



Nonlocal deep material network for material constitutive models with damage

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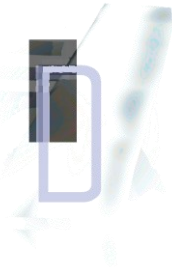
Computational & Multiscale Mechanics of Materials – CM3

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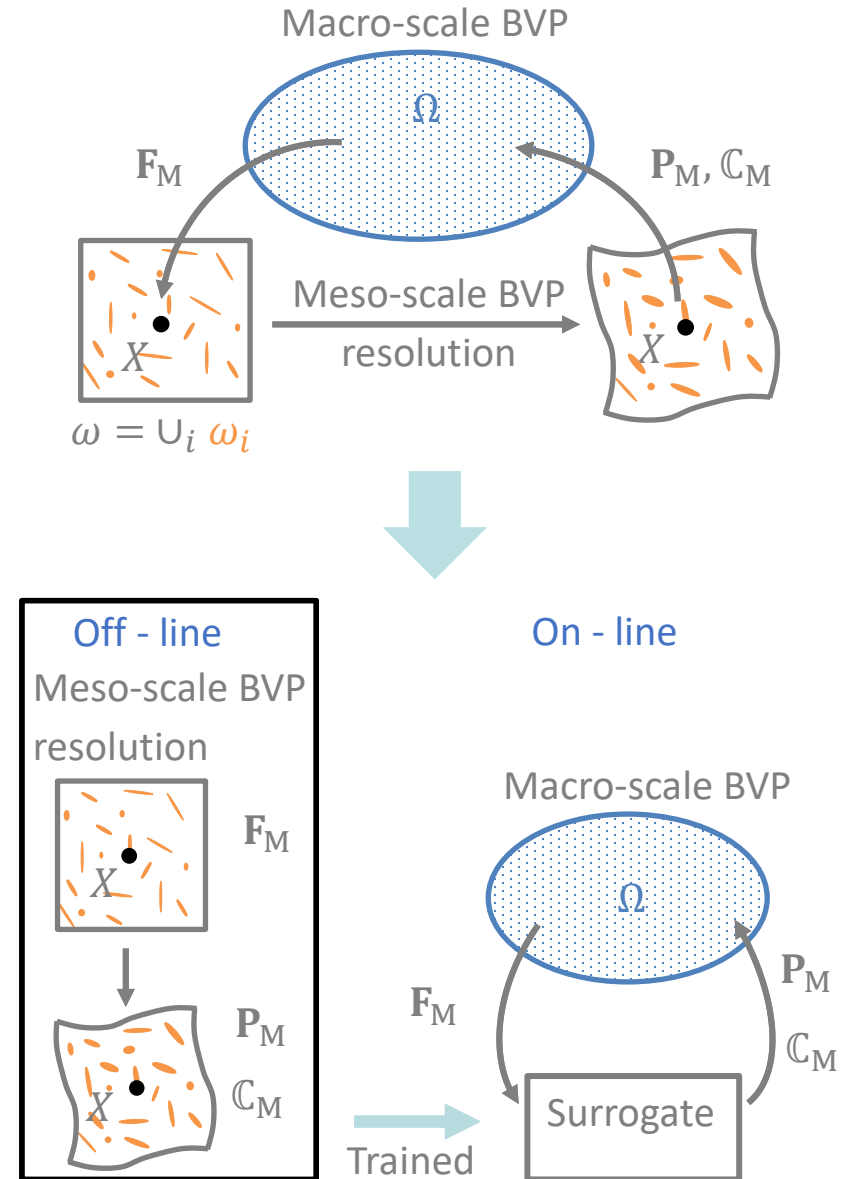
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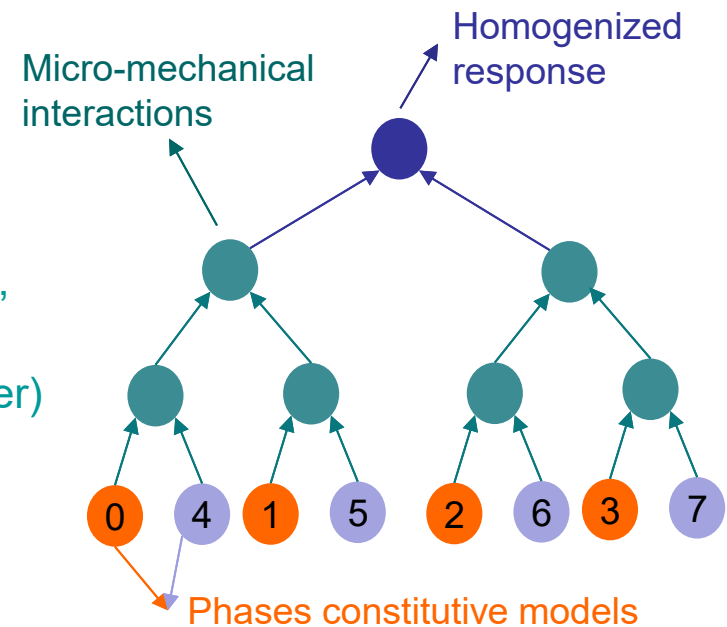


Interaction-Based Deep Material Network

- Introduction to non-linear multi-scale simulations
 - FE multi-scale simulations
 - Problems to be solved at two scales
 - Requires Newton-Raphson iterations at both scales
 - Use of surrogate models
 - Train a meso-scale surrogate model (off-line)
 - Requires extensive data
 - Obtained from RVE simulations
 - Use the trained surrogate model during analyses (on-line)
 - Surrogate acts as a homogenised constitutive law
 - Expected speed-up of several orders



- 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
- 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)
 - ...
 - 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

- Micro-scale interactions

- Subdivision in sub-domains Ω_i

$$v_i = \frac{V_i}{V_M}$$

- Stress-strain averaging

$$\mathbf{F}_M = \sum_{i=0}^{Np-1} v_i \mathbf{F}_i, \quad \text{and}$$

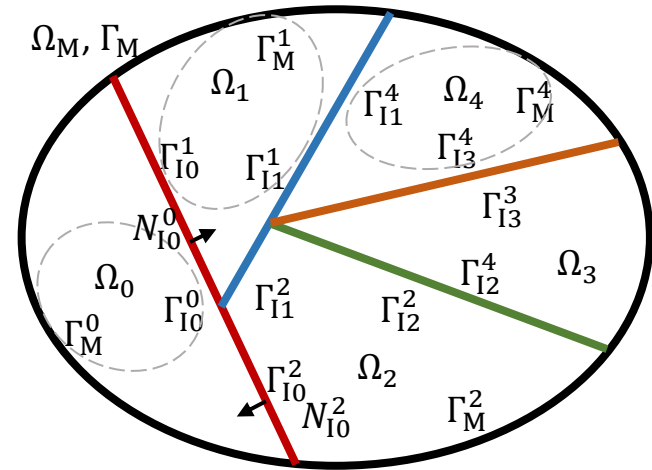
$$\mathbf{P}_M = \sum_{i=0}^{Np-1} v_i \mathbf{P}_i$$

- Introduction of fluctuations

$$\mathbf{F}_m(\mathbf{X}_m) = \mathbf{u}_m(\mathbf{X}_m) \otimes \nabla_0 = \mathbf{F}_M + \mathbf{u}'(\mathbf{X}_m) \otimes \nabla_0, \quad \mathbf{X}_m \in \Omega_M$$

$$\Rightarrow \mathbf{F}_i = \mathbf{F}_M + \frac{1}{V_i} \sum_{\forall \Gamma_{I_j}^i \neq \emptyset} \int_{\Gamma_{I_j}^i} \mathbf{u}'(\mathbf{X}_m) \otimes \mathbf{N}_{I_j}^i dS \quad s_j^i = \int_{\Gamma_{I_j}^i} dS$$

$$\Rightarrow \boxed{\mathbf{F}_i \simeq \mathbf{F}_M + \frac{1}{V_i} \sum_{\forall \Gamma_{I_j}^i \neq \emptyset} s_j^i \mathbf{u}'_j \otimes \mathbf{N}_{I_j}^i}$$



Interactions

- Introduction of fluctuations

$$\mathbf{F}_i \simeq \mathbf{F}_M + \frac{1}{V_i} \sum_{\forall \Gamma_{I_j}^i \neq \emptyset} s_j^i \mathbf{N}_{I_j}^i \otimes \mathbf{u}'_j$$

- Assume constitutive model in each sub-domain

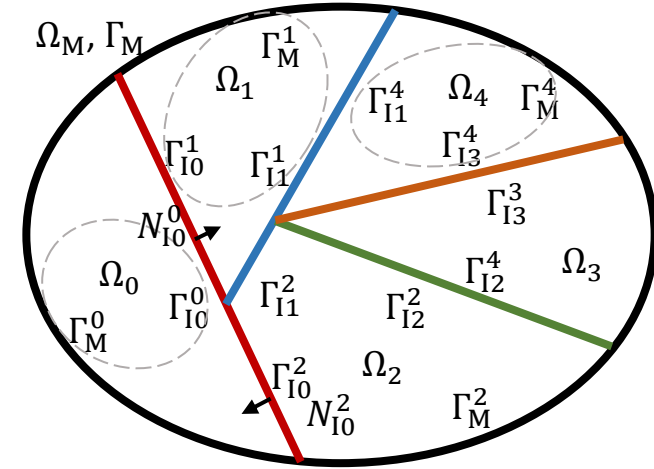
$$\mathbf{P}_i = \mathbf{P}^p(\mathbf{F}_i(\mathbf{u}'_j); \boldsymbol{\psi}_i), \text{ for } i = 0, \dots, N_p - 1$$

- Hill-Mandel Condition

$$\begin{aligned} \mathbf{P}_M : \delta \mathbf{F}_M &= \sum_{i=0}^{N_p-1} v_i \mathbf{P}_i : \delta \mathbf{F}_i \\ \Rightarrow \sum_{i=0}^{N_p-1} \sum_{\forall \Gamma_{I_j}^i \neq \emptyset} \frac{v_i s_j^i}{V_i} \mathbf{P}_i : (\delta \mathbf{u}'_j \otimes \mathbf{N}_{I_j}^i) &= 0 \end{aligned}$$

- Weak form is the interface equation

$$\Rightarrow \sum_{i=0}^{N_p-1} \int_{\Gamma_{I_j}^i} \mathbf{P}_i \cdot \mathbf{N}_{I_j}^i dS = \sum_{i=0}^{N_p-1} s_j^i \mathbf{P}_i \cdot \mathbf{N}_{I_j}^i = \mathbf{0}, \text{ for } j = 0, \dots, N_I - 1$$



- Interactions

- Weak form

$$\sum_{i=0}^{N_p-1} \int_{\Gamma_{I_j}^i} \mathbf{P}_i \cdot \mathbf{N}_{I_j}^i ds = \sum_{i=0}^{N_p-1} s_j^i \mathbf{P}_i \cdot \mathbf{N}_{I_j}^i = \mathbf{0}, \text{ for } j = 0, \dots, N_I - 1$$

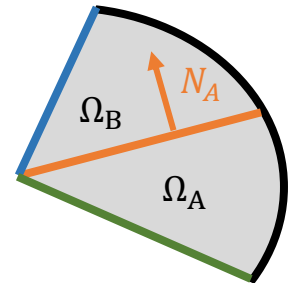
- With $\mathbf{P}_i = \mathbf{P}^p(\mathbf{F}_i(\mathbf{u}'_j); \boldsymbol{\psi}_i)$, for $i = 0, \dots, N_p - 1$

- One-level two-phase interaction

- Strain tensors

$$\mathbf{F}_A = \mathbf{F}_M + \frac{1}{v_A} \frac{s_{AB}}{V_M} \mathbf{u}' \otimes \mathbf{N}_A \text{ and } \mathbf{F}_B = \mathbf{F}_M - \frac{1}{v_B} \frac{s_{AB}}{V_M} \mathbf{u}' \otimes \mathbf{N}_A$$

$$\hat{\mathbf{a}} = \frac{s_{AB}}{V_M} \mathbf{u}'$$



- In linear elasticity the weak form becomes

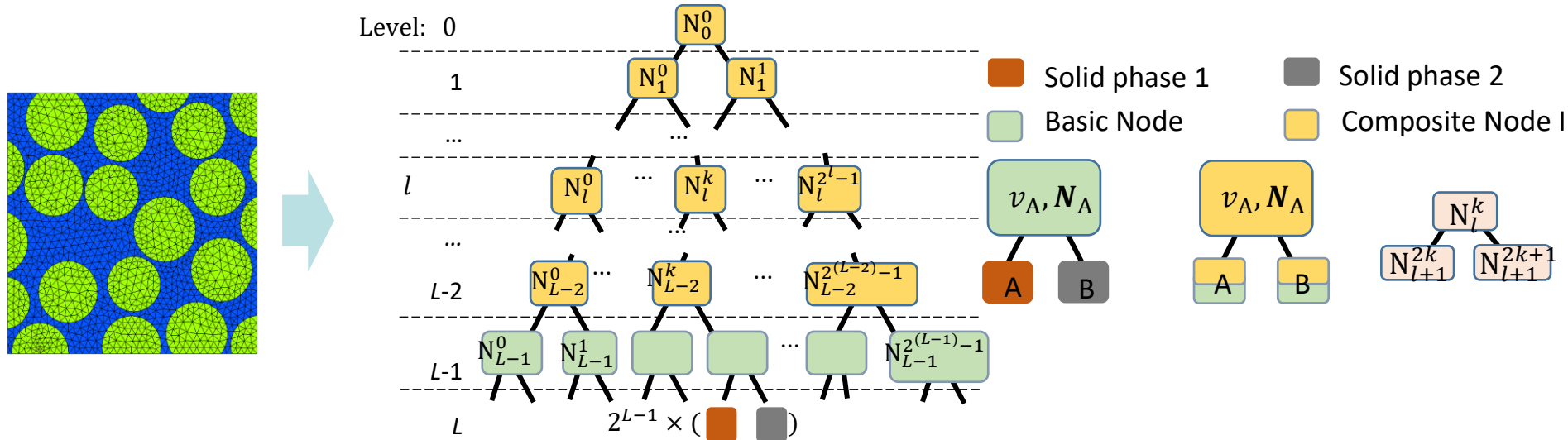
$$\mathbb{C}_M = v_A \mathbb{C}_A + (1.0 - v_A) \mathbb{C}_B + (\mathbb{C}_A - \mathbb{C}_B) \cdot \mathbf{N}_A \otimes^s [\mathcal{K}^{-1}(v_A, \mathbf{N}_A) \cdot \mathcal{F}(v_A, \mathbf{N}_A)]$$



Topology parameters to be defined $\mathcal{G}^2 = \{v_A, \mathbf{N}_A\}$

Interaction-Based Deep Material Network

- Simple network of material nodes with interactions to Replace volume element



- Elasticity tensor

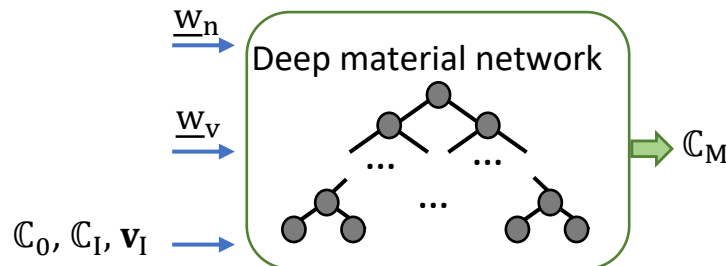
- From material tensor evaluation $\mathbb{C}(N_l^k) = \text{FUN}(l, \mathbb{C}_0, \mathbb{C}_l, \mathcal{G}^2(N_l^k))$
- Requires

$$\begin{cases} \mathbb{C}(N_{l+1}^{2k}) = \text{FUN}(l+1, \mathbb{C}_0, \mathbb{C}_l, \mathcal{G}^2(N_{l+1}^{2k})) \\ \mathbb{C}(N_{l+1}^{2k+1}) = \text{FUN}(l+1, \mathbb{C}_0, \mathbb{C}_l, \mathcal{G}^2(N_{l+1}^{2k+1})) \end{cases}$$

➡ Recursively $\mathbb{C}_M = \text{FUN}(l=0, \mathbb{C}_0, \mathbb{C}_l, \mathcal{G}^2(N_0^0))$

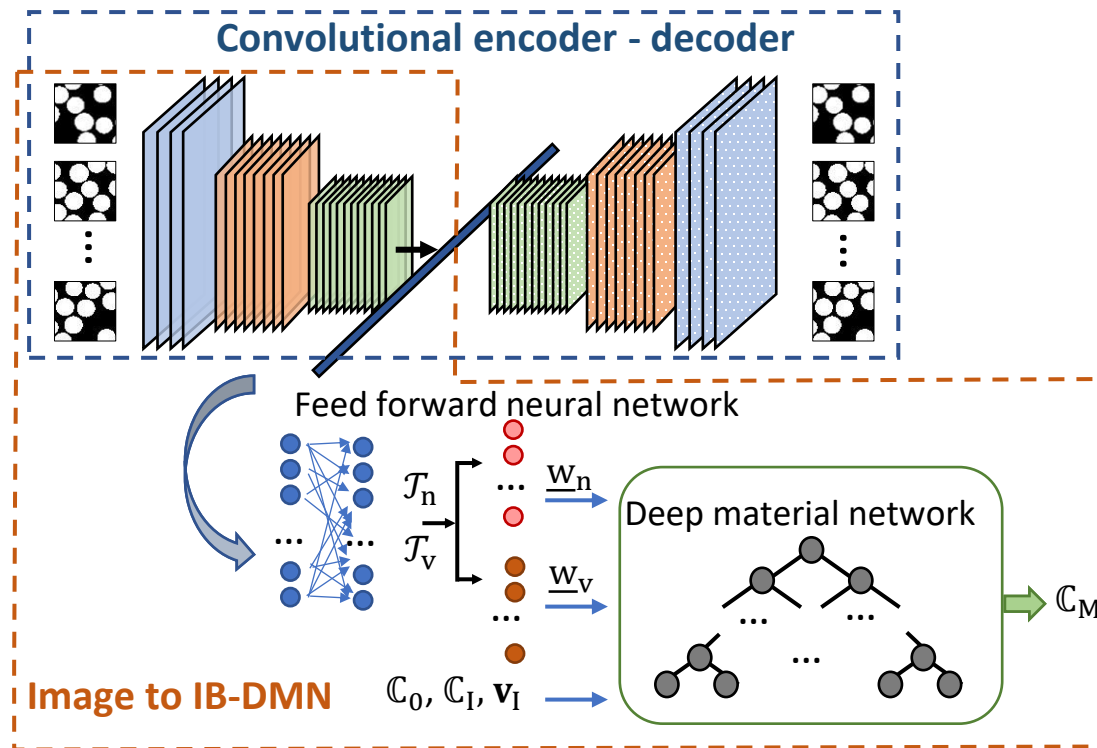
- Micro-structure topological parameters $\mathcal{G}^2(N_0^0), \mathcal{G}^2(N_1^0), \mathcal{G}^2(N_1^1), \dots, \mathcal{G}^2(N_{L-1}^{2^{L-1}-1})$

- Determination of Micro-structure topological parameters



- "Stochastic deep material networks as efficient surrogates for stochastic homogenisation of non-linear heterogeneous materials." Computer Methods in Applied Mechanics and Engineering, 441 (01 June 2025): 117994,

- Determination of Micro-structure topological parameters



- "Stochastic deep material networks as efficient surrogates for stochastic homogenisation of non-linear heterogeneous materials." Computer Methods in Applied Mechanics and Engineering, 441 (01 June 2025): 117994
- "Convolutional neural network-based mapping of material micro-structures to deep material networks for non-linear mechanical response prediction." Computer Methods in Applied Mechanics and Engineering, 449 (01 February 2026): 118554

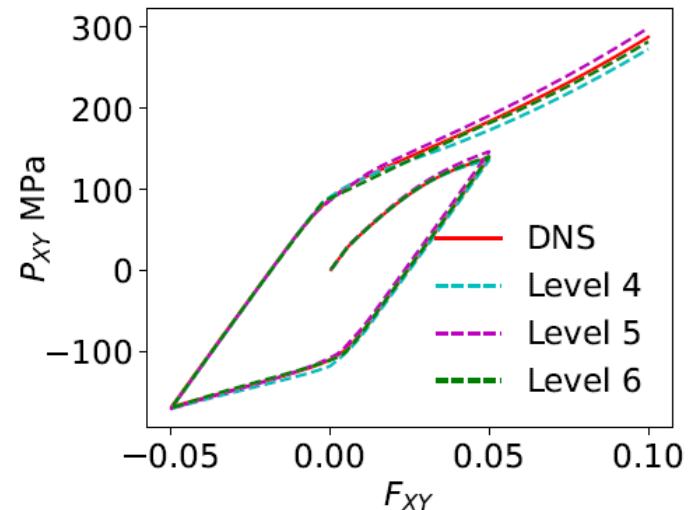
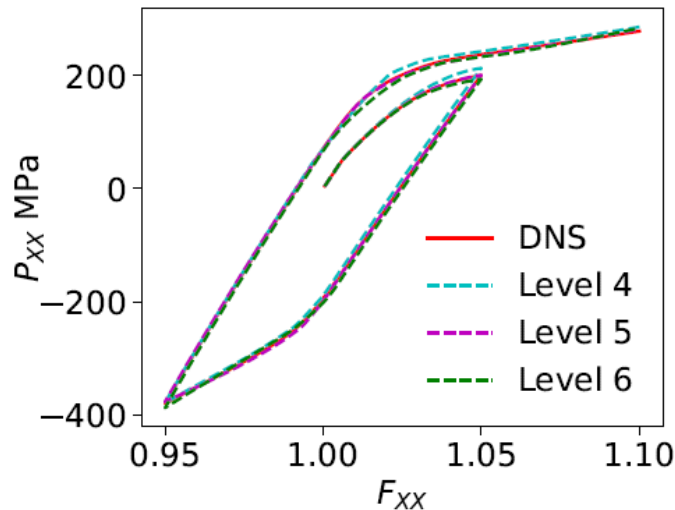
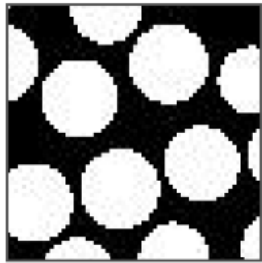
- Testing of Interaction-Based Deep Material Networks

- For one micro-structure infer one set of topological parameters

➡ $\left\{ \mathcal{G}^2(N_0^0), \mathcal{G}^2(N_1^0), \mathcal{G}^2(N_1^1), \dots, \mathcal{G}^2\left(N_{L-1}^{2^{(L-1)}-1}\right) \right\}$

- Testing on complex elasto-plasticity

- Non-associated pressure-dependent plasticity
- Extrapolation in terms of loading path
- Extrapolation in terms of constitutive model



Can we extrapolate with damage-enhanced model at the material nodes?

Damage-enhanced Interaction-Based Deep Material Network

- Can we extrapolate with damage-enhanced model at the material nodes?

- Train 6 DMNs of different volume fractions

$$v_I = 0.330$$

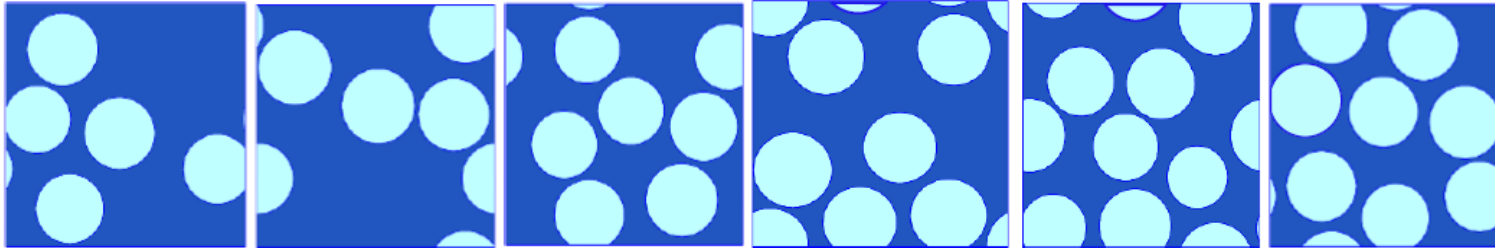
$$v_I = 0.361$$

$$v_I = 0.450$$

$$v_I = 0.486$$

$$v_I = 0.526$$

$$v_I = 0.554$$

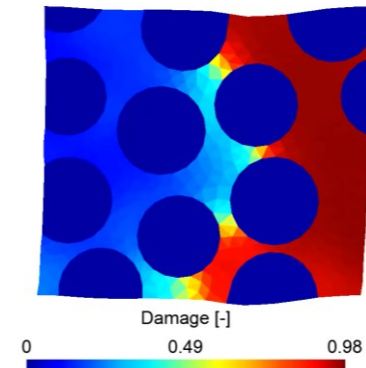
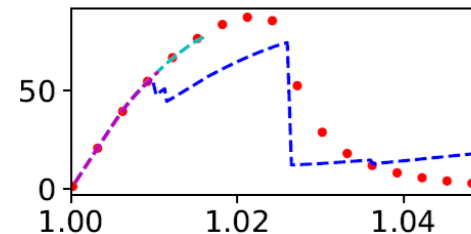
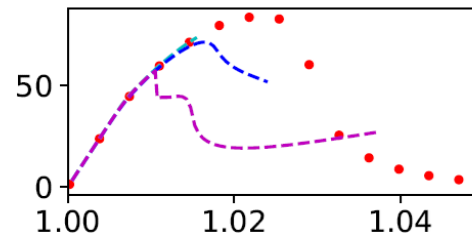
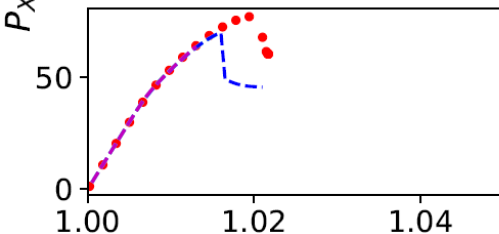
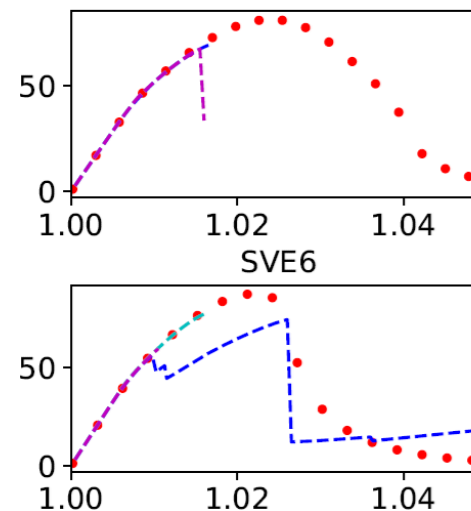
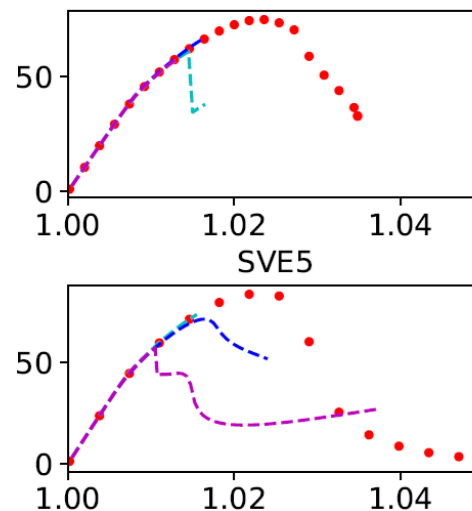
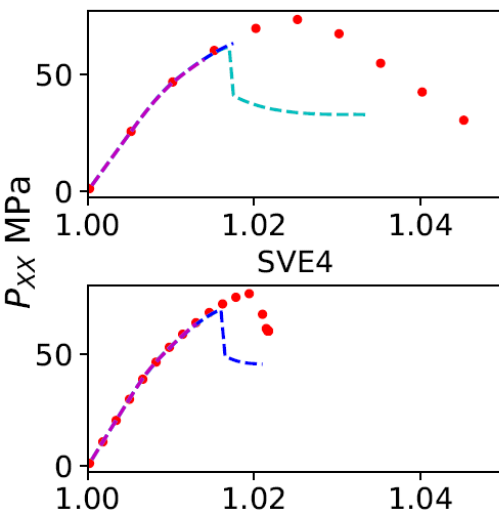


- Introduction of damage in the matrix model

DNS: $\bullet$ $l_c = 3\mu\text{m}$
SVE1

DMN of 5 Level with local damage: ---
SVE2

SVE3



DMN exhibits strain localization at some material nodes (like local FEM)

Discrete Non-Local Damage Deep Material Network

- Regularisation of the IB-DMN

- Classical non-local form

- $D(\tilde{\psi})$ with $\tilde{\psi}(x_0) = \int_V w(x - x_0) \psi(x) dx$

- $\mathbf{P} = \mathbf{P}^p(\mathbf{F}; \boldsymbol{\psi}) \rightarrow \mathbf{P} = \mathbf{P}^p(\mathbf{F}; \boldsymbol{\psi}, \tilde{\boldsymbol{\psi}})$

- Equivalent discrete form for the IB-DMB

$$\tilde{\psi}_i = \sum_{j=1}^n w_{ij} v_j \psi_j$$

- Under the constraints

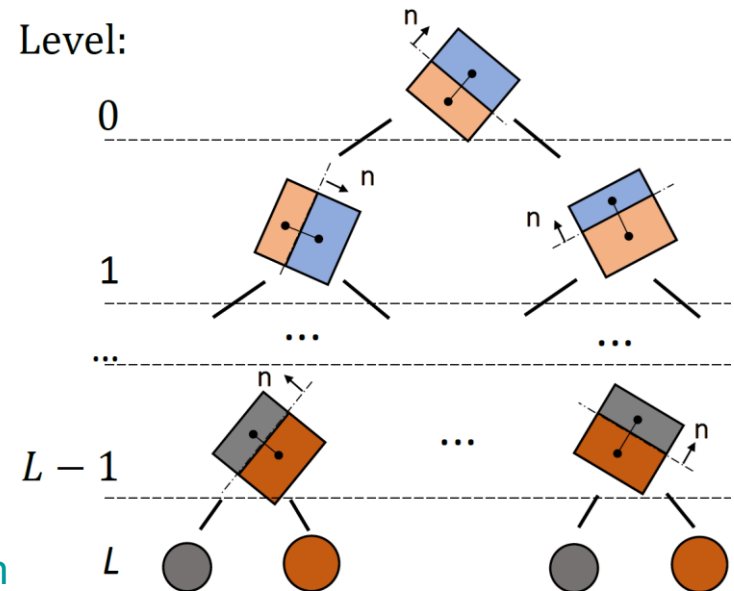
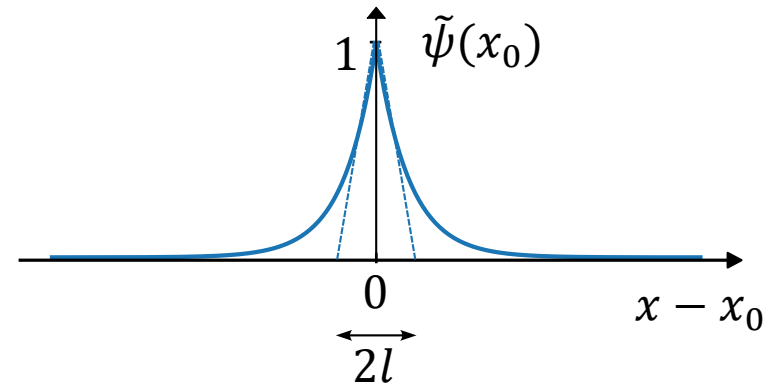
$$\left\{ \begin{array}{l} w_{ij} = w_{ji} \quad \sum_{j=1}^n w_{ij} v_j = 1 \\ \psi_i = \sum_{j=1}^n w_{ij} v_j \tilde{\psi}_j \end{array} \right.$$

- Satisfied by introducing auxiliary function

$$w_{ij} \propto \exp(-\sqrt{d_{ij} \cdot \mathbf{c}^{-1} \cdot d_{ij}})$$

Squared length scales

How to evaluate the distance in an abstract tree ?



- Implementation of discrete non-local IB-DMN

- Discrete Nonlocal form

- $$\tilde{\psi}_i = \sum_{j=1}^n w_{ij} v_j \psi_j \quad \Rightarrow \quad \mathbf{P} = \mathbf{P}^p(\mathbf{F}); \quad \boldsymbol{\psi}, \tilde{\boldsymbol{\psi}}$$

- w_{ij} under constraints

- $w_{ij} \propto \exp(-\sqrt{\mathbf{d}_{ij} \cdot \mathbf{c}^{-1} \cdot \mathbf{d}_{ij}})$

- Auxiliary function

- $g_{ij} = \exp(-\sqrt{\mathbf{d}_{ij} \cdot \mathbf{c}^{-1} \cdot \mathbf{d}_{ij}})$

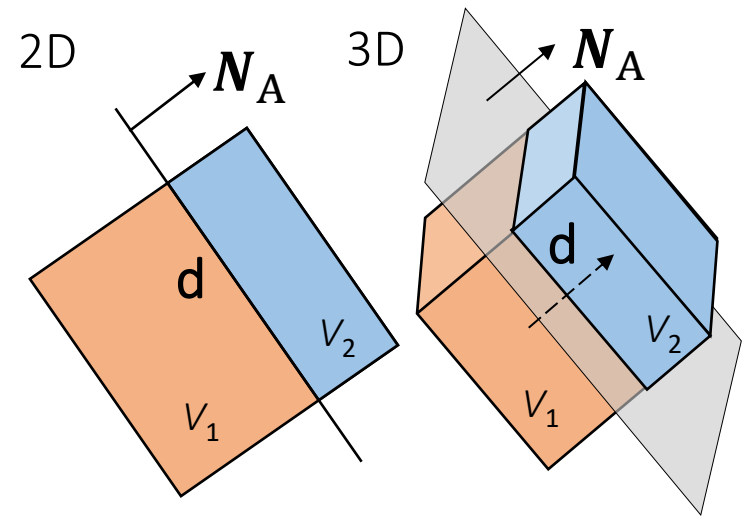
- Characteristic lengths $\mathbf{c} = \text{diag}(l_0^2, l_1^2, l_2^2)$

- $\mathbf{d}_{ij} = \frac{\dim \sqrt{V_i + V_j}}{2} \mathbf{N}$

- Evaluation of the coefficients (only once)

$\Rightarrow w_{ij} = \alpha_i g_{ij} \alpha_j$

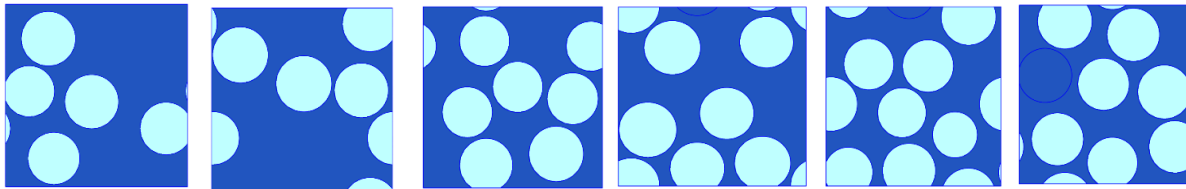
$\Rightarrow \alpha_i$ is solved to satisfy the constraints on w_{ij}



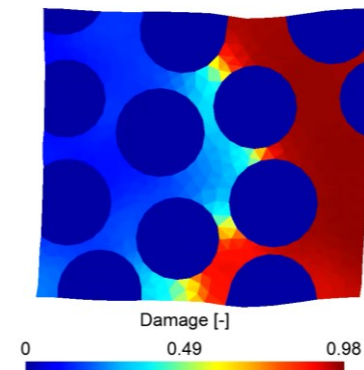
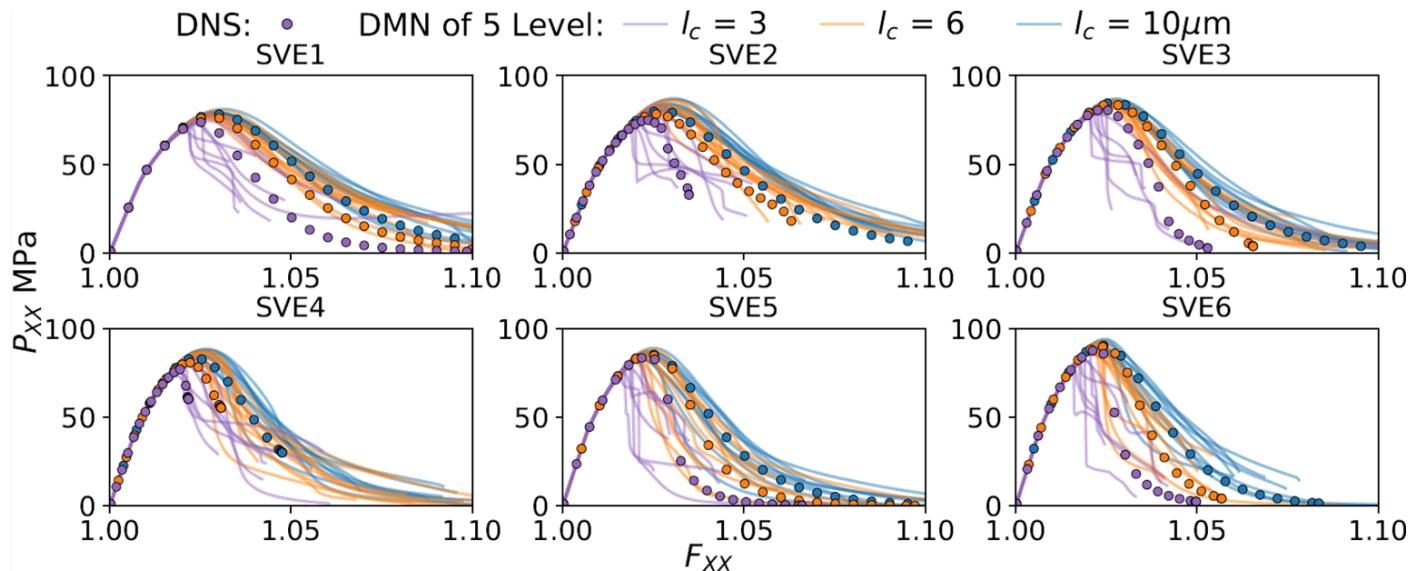
Damage-enhanced Interaction-Based Deep Material Network

- Test: Simple J2 plasticity with saturating damage model in the matrix phase
 - Train 6 DMNs of different volume fractions

$v_I = 0.330$ $v_I = 0.360$ $v_I = 0.450$ $v_I = 0.486$ $v_I = 0.526$ $v_I = 0.554$

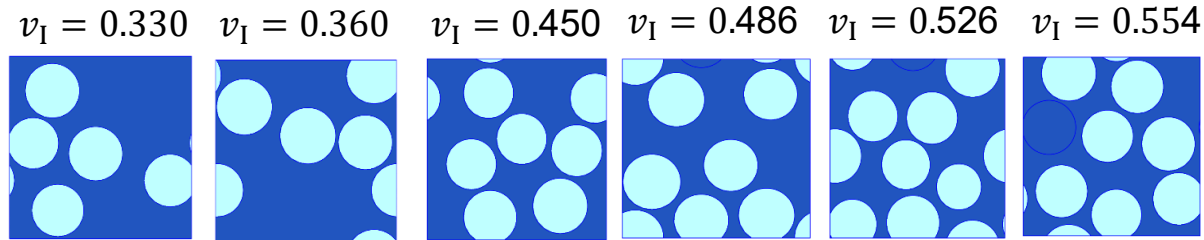


- 10 training initialisations per volume element

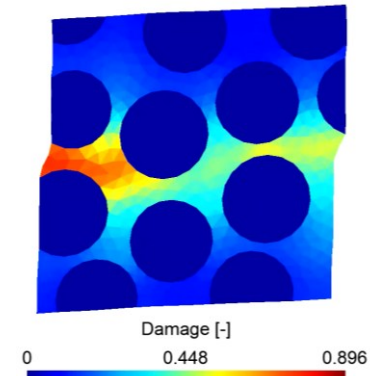
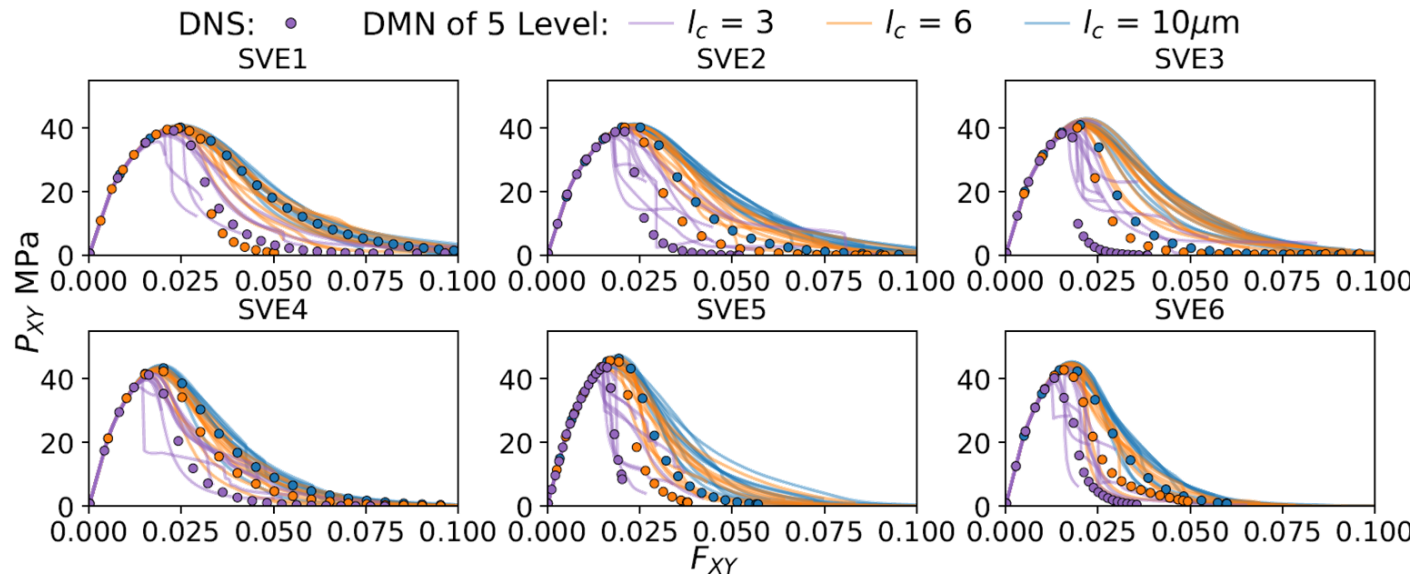


Damage-enhanced Interaction-Based Deep Material Network

- Test: Simple J2 plasticity with saturating damage model in the matrix phase
 - Train 6 DMNs of different volume fractions



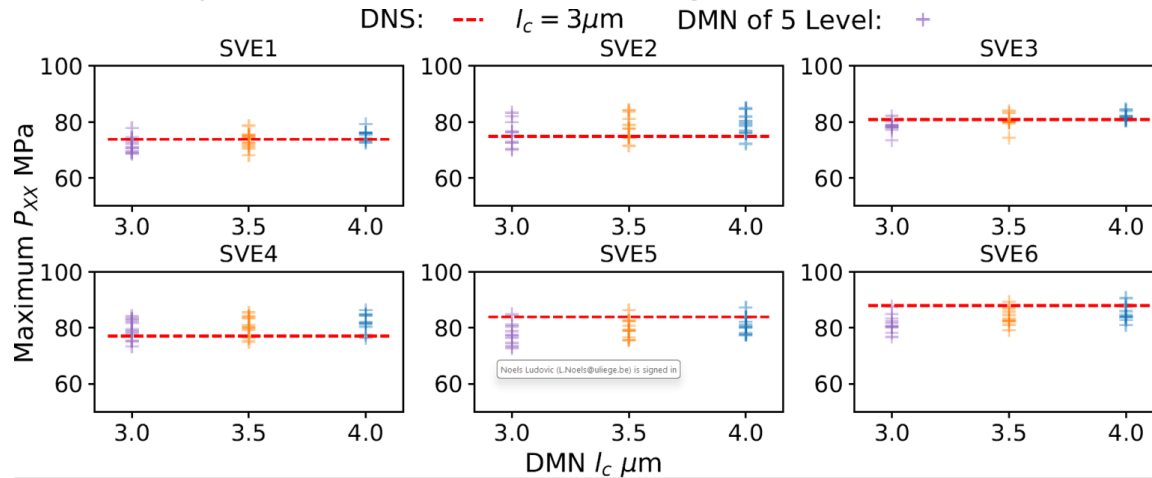
- 10 training initialisations per volume element



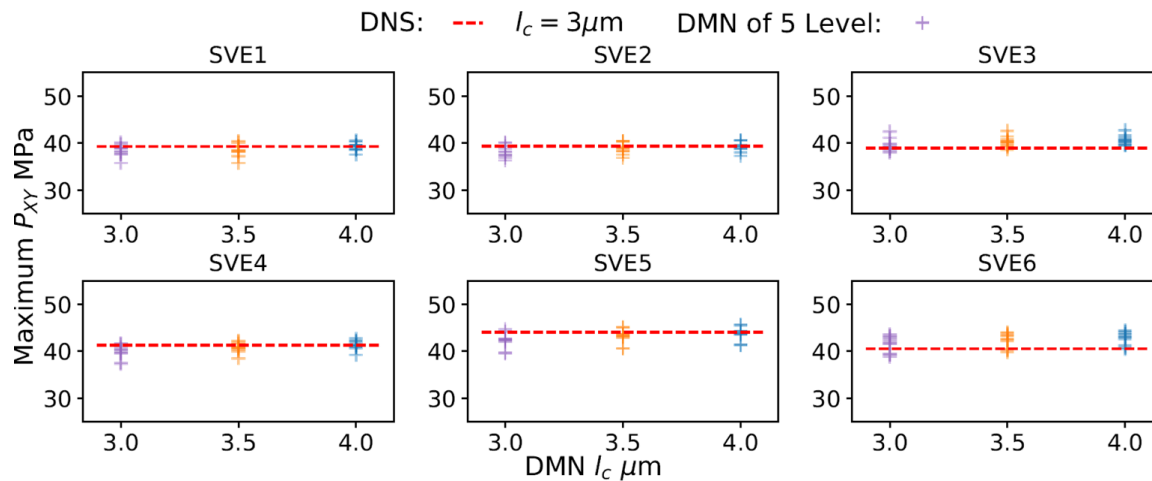
Damage-enhanced Interaction-Based Deep Material Network

- Test: Simple J2 plasticity with saturating damage model in the matrix phase
 - Analysis of the predicted strength

Uniaxial-stress



Shearing



→ DNS strength is recovered

→ Post-softening curve is not physical anyway (depends on the RVE size)

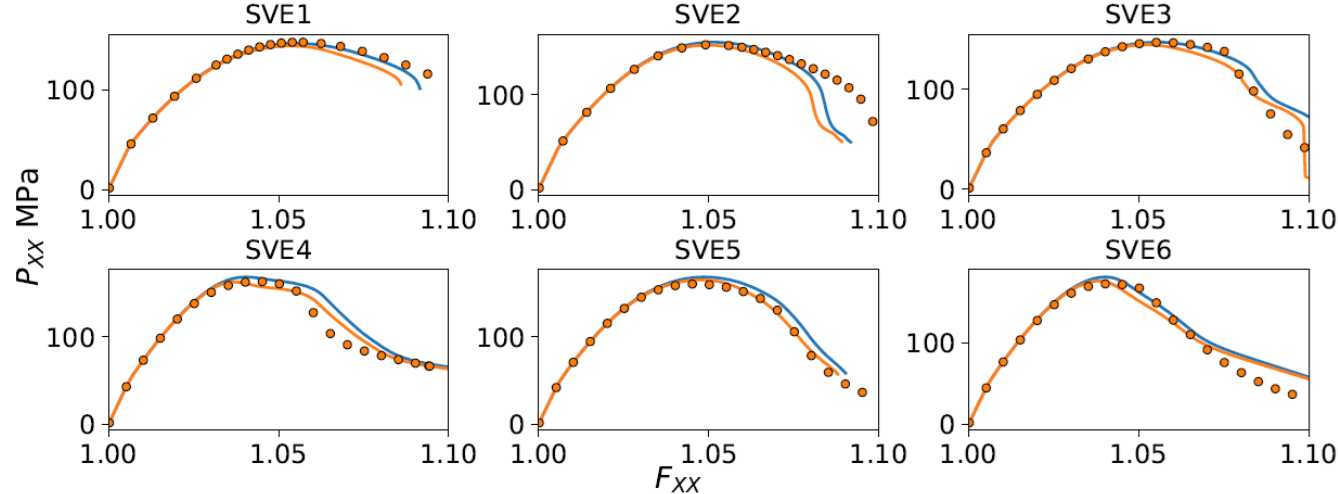
Damage-enhanced Interaction-Based Deep Material Network

- Test: Multi-damage-enhanced non-associated model in the matrix phase

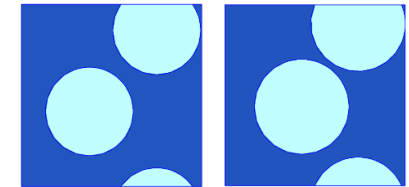
- Train 6 (smaller) DMNs of different volume fractions
- Best training for each volume element

DNS: • DMN of 5 Level: — $l_c^s = 2, l_c^f = 3$; — $l_c^s = 3, l_c^f = 3\mu\text{m}$

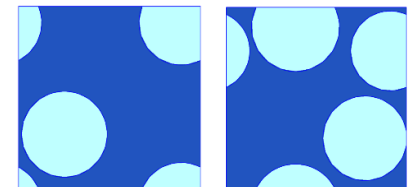
Uniaxial-stress



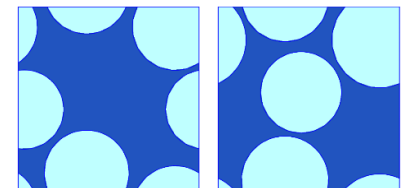
$v_I = 0.372$ $v_I = 0.432$



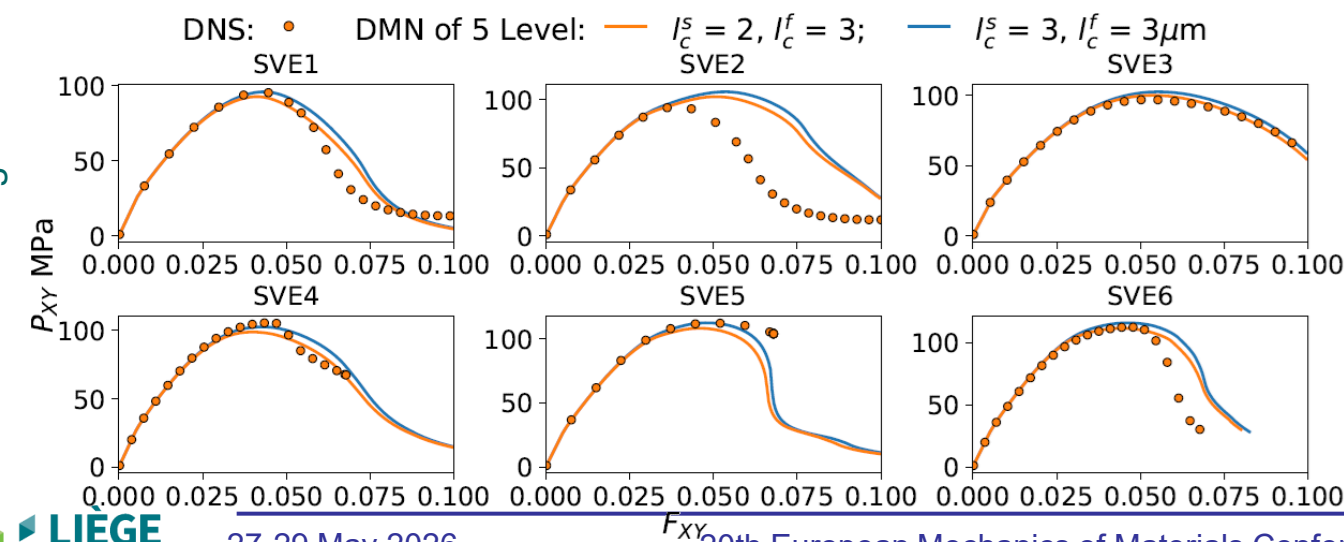
$v_I = 0.344$ $v_I = 0.510$



$v_I = 0.499$ $v_I = 0.556$



Shearing



- Publications

- L. Wu and L. Noels. "Convolutional neural network-based mapping of material micro-structures to deep material networks for non-linear mechanical response prediction." Computer Methods in Applied Mechanics and Engineering, 449 (01 February 2026): 118554. doi: <https://doi.org/10.1016/j.cma.2025.118554>
- L. Wu and L. Noels. "Stochastic deep material networks as efficient surrogates for stochastic homogenisation of non-linear heterogeneous materials." Computer Methods in Applied Mechanics and Engineering, 441 (01 June 2025): 117994. doi: <https://doi.org/10.1016/j.cma.2025.117994>
- L. Wu and L. Noels. "Discrete non-local interactions formulation of deep material networks for damage-enhanced constitutive material models". Available at SSRN: <http://dx.doi.org/10.2139/ssrn.6539687>

- Data and code on

- Repository: https://gitlab.uliege.be/didearot/didearotPublic/publicationsData/2025_StochasticBDMN
- Doi: <http://dx.doi.org/10.5281/zenodo.15120313>
- Repository: https://gitlab.onelab.info/cm3/carbobrake/-/tree/main/cmame_2025_cnn_dmn
- Doi: <https://doi.org/10.5281/zenodo.17182395>