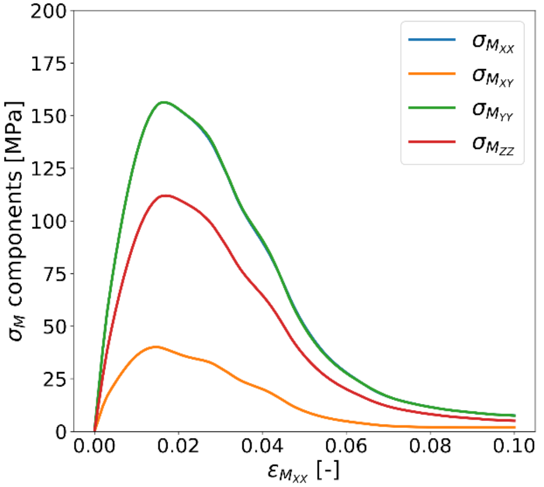


AI-accelerated multi-scale analysis of composite failure

- Challenges to develop the AI surrogate:
  - We need an extensive data-base
    - Simulations should reach total failure
    - Resin is brittle ➡ snapback

➡ (R)VE size is reduced





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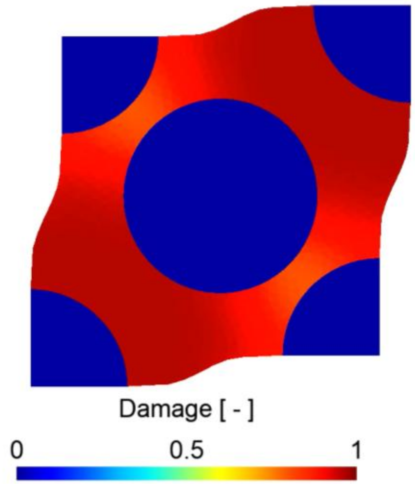
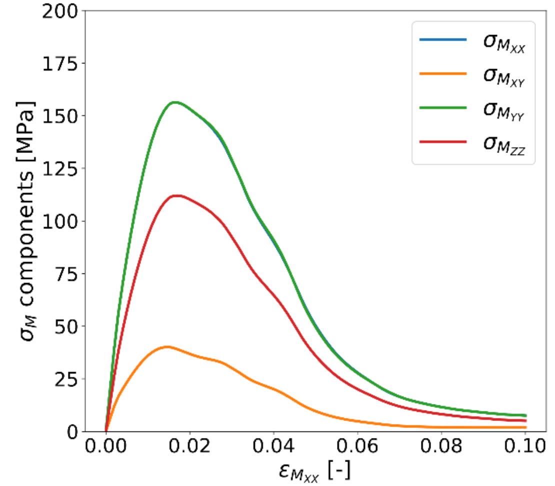
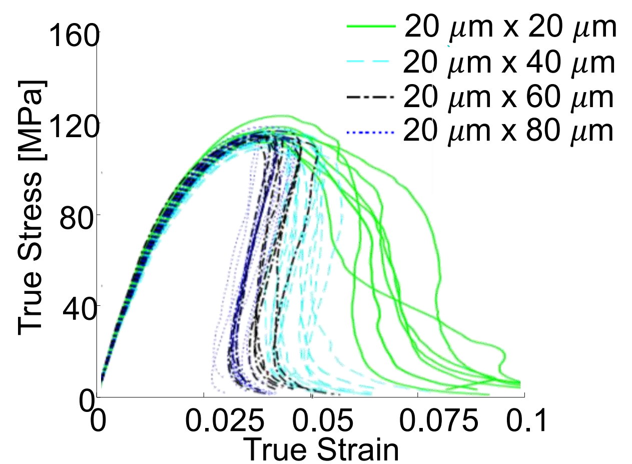




  - Homogenized curves are meaningless
    - They exhibit a strain softening
    - Softening depends on the RVE size
    - Only physical value is fracture energy G_c
  - ➔ We need to regularize the homogenized response

$$\tilde{\alpha} - l_c^2 \, \nabla^2 \tilde{\alpha} = \alpha$$



↳ Parameter tuned to recover the fracture energy G_c

- Development of an embedding non-local framework:
  - Identification of local/non-local variables
    - Plastic strain tensor (from unloading in apparent space)

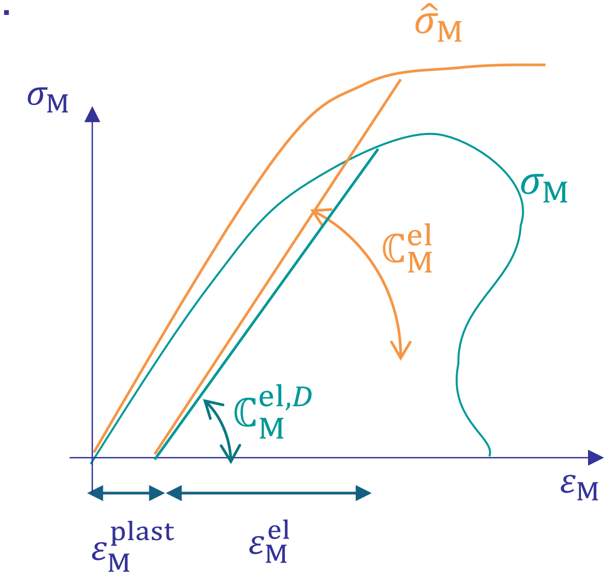
$$\boldsymbol{\varepsilon}_{\mathrm{M}}^{\mathrm{plast}} = \boldsymbol{\varepsilon}_{\mathrm{M}} - \mathbb{C}_{\mathrm{M}}^{\mathrm{el},D^{-1}} : \boldsymbol{\sigma}_{\mathrm{M}}$$

    - Component-wise damage (to be reduced*)

$$D_{\mathrm{M}_{ijkl}} = 1 - \frac{C_{\mathrm{M}_{ijkl}}^{\mathrm{el},D}}{C_{\mathrm{M}_{ijkl}}^{\mathrm{el}}}$$

    - New macro-scale Helmholtz equations

$$D_{\mathrm{M}_a} - l_d^2 \boldsymbol{\nabla}^2 \widetilde{D}_{\mathrm{M}_a} = D_{\mathrm{M}_a}$$
$$\tilde{\varepsilon}_{\mathrm{M}_b}^{\mathrm{plast}} - l_p^2 \boldsymbol{\nabla}^2 \tilde{\varepsilon}_{\mathrm{M}_b}^{\mathrm{plast}} = \varepsilon_{\mathrm{M}_b}^{\mathrm{plast}}$$



*J. Yvonnet, Q-C. He, P. Li, Reducing internal variables and improving efficiency in data-driven modelling of anisotropic damage from RVE simulations, Computational Mechanics 72 (2023), p 37-55

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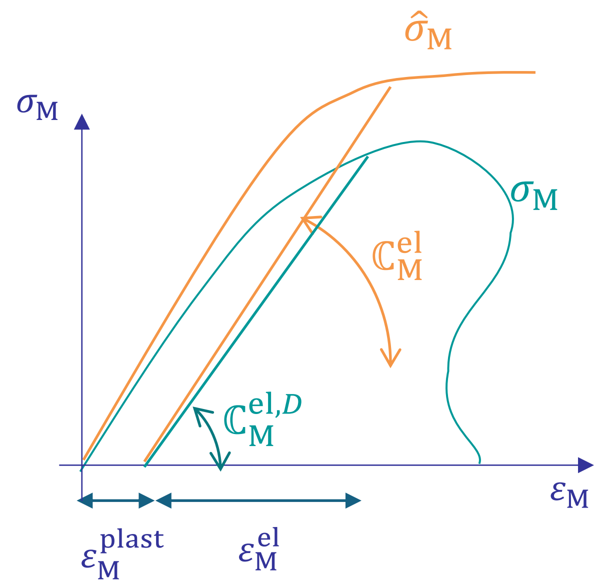
  - Reconstructed (mesh-insensitive) apparent stress

    $$\boldsymbol{\sigma}_{\mathrm{M}_{\mathrm{rec}}} = \left[(1 - \widetilde{\mathbb{D}}_{\mathrm{M}}) \odot \mathbb{C}_{\mathrm{M}}^{\mathrm{el}}\right] : \left(\boldsymbol{\varepsilon}_{\mathrm{M}} - \tilde{\boldsymbol{\varepsilon}}_{\mathrm{M}}^{\mathrm{plast}}\right)$$



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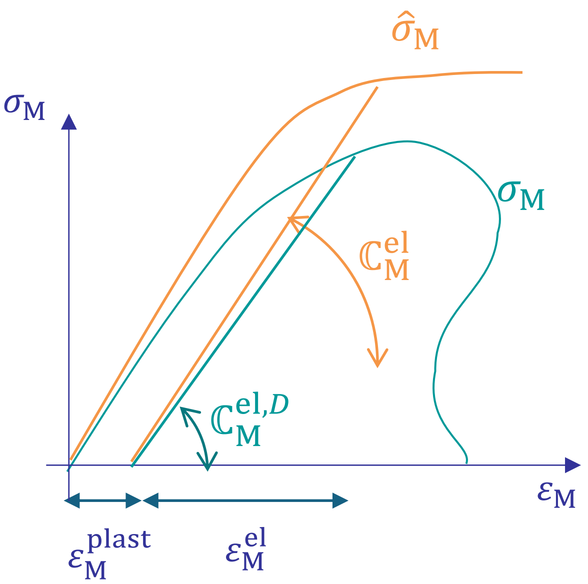


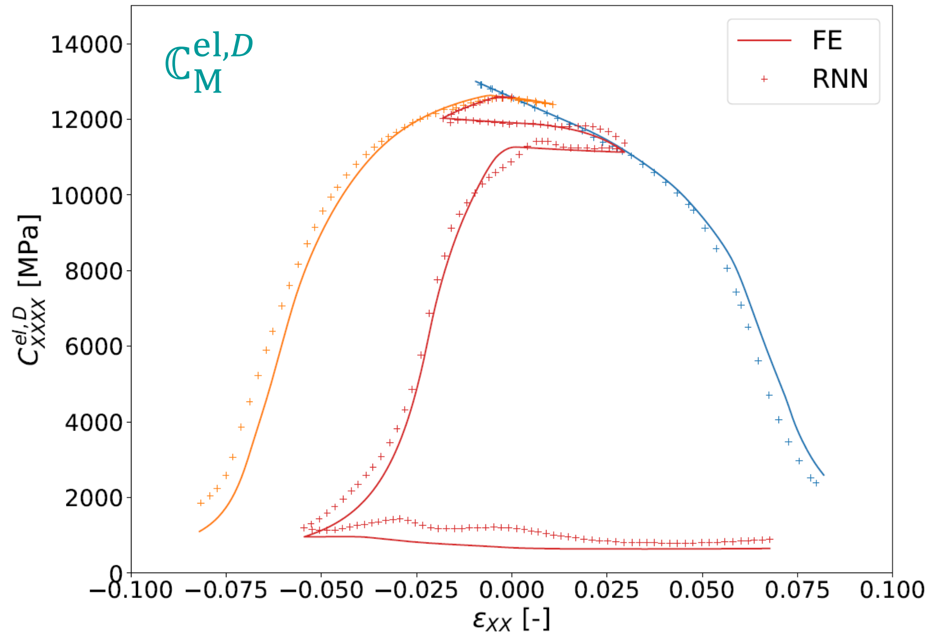
Neural networks to be developed:

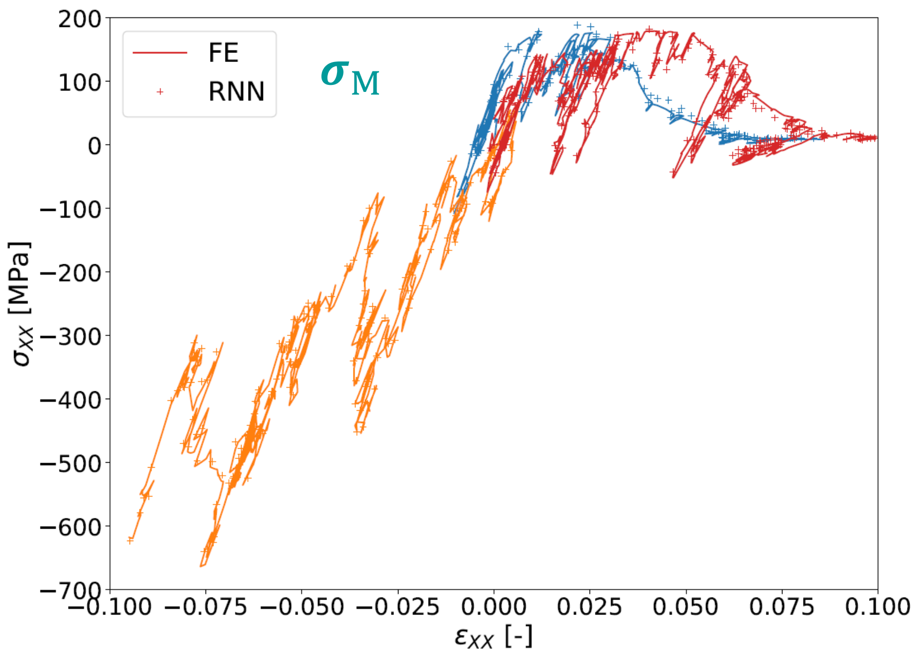
- Inputs: $\underline{\boldsymbol{u}}_t = \{\boldsymbol{\varepsilon}_{\mathrm{M}}\}_t$
- Outputs: $\underline{\boldsymbol{v}}_t = \left\{\boldsymbol{\sigma}_{\mathrm{M}}, \mathbb{C}_{\mathrm{M}}^{\mathrm{el},D}, \mathbb{C}_{\mathrm{M}}^{\mathrm{el}}\right\}_t$

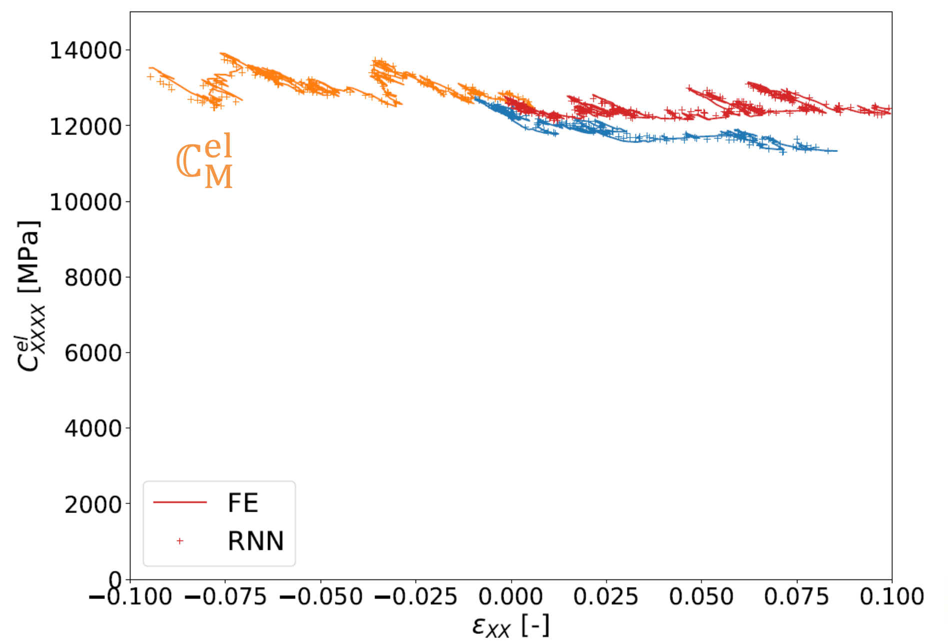
*J. Yvonnet, Q-C. He, P. Li, Reducing internal variables and improving efficiency in data-driven modelling of anisotropic damage from RVE simulations, Computational Mechanics 72 (2023), p 37-55

AI-accelerated multi-scale analysis of composite failure

- Training data-base
  - ~10 000 random paths
  - ~ 5000 cyclic paths
- Testing the neural networks
  - Inputs: $\underline{\boldsymbol{u}}_t = \{\boldsymbol{\varepsilon}_{\mathrm{M}}\}_t$
  - Outputs: $\underline{\boldsymbol{v}}_t = \left\{\boldsymbol{\sigma}_{\mathrm{M}}, \mathbb{C}_{\mathrm{M}}^{\mathrm{el},D}, \mathbb{C}_{\mathrm{M}}^{\mathrm{el}}\right\}_t$

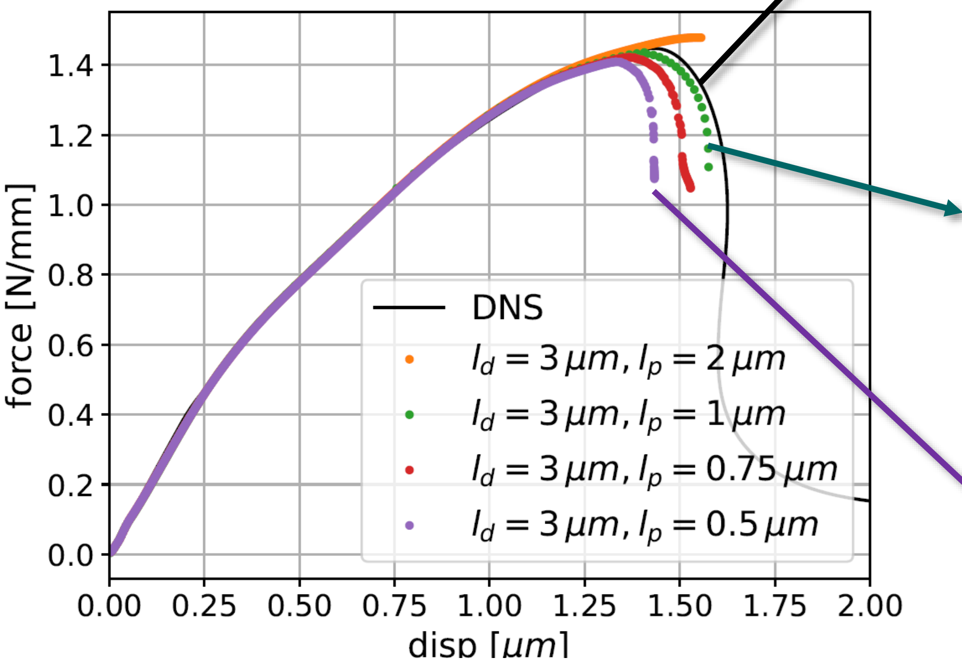


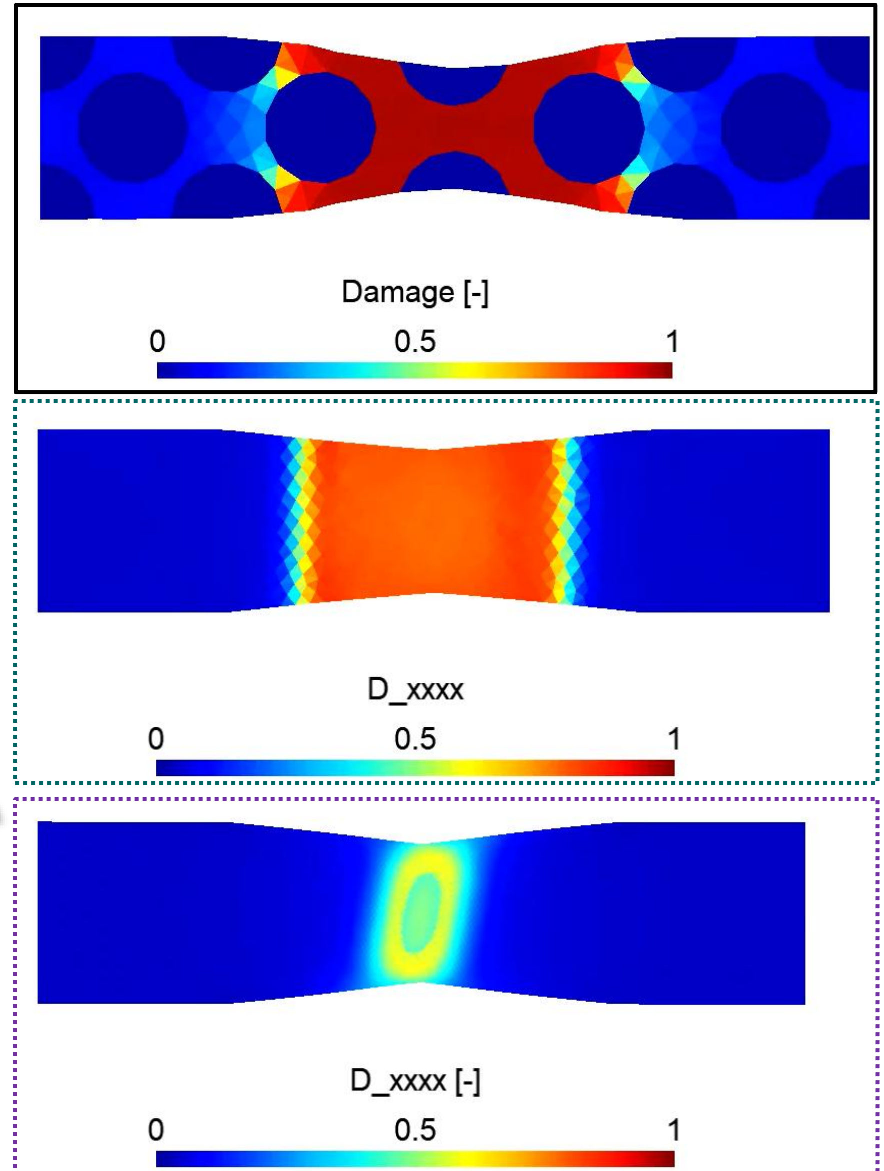




AI-accelerated multi-scale analysis of composite failure

- Non-local lengths
  - $$\begin{cases} D_{\mathrm{M}_a} - l_d^2 \nabla^2 \widetilde{D}_{\mathrm{M}_a} = D_{\mathrm{M}_a} \\ \tilde{\varepsilon}_{\mathrm{M}_b}^{\mathrm{plast}} - l_p^2 \nabla^2 \tilde{\varepsilon}_{\mathrm{M}_b}^{\mathrm{plast}} = \varepsilon_{\mathrm{M}_b}^{\mathrm{plast}} \end{cases}$$
  - Calibration from DNS





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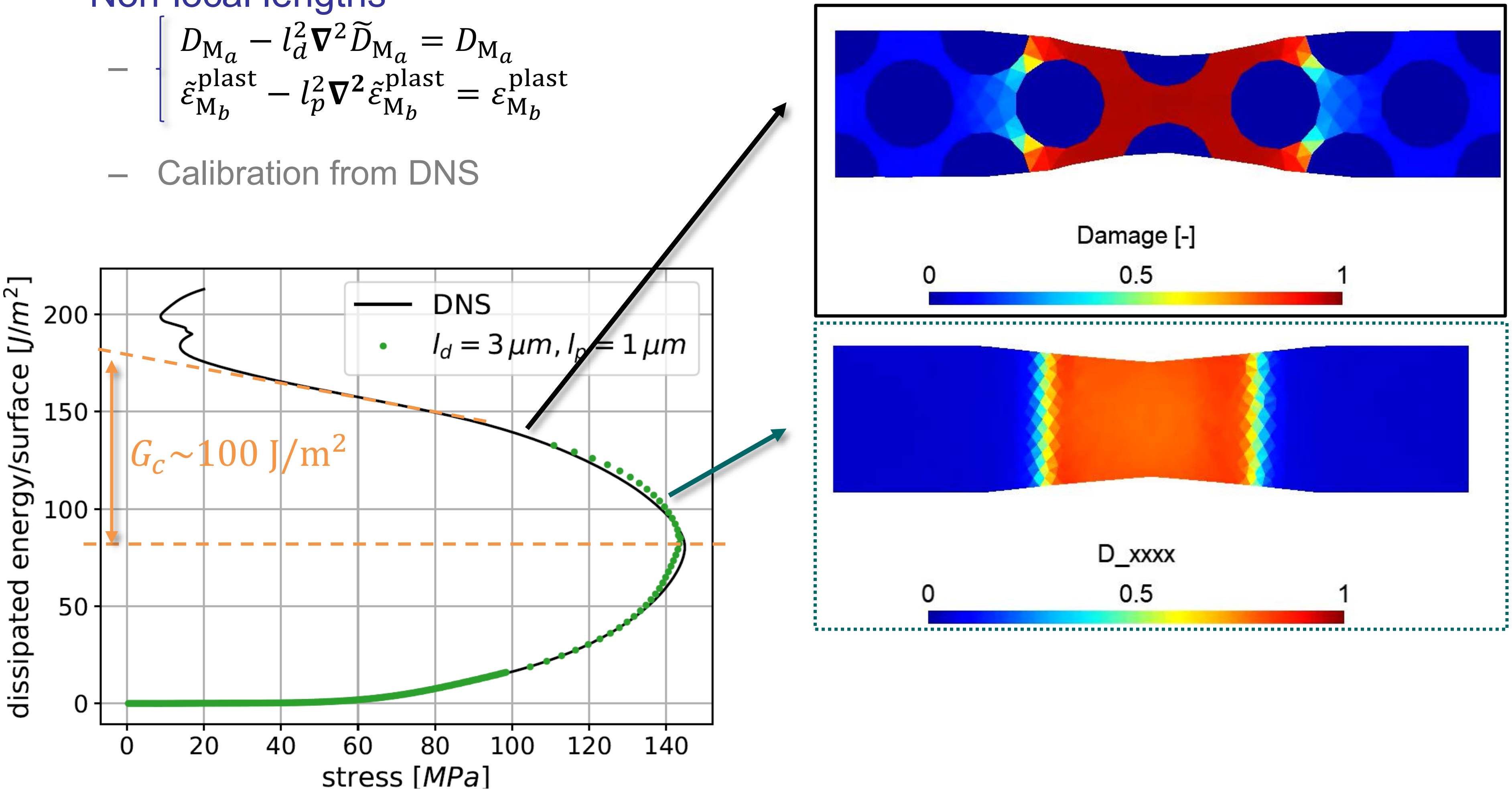
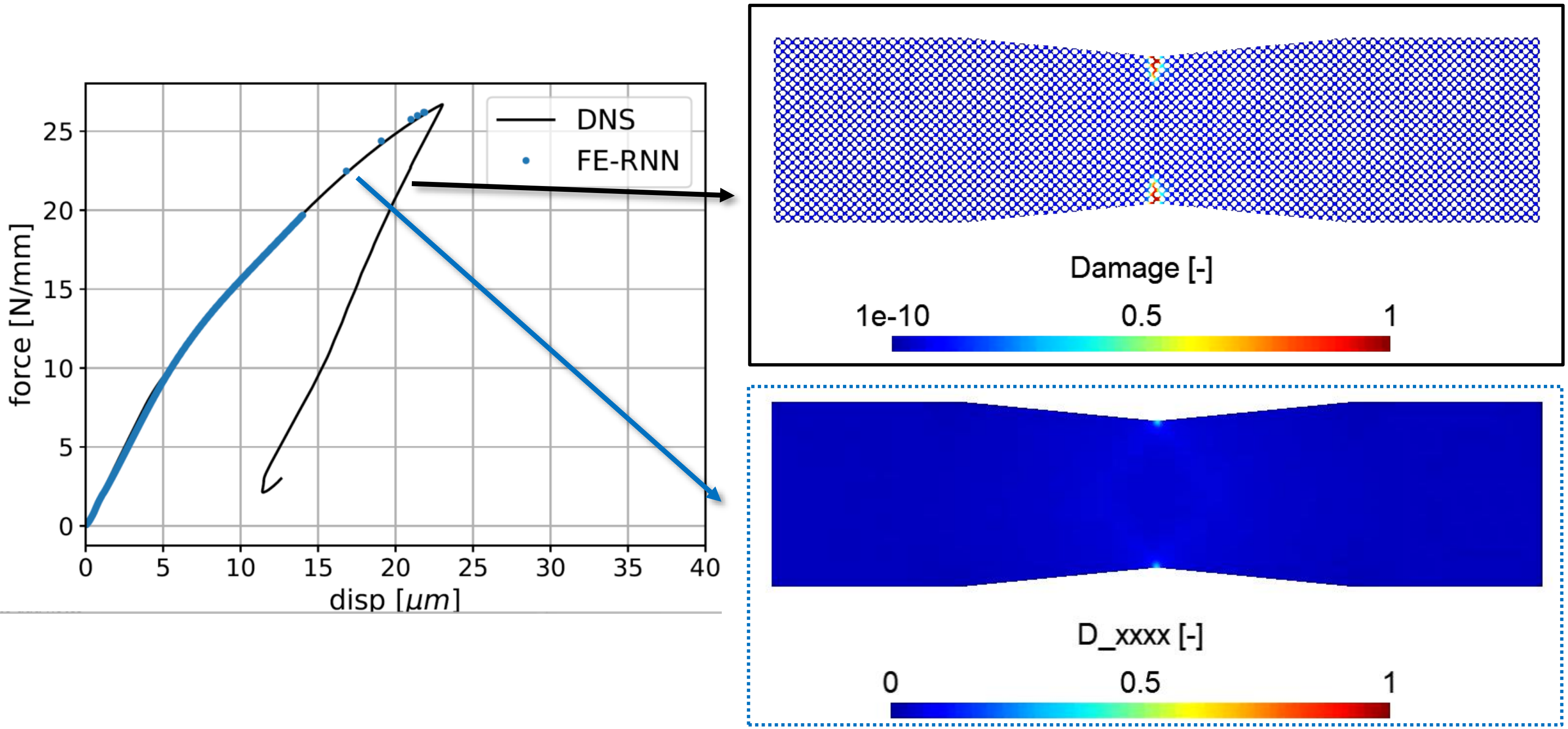


AI-accelerated multi-scale analysis of composite failure

- Larger sample
  - DNS vs. RNN
    - RNN trained on volume elements
    - Calibrated macro-scale non-local lengths



- Use of RNN
  - Good accuracy/performance for RNN
    - When designed for computational mechanics
    - Trained with adequate synthetic data base
  - Limitations: No extrapolation capabilities
    - Requires extensive synthetic data base
    - Generalizing for arbitrary micro-structure/phase response requires unreachable data bases
    - Validity range is limited

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- Can we limit the size of the data base?
  - Introduce Physics in neural networks
    - Predicting energy potentials (Yvonnet, Masi, Stefanou, …)
    - Introducing material laws (Maia, van der Meer, …
    - Modifying loss function (Cueto, …)
    - ….

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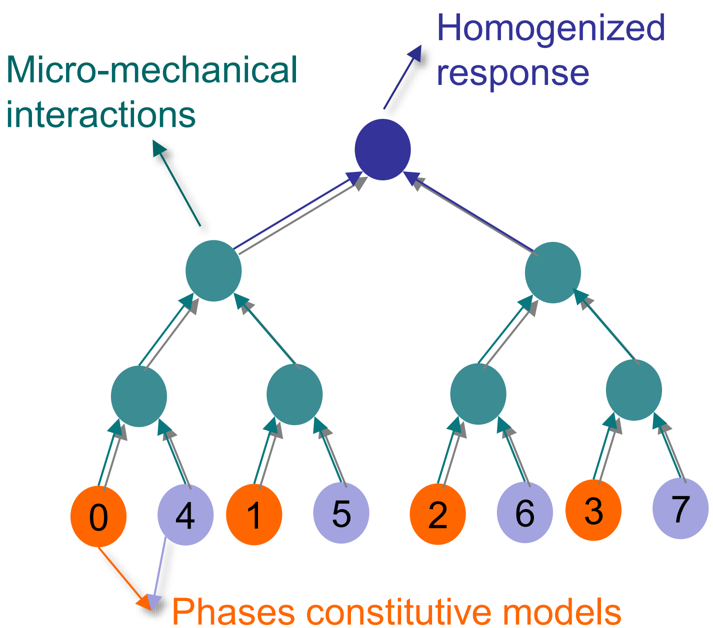
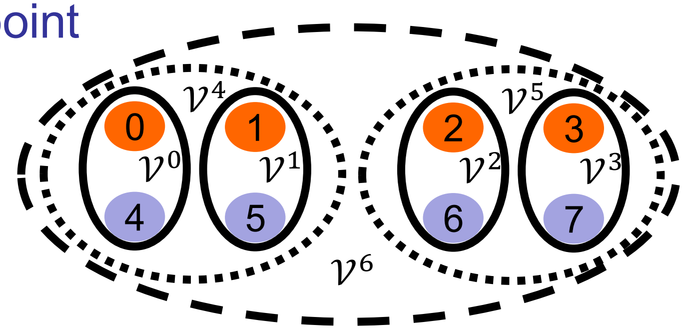
    - ….
  - Alternative solution: build a network of physical blocks
    - Deep Material Network (Liu, …)*



*Z. Liu, C. Wu, M. Koishi, A deep material network for multiscale topology learning and accelerated nonlinear modeling of heterogeneous materials, Comput. Methods Appl. Mech. Engrg. 345 (2019) 1138–1168

- Deep Material Networks from the interaction viewpoint
  - Strain/Stress averaging

$$\mathbf{P}_{\mathrm{M}}(t) = \sum_{i=0}^{7} v_i \, \mathbf{P}_i(t)$$
$$\mathbf{F}_{\mathrm{M}}(t) = \sum_{i=0}^{7} v_i \, \mathbf{F}_i(t)$$
$$v_i = \frac{V_i}{V_{\mathrm{M}}}$$



  - Fluctuation filed $\boldsymbol{u}'$

$$\mathbf{F}_{\mathrm{m}}(\boldsymbol{X}_{\mathrm{m}}) = \mathbf{F}_{\mathrm{M}} + \boldsymbol{u}'(\boldsymbol{X}_{\mathrm{m}}) \otimes \nabla_0$$

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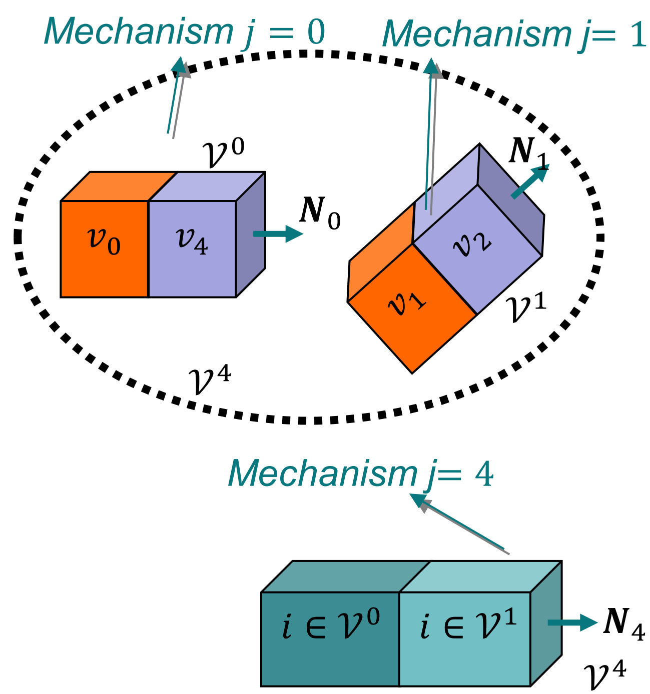

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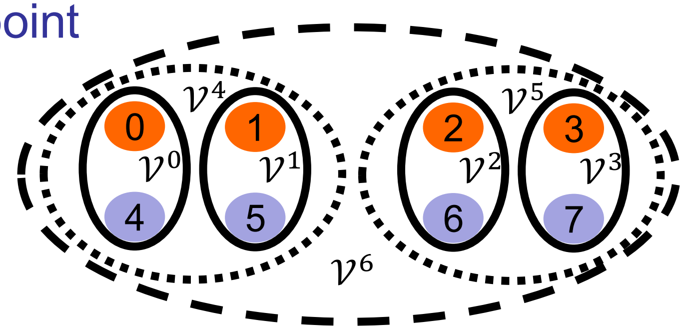

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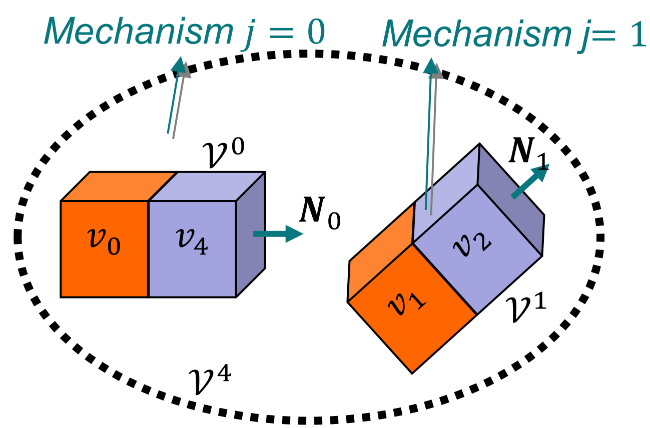
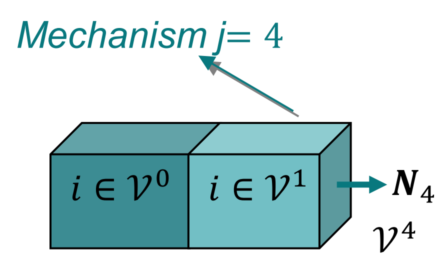


  - Weak form from Hill Mandel condition

$$\mathbf{P}_{\mathrm{M}} : \delta \mathbf{F}_{\mathrm{M}} = \sum_i v_i \, \mathbf{P}_i : \delta \mathbf{F}_i$$

$$\Rightarrow \left[\sum_j \left(\sum_i \frac{v_i s_j^i}{V_i} \mathbf{P}_i(\boldsymbol{u}_k') \right) \cdot \boldsymbol{N}_j^i \right] \cdot \delta \boldsymbol{u}_j' = 0$$

$$\Rightarrow \sum_i s_j^i \, \mathbf{P}_i(\boldsymbol{u}_k') \cdot \boldsymbol{N}_j^i = 0, \qquad j = 0, \ldots, 6$$



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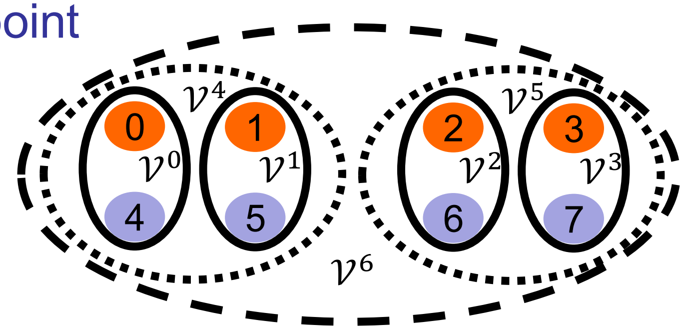
Weight of node i (parameter)



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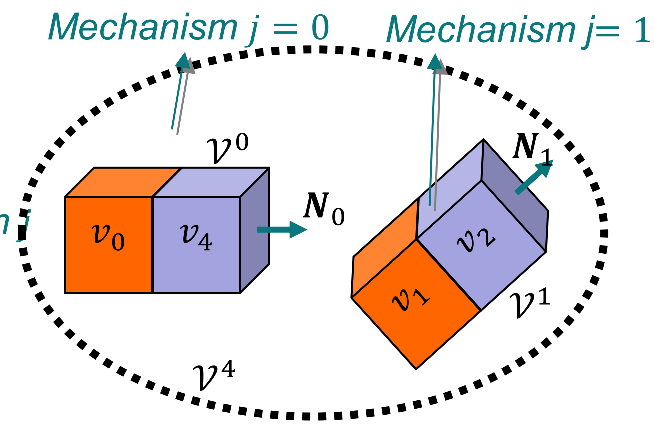
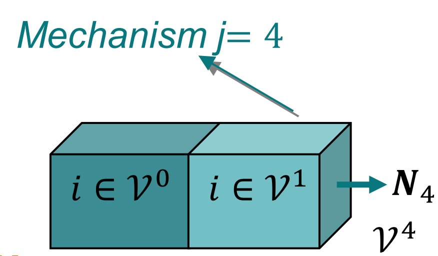
Contribution of node i in mechanism j (parameter)

Direction of mechanism j (parameter)



  - Offline stage: Parameters $(v_i, s_j^i, \boldsymbol{N}_j^i)$
    - Obtained by training ⇒ data driven approach
    - Should be independent from the constitutive behaviours
    - Should be independent from load paths

⇒ **Representative of the micro-structure organisation only**



AI-accelerated multi-scale analysis of composites

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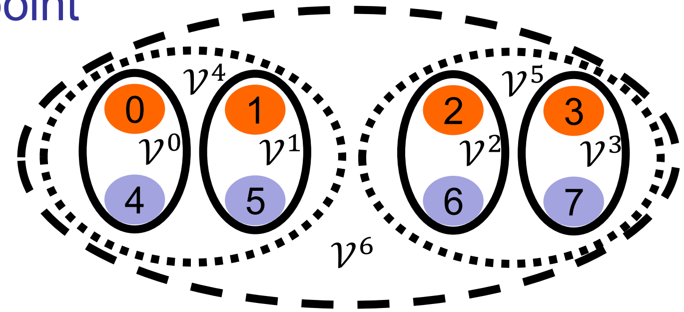

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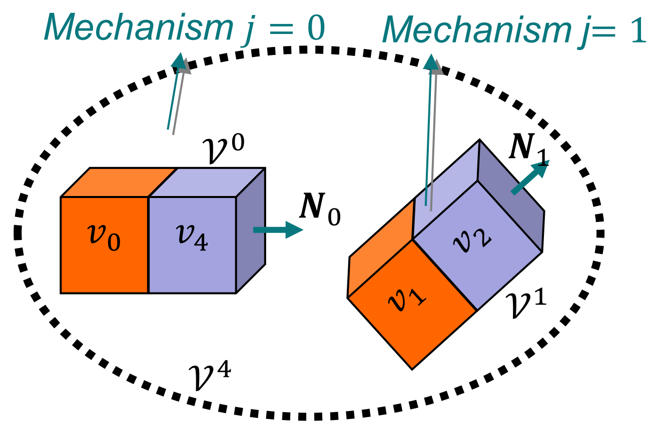
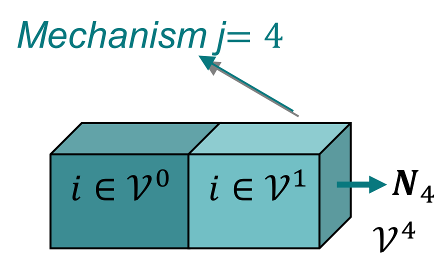
Degrees of freedom of mechanism j defining the strain fluctuation



  - Online stage: Weak form from Hill Mandel condition

$$\sum_i s_j^i \, \mathbf{P}_i(\boldsymbol{u}_k') \cdot \boldsymbol{N}_j^i = 0, \qquad j = 0, \ldots, 6$$

with $\mathbf{P}_i = \mathbf{P}^p(\mathbf{F}_i(\boldsymbol{u}'_k);\ \boldsymbol{Z}_i)$, for $i = 0, \ldots, 7$



⇒ Non-linear problem for given loading/material models

- Training of Interaction-Based Deep Material Networks
  - Summary

$$\begin{cases} \mathbf{F}_i = \mathbf{F}_\mathrm{M} + \frac{1}{V_i}\sum_{(i,j)} s_j^i\, \boldsymbol{u}'_j \otimes \boldsymbol{N}_j^i\;, \quad i = 0..7 \\ \sum_i s_j^i\, \mathbf{P}_i\,(\boldsymbol{u}'_k) \cdot \boldsymbol{N}_j^i = 0, \qquad j = 0,\ldots,6 \\ \mathbf{P}_i = \mathbf{P}^p(\mathbf{F}_i(\boldsymbol{u}'_k);\; \boldsymbol{Z}_i)\;, \text{ for } i = 0,\ldots,7 \\ \mathbf{P}_\mathbf{M}(t) = \sum_{i=0}^{7} v_i\, \mathbf{P}_i(t) \end{cases}$$

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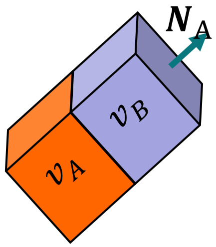
  - Elasticity with only two pseudo-grains (1-level)
    - Analytical solution



New dof: $\hat{\mathrm{a}} = \frac{s_\mathrm{AB}}{V_\mathrm{M}}\boldsymbol{u}'$

$$\begin{cases} \boldsymbol{\varepsilon}_\mathrm{A} = \boldsymbol{\varepsilon}_\mathrm{M} + \frac{1}{v_\mathrm{A}}\frac{s_\mathrm{AB}}{V_\mathrm{M}}\boldsymbol{u}' \otimes^s \boldsymbol{N}_\mathrm{A} \text{ and} \\ \boldsymbol{\varepsilon}_\mathrm{B} = \boldsymbol{\varepsilon}_\mathrm{M} - \frac{1}{v_\mathrm{B}}\frac{s_\mathrm{AB}}{V_\mathrm{M}}\boldsymbol{u}' \otimes^s \boldsymbol{N}_\mathrm{A} \\ \mathbb{C}_\mathrm{M} = v_\mathrm{A}\mathbb{C}_\mathrm{A} + (1.0 - v_\mathrm{A})\mathbb{C}_\mathrm{B} + (\mathbb{C}_\mathrm{A} - \mathbb{C}_\mathrm{B}) \cdot \boldsymbol{N}_\mathrm{A} \otimes^s [\mathcal{K}^{-1}(v_\mathrm{A}, \boldsymbol{N}_\mathrm{A}) \cdot \mathcal{F}_\mathrm{M}(v_\mathrm{A}, \boldsymbol{N}_\mathrm{A})] \end{cases}$$

Topology parameters to be defined $\mathcal{G}^2 = \{v_\mathrm{A}, \boldsymbol{N}_\mathrm{A}\}$

$$\mathbb{C}_\mathrm{M} = \mathrm{FUN}\left(\mathbb{C}_\mathrm{A}, \mathbb{C}_\mathrm{B}, \mathcal{G}^2(v_\mathrm{A}, \boldsymbol{N}_\mathrm{A})\right)$$

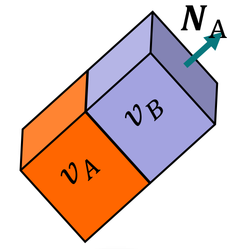
AI-accelerated multi-scale analysis of composites

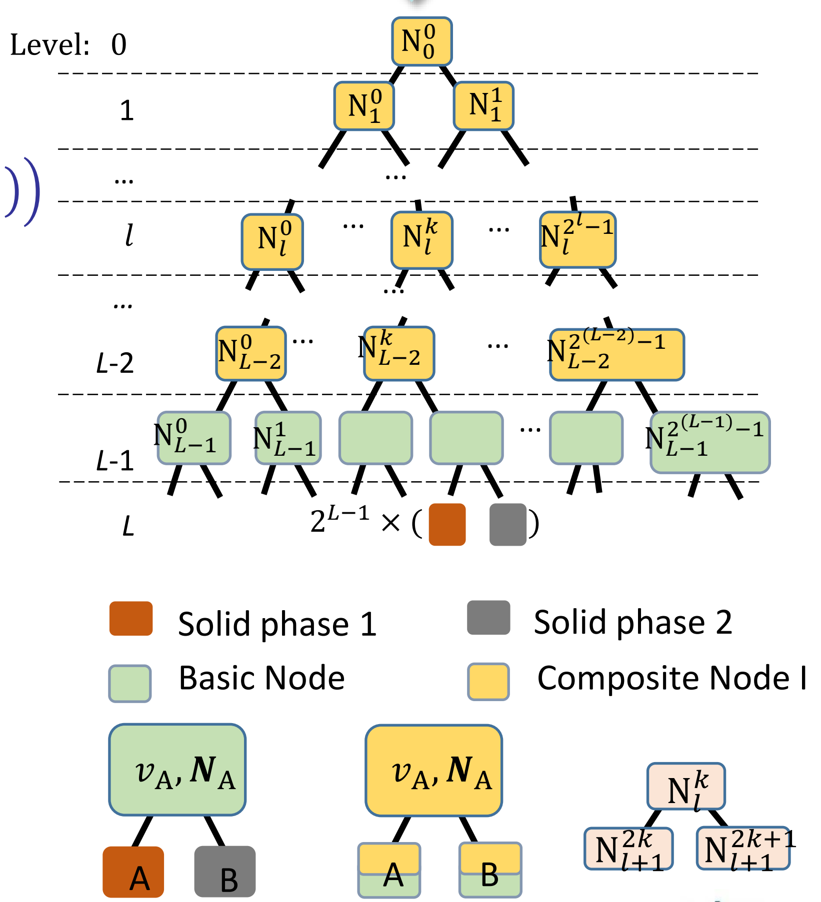
- Training of Interaction-Based Deep Material Networks
  - Elasticity with multi-level tree
    - Generalizing $\mathbb{C}_{\mathrm{M}} = \mathrm{FUN}\left(\mathbb{C}_{\mathrm{A}}, \mathbb{C}_{\mathrm{B}}, \mathcal{G}^2(v_{\mathrm{A}}, \boldsymbol{N}_{\mathrm{A}})\right)$

$$\mathbb{C}(\mathrm{N}_l^k) = \mathrm{FUN}\left(l, \mathbb{C}_0, \mathbb{C}_{\mathrm{I}}, \mathcal{G}^2(\mathrm{N}_l^k)\right)$$

with

$$\begin{cases} \mathbb{C}(\mathrm{N}_{l+1}^{2k}) = \mathrm{FUN}\left(l+1, \mathbb{C}_0, \mathbb{C}_{\mathrm{I}}, \mathcal{G}^2(\mathrm{N}_{l+1}^{2k})\right) \\ \mathbb{C}(\mathrm{N}_{l+1}^{2k+1}) = \mathrm{FUN}\left(l+1, \mathbb{C}_0, \mathbb{C}_{\mathrm{I}}, \mathcal{G}^2(\mathrm{N}_{l+1}^{2k+1})\right) \end{cases}$$





- Training of Interaction-Based Deep Material Networks
  - Elasticity with multi-level tree
    - Generalizing $\mathbb{C}_M = \text{FUN}\left(\mathbb{C}_A, \mathbb{C}_B, \mathcal{G}^2(v_A, \boldsymbol{N}_A)\right)$

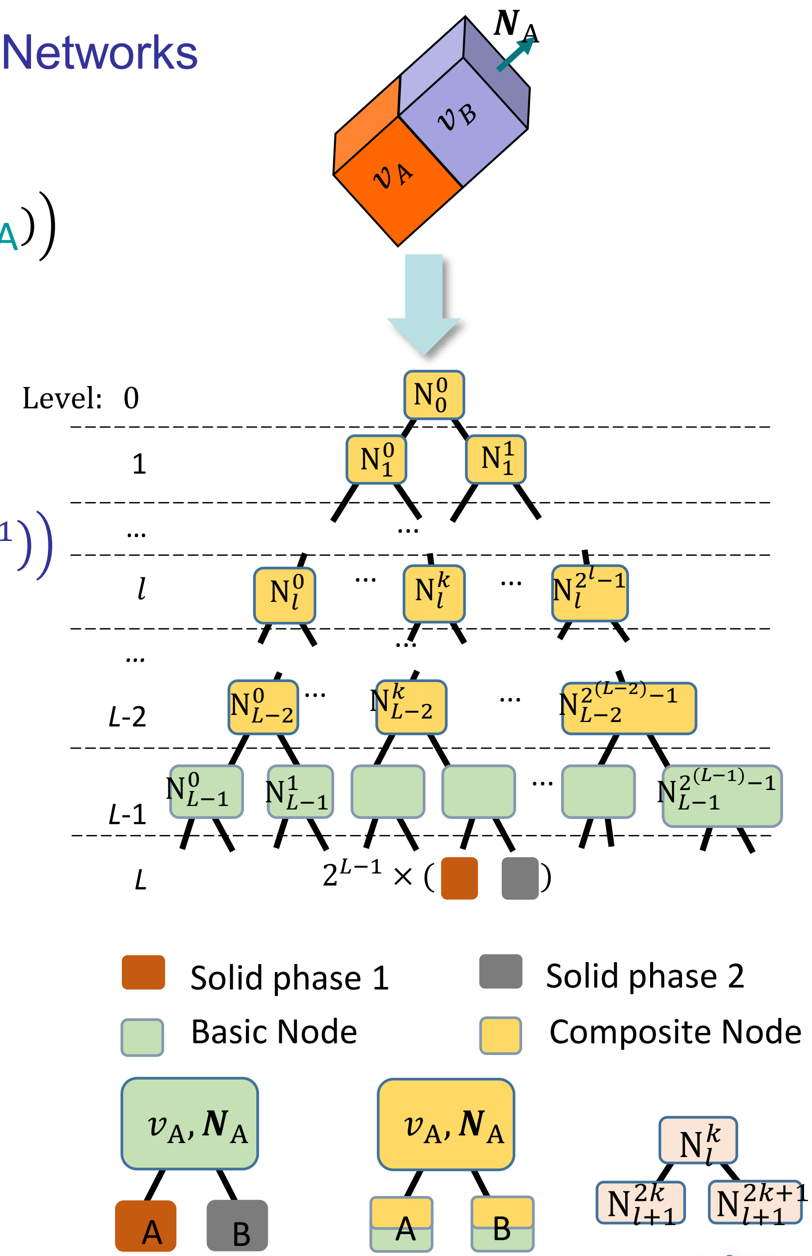
$$\mathbb{C}(\text{N}_l^k) = \text{FUN}\left(l, \mathbb{C}_0, \mathbb{C}_\text{I}, \mathcal{G}^2(\text{N}_l^k)\right)$$

with

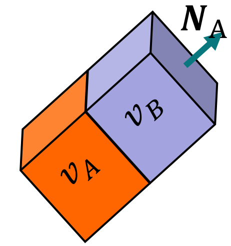
$$\begin{cases} \mathbb{C}(\text{N}_{l+1}^{2k}) = \text{FUN}\left(l+1, \mathbb{C}_0, \mathbb{C}_\text{I}, \mathcal{G}^2(\text{N}_{l+1}^{2k})\right) \\ \mathbb{C}(\text{N}_{l+1}^{2k+1}) = \text{FUN}\left(l+1, \mathbb{C}_0, \mathbb{C}_\text{I}, \mathcal{G}^2(\text{N}_{l+1}^{2k+1})\right) \end{cases}$$

- Recursive analytical solution

$$\mathbb{C}_M = \text{FUN}\left(l = 0, \mathbb{C}_0, \mathbb{C}_\text{I}, \mathcal{G}^2(\text{N}_0^0)\right)$$



- Training of Interaction-Based Deep Material Networks
  - Elasticity with multi-level tree



- Generalizing $\mathbb{C}_\mathrm{M} = \mathrm{FUN}\left(\mathbb{C}_\mathrm{A}, \mathbb{C}_\mathrm{B}, \mathcal{G}^2(v_\mathrm{A}, \boldsymbol{N}_\mathrm{A})\right)$

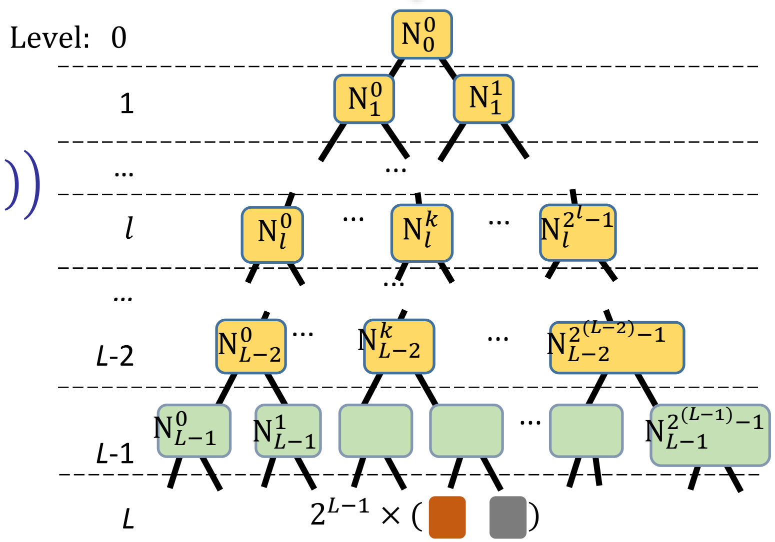
$$\mathbb{C}(\mathrm{N}_l^k) = \mathrm{FUN}\left(l, \mathbb{C}_0, \mathbb{C}_\mathrm{I}, \mathcal{G}^2(\mathrm{N}_l^k)\right)$$

with

$$\begin{cases} \mathbb{C}(\mathrm{N}_{l+1}^{2k}) = \mathrm{FUN}\left(l+1, \mathbb{C}_0, \mathbb{C}_\mathrm{I}, \mathcal{G}^2(\mathrm{N}_{l+1}^{2k})\right) \\ \mathbb{C}(\mathrm{N}_{l+1}^{2k+1}) = \mathrm{FUN}\left(l+1, \mathbb{C}_0, \mathbb{C}_\mathrm{I}, \mathcal{G}^2(\mathrm{N}_{l+1}^{2k+1})\right) \end{cases}$$

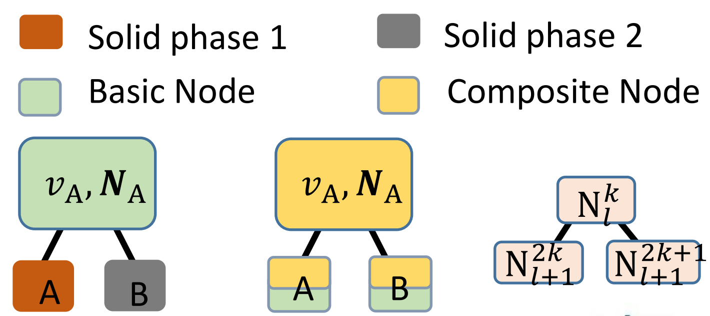
- Recursive analytical solution

$$\mathbb{C}_\mathrm{M} = \mathrm{FUN}\left(l=0, \mathbb{C}_0, \mathbb{C}_\mathrm{I}, \mathcal{G}^2(\mathrm{N}_0^0)\right)$$



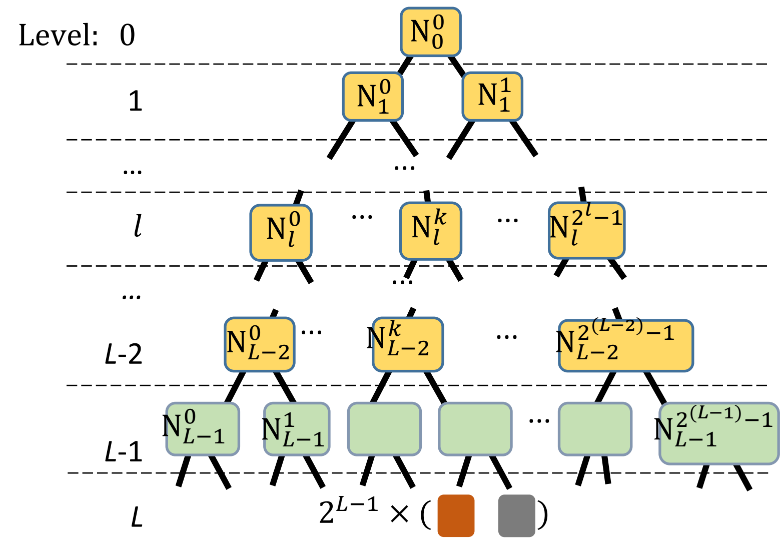
Topology parameters to be defined:

$\mathcal{G}^2(\mathrm{N}_0^0), \mathcal{G}^2(\mathrm{N}_1^0), \mathcal{G}^2(\mathrm{N}_1^1), \dots, \mathcal{G}^2\left(\mathrm{N}_{L-1}^{2^{(L-1)}-1}\right)$



- Training of Interaction-Based Deep Material Networks
  - Summary

$$
\begin{cases}
\mathbf{F}_i = \mathbf{F}_\mathrm{M} + \frac{1}{V_i}\sum_{(i,j)} s_j^i \, \boldsymbol{u}'_j \otimes \boldsymbol{N}_j^i \ , \quad i = 0..7 \\
\sum_i s_j^i \, \mathbf{P}_i\left(\boldsymbol{u}'_k\right) \cdot \boldsymbol{N}_j^i = 0, \qquad j = 0, \ldots, 6 \\
\mathbf{P}_i = \mathbf{P}^p\left(\mathbf{F}_i(\boldsymbol{u}'_k);\ \boldsymbol{Z}_i\right) \text{, for } i = 0, \ldots, 7 \\
\mathbf{P}_\mathrm{M}(t) = \sum_{i=0}^{7} v_i \, \mathbf{P}_i(t)
\end{cases}
$$



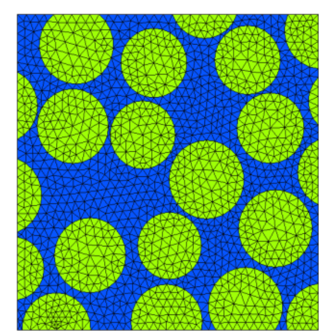
  - Analytical solution in linear elasticity
    - Recursively

$$\mathbb{C}_\mathrm{M} = \mathrm{FUN}\left(l = 0, \mathbb{C}_0, \mathbb{C}_\mathrm{I}, \mathcal{G}^2(\mathrm{N}_0^0)\right)$$

    - Topological parameters

$$\mathcal{G}^2(\mathrm{N}_0^0), \mathcal{G}^2(\mathrm{N}_1^0), \mathcal{G}^2(\mathrm{N}_1^1), \ldots, \mathcal{G}^2\left(\mathrm{N}_{L-1}^{2^{(L-1)}-1}\right)$$

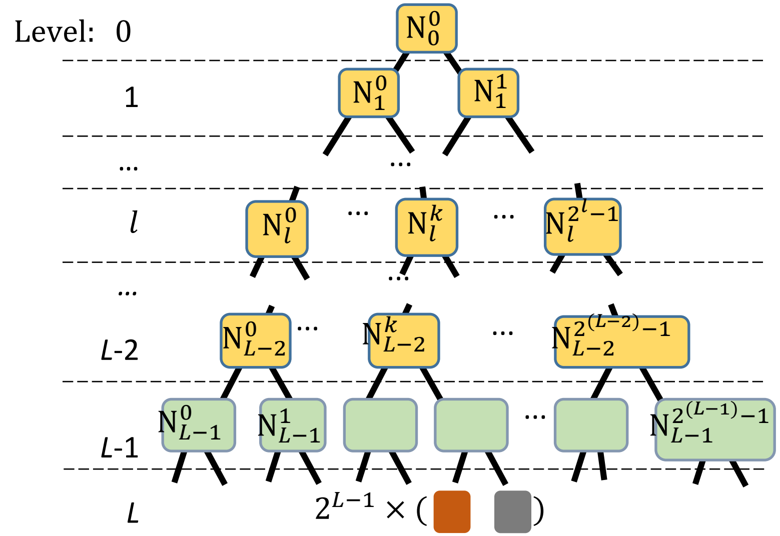
To be identified for a given micro-structure



AI-accelerated multi-scale analysis of composites

- Training of Interaction-Based Deep Material Networks
  - Summary

$$\begin{cases} \mathbf{F}_i = \mathbf{F}_\mathrm{M} + \frac{1}{V_i}\sum_{(i,j)} s_j^i\, \boldsymbol{u}'_j \otimes \boldsymbol{N}_j^i \;, \quad i = 0..7 \\ \sum_i s_j^i\, \mathbf{P}_i\,(\boldsymbol{u}'_k)\cdot \boldsymbol{N}_j^i = 0, \qquad j = 0,\dots,6 \\ \mathbf{P}_i = \mathbf{P}^p(\mathbf{F}_i(\boldsymbol{u}'_k);\; \boldsymbol{Z}_i)\;, \text{ for } i = 0, \dots, 7 \\ \mathbf{P}_\mathrm{M}(t) = \sum_{i=0}^{7} v_i\, \mathbf{P}_i(t) \end{cases}$$

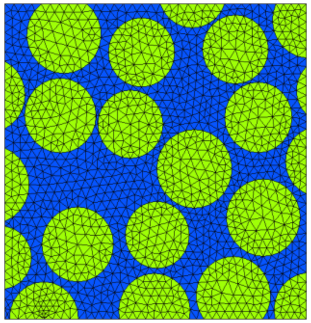


  - Analytical solution in linear elasticity
    - Recursively

$$\mathbb{C}_\mathrm{M} = \mathrm{FUN}\left(l = 0,\, \mathbb{C}_0,\, \mathbb{C}_\mathrm{I},\, \mathcal{G}^2(\mathrm{N}_0^0)\right)$$

    - Topological parameters

$$\mathcal{G}^2(\mathrm{N}_0^0), \mathcal{G}^2(\mathrm{N}_1^0), \mathcal{G}^2(\mathrm{N}_1^1), \dots, \mathcal{G}^2\left(\mathrm{N}_{L-1}^{2^{(L-1)}-1}\right)$$



  - Data driven approach:
    - Generate observations $\{\hat{\mathbb{C}}_\mathrm{M}(\mathbb{C}_0^s, \mathbb{C}_\mathrm{I}^s)\}$ by full DNS using random $\mathbb{C}_0^s$, $\mathbb{C}_\mathrm{I}^s$
    - Identify topological parameters from loss function (knowing real volume fraction $\hat{\mathrm{v}}_\mathrm{I}$ of phase I)

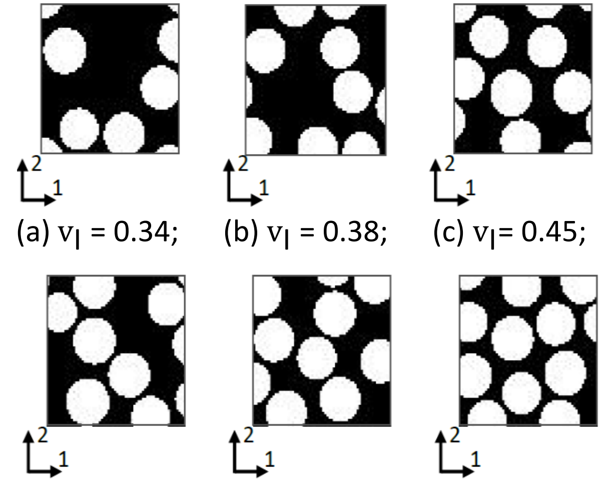
$$Loss(\hat{\mathbb{C}}_\mathrm{M}, \mathbb{C}_\mathrm{M}) = \frac{1}{n}\sum_{s=0}^{n-1} \frac{\|\hat{\mathbb{C}}_\mathrm{M}(\mathbb{C}_0^s, \mathbb{C}_\mathrm{I}^s) - \mathbb{C}_\mathrm{M}(\mathbb{C}_0^s, \mathbb{C}_\mathrm{I}^s; \mathcal{G}^2)\|}{\|\hat{\mathbb{C}}_\mathrm{M}(\mathbb{C}_0^s, \mathbb{C}_\mathrm{I}^s)\|} + \frac{\lambda}{2}(\hat{\mathrm{v}}_\mathrm{I} - \mathrm{v}_\mathrm{I})^2$$

AI-accelerated multi-scale analysis of composites

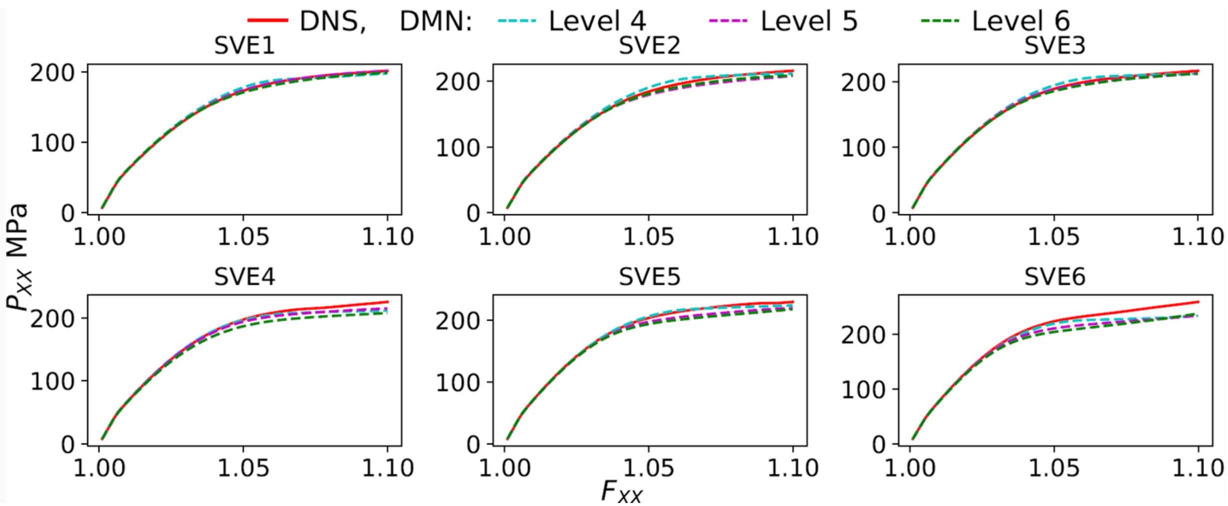
- Testing of Interaction-Based Deep Material Networks
  - Six micro-structure realizations
  - ➡ Six IB-DMNs to be trained in linear elasticity
    - For each micro-structure new set of topological parameters

$$\left\{ \mathcal{G}^2(\mathrm{N}_0^0), \mathcal{G}^2(\mathrm{N}_1^0), \mathcal{G}^2(\mathrm{N}_1^1), \ldots, \mathcal{G}^2\left(\mathrm{N}_{L-1}^{2^{(L-1)}-1}\right) \right\}$$

  - Testing on complex elasto-plasticity
    - Non-associated pressure-dependent plasticity
    - Extrapolation in terms of loading path
    - Extrapolation in terms of constitutive model



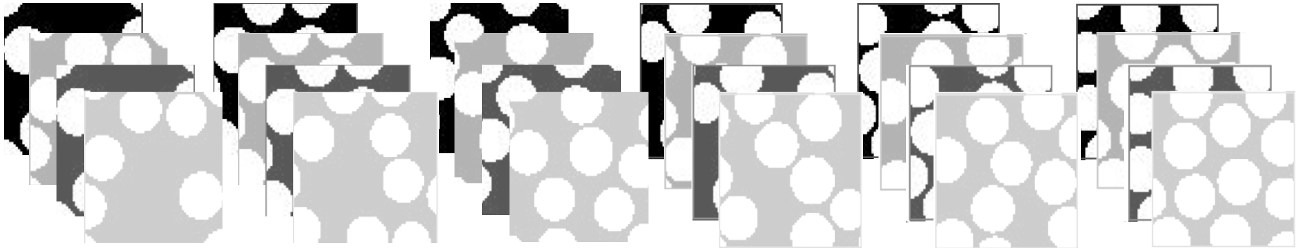
(a) $v_I = 0.34$; (b) $v_I = 0.38$; (c) $v_I = 0.45$; (d) $v_I = 0.47$; (e) $v_I = 0.52$; (f) $v_I = 0.58$



➡ For a new micro-structure: new training required

- Stochastic Interaction-Based Deep Material Networks
  - For a new micro-structure:
    - New training needed
  - When separation of scale not satisfied

$$l_{\mathrm{M}} >> l_{\mathrm{SVE}} \sim l_{\mathrm{m}}$$



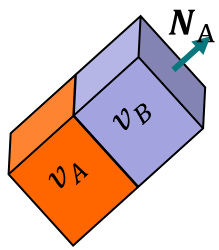
    - For the same composite volume fraction v_{I} the response depends on the micro-structure realisation

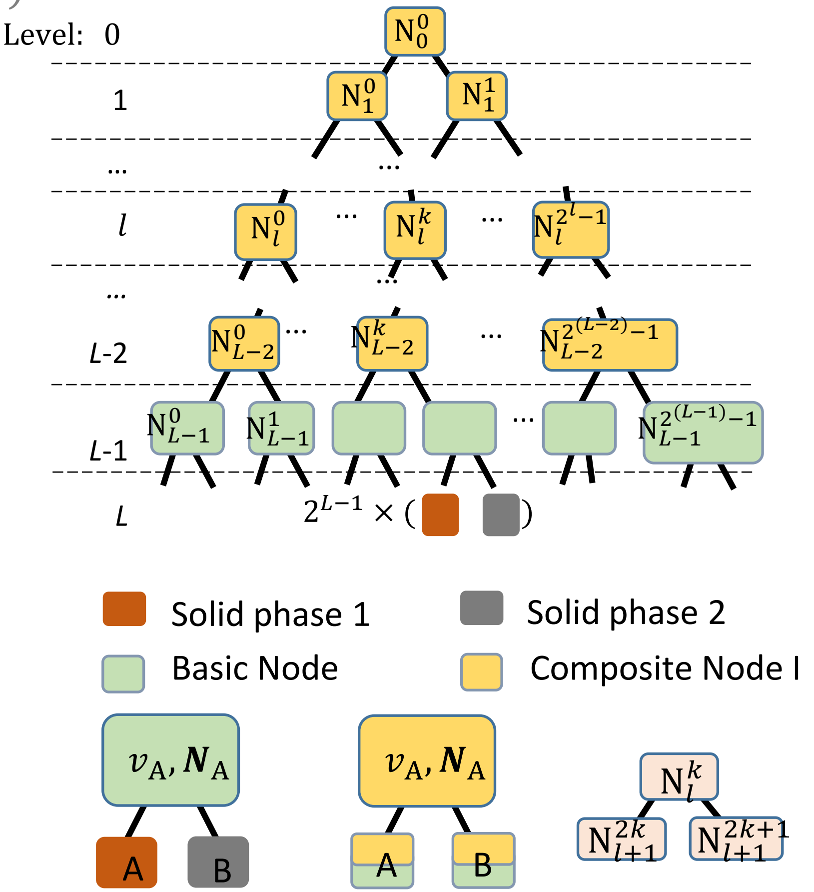
Can we interpolate the IB-DMN in terms of the micro-structure?

- Stage 1: arbitrary volume fraction v_l by reformulating $\mathcal{G}^2 = \{v_A, \boldsymbol{N}_A\}$ at node N_l^k
  - Normal $\boldsymbol{N}_A(N_l^k)$ from angles $\theta_1(N_l^k)$ and $\theta_2(N_l^k)$

$$\theta_1 = 2\pi w_{\theta_1}(N_l^k),\ \theta_2 = \pi w_{\theta_2}(N_l^k)$$

$$w_{\theta_1}(N_l^k), w_{\theta_2}(N_l^k) \in [0,\ 1)$$

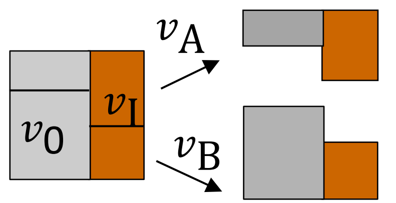




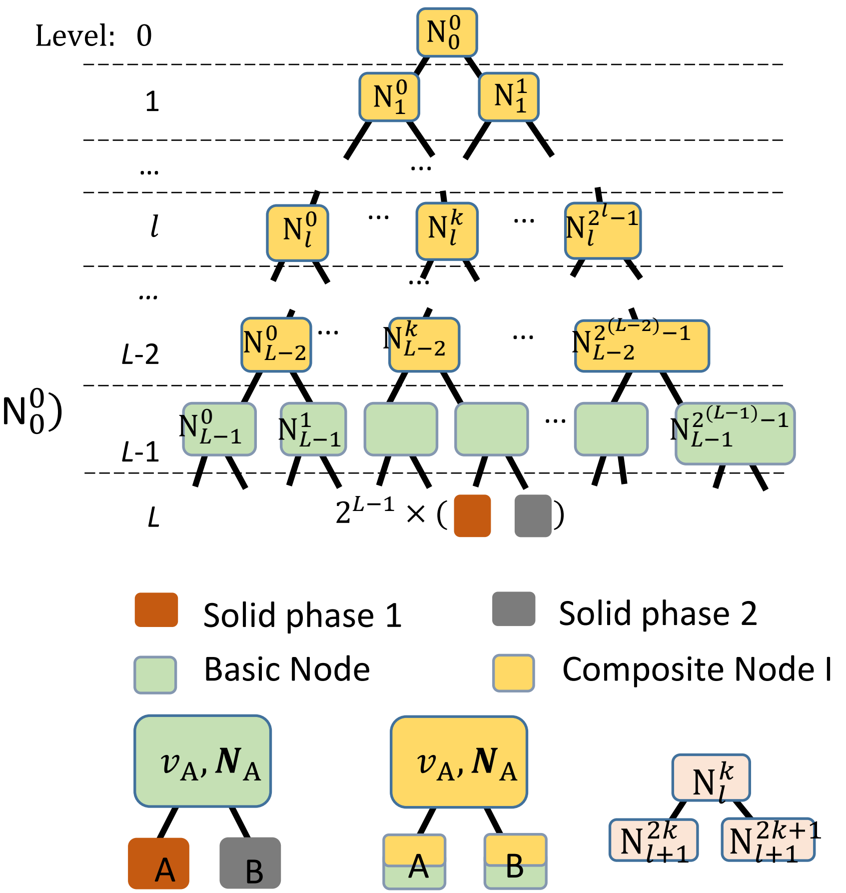
Redefinition of topological parameters to be defined:

$$\underline{w}_n = \{w_{\theta_1}, w_{\theta_2}\} = \text{sigmoid}(\mathcal{T}_n)$$

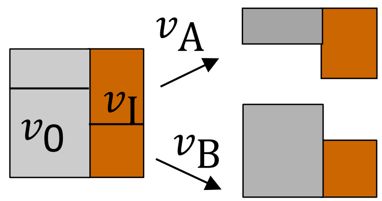
- Stage 1: arbitrary volume fraction v_I by reformulating $\mathcal{G}^2 = \{v_A, \boldsymbol{N}_A\}$ at node N_l^k
  - Volume fraction $v_A(N_l^k)$
    1) "Yellow" Node at level $l = 0$:
       $v_I(N_0^0) = v_I$ and $v_0(N_0^0) = 1 - v_I$ known



$$\begin{cases} v_A(N_0^0) = w_{v0}(N_0^0)\, v_0(N_0^0) + w_{vI}(N_0^0)\, v_I(N_0^0) \\ v_B(N_0^0) = 1.0 - v_A(N_0^0) \end{cases}$$



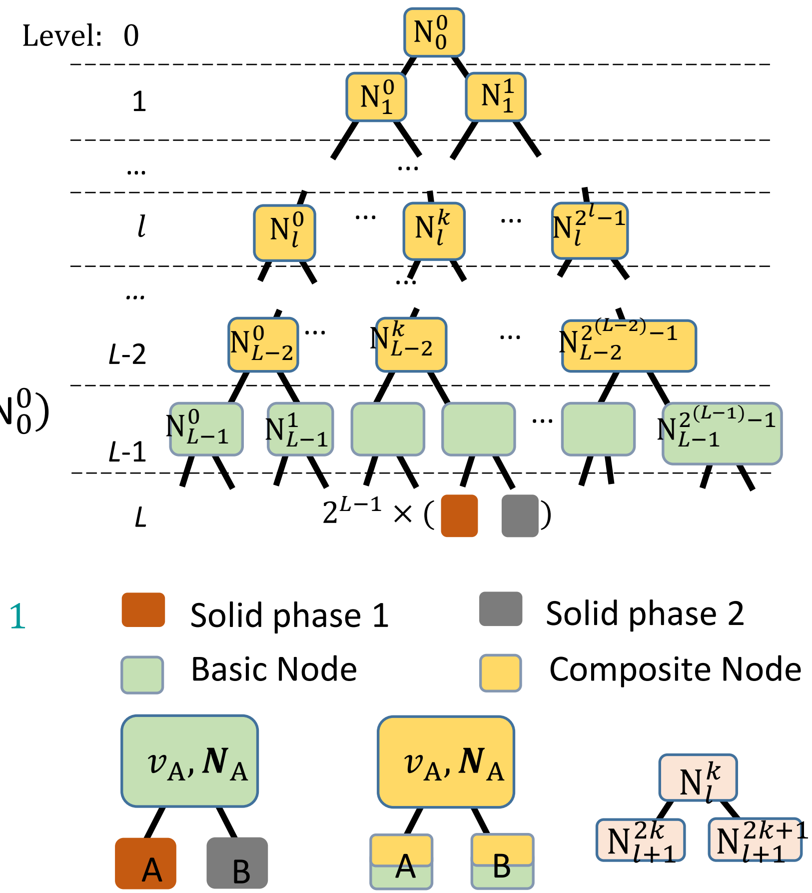
- Stage 1: arbitrary volume fraction v_I by reformulating $\mathcal{G}^2 = \{v_A, \boldsymbol{N}_A\}$ at node N_l^k
  - Volume fraction $v_A(N_l^k)$
    1) "Yellow" Node at level $l = 0$:
       $v_I(N_0^0) = v_I$ and $v_0(N_0^0) = 1 - v_I$ known



$$\begin{cases} v_A(N_0^0) = w_{v0}(N_0^0)v_0(N_0^0) + w_{vI}(N_0^0)v_I(N_0^0) \\ v_B(N_0^0) = 1.0 - v_A(N_0^0) \end{cases}$$

    2) Recursively for "Yellow" Node at level $0 < l < L - 1$

$$w_{v0}(N_l^k), w_{vI}(N_l^k) \in [0, 1)$$

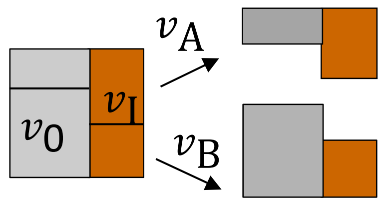


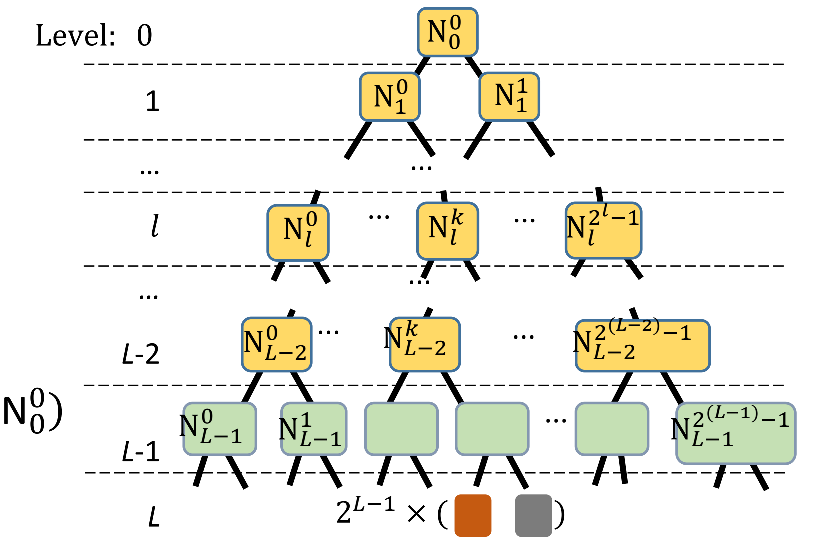
AI-accelerated stochastic multi-scale analysis of composites

- Stage 1: arbitrary volume fraction $\mathrm{v_I}$ by reformulating $\mathcal{G}^2 = \{v_\mathrm{A}, \boldsymbol{N}_\mathrm{A}\}$ at node N_l^k
  - Volume fraction $v_\mathrm{A}(\mathrm{N}_l^k)$

1) "Yellow" Node at level $l = 0$:

$v_\mathrm{I}(\mathrm{N}_0^0) = \mathrm{v_I}$ and $v_0(\mathrm{N}_0^0) = 1 - \mathrm{v_I}$ known

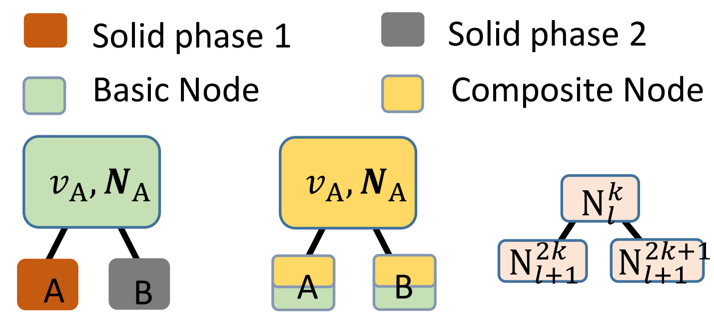




$$\begin{cases} v_\mathrm{A}(\mathrm{N}_0^0) = \mathrm{w}_{\mathrm{v}0}(\mathrm{N}_0^0) v_0(\mathrm{N}_0^0) + \mathrm{w}_{\mathrm{vI}}(\mathrm{N}_0^0) v_\mathrm{I}(\mathrm{N}_0^0) \\ v_\mathrm{B}(\mathrm{N}_0^0) = 1.0 - v_\mathrm{A}(\mathrm{N}_0^0) \end{cases}$$

2) Recursively for "Yellow" Node at level $0 < l < L-1$

$$\mathrm{w}_{\mathrm{v}0}(\mathrm{N}_l^k), \mathrm{w}_{\mathrm{vI}}(\mathrm{N}_l^k) \in [0, 1)$$



3) Basic "Green" Node at level $L - 1$:

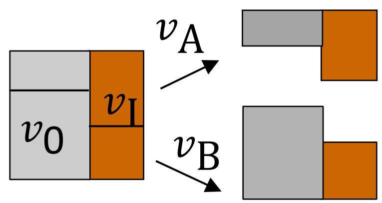
$$v_\mathrm{A} = 1.0 - v_\mathrm{I}(\mathrm{N}_{L-1}^k) \text{ and } v_\mathrm{B} = v_\mathrm{I}(\mathrm{N}_{L-1}^k)$$

AI-accelerated stochastic multi-scale analysis of composites

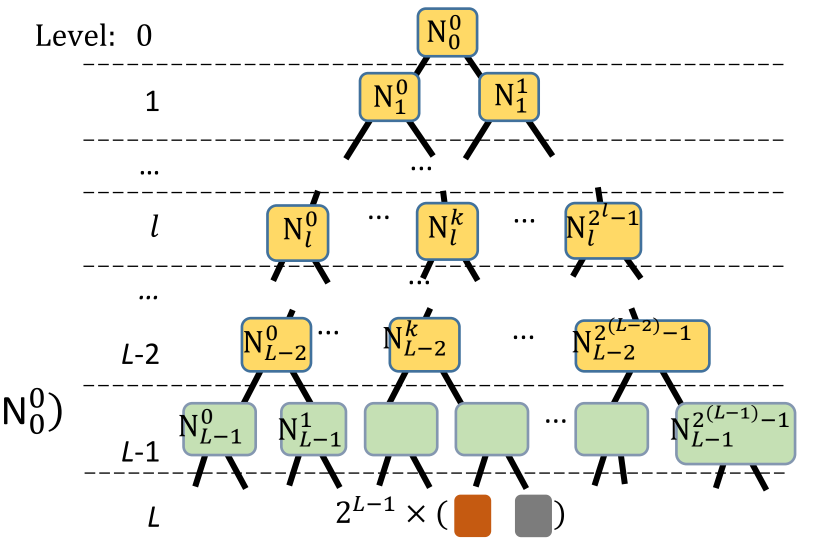
- Stage 1: arbitrary volume fraction v_I by reformulating $\mathcal{G}^2 = \{v_A, \boldsymbol{N}_A\}$ at node N_l^k
  - Volume fraction $v_A(N_l^k)$

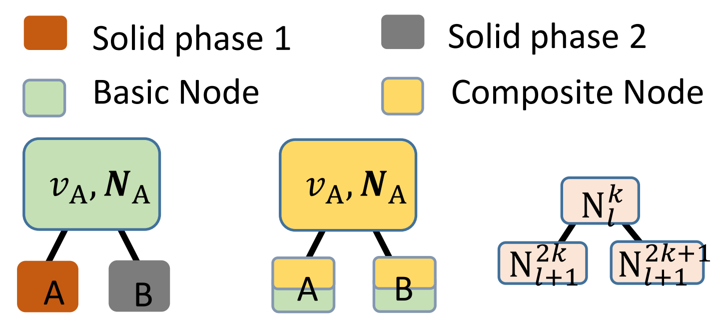
1) “Yellow” Node at level $l = 0$:

$v_I(N_0^0) = v_I$ and $v_0(N_0^0) = 1 - v_I$ known



$$\begin{cases} v_A(N_0^0) = w_{v0}(N_0^0)v_0(N_0^0) + w_{vI}(N_0^0)v_I(N_0^0) \\ v_B(N_0^0) = 1.0 - v_A(N_0^0) \end{cases}$$





2) Recursively for “Yellow” Node at level $0 < l < L - 1$

$$w_{v0}(N_l^k), w_{vI}(N_l^k) \in [0, 1)$$

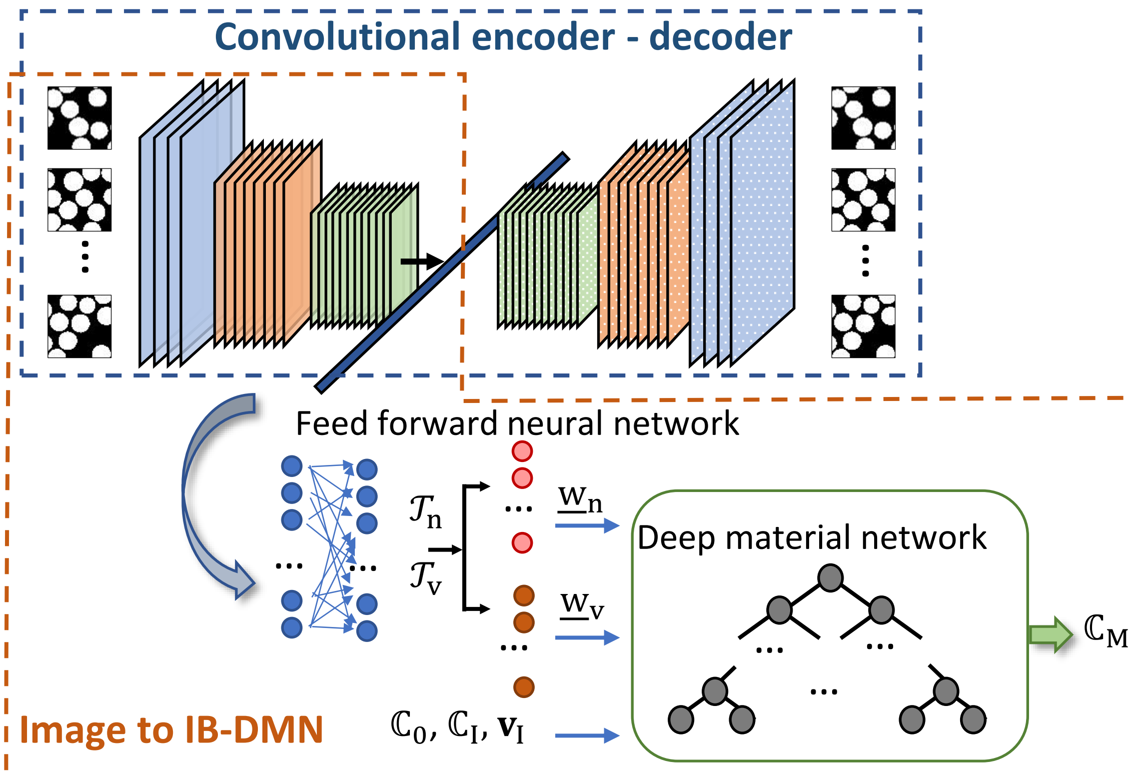
3) Basic “Green” Node at level $L - 1$:

$v_A = 1.0 - v_I(N_{L-1}^k)$ and $v_B = v_I(N_{L-1}^k)$

Redefinition of topological parameters to be defined: $\underline{w}_v = \{w_{v0}, w_{v1}\} = \text{sigmoid}(\mathcal{J}_v)$

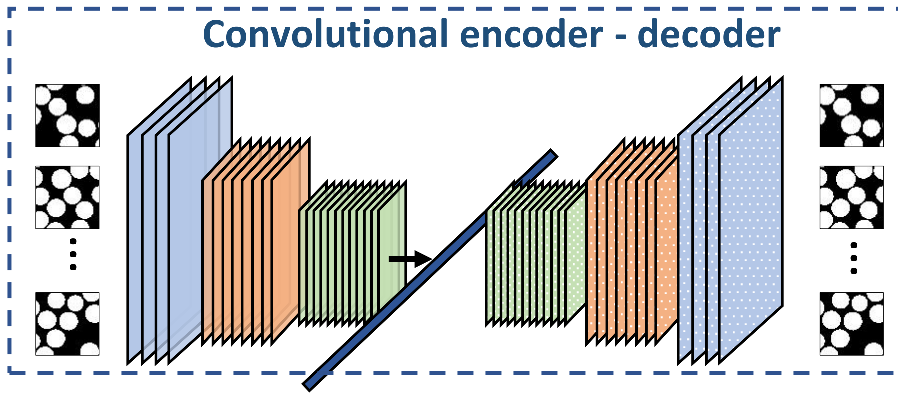
AI-accelerated stochastic multi-scale analysis of composites

- Stage 2: Predict topological parameters $\underline{w}_n = \text{sigmoid}(\mathcal{T}_n)$ & $\underline{w}_v = \text{sigmoid}(\mathcal{T}_v)$
  - Volume fraction v_I already extracted
  - $\mathcal{T}_n$ & $\mathcal{T}_v$ represent the micro-structure organisation → to be predicted from images
    - Trained Convolutional encoder-decoder: encoder predicts a features vector from image
    - Trained Feed-forward neural network: predicts topological parameters from features vector

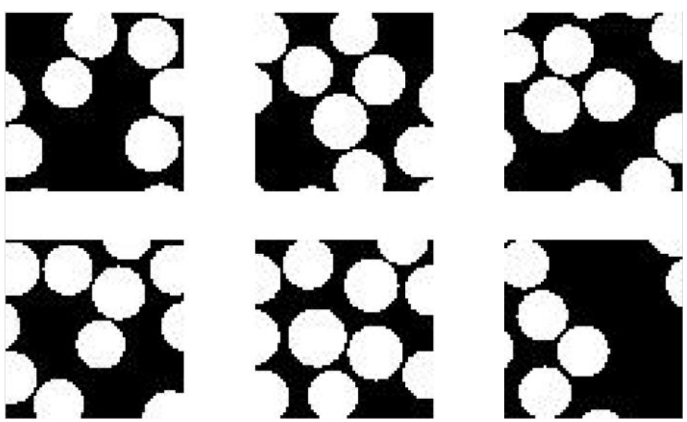


AI-accelerated stochastic multi-scale analysis of composites

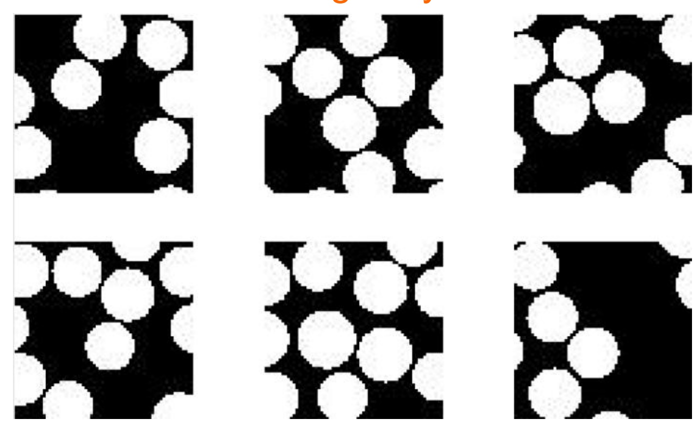
- Stage 2: Predict topological parameters $\underline{w}_n = \mathrm{sigmoid}(\mathcal{J}_n) \;\&\; \underline{w}_v = \mathrm{sigmoid}(\mathcal{J}_v)$
  - Convolutional encoder-decoder
    - Inputs: Reference images from SEM analyses
    - Output: reconstructed image
    - Trained with 10,000 reference images



Reference testing images



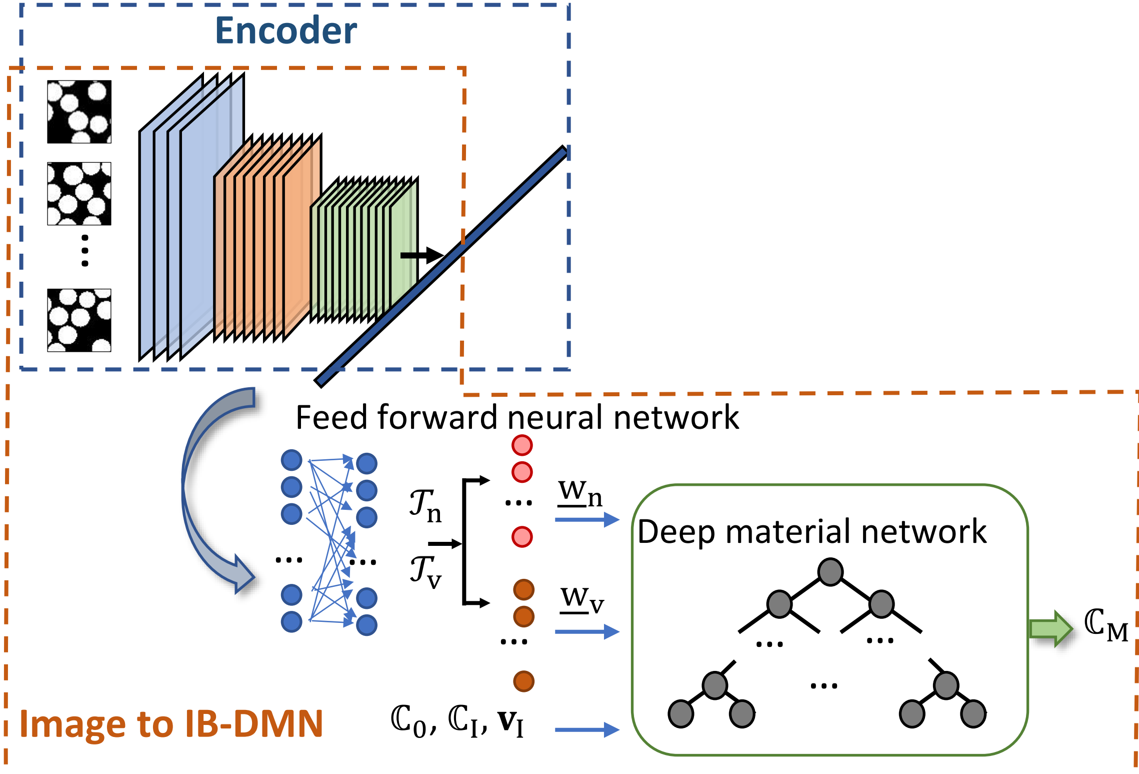
Predicted images by decoder

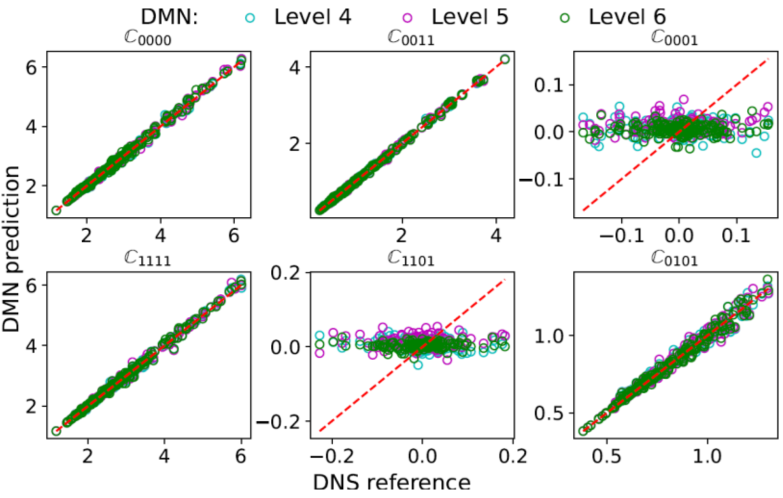


Once trained, the encoder gives a features vector of a micro-structure image

AI-accelerated stochastic multi-scale analysis of composites

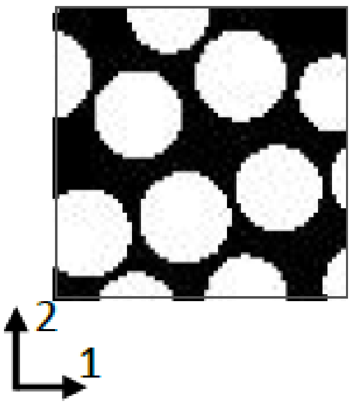
- Stage 2: Predict topological parameters $\underline{w_n} = \text{sigmoid}(\mathcal{T}_n)$ & $\underline{w_v} = \text{sigmoid}(\mathcal{T}_v)$
  - Feed forward neural network
    - Input: features vector of encoder
    - Output: topological parameters $\mathcal{T}_n$ & $\mathcal{T}_v$ representing the micro-structure
    - Trained so that the IB-DMN predicts the elasticity tensor of DNS

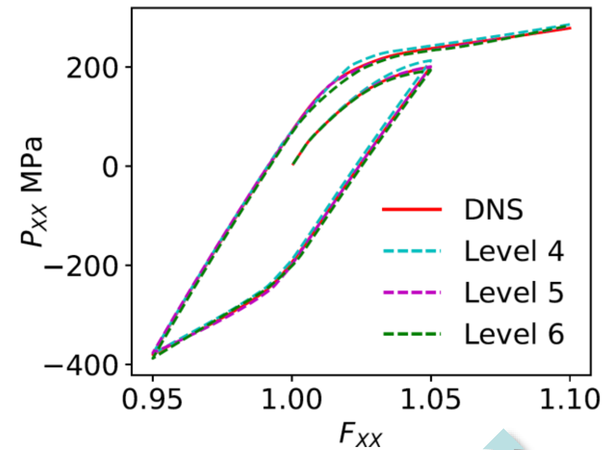


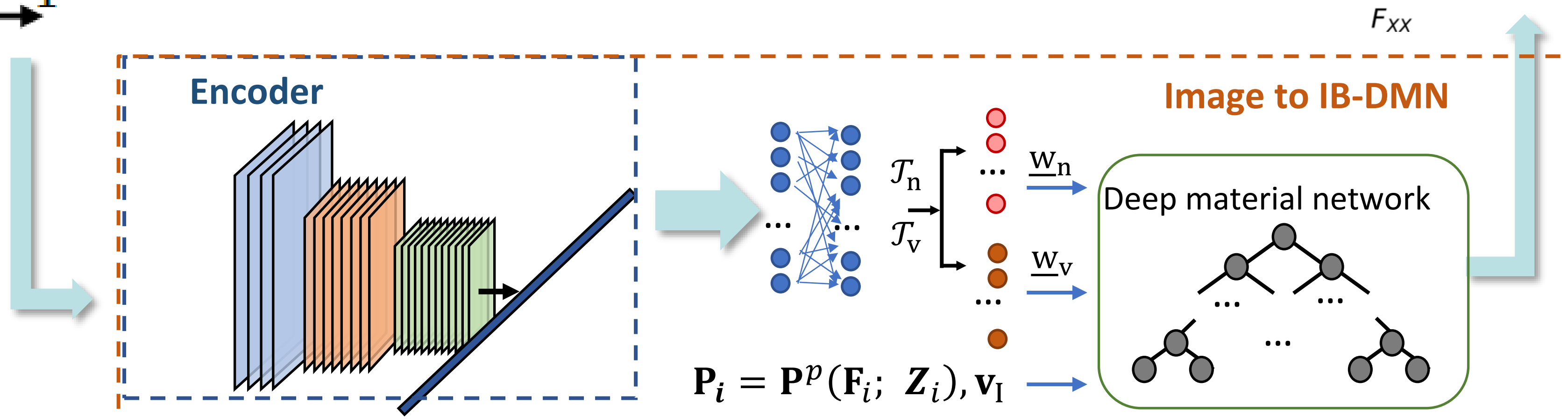


AI-accelerated stochastic multi-scale analysis of composites

- Stochastic IB-DMN prediction
  - New micro-structure realisation
  - Non-linear phase material model
  - Cyclic loading case







Conclusions & available materials

- Conclusions
  - Collection of powerful AI tools for many complex engineering applications
  - Right tool needs to be selected/developed for a given problem

- **Open positions (PhD students & post-doc)**

- Materials
  - Open source code : http://www.ltas-cm3.ulg.ac.be/openSource.htm
  - Publications http://www.ltas-cm3.ulg.ac.be/publications.htm
  - Data: http://www.ltas-cm3.ulg.ac.be/openSource.htm

- Credits

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