

Stochastic Interaction-Based Deep Material Networks for composites

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Computational & Multiscale Mechanics of Materials – CM3

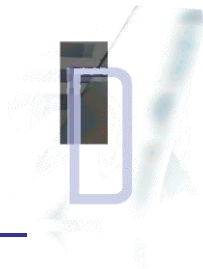
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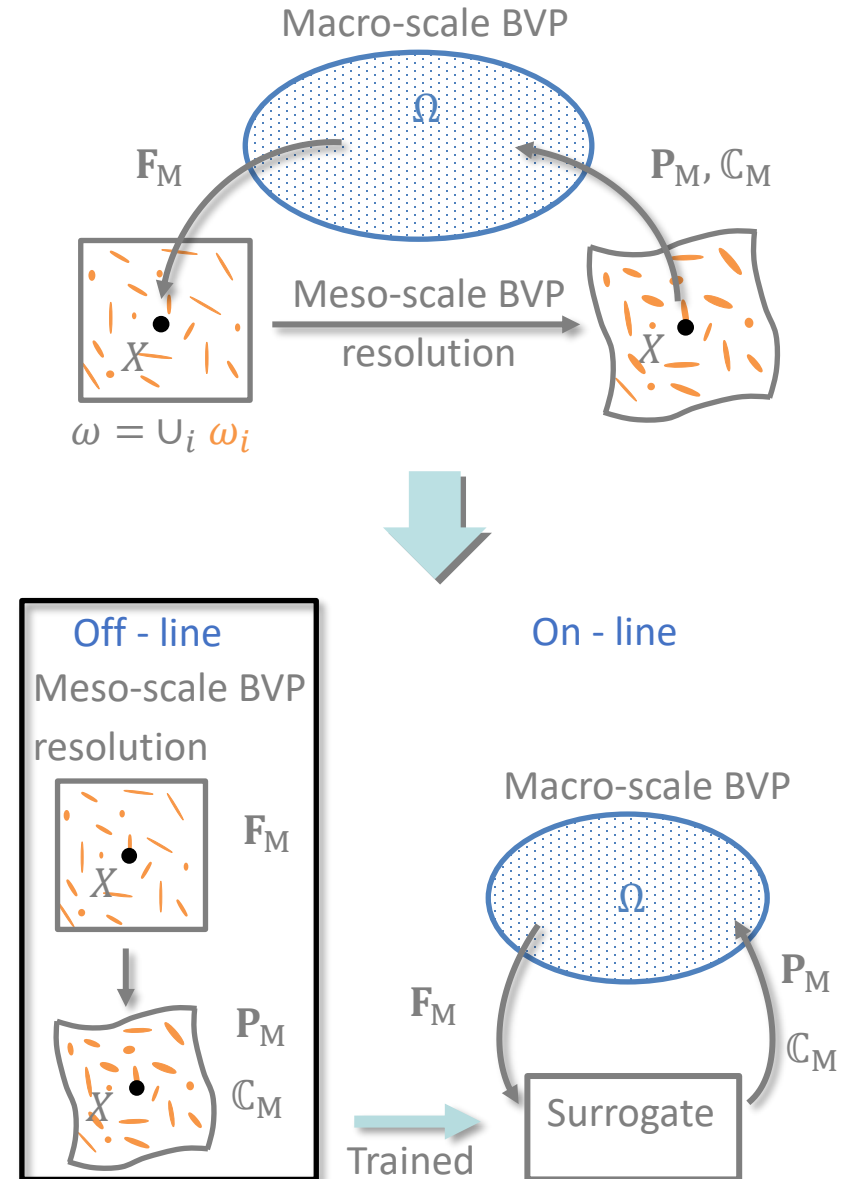


Advances in Applied Mechanics 2026, 5-9th January 2026 - Meloneras



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

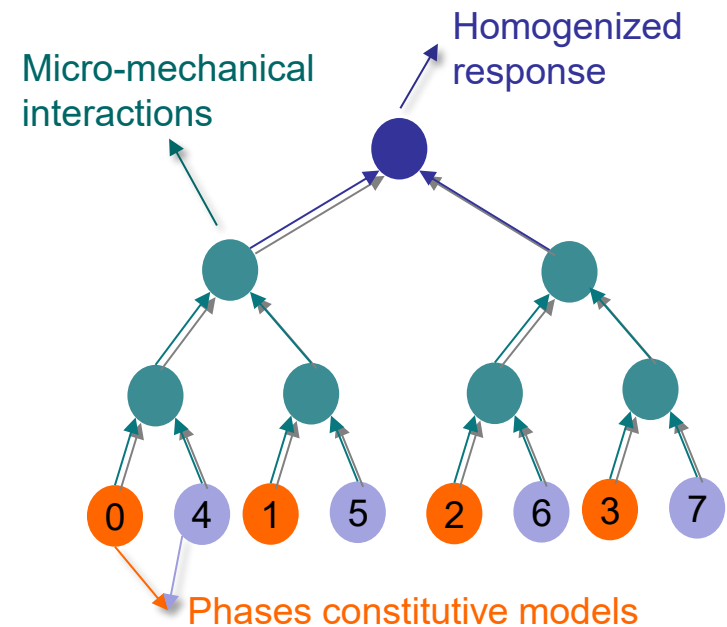


- Use of RNN

- 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

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

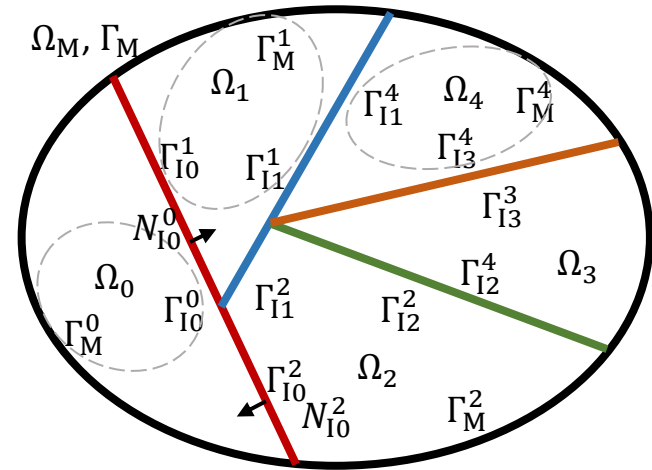
$$\boldsymbol{\sigma}_M = \sum_{i=0}^{Np-1} v_i \boldsymbol{\sigma}_i$$

- Introduction of fluctuations

$$\boldsymbol{\varepsilon}_m(\mathbf{X}_m) = \nabla \otimes^s \mathbf{u}_m(\mathbf{X}_m) = \boldsymbol{\varepsilon}_M + \nabla \otimes^s \mathbf{u}'(\mathbf{X}_m), \quad \mathbf{X}_m \in \Omega_M$$

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

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



Interactions

- Introduction of fluctuations

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

- Assume constitutive model in each sub-domain

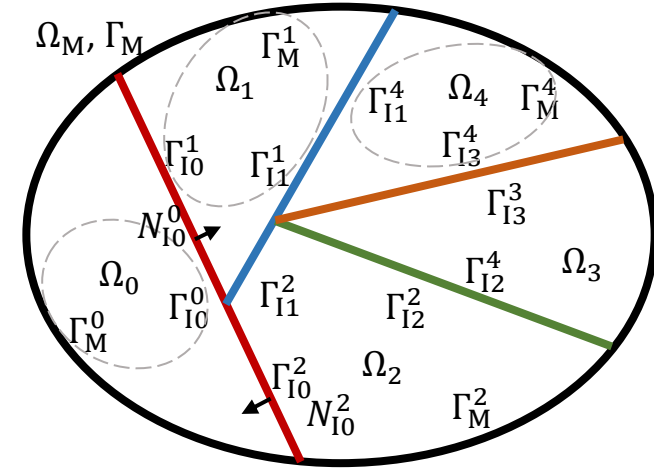
$$\boldsymbol{\sigma}_i = \boldsymbol{\sigma}^p(\boldsymbol{\varepsilon}_i(\mathbf{u}'_j); \mathbf{Z}_i), \text{ for } i = 0, \dots, N_p - 1$$

- Hill-Mandel Condition

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

- Weak form is the interface equation

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



- Interactions

- Weak form

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

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

- One-level two-phase interaction

- Strain tensors

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

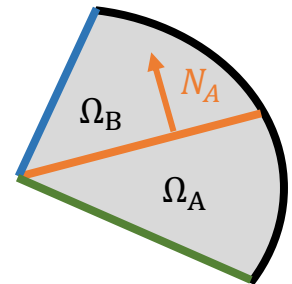
$$\hat{\mathbf{a}} = \frac{s_{AB}}{V_M} \mathbf{u}'$$

- In linear elasticity the weak form becomes

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

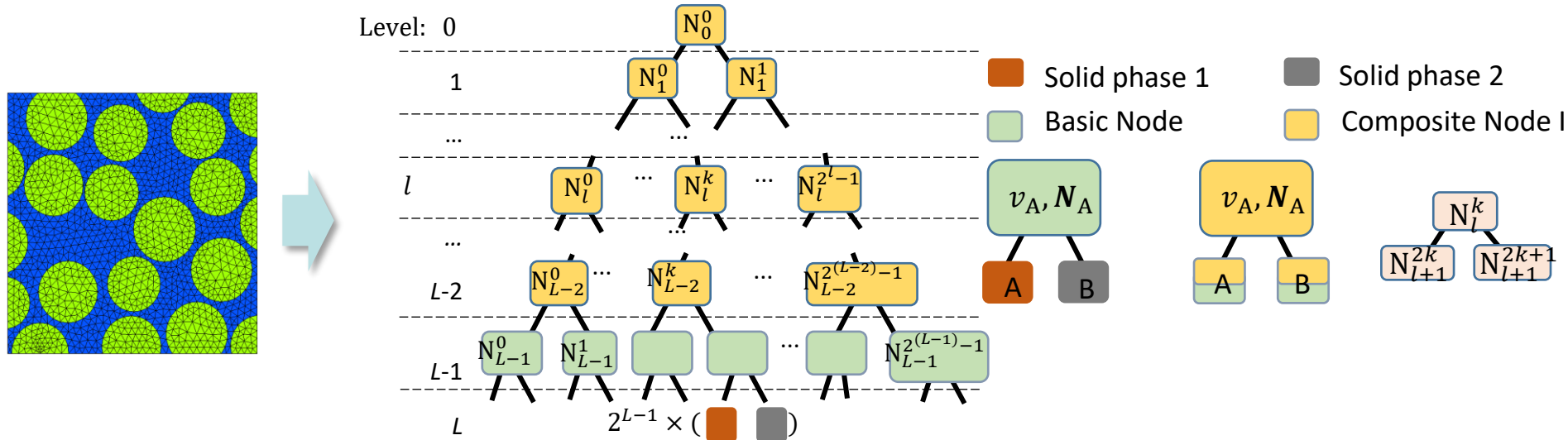


Topology parameters to be defined $\mathcal{G}^2 = \{v_A, \mathbf{N}_A\}$



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

Interaction-Based Deep Material Network

• Testing of Interaction-Based Deep Material Networks

- Six micro-structure realizations



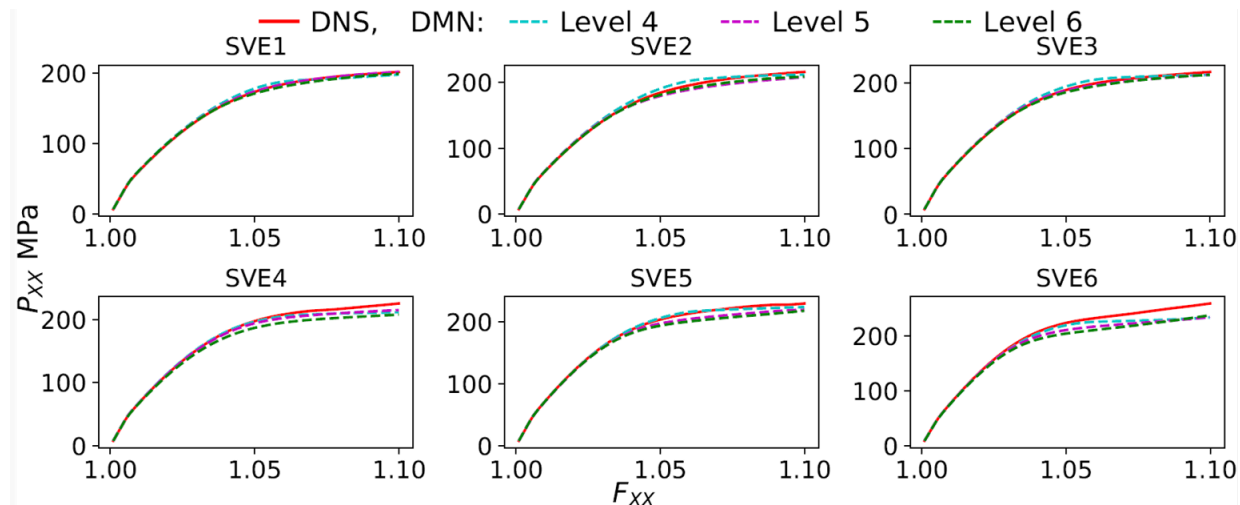
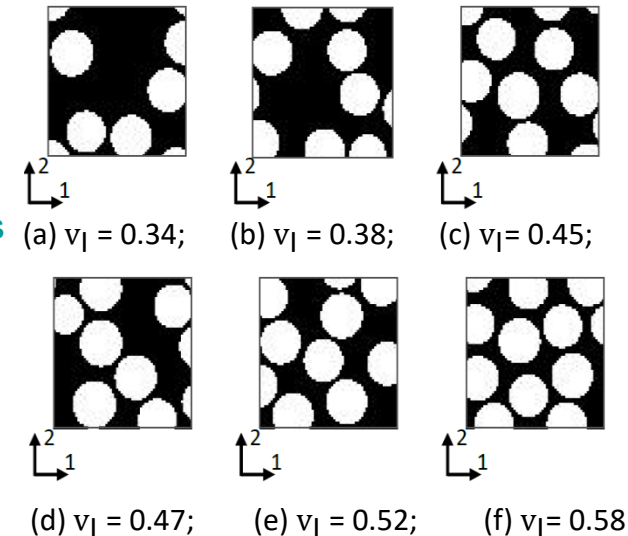
Six IB-DMNs to be trained in linear elasticity

- For each micro-structure new set of topological parameters

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

- Testing on complex elasto-plasticity

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



Can we predict for arbitrary volume fraction?

Parameter Reformulation of Interaction-Based Deep Material Network

- Reformulation of parameters $\mathcal{G}^2 = \{v_A, N_A\}$ at node N_l^k

- Normal $N_A(N_l^k)$ from angles $\theta_1(N_l^k)$ and $\theta_2(N_l^k)$

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

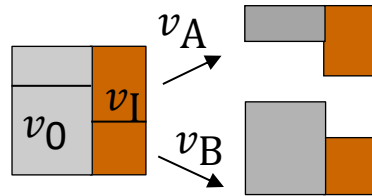
$$\Rightarrow w_{\theta_1}(N_l^k), w_{\theta_2}(N_l^k) \in [0, 1]$$

- Volume fraction $v_A(N_l^k)$

1) “Yellow” Node at level $l = 0$:

$$v_l(N_0^0) = v_l \text{ and } v_0(N_0^0) = 1 - v_l \text{ known}$$

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

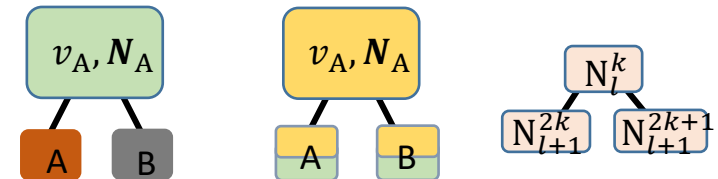
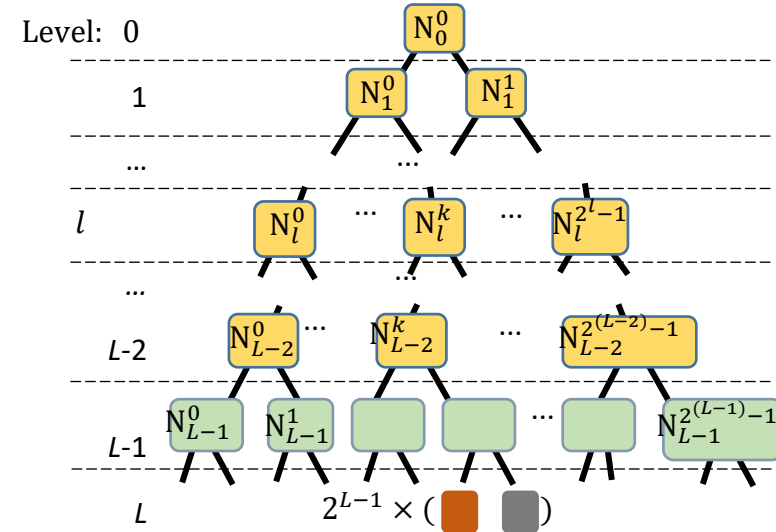


2) Recursively for “Yellow” Node at level $0 < l < L$

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

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

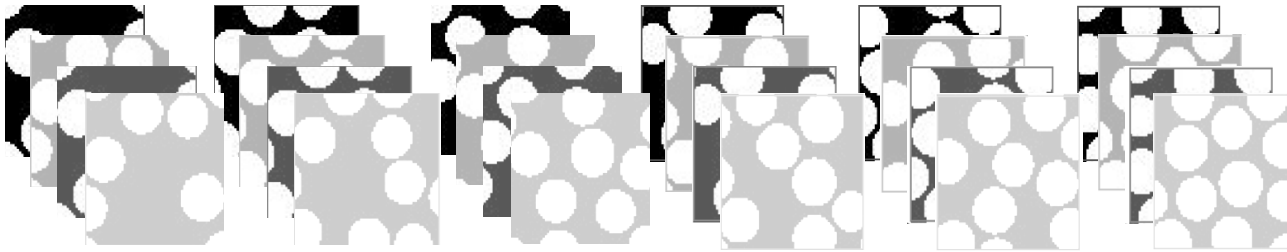
$$v_A = 1.0 - v_l(N_{L-1}^k) \text{ and } v_B = v_l(N_{L-1}^k)$$



Parameter Reformulation of Interaction-Based Deep Material Network

- SVEs batch training

- New parameters $\tilde{\mathcal{T}}_{\mathbf{n}} = \{w_{\theta_1}(\mathbf{N}_l^k), w_{\theta_2}(\mathbf{N}_l^k)\}$ and $\tilde{\mathcal{T}}_{\mathbf{v}} = \{w_{v0}(\mathbf{N}_l^k), w_{v1}(\mathbf{N}_l^k)\}$
- Train a generic DMN
 - Random micro-topologies and volume fractions,
 - Random phase properties



➡ $\{\hat{\mathbb{C}}_{\mathbf{M}}(\mathbb{C}_0^s, \mathbb{C}_1^s)\}$

- New loss function in which v_1^s is known for each SVE

$$Loss(\hat{\mathbb{C}}_{\mathbf{M}}, \mathbb{C}_{\mathbf{M}}) = \frac{1}{n} \sum_{s=1}^n \frac{\|\hat{\mathbb{C}}_{\mathbf{M}}(\mathbb{C}_0^s, \mathbb{C}_1^s) - \mathbb{C}_{\mathbf{M}}(\mathbb{C}_0^s, \mathbb{C}_1^s, v_1^s; \tilde{\mathcal{T}}_{\mathbf{n}}, \tilde{\mathcal{T}}_{\mathbf{v}})\|}{\|\hat{\mathbb{C}}_{\mathbf{M}}(\mathbb{C}_0^s, \mathbb{C}_1^s)\|}$$

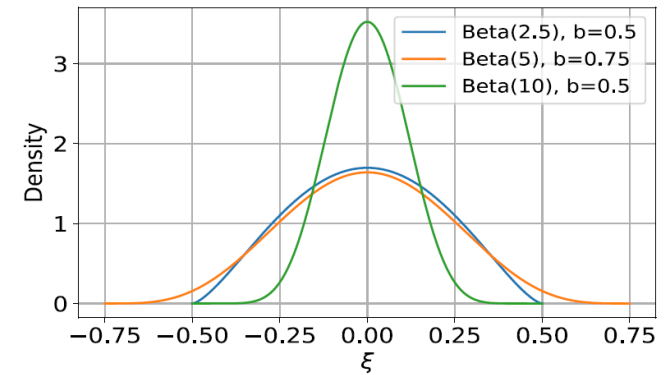
➡ Identify the generic DMN parameter $\tilde{P}_{\mathbf{n}}, \tilde{P}_{\mathbf{v}}$,
 where $\tilde{\mathcal{T}}_{\mathbf{n}} = \text{sigmoid}(\tilde{P}_{\mathbf{n}})$ and $\tilde{\mathcal{T}}_{\mathbf{v}} = \text{sigmoid}(\tilde{P}_{\mathbf{v}})$

- Perturbate generic DMN

- $\tilde{\mathcal{T}}_{\mathbf{n}}, \tilde{\mathcal{T}}_{\mathbf{v}}$ define a generic deterministic DMN with volume fraction $v_{\mathbf{I}}$ as input
- We can perturbate the parameters $\tilde{\mathcal{T}}_{\mathbf{n}}, \tilde{\mathcal{T}}_{\mathbf{v}}$ to have a stochastic DMN

$$\begin{cases} P_{\mathbf{n}} = (1 + \xi) \odot \tilde{P}_{\mathbf{n}} \\ P_{\mathbf{v}} = (1 + \xi) \odot \tilde{P}_{\mathbf{v}} \end{cases} \quad \begin{aligned} \xi &= 2b(\chi - 0.5) \\ \chi &\sim \text{Beta}(\alpha) \end{aligned}$$

- $\mathcal{T}_{\mathbf{n}} = \text{sigmoid}(P_{\mathbf{n}})$ and $\mathcal{T}_{\mathbf{v}} = \text{sigmoid}(P_{\mathbf{v}})$



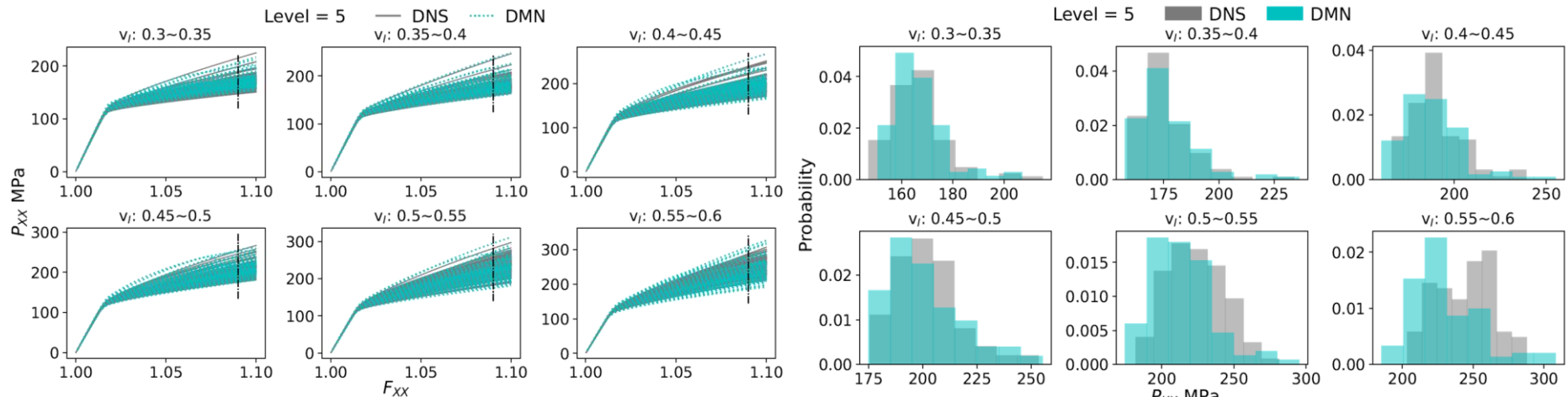
Stochastic Interaction-Based Deep Material Network

- Perturbate generic DMN

$$P_n = (1 + \xi) \odot \tilde{P}_n \quad P_v = (1 + \xi) \odot P_v$$

$$\xi = (\chi - 0.5)$$

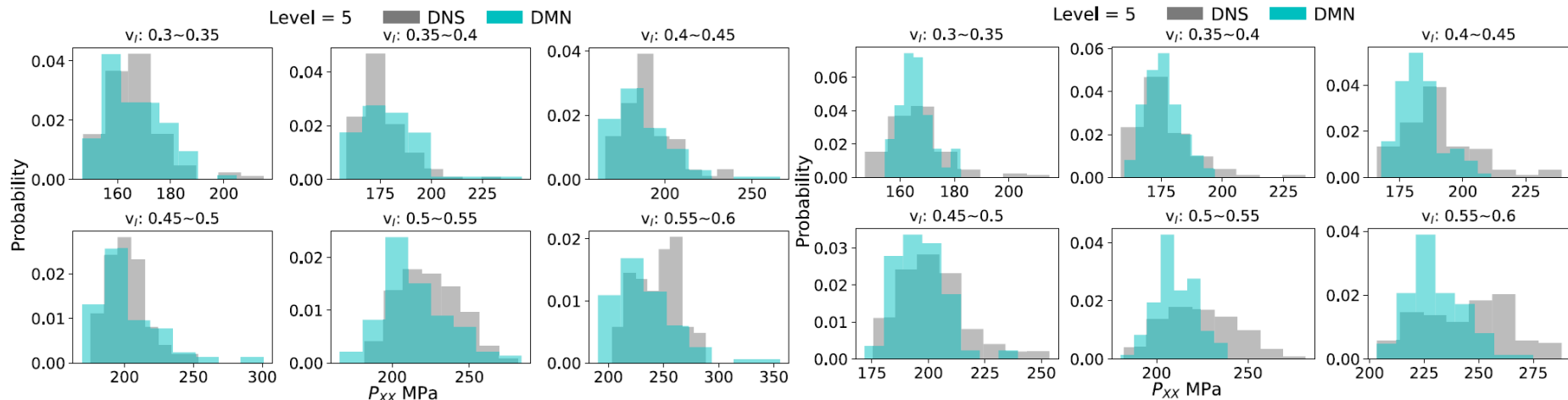
$$\chi \sim \text{Beta}(2.5)$$



$$\xi = 1.5(\chi - 0.5) \quad \chi \sim \text{Beta}(5)$$

$$\xi = (\chi - 0.5)$$

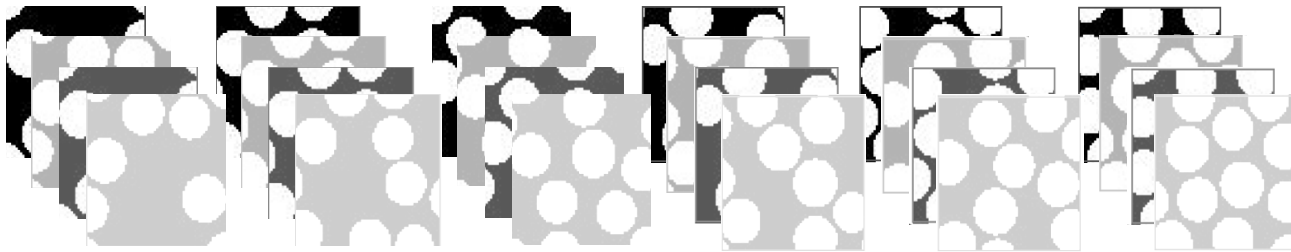
$$\chi \sim \text{Beta}(10)$$



- We still need to find a proper way to infer the perturbation

- Stochastic Interaction-Based Deep Material Networks

- How to link the parameters $\mathcal{T}_n = \text{sigmoid}(P_n)$ and $\mathcal{T}_V = \text{sigmoid}(P_V)$ to a given micro-structure realization without requiring a new training for a new micro-structure
- When separation of scale not satisfied $l_M \gg l_{SVE} \sim l_m$



- For the same volume fraction v_f the response depends on the micro-structure realisation

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

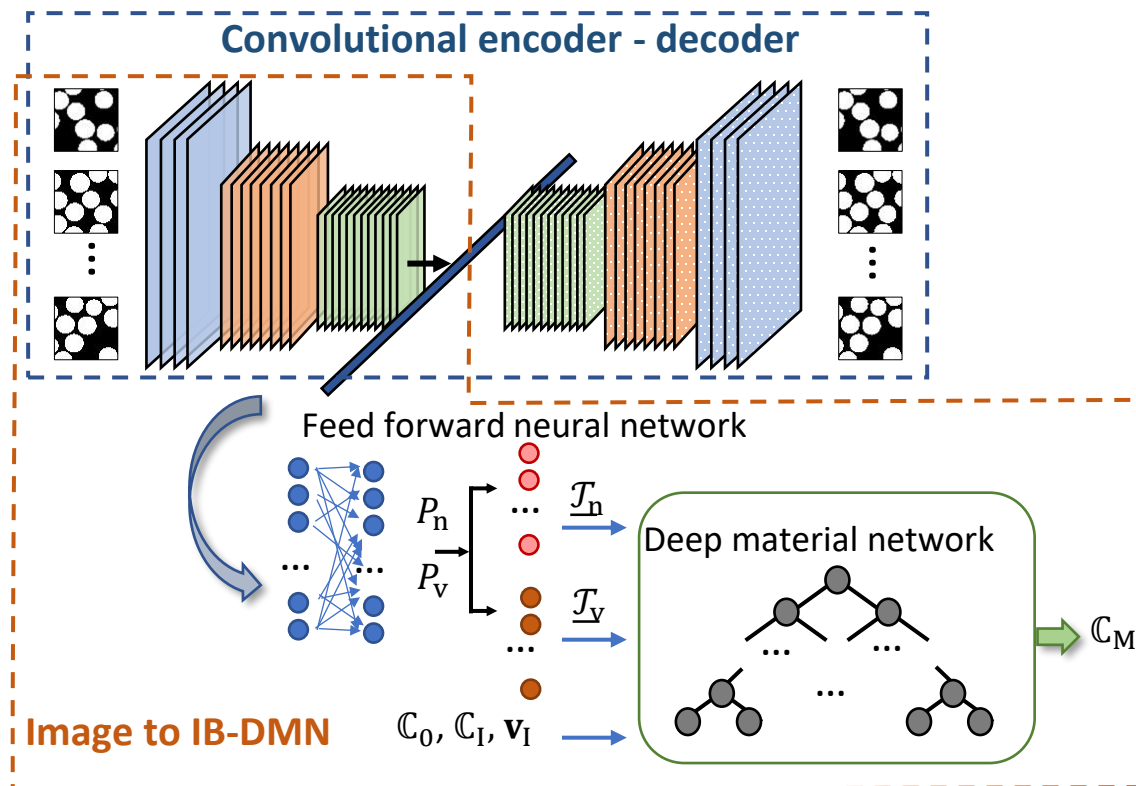
- Composite response also depends on the inclusions shape



➡ Can we handle different inclusions shapes at the same time?

“Image to IB-DMN” framework

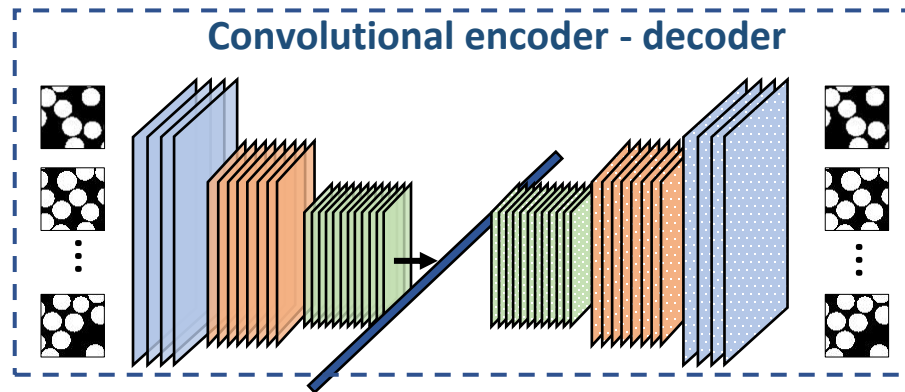
- Prediction of topological parameters $\mathcal{T}_n = \text{sigmoid}(P_n)$ and $\mathcal{T}_v = \text{sigmoid}(P_v)$
 - Volume fraction v_I already extracted
 - P_n & P_v represent the micro-structure organisation  to be predicted from images
 - Trained Convolutional encoder-decoder: encoder predicts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



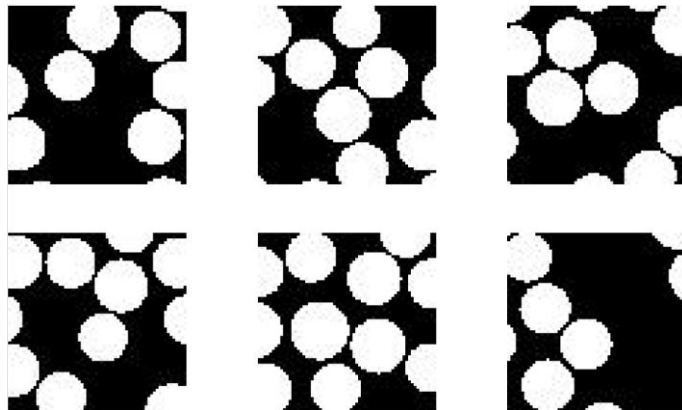
“Image to IB-DMN” framework

- Prediction of topological parameters $\mathcal{T}_h = \text{sigmoid}(P_h)$ and $\mathcal{T}_v = \text{sigmoid}(P_v)$
 - Convolutional encoder-decoder

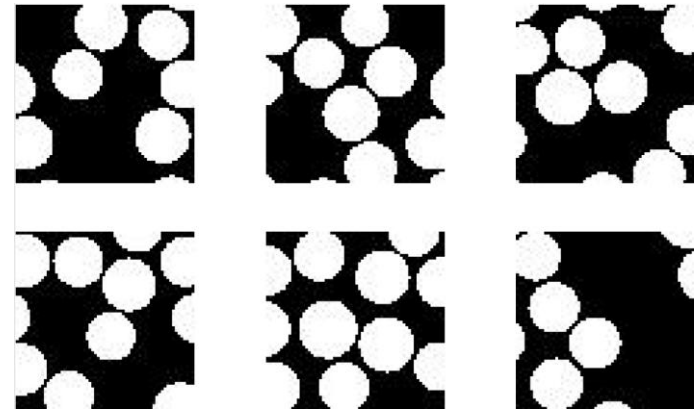
- Inputs: Reference images from SEM analyses
- Output: reconstructed image
- Trained with 10,000 reference images



Reference testing images



Predicted images by decoder



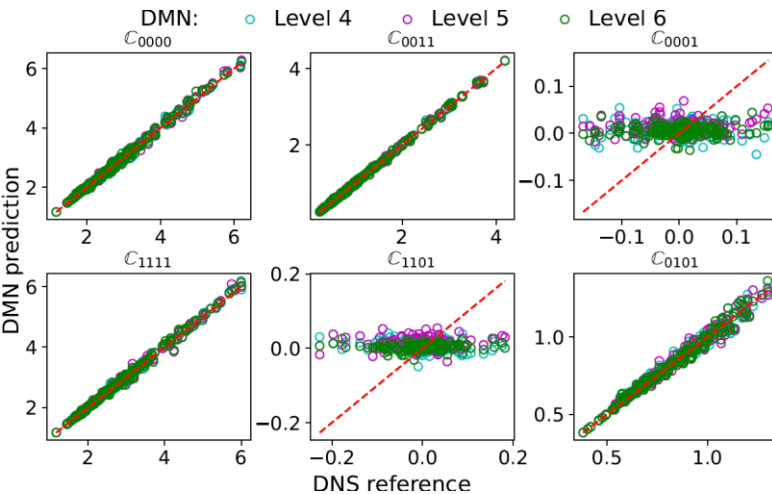
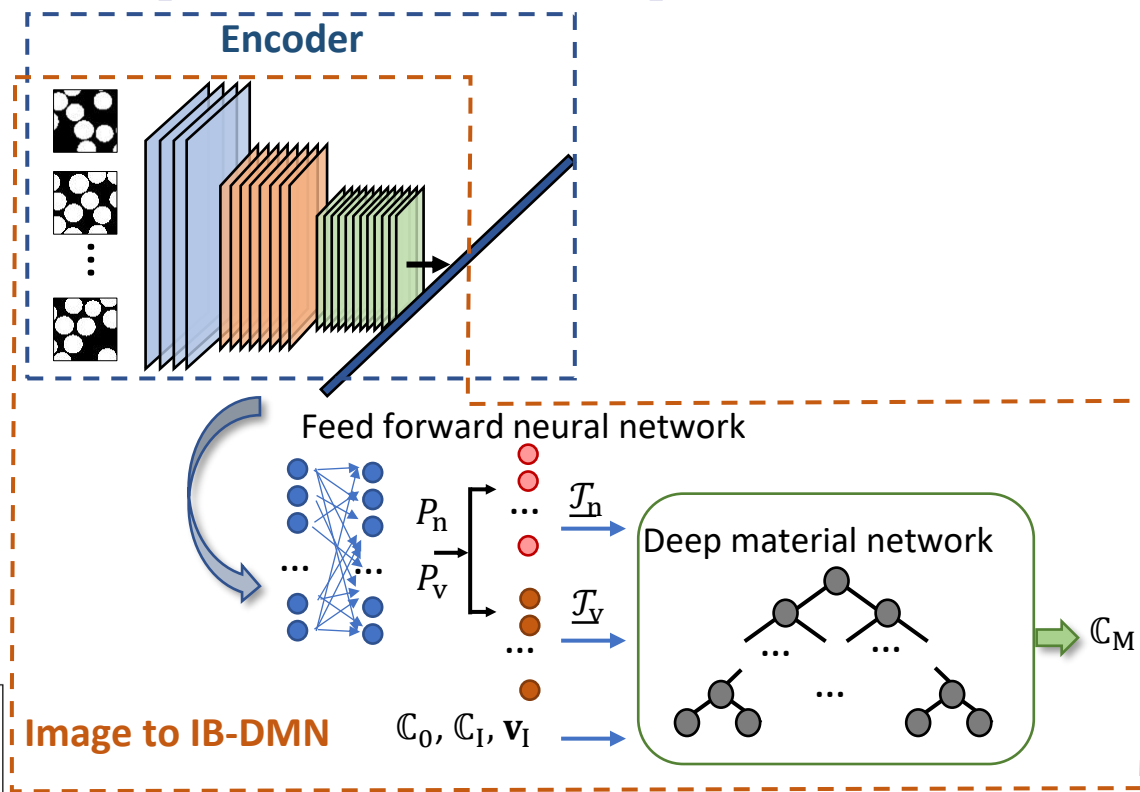
Once trained, the encoder gives a features vector of a micro-structure image

“Image to IB-DMN” framework

- Prediction of topological parameters $\mathcal{T}_h = \text{sigmoid}(P_h)$ and $\mathcal{T}_v = \text{sigmoid}(P_v)$

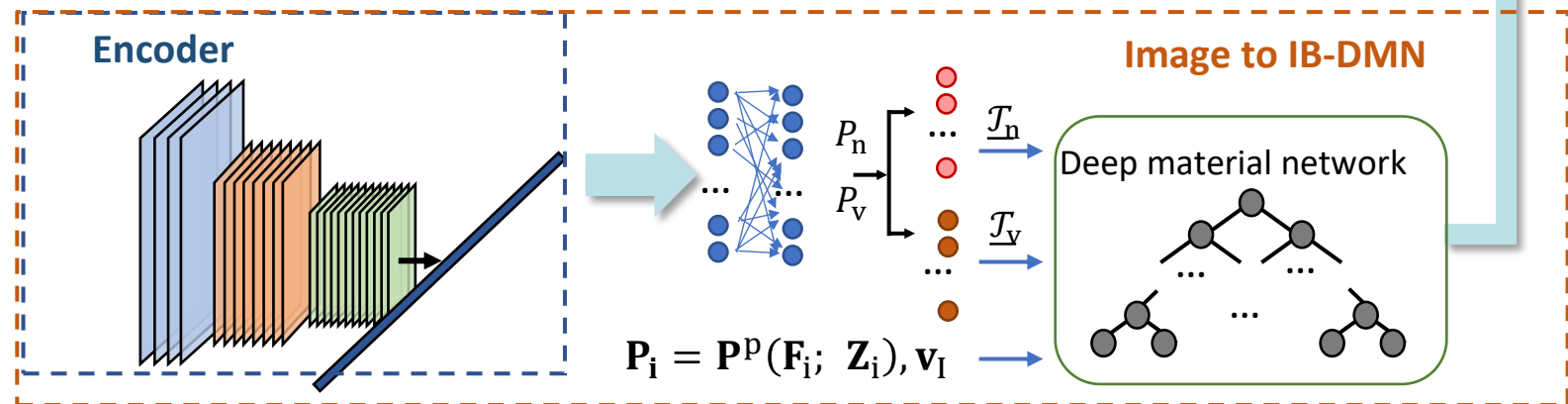
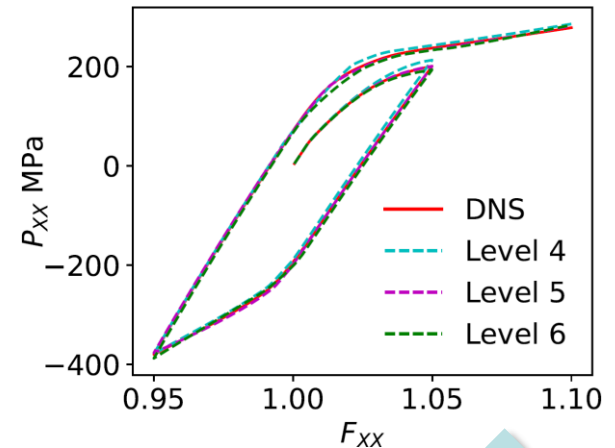
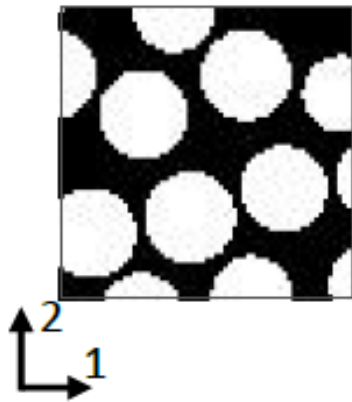
- Feed forward neural network

- Input: features vector of encoder
- Output: topological parameters $\mathcal{T}_h$ & $\mathcal{T}_v$ representing the micro-structure
- Trained so that the IB-DMN predicts the elasticity tensor of DNS



“Image to IB-DMN” framework

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

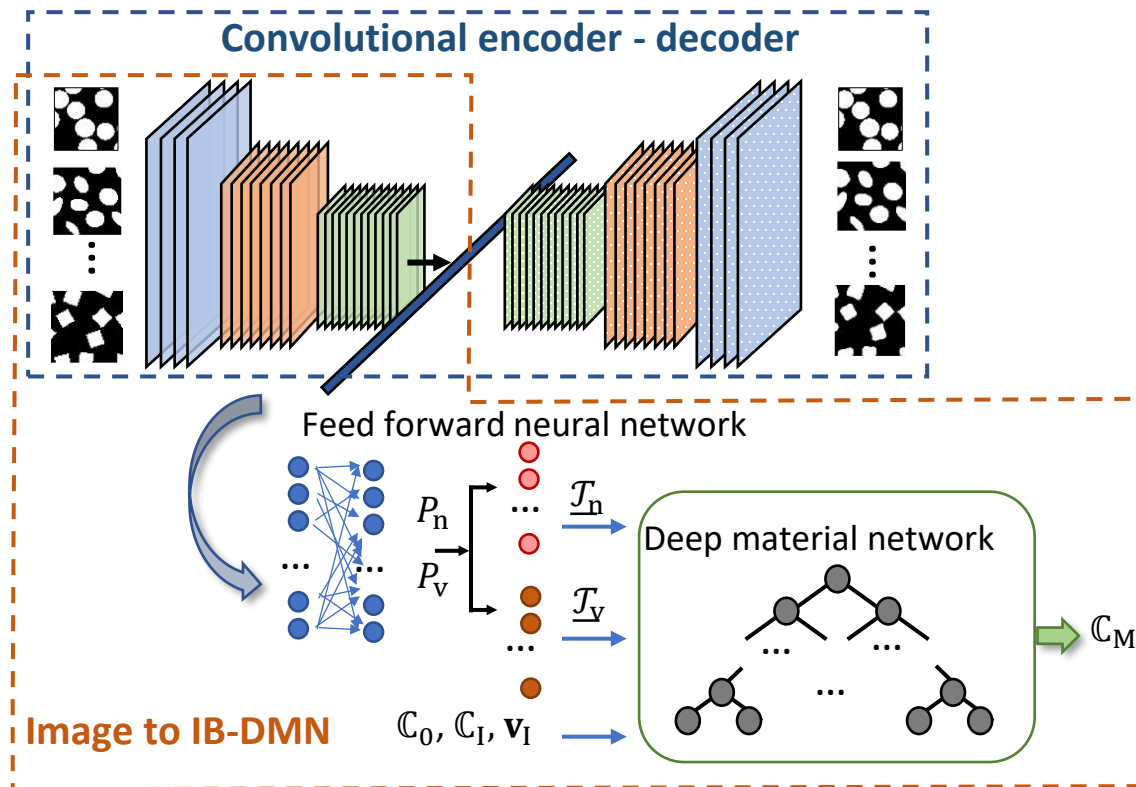


“Image to IB-DMN” framework

- Multiple-composite family “image to IB-DMN” framework

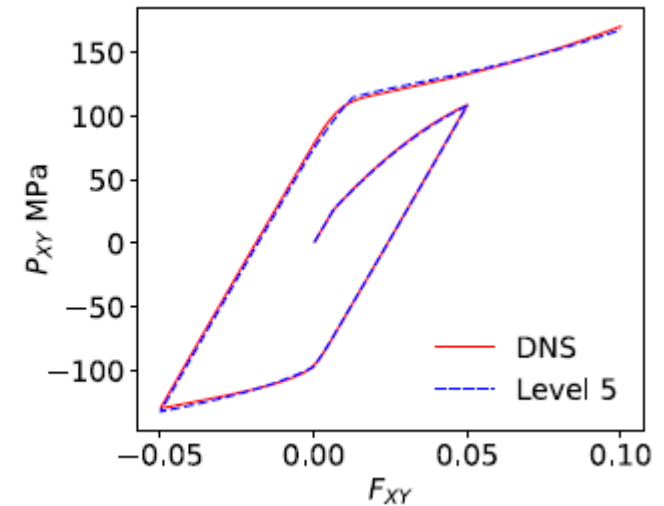
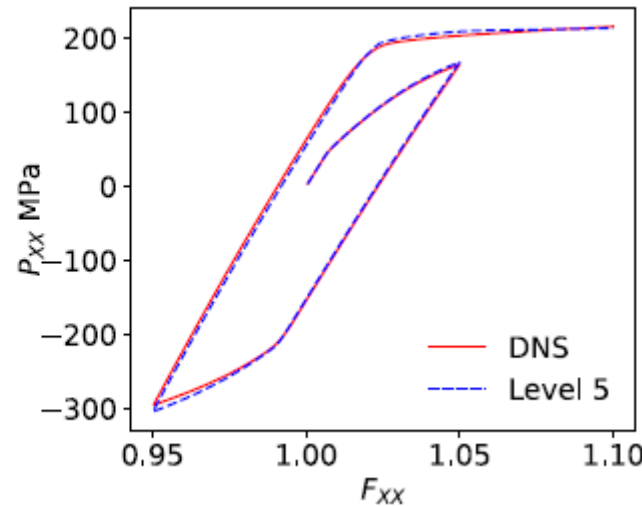
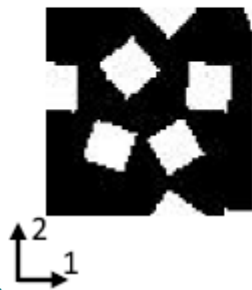
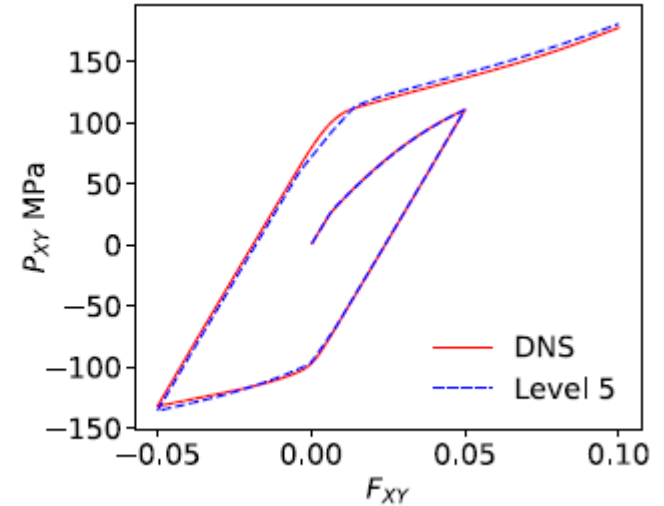
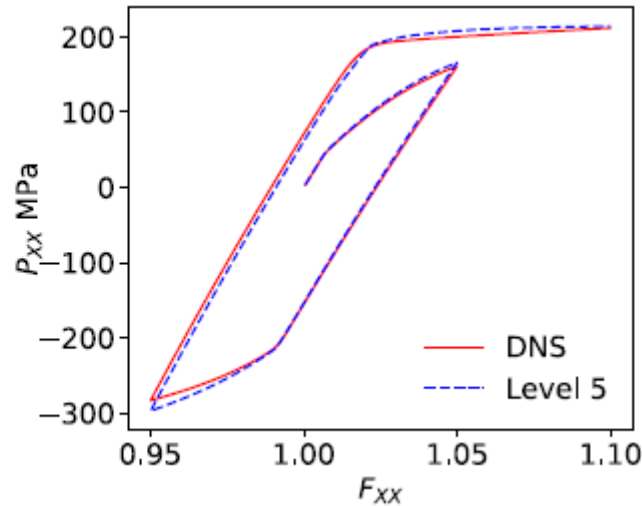
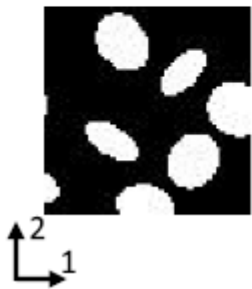


- Train the encoder-decoder & the feed-forward neural network considering all realisations at the same time



“Image to IB-DMN” framework

- Multiple-composite family “image to IB-DMN” framework



- Publications

- L. Wu and L. Noels. "Convolutional neural network-based mapping of material microstructures 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>

- Data and code on

- Repository:
https://gitlab.uliege.be/didearot/didearotPublic/publicationsData/2025_StochasticIBDMN
- 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>