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Mechanics of Materials

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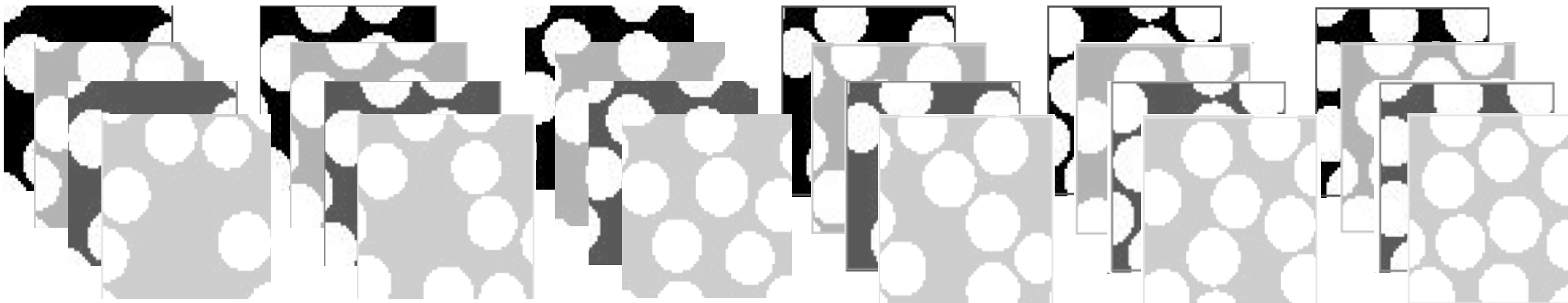

Stochastic Deep Material Networks as efficient surrogates for composites & Deep Material Networks performance for damaging processes

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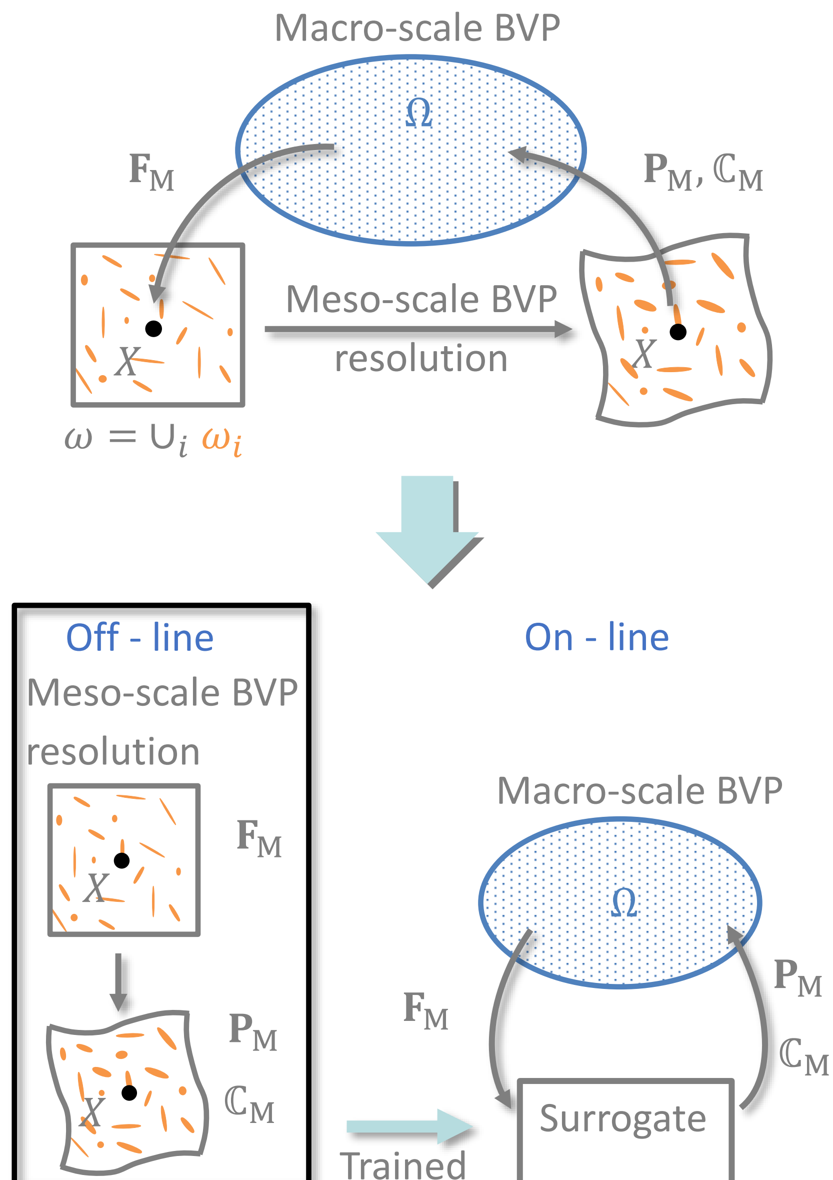
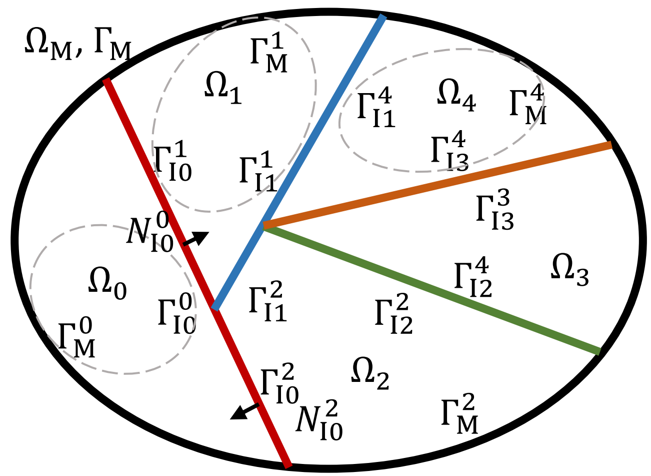
- Introduction to non-linear multi-scale simulations
  - FE multi-scale simulations
    - Problems to be solved at two scales
    - Requires Newton-Raphson iterations at both scales
  - Use of surrogate models
    - Train a meso-scale surrogate model (off-line)
      - Requires extensive data
      - 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



- Micro-scale interactions
  - Subdivision in sub-domains Ω_i

$$v_i = \frac{V_i}{V_\mathrm{M}}$$



  - Stress-strain averaging

$$\boldsymbol{\varepsilon}_\mathrm{M} = \sum_{i=0}^{N_\mathrm{p}-1} v_i\, \boldsymbol{\varepsilon}_i\,, \quad \text{and}$$

$$\boldsymbol{\sigma}_\mathrm{M} = \sum_{i=0}^{N_\mathrm{p}-1} v_i\, \boldsymbol{\sigma}_i$$

  - Introduction of fluctuations

$$\boldsymbol{\varepsilon}_\mathrm{m}(\boldsymbol{X}_\mathrm{m}) = \boldsymbol{\nabla} \otimes^s \boldsymbol{u}_\mathrm{m}(\boldsymbol{X}_\mathrm{m}) = \boldsymbol{\varepsilon}_\mathrm{M} + \boldsymbol{\nabla} \otimes^s \boldsymbol{u}'(\boldsymbol{X}_\mathrm{m}), \quad \boldsymbol{X}_\mathrm{m} \in \Omega_\mathrm{M}$$

$$\boldsymbol{\varepsilon}_i = \boldsymbol{\varepsilon}_\mathrm{M} + \frac{1}{V_i} \sum_{\forall \Gamma_{\mathrm{I}_j}^i \neq \emptyset} \int_{\Gamma_{\mathrm{I}_j}^i} \boldsymbol{u}'(\boldsymbol{X}_\mathrm{m}) \otimes^s \boldsymbol{N}_{\mathrm{I}_j}^i \mathrm{d}s \qquad s_j^i = \int_{\Gamma_{\mathrm{I}_j}^i} \mathrm{d}\,s$$

$$\boxed{\boldsymbol{\varepsilon}_i \simeq \boldsymbol{\varepsilon}_\mathrm{M} + \frac{1}{V_i} \sum_{\forall \Gamma_{\mathrm{I}_j}^i \neq \emptyset} s_j^i\, \boldsymbol{u}'_j \otimes^s \boldsymbol{N}_{\mathrm{I}_j}^i}$$

- Interactions
  - Introduction of fluctuations

$$\boldsymbol{\varepsilon}_i \simeq \boldsymbol{\varepsilon}_\mathrm{M} + \frac{1}{V_i} \sum_{\forall \Gamma_{\mathrm{I}_j}^{\,i} \neq \emptyset} s_j^i \, \boldsymbol{u}'_j \otimes^s \boldsymbol{N}_{\mathrm{I}_j}^{\,i}$$

  - Assume constitutive model in each sub-domain

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

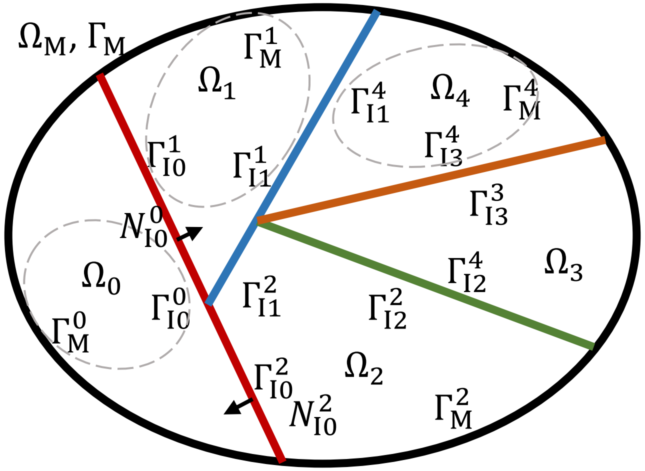
  - Hill-Mandel Condition

$$\boldsymbol{\sigma}_\mathrm{M} : \delta\boldsymbol{\varepsilon}_\mathrm{M} = \sum_{i=0}^{N_\mathrm{p}-1} v_i \, \boldsymbol{\sigma}_i : \delta\boldsymbol{\varepsilon}_i$$

$$\Rightarrow \sum_{i=0}^{N_\mathrm{p}-1} \sum_{\forall \Gamma_{\mathrm{I}_j}^{\,i} \neq \emptyset} \frac{v_i s_j^i}{V_i} \boldsymbol{\sigma}_i : \left(\boldsymbol{N}_{\mathrm{I}_j}^{\,i} \otimes^s \delta\boldsymbol{u}'_j\right) = 0$$

  - Weak form is the interface equation

$$\Rightarrow \sum_{i=0}^{N_\mathrm{p}-1} \int_{\Gamma_{\mathrm{I}_j}^{\,i}} \boldsymbol{\sigma}_i \cdot \boldsymbol{N}_{\mathrm{I}_j}^{\,i} \mathrm{d}s = \sum_{i=0}^{N_\mathrm{p}-1} s_j^i \, \boldsymbol{\sigma}_i \cdot \boldsymbol{N}_{\mathrm{I}_j}^{\,i} = \boldsymbol{0}, \text{ for } j = 0, \dots, N_\mathrm{I} - 1$$



Stochastic Interaction-Based Deep Material Network

- Interactions
  - Weak form

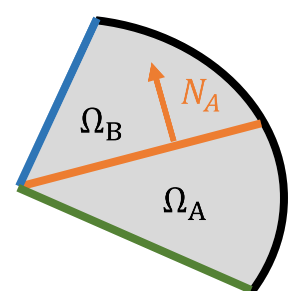
$$\sum_{i=0}^{N_{\mathsf{p}}-1}\int_{\Gamma_{\mathsf{I}_j}^{i}}\boldsymbol{\sigma}_i\cdot\boldsymbol{N}_{\mathsf{I}_j}^{i}\mathrm{d}s=\sum_{i=0}^{N_{\mathsf{p}}-1}s_j^i\,\boldsymbol{\sigma}_i\cdot\boldsymbol{N}_{\mathsf{I}_j}^{i}=\mathbf{0}\text{, for } j=0,\dots,N_{\mathsf{I}}-1$$

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

- One-level two-phase interaction
  - Strain tensors

$$\boldsymbol{\varepsilon}_{\mathsf{A}}=\boldsymbol{\varepsilon}_{\mathsf{M}}+\frac{1}{v_{\mathsf{A}}}\frac{s_{\mathsf{AB}}}{V_{\mathsf{M}}}\boldsymbol{u}'\otimes^s\boldsymbol{N}_{\mathsf{A}}\text{ and }\boldsymbol{\varepsilon}_{\mathsf{B}}=\boldsymbol{\varepsilon}_{\mathsf{M}}-\frac{1}{v_{\mathsf{B}}}\frac{s_{\mathsf{AB}}}{V_{\mathsf{M}}}\boldsymbol{u}'\otimes^s\boldsymbol{N}_{\mathsf{A}}$$

$$\hat{\mathbf{a}}=\frac{s_{\mathsf{AB}}}{V_{\mathsf{M}}}\boldsymbol{u}'$$



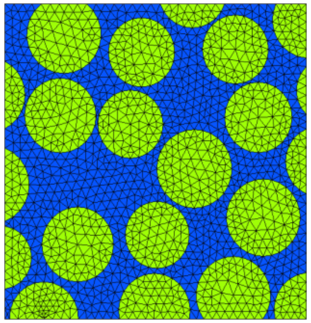
  - In linear elasticity the weak form becomes

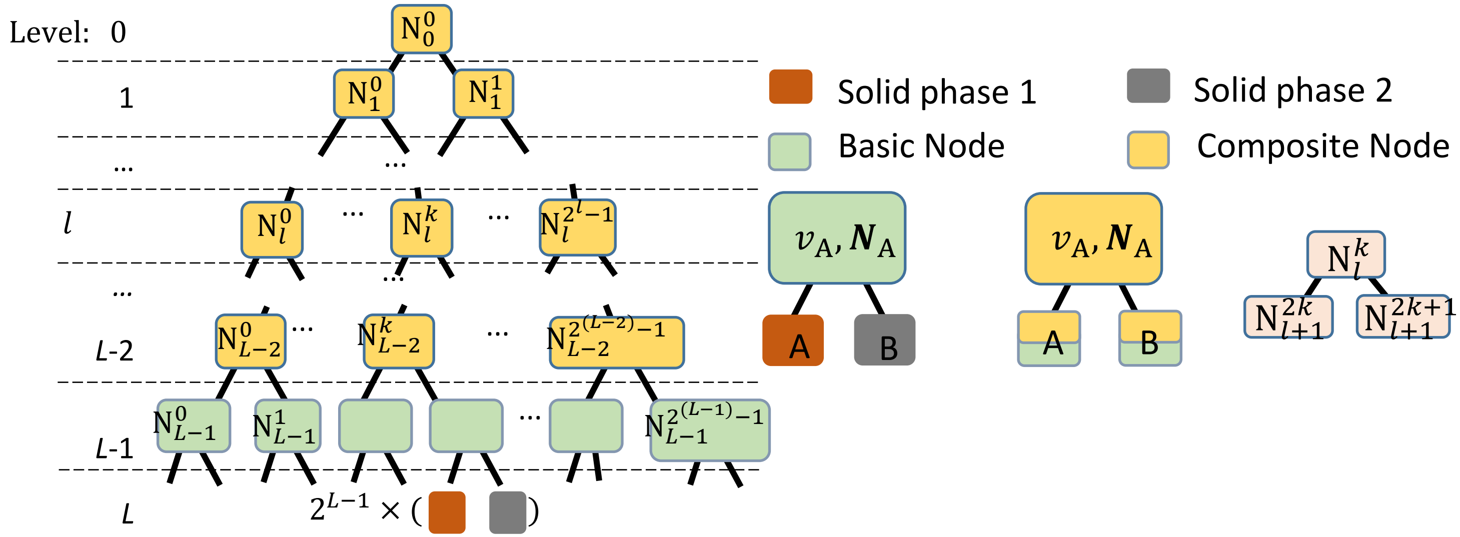
$$\mathbb{C}_{\mathsf{M}}=v_{\mathsf{A}}\mathbb{C}_{\mathsf{A}}+(1.0-v_{\mathsf{A}})\mathbb{C}_{\mathsf{B}}+(\mathbb{C}_{\mathsf{A}}-\mathbb{C}_{\mathsf{B}})\cdot\boldsymbol{N}_{\mathsf{A}}\otimes^s\left[\mathcal{K}^{-1}(v_{\mathsf{A}},\boldsymbol{N}_{\mathsf{A}})\cdot\mathcal{F}(v_{\mathsf{A}},\boldsymbol{N}_{\mathsf{A}})\right]$$

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

Stochastic Interaction-Based Deep Material Network

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





- Elasticity tensor
  - From material tensor evaluation $\mathbb{C}\left(\mathrm{N}_l^k\right) = \mathrm{FUN}\left(l, \mathbb{C}_0, \mathbb{C}_\mathrm{I}, \mathcal{G}^2\left(\mathrm{N}_l^k\right)\right)$
    - Requires

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

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

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

Stochastic Interaction-Based Deep Material Network

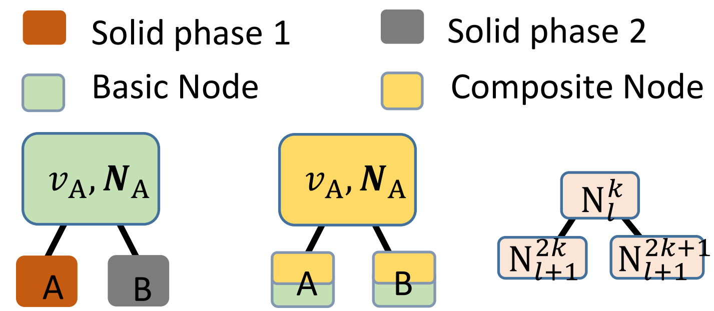
- Micro-structure topological parameters

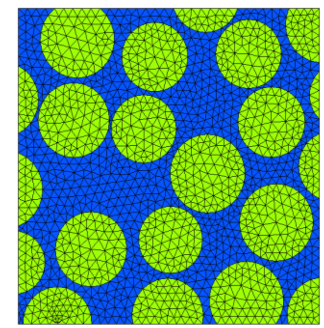
$$\boxed{\mathcal{G}^2(\mathrm{N}_0^0), \mathcal{G}^2(\mathrm{N}_1^0), \mathcal{G}^2(\mathrm{N}_1^1), \ldots, \mathcal{G}^2\left(\mathrm{N}_{L-1}^{2^{(L-1)}-1}\right)}$$

- Elastic training
  - From material tensor evaluation

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

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





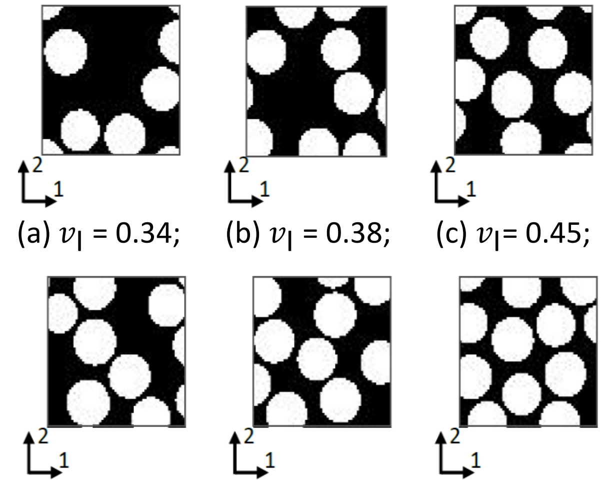
$$Loss(\hat{\mathbb{C}}_{\mathsf{M}}, \mathbb{C}_{\mathsf{M}}) = \frac{1}{n}\sum_{s=0}^{n-1} \frac{\|\hat{\mathbb{C}}_{\mathsf{M}}(\mathbb{C}_0^s, \mathbb{C}_{\mathsf{I}}^s) - \mathbb{C}_{\mathsf{M}}(\mathbb{C}_0^s, \mathbb{C}_{\mathsf{I}}^s; \mathcal{G}^2)\|}{\|\hat{\mathbb{C}}_{\mathsf{M}}(\mathbb{C}_0^s,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

Stochastic Interaction-Based Deep Material Network

- Once topological parameters knowns

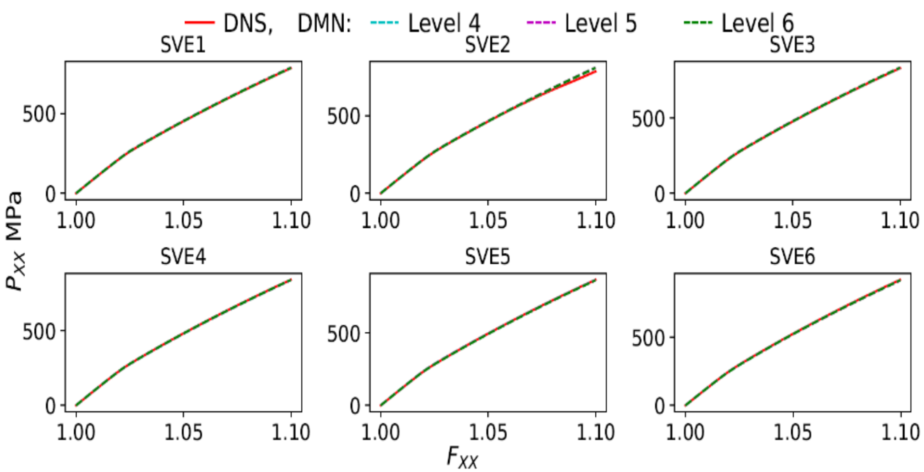
$$\mathcal{G}^2(\mathrm{N}_0^0), \mathcal{G}^2(\mathrm{N}_1^0), \mathcal{G}^2(\mathrm{N}_1^1), \dots, \mathcal{G}^2\left(\mathrm{N}_{L-1}^{2^{(L-1)}-1}\right)$$

- Online simulations in the non-linear range
  - $\boldsymbol{\varepsilon} \rightarrow \mathbf{F},\ \boldsymbol{\sigma} \rightarrow \mathbf{P},\ \mathbf{P}_i = \mathbf{P}^p\left(\mathbf{F}_i\left(\boldsymbol{u}'_j\right);\ \boldsymbol{Z}_i\right)$
  - Isotropic hardening $f = \tau_{\mathrm{eq}} - \tau_{\mathrm{y}}^0 - h\gamma \leq 0$,
  - Tests on 6 SVEs

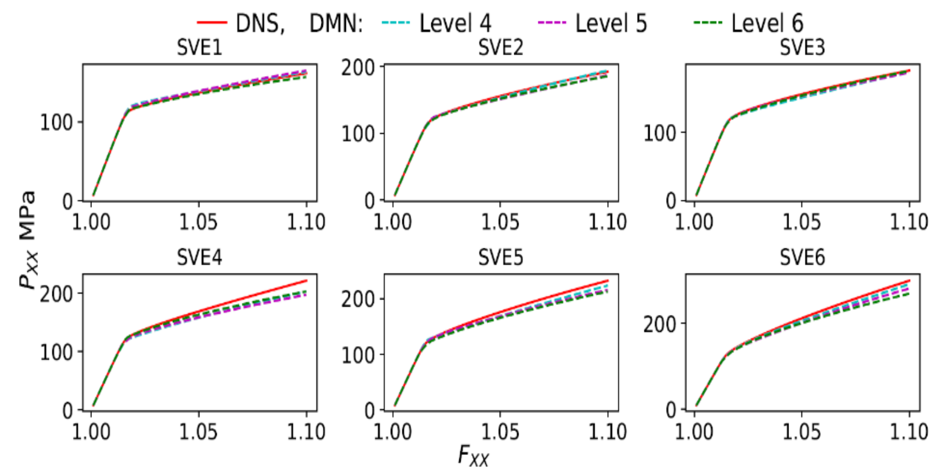


(a) v_{I} = 0.34; (b) v_{I} = 0.38; (c) v_{I}= 0.45;

(d) v_{I} = 0.47; (e) v_{I} = 0.52; (f) v_{I}= 0.58



(a) Uni-axial strain



(b) In-plane uni-axial stress

- Reformulation of parameters $\mathcal{G}^2 = \{v_\mathrm{A}, \boldsymbol{N}_\mathrm{A}\}$ at node N_l^k
  - Normal $\boldsymbol{N}_\mathrm{A}(\mathrm{N}_l^k)$ from angles $\theta_1(\mathrm{N}_l^k)$ and $\theta_2(\mathrm{N}_l^k)$

$$\theta_1 = 2\pi \mathrm{w}_{\theta_1}(\mathrm{N}_l^k),\ \theta_2 = \pi \mathrm{w}_{\theta_2}(\mathrm{N}_l^k)$$

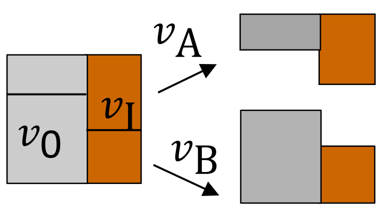
$$\Rightarrow \boxed{\mathrm{w}_{\theta_1}(\mathrm{N}_l^k), \mathrm{w}_{\theta_2}(\mathrm{N}_l^k) \in [0,\ 1)}$$

  - Volume fraction $v_\mathrm{A}(\mathrm{N}_l^k)$

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

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

$$\Rightarrow \begin{cases} v_\mathrm{A}(\mathrm{N}_0^0) = \mathrm{w}_{v0}(\mathrm{N}_0^0) v_0(\mathrm{N}_0^0) + \mathrm{w}_{v\mathrm{I}}(\mathrm{N}_0^0) v_\mathrm{I}(\mathrm{N}_0^0) \\ v_\mathrm{B}(\mathrm{N}_0^0) = 1.0 - v_\mathrm{A}(\mathrm{N}_0^0) \end{cases}$$

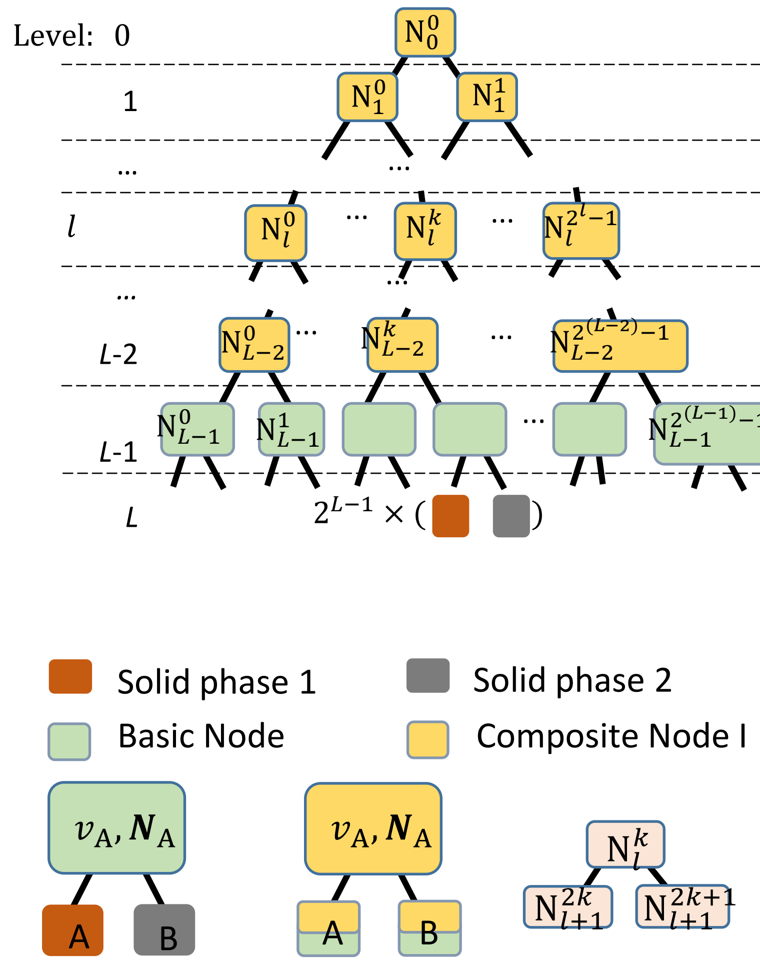


2) Recursively for "Yellow" Node at level $0 < l < L$

$$\Rightarrow \boxed{\mathrm{w}_{v0}(\mathrm{N}_l^k), \mathrm{w}_{v\mathrm{I}}(\mathrm{N}_l^k) \in [0,\ 1)}$$

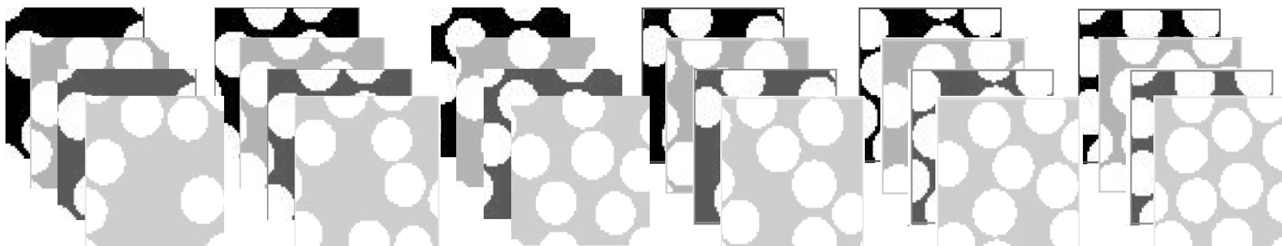
3) Basic "Green" Node at level $L - 1$:

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



Stochastic Interaction-Based Deep Material Network

- SVEs batch training
  - New parameters $\underline{\tilde{\mathcal{T}}}_{\mathrm{n}} = \{w_{\theta_1}(\mathrm{N}_l^k), w_{\theta_2}(\mathrm{N}_l^k)\}$ and $\underline{\tilde{\mathcal{T}}}_{\mathrm{V}} = \{w_{\mathrm{V}0}(\mathrm{N}_l^k), w_{\mathrm{VI}}(\mathrm{N}_l^k)\}$
  - Train a generic DMN
    - Random micro-topologies and volume fractions,
    - Random phase properties



$\{\hat{\mathbb{C}}_{\mathrm{M}}(\mathbb{C}_0^s, \mathbb{C}_{\mathrm{I}}^s)\}$

  - New loss function in which v_{I}^s is known for each SVE

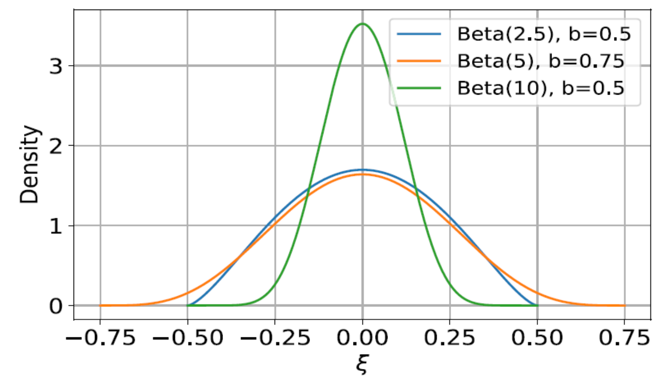
$$Loss(\hat{\mathbb{C}}_{\mathrm{M}}, \mathbb{C}_{\mathrm{M}}) = \frac{1}{n}\sum_{s=1}^{n} \frac{\|\hat{\mathbb{C}}_{\mathrm{M}}(\mathbb{C}_0^s, \mathbb{C}_{\mathrm{I}}^s) - \mathbb{C}_{\mathrm{M}}(\mathbb{C}_0^s, \mathbb{C}_{\mathrm{I}}^s, v_{\mathrm{I}}^s; \underline{\tilde{\mathcal{T}}}_{\mathrm{n}}, \underline{\tilde{\mathcal{T}}}_{\mathrm{V}})\|}{\|\hat{\mathbb{C}}_{\mathrm{M}}(\mathbb{C}_0^s, \mathbb{C}_{\mathrm{I}}^s)\|}$$

Identify the generic DMN parameters $\underline{\tilde{\mathcal{P}}}_{\mathrm{n}}, \underline{\tilde{\mathcal{P}}}_{\mathrm{V}}$,

where $\underline{\tilde{\mathcal{T}}}_{\mathrm{n}} = sigmoid(\underline{\tilde{\mathcal{P}}}_{\mathrm{n}})$ and $\underline{\tilde{\mathcal{T}}}_{\mathrm{V}} = sigmoid(\underline{\tilde{\mathcal{P}}}_{\mathrm{V}})$

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

$$\begin{cases} \underline{\mathcal{P}}_{\mathrm{n}} = (1+\xi)\odot\underline{\tilde{\mathcal{P}}}_{\mathrm{n}} \\ \underline{\mathcal{P}}_{\mathrm{v}} = (1+\xi)\odot\underline{\tilde{\mathcal{P}}}_{\mathrm{v}} \end{cases} \qquad \begin{aligned} &\xi = 2b(\chi - 0.5) \\ &\chi \sim \mathrm{Beta}(\alpha) \end{aligned}$$

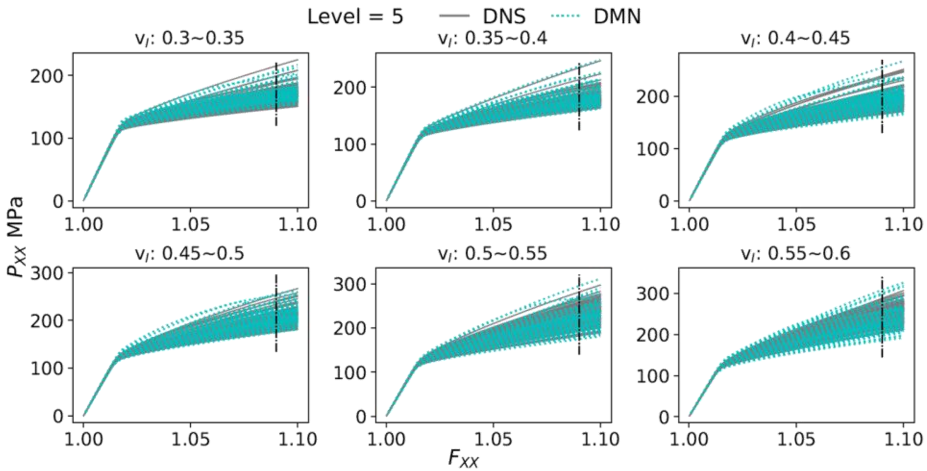


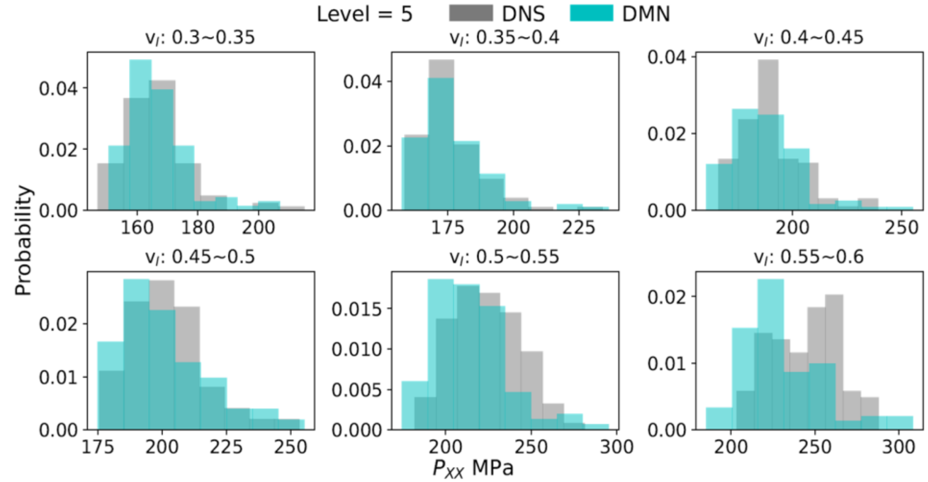
  - $\underline{\mathcal{T}}_{\mathrm{n}} = sigmoid\left(\underline{\mathcal{P}}_{\mathrm{n}}\right)$ *and* $\underline{\mathcal{T}}_{\mathrm{v}} = sigmoid\left(\underline{\mathcal{P}}_{\mathrm{v}}\right)$

Stochastic Interaction-Based Deep Material Network

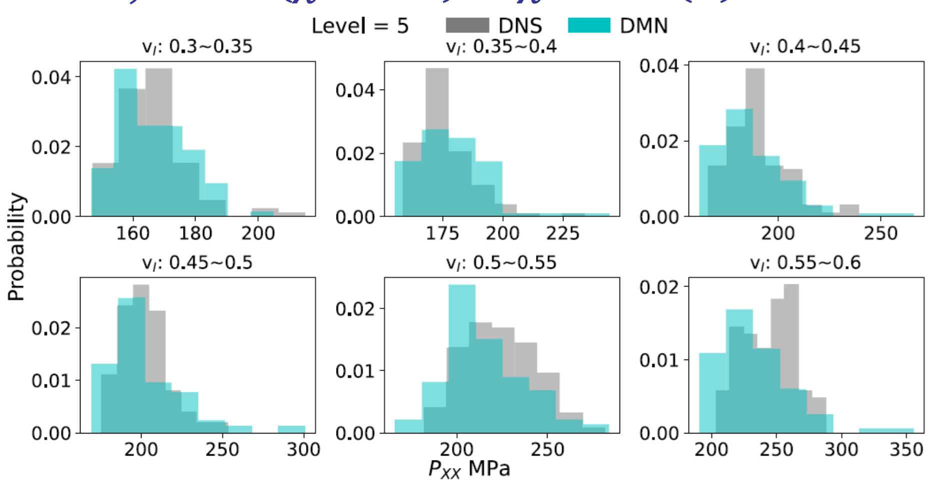
- Perturbate generic DMN

$$\underline{\mathcal{P}}_{\mathrm{n}} = (1+\xi)\odot\underline{\tilde{\mathcal{P}}}_{\mathrm{n}} \qquad \underline{\mathcal{P}}_{\mathrm{v}} = (1+\xi)\odot\underline{\tilde{\mathcal{P}}}_{\mathrm{v}} \qquad \xi = (\chi - 0.5) \qquad \chi \sim \mathrm{Beta}(2.5)$$

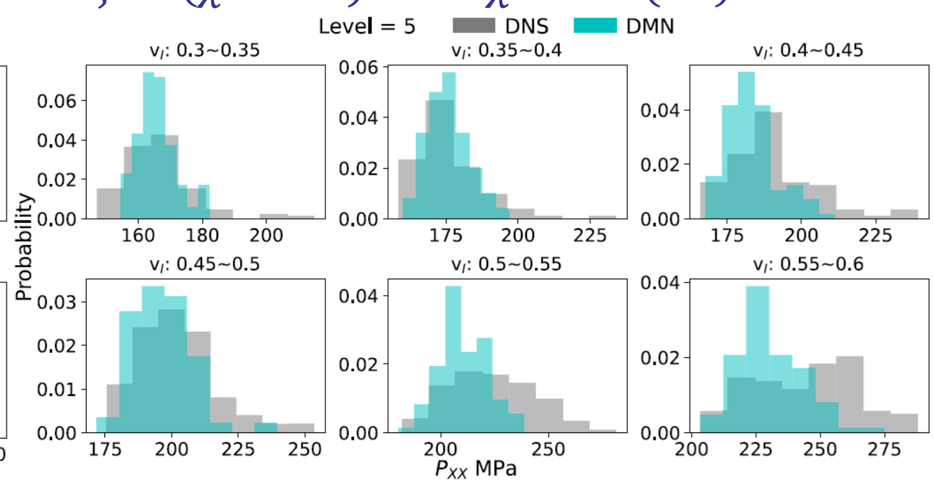




$$\xi = 1.5(\chi - 0.5) \qquad \chi \sim \mathrm{Beta}(5)$$



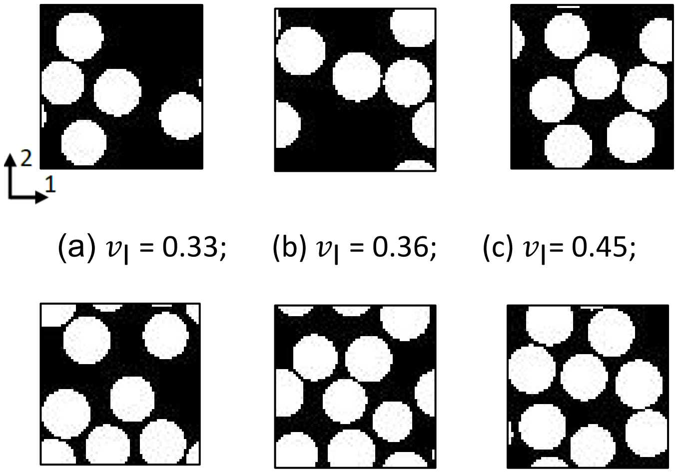
$$\xi = (\chi - 0.5) \qquad \chi \sim \mathrm{Beta}(10)$$



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

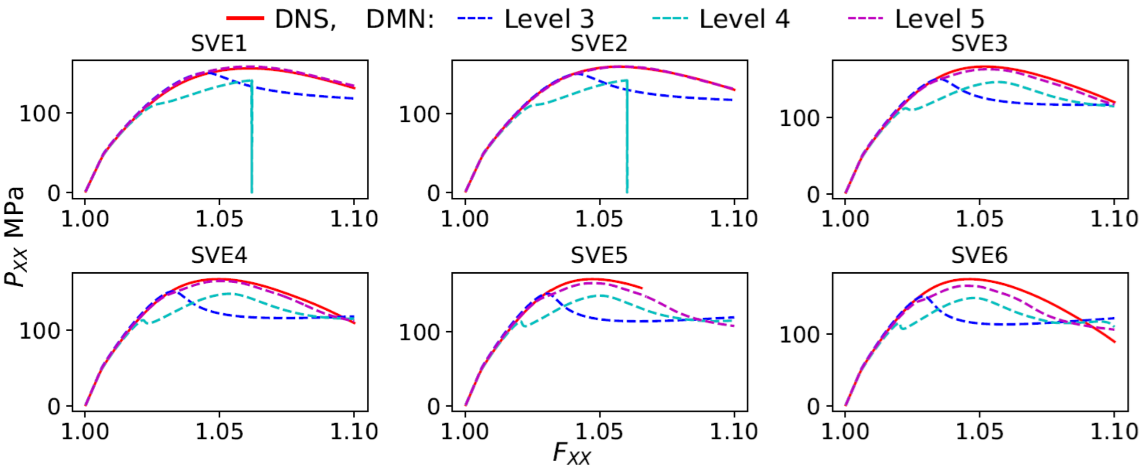
Stochastic Interaction-Based Deep Material Network

- DMN extrapolates constitutive model ➡ introduction of damage straightforward



(a) v_{I} = 0.33; (b) v_{I} = 0.36; (c) v_{I}= 0.45;

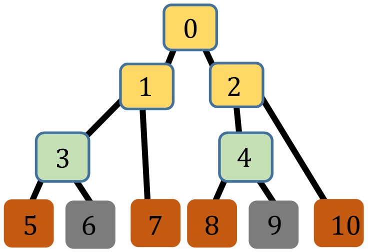
(d) v_{I} = 0.49; (e) v_{I} = 0.53; (f) v_{I}= 0.55



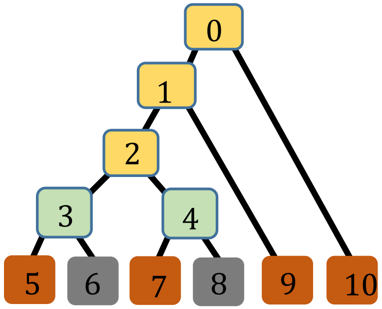
➡ Damage localises in a material node but is spread in the tree

Stochastic Interaction-Based Deep Material Network

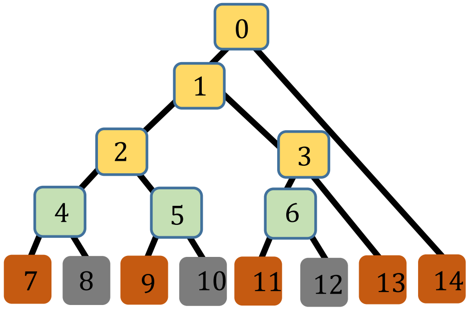
- Damage localises in a material node ➡ shorten the information path for matrix



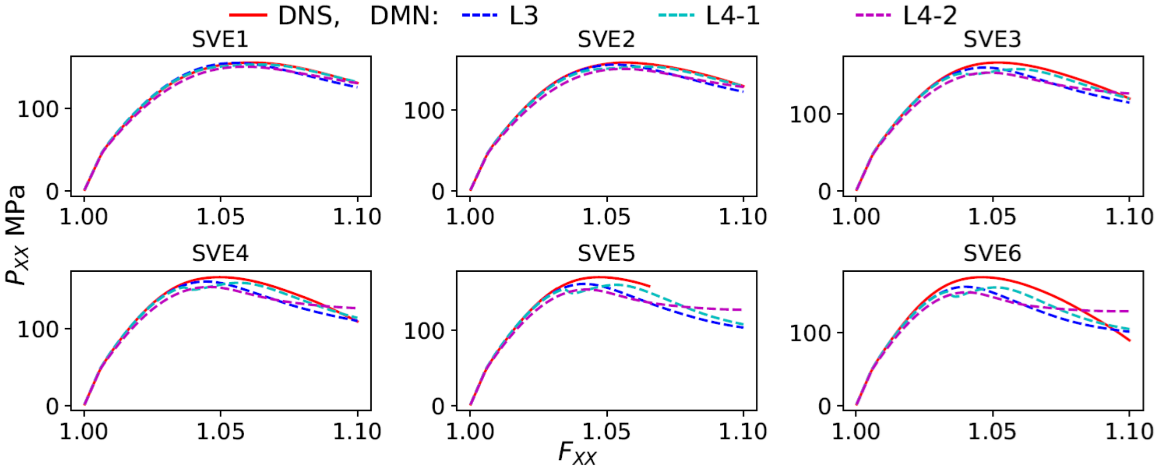
(a) L3



(b) L4-1



(c) L4-2



Better but not enough ➡ need for non-locality

References

- DIDEAROT project (https://www.didearot-project.eu/)
  - CENAERO, HEXAGON, SONACA, ULiège (Belgium)
  - Tecnalia, Aernnova, Barcelona Supercomputing Center (Spain)
  - Inegi (Portugal)

- Publication

  - 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