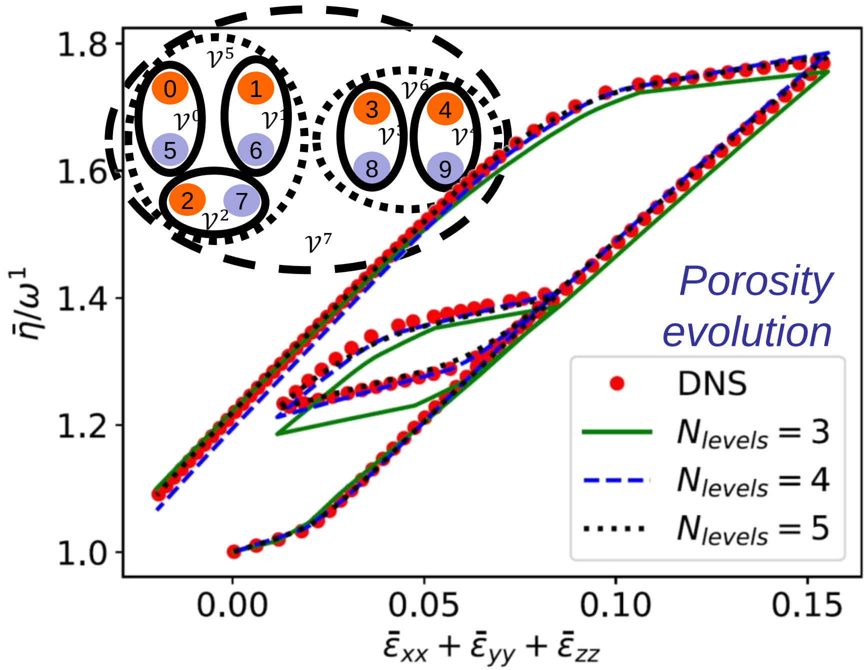
Redefinition of the interactions in Deep-Material-Networks

Noels Ludovic, Wu Ling, Nguyen Van Dung



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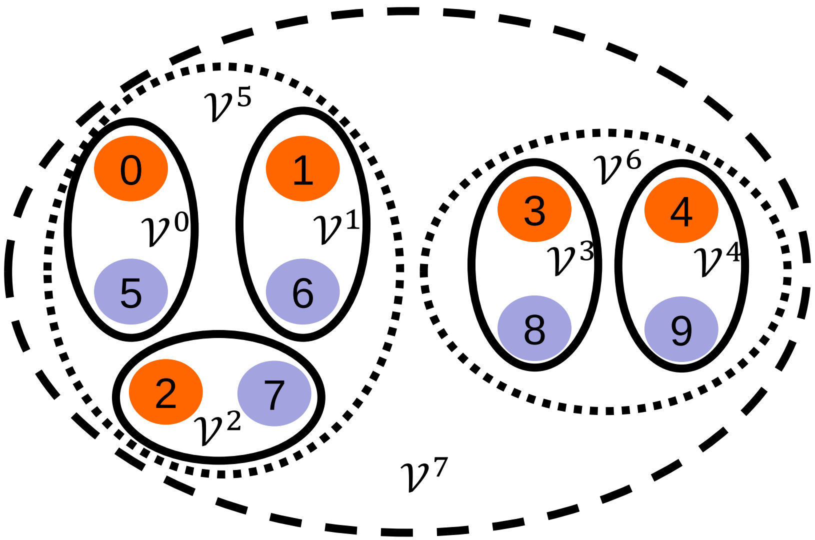
Deep Material Networks with laminate building blocks

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



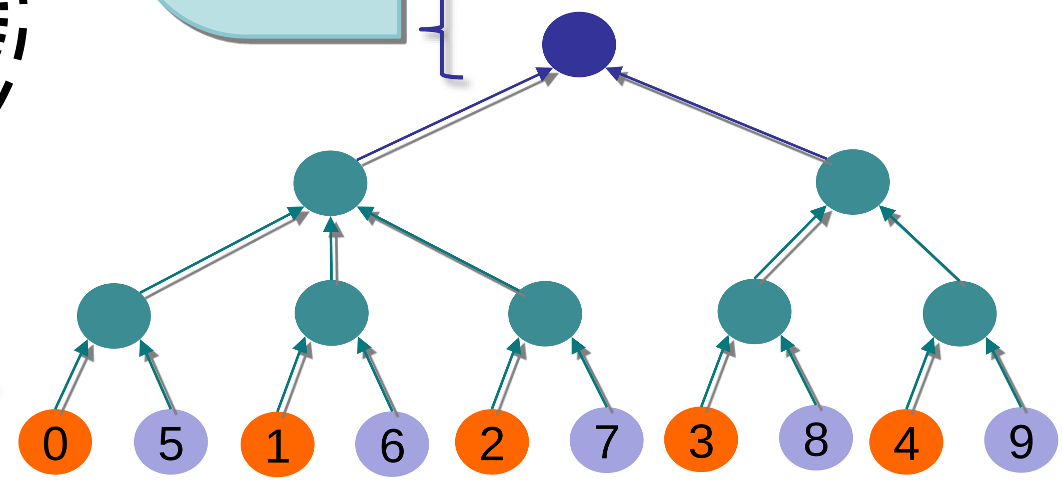
Homogenised behaviour

$$\bar{\boldsymbol{P}}(t) = \bar{\boldsymbol{P}}(\bar{\boldsymbol{F}}(t), z(\tau \leq t))$$

$$\bar{\boldsymbol{P}}(t) = \sum_{i=0}^{9} W^i\, \boldsymbol{P}^i(t)$$

$$\bar{\boldsymbol{F}}(t) = \sum_{i=0}^{9} W^i\, \boldsymbol{F}^i(t)$$

Weight of node i (parameter)



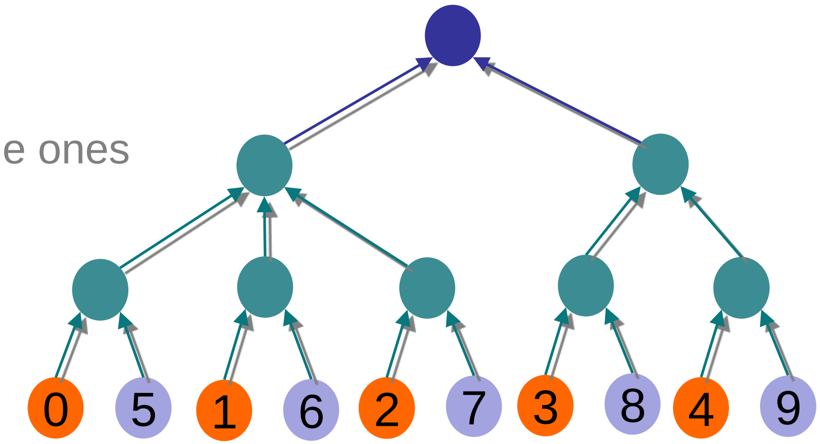
Material node i =0..9, of weight W^i

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

if node $i \in$ *phase* p *for material p=0 or p=1*

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

Deep Material Networks with laminate building blocks



- Mechanism $k = 0..M-1$
  - Link homogenised deformation gradient to node ones
    - Construction of a strain fluctuation field

$$\overline{\boldsymbol{F}} + \sum_{k=0}^{M-1} \alpha^{i,k}\, \boldsymbol{a}^k \otimes \boldsymbol{G}^k = \boldsymbol{F}^i\,, \quad i = 0..9$$

Contribution of node i in mechanism k (parameter?)

Degrees of freedom of mechanism k defining the strain fluctuation

Direction of mechanism k (parameter)

  - Constraints from strain averaging
    - $\overline{\boldsymbol{F}} = \sum_i W^i \boldsymbol{F}^i \Rightarrow \sum_k \left(\sum_i W^i \alpha^{i,k} \right) \boldsymbol{a}^k \otimes \boldsymbol{G}^k = 0 \Rightarrow \sum_i W^i \alpha^{i,k} = 0$

Weight of node i (parameter)

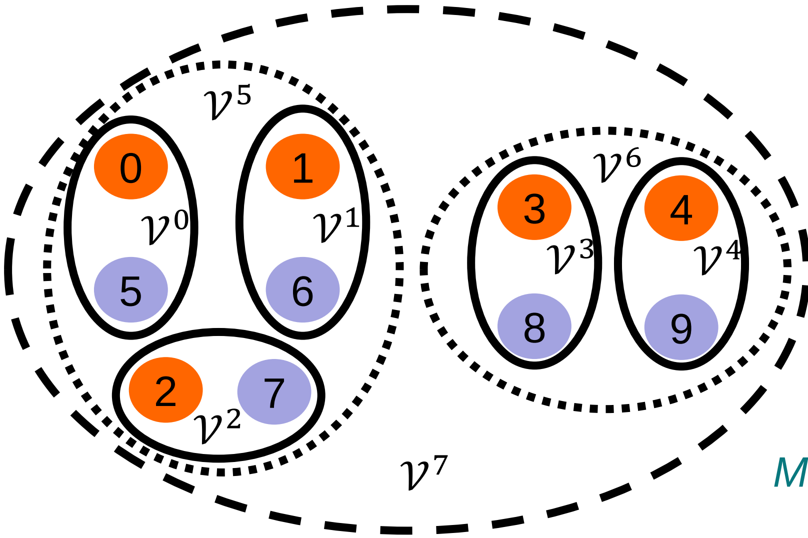
  - Weak form from Hill-Mandel
    - $\overline{\boldsymbol{P}} : \delta \overline{\boldsymbol{F}} = \sum_i W^i \boldsymbol{P}^i : \delta \boldsymbol{F}^i \Rightarrow \left[\sum_k \left(\sum_i W^i \boldsymbol{P}^i \alpha^{i,k} \right) \cdot \boldsymbol{G}^k \right] \cdot \delta \boldsymbol{a}^k = 0$

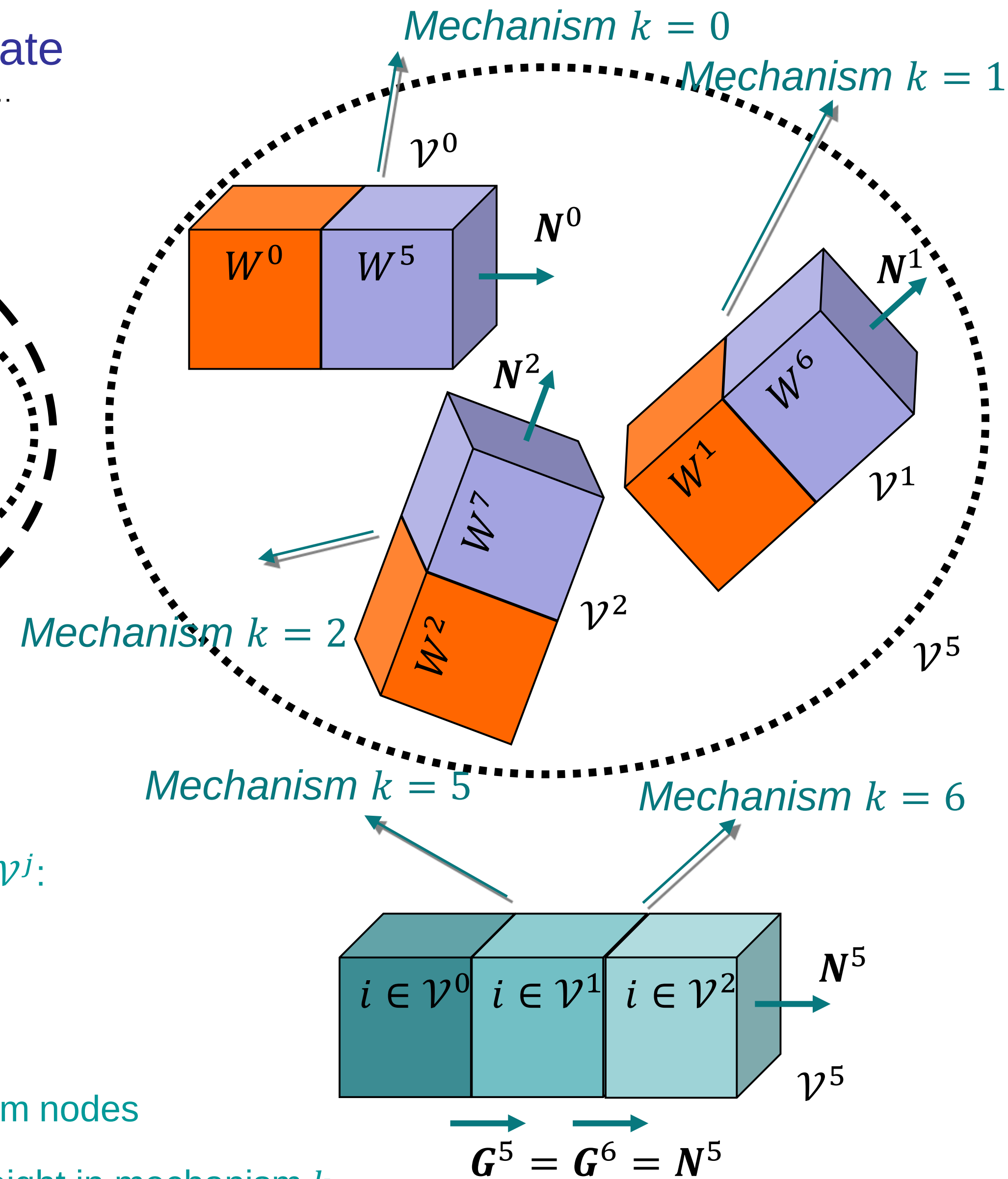
Deep Material Networks with laminate building blocks

- Mechanistic building blocks: Laminate

  Z. Liu, C. Wu, M. Koishi, A deep material network for …

  – Interaction $\mathcal{V}^j$ as a laminate





  – Parameters

    - Weight: $W^i,\ i = 0..9$
    - Unique direction for an interaction $\mathcal{V}^j$:

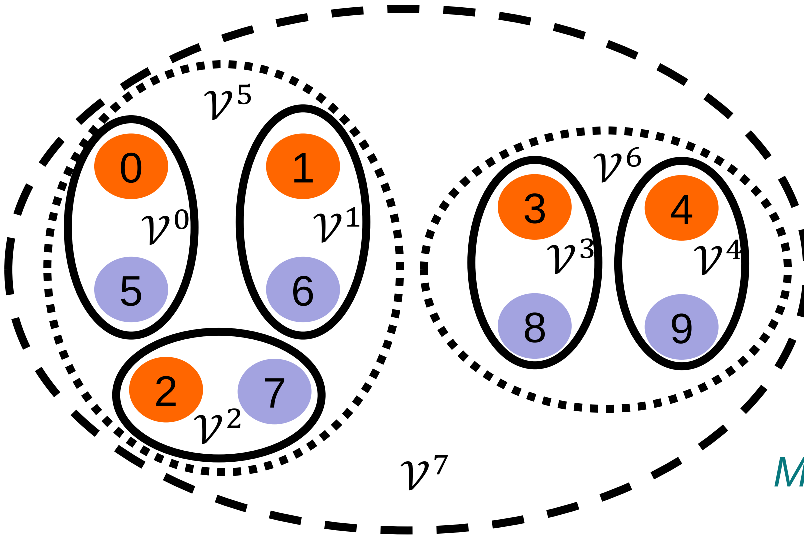
      $\boldsymbol{G}^k$ ⇨ $\boldsymbol{N}^j,\ j = 0..7$

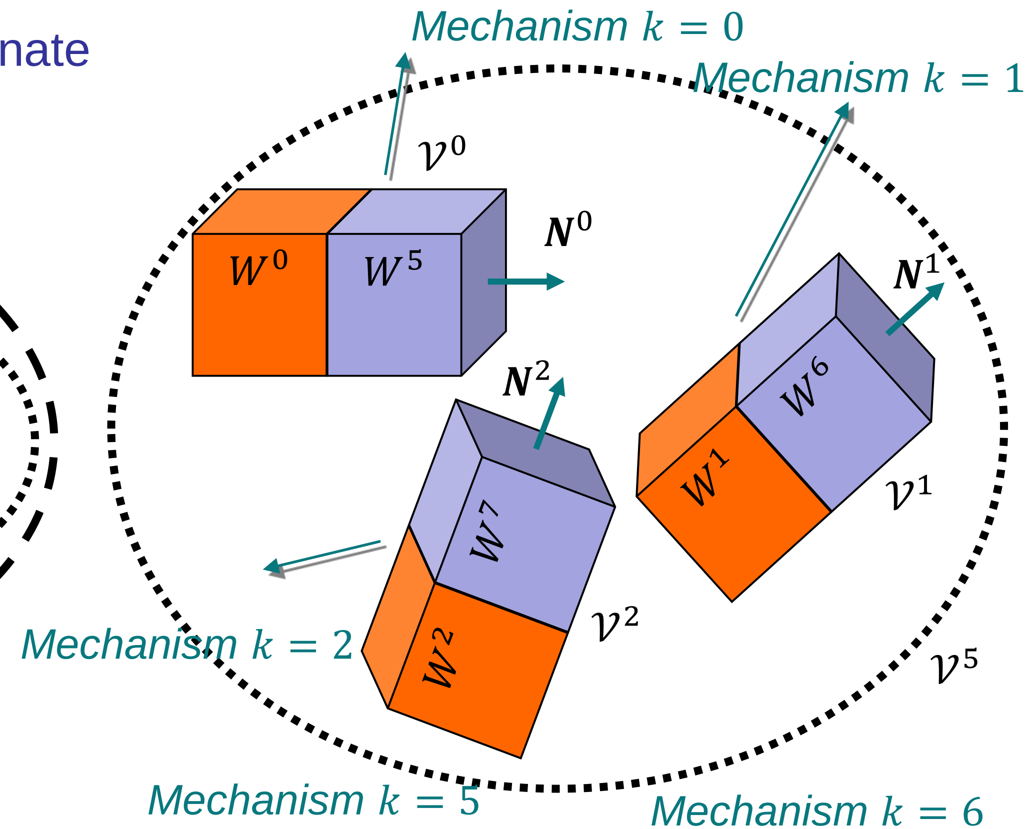
  – Constraint

    - $\sum_i W^i \alpha^{i,k} = 0$ ⇨ $\alpha^{i,k}$ from nodes weight in mechanism k

Deep Material Networks with laminate building blocks

- Mechanistic building blocks: Laminate
  - Interaction $\mathcal{V}^j$ as a laminate

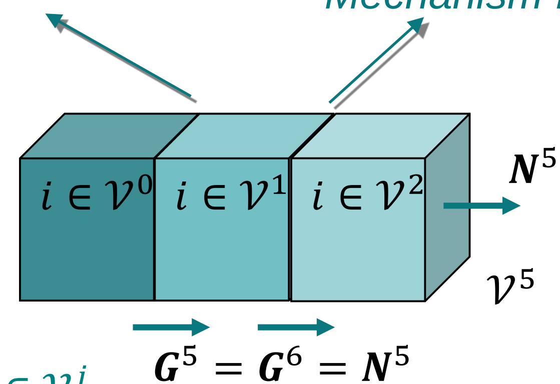




  - Weak form

$$\left[\sum_k \left(\sum_i W^i \boldsymbol{P}^i \alpha^{i,k}\right) \cdot \boldsymbol{G}^k\right] \cdot \delta \boldsymbol{a}^k = 0$$

$$\left(\frac{1}{W(\mathcal{V}^m)} \sum_{i \in \mathcal{V}^m} W^i \boldsymbol{P}^i - \frac{1}{W(\mathcal{V}^{m+1})} \sum_{i \in \mathcal{V}^{m+1}} W^i \boldsymbol{P}^i\right) \cdot \boldsymbol{N}^j = 0$$



$j = 0..7$, $\mathcal{V}^m$ and $\mathcal{V}^{m+1}$ interactions of mechanism $k \in \mathcal{V}^j$

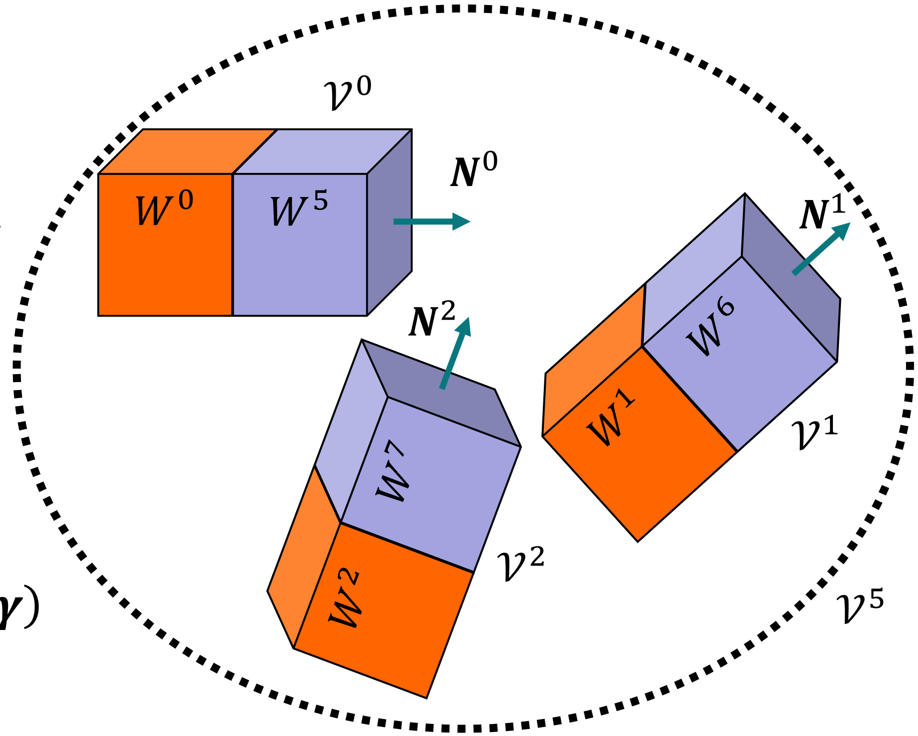
- Offline stage on a p-phase RVE
  - Topological parameters $\boldsymbol{\chi}$
    - Weight: $W^i,\ i = 0..9$
    - Direction of interaction $\mathcal{V}^j$: $\boldsymbol{N}^j, j = 0..7$

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

  - Using elastic data
    - Random properties on RVE

$$\boldsymbol{\gamma} = [E_0, \nu_0, E_1, \nu_1 \dots E_p, \nu_p,]$$

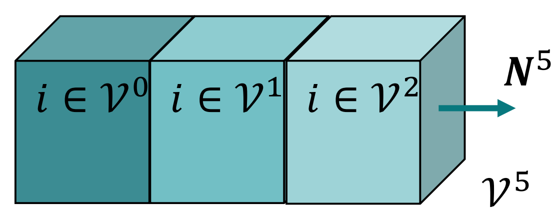
Direct simulations on RVE $\hat{\mathbb{C}}(\boldsymbol{\gamma})$



    - Cost functions to minimise

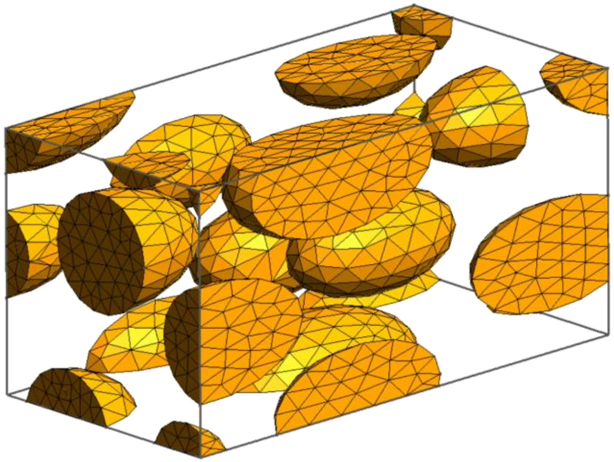
$$L(\hat{\mathbb{C}}, \bar{\mathbb{C}}(\boldsymbol{\chi})) = \frac{1}{n}\sum_{s=1}^{n} \frac{\|\hat{\mathbb{C}}(\boldsymbol{\gamma}_s) - \bar{\mathbb{C}}(\boldsymbol{\chi}|\boldsymbol{\gamma}_s)\|}{\|\hat{\mathbb{C}}(\boldsymbol{\gamma}_s)\|}$$

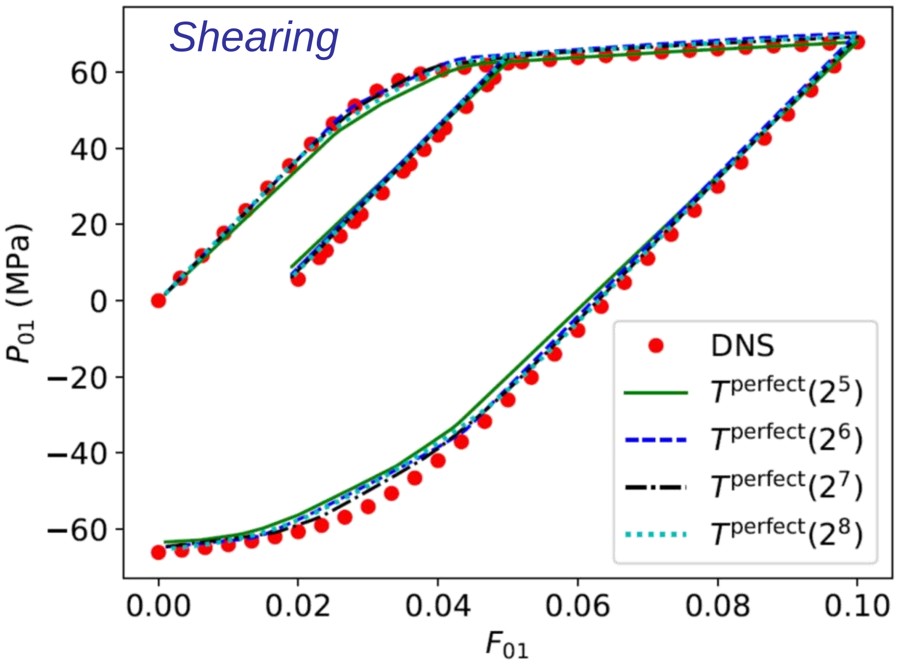
    - « Stochastic gradient descent (SGD) » algorithm

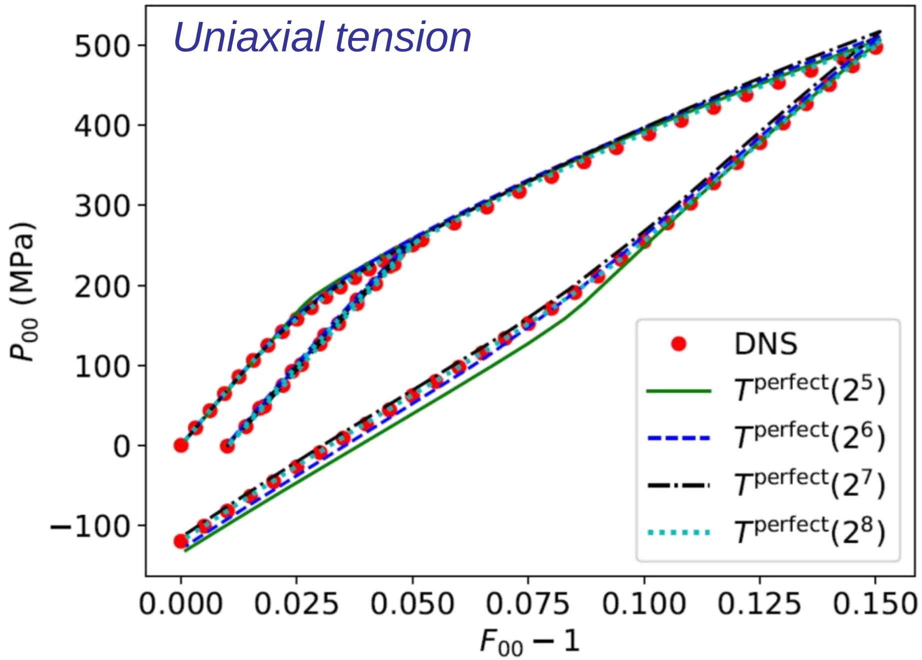


Deep Material Networks with laminate building blocks

- Online stage on a particle-reinforced composite
  - Properties
    - Elastic inclusions
    - Elasto-plastic matrix



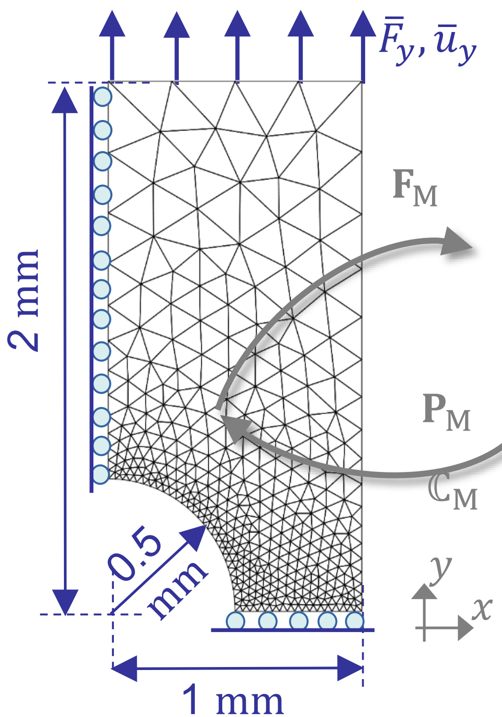


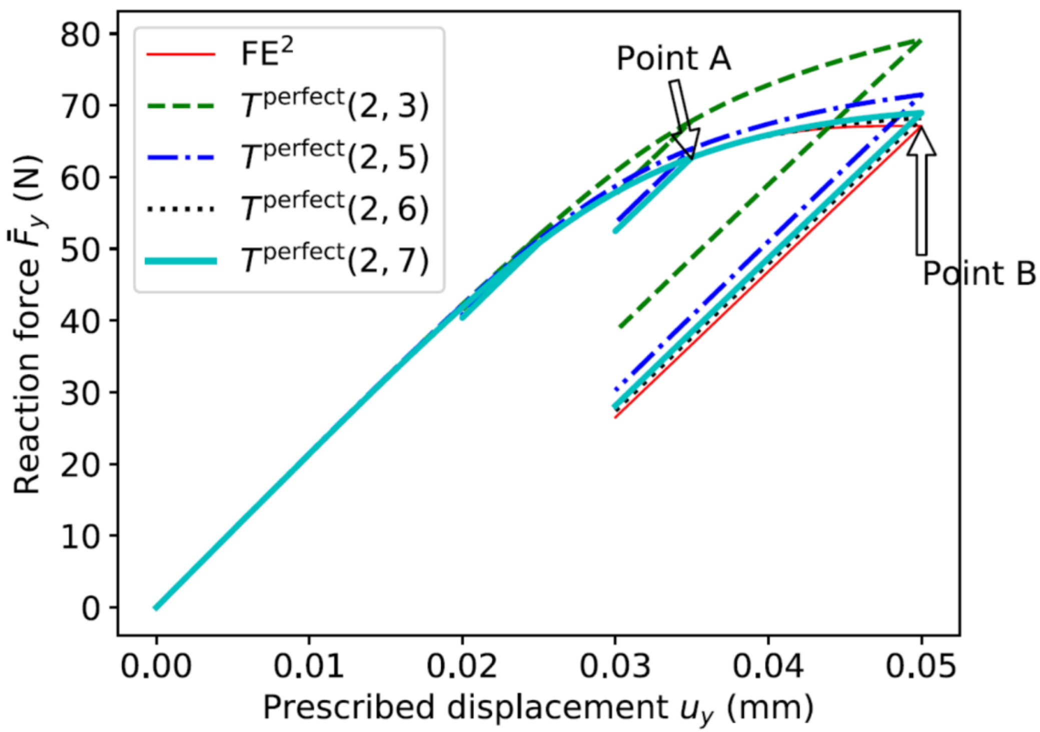


Deep Material Networks with laminate building blocks

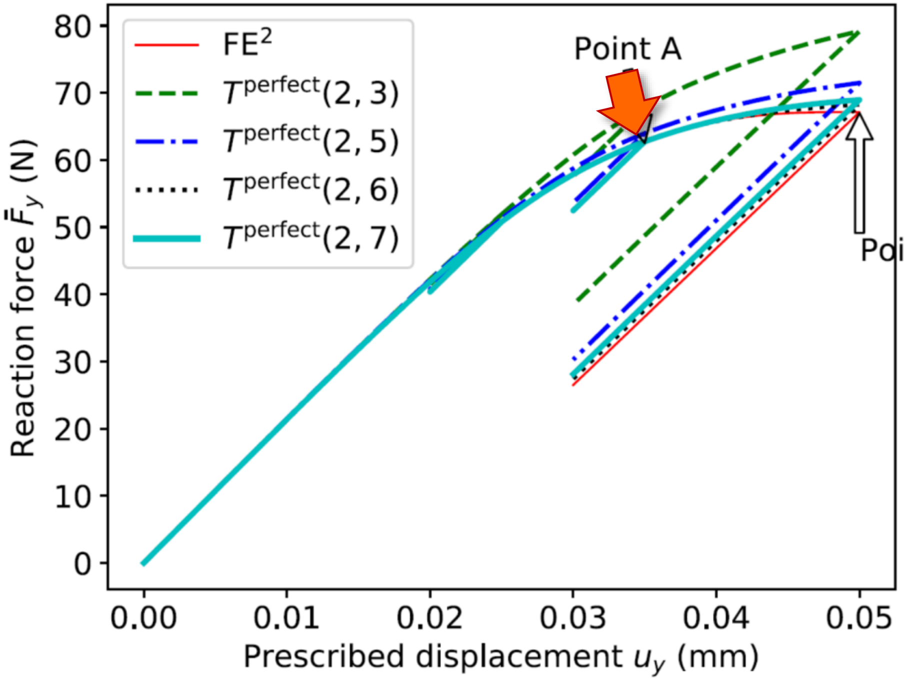
- Multiscale simulation
  - Elasto-plastic composite RVE
  - Comparison FE² vs. DMN-surrogate

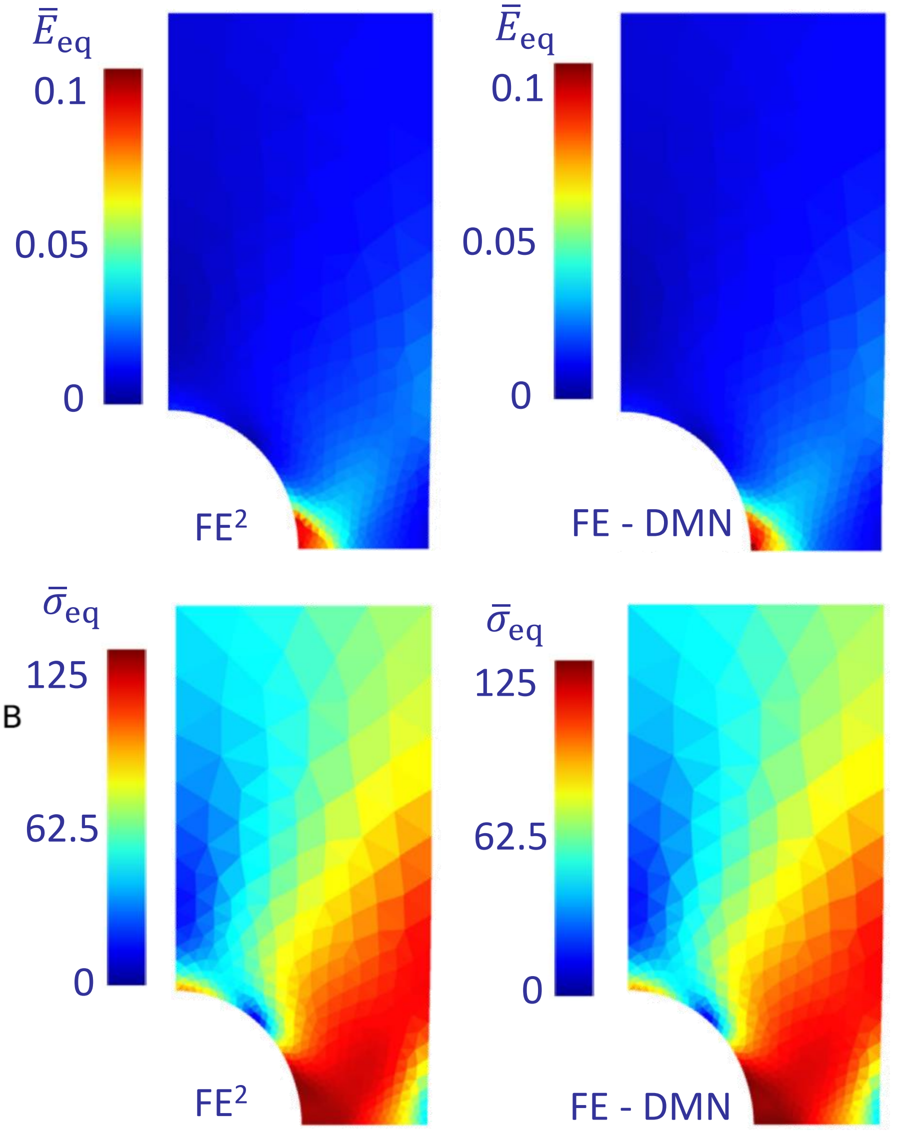
Off-line	FE²	FE-DMN
Data generation	-	10 min.-cpu
Training	-	2 min.-cpu
On-line	**FE²**	**FE-DMN**
Simulation	18000 h-cpu	½ to 34 h-cpu





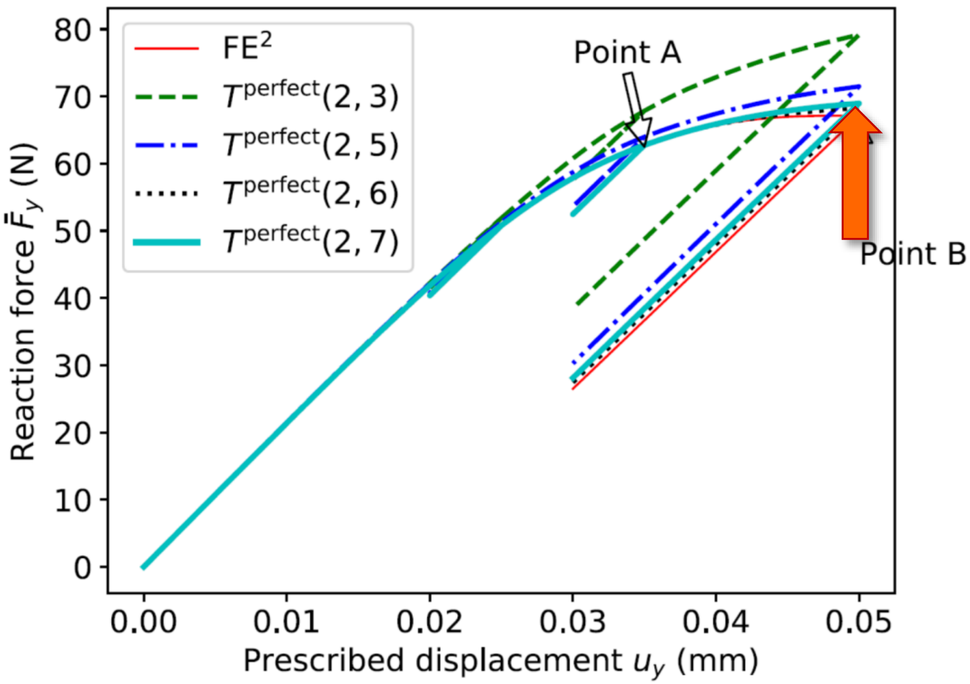
- Multiscale simulation
  - Stress-strain distribution at point A
  - For 2^7 material nodes

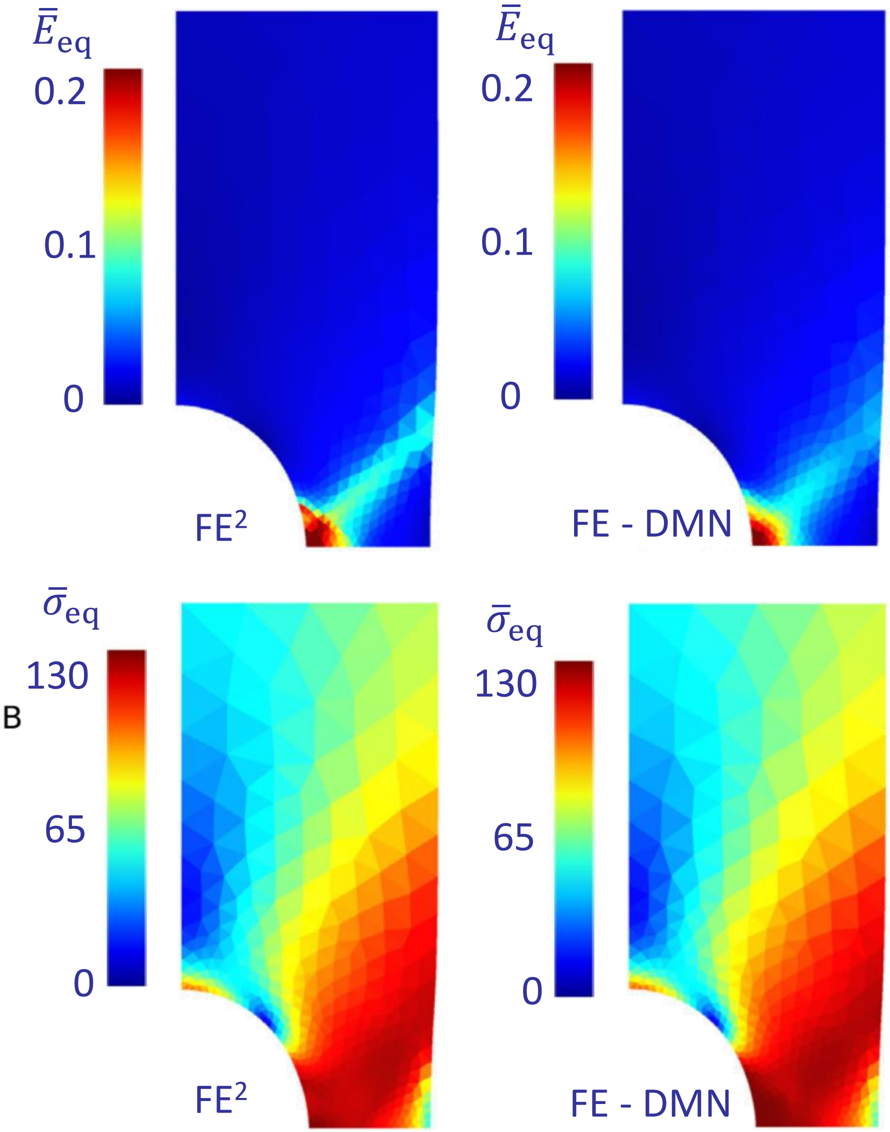




Deep Material Networks with laminate building blocks

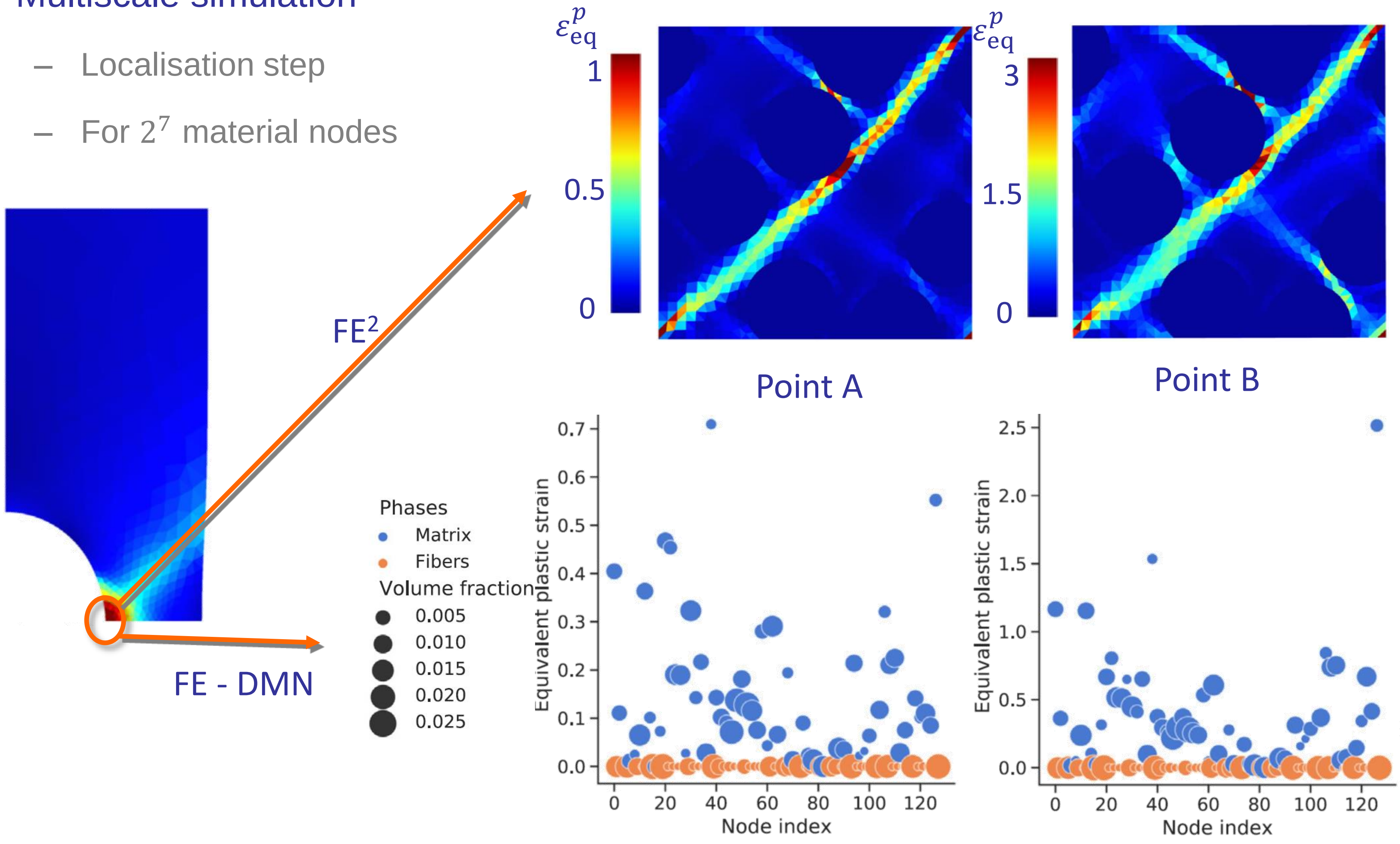
- Multiscale simulation
  - Stress-strain distribution at point B
  - For 2^7 material nodes



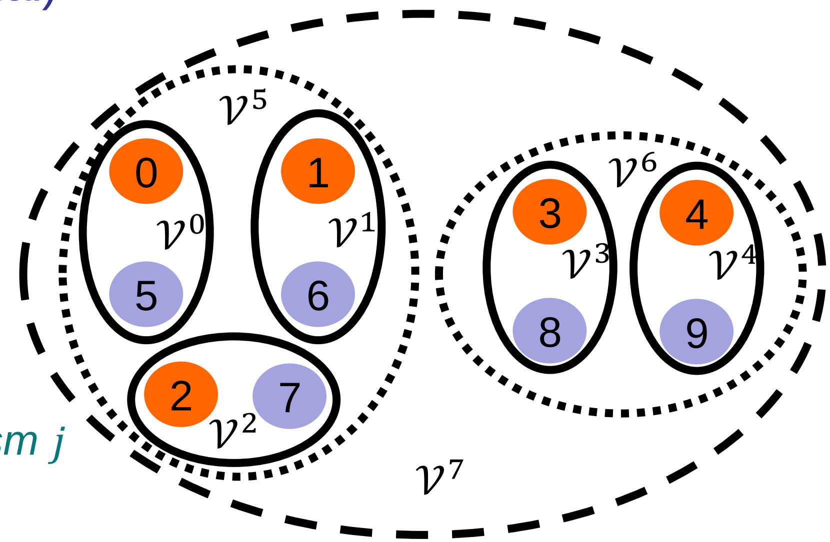


Deep Material Networks with laminate building blocks

- Multiscale simulation
  - Localisation step
  - For 2^7 material nodes



- Alternative to laminate (e.g. for porous material)
- Mechanism $j = 0..M-1$ of interaction $\mathcal{V}^j$



  – Homogenised deformation gradient
    - Construction of a strain fluctuation field

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

Contribution of node i in mechanism j (parameter?)

Degrees of freedom of mechanism j defining the strain fluctuation

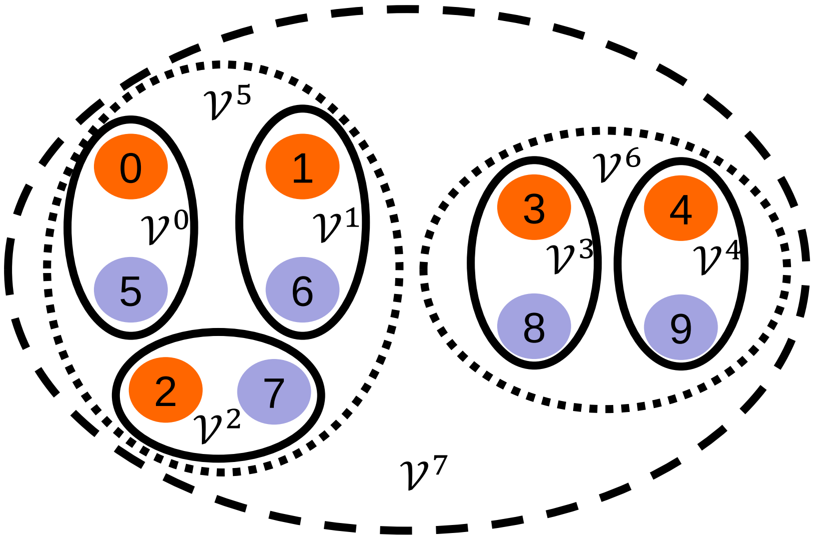
Direction of mechanism j (parameter)

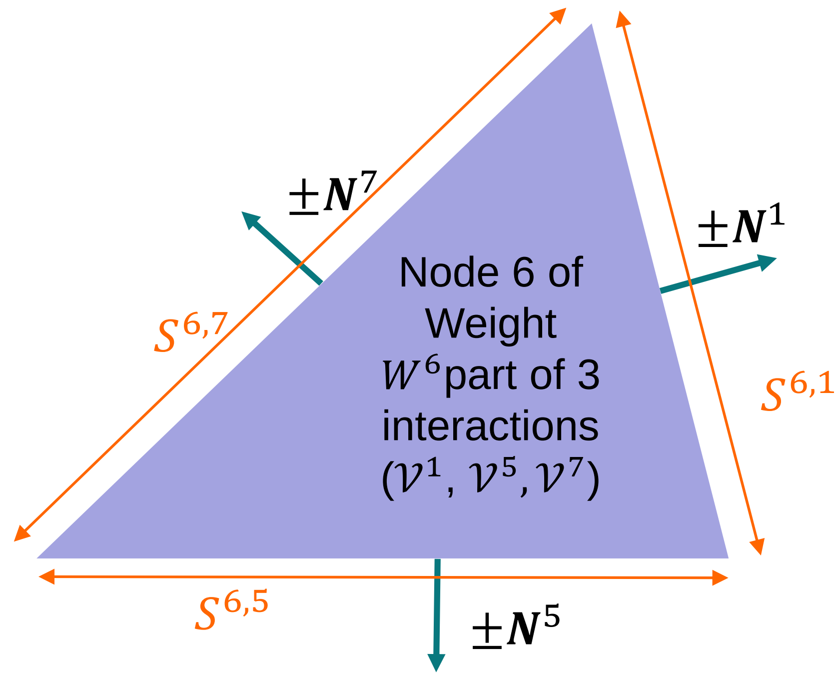
Weight of node i (parameter)

  – Constraints from strain averaging
    - $\overline{\boldsymbol{F}} = \sum_i W^i \boldsymbol{F}^i$ ⇒ $\sum_j \left(\sum_{i\in\mathcal{V}^j} W^i \alpha^{i,j} \right) \boldsymbol{a}^j \otimes \boldsymbol{N}^j = 0$ ⇒ $\sum_{i\in\mathcal{V}^j} W^i \alpha^{i,j} = 0$

  – Weak form from Hill-Mandel
    - $\overline{\boldsymbol{P}} : \delta\overline{\boldsymbol{F}} = \sum_i W^i\, \boldsymbol{P}^i : \delta\boldsymbol{F}^i$ ⇒ $\left[\sum_j \left(\sum_{i\in\mathcal{V}^j} W^i \boldsymbol{P}^i \alpha^{i,j} \right) \cdot \boldsymbol{N}^j \right] \cdot\, \delta\boldsymbol{a}^j = 0$

- Mechanistic building blocks: Polyhedra
  - Interaction $\mathcal{V}^j$, $j = 0..M-1$





  - Fluctuation field
    - Integration by parts on a polyhedron of volume V^i associated to node i

$$\overline{\boldsymbol{F}} + \frac{1}{V^i}\int_{V^i} \mathbf{w} \otimes \nabla \, dV = \boldsymbol{F}^i \quad \Rightarrow \quad \overline{\boldsymbol{F}} + \sum_{j:i\in\mathcal{V}^j} \frac{S^{i,j}}{V^i} \mathbf{w} \otimes (\pm \mathbf{N}^j) = \boldsymbol{F}^i$$

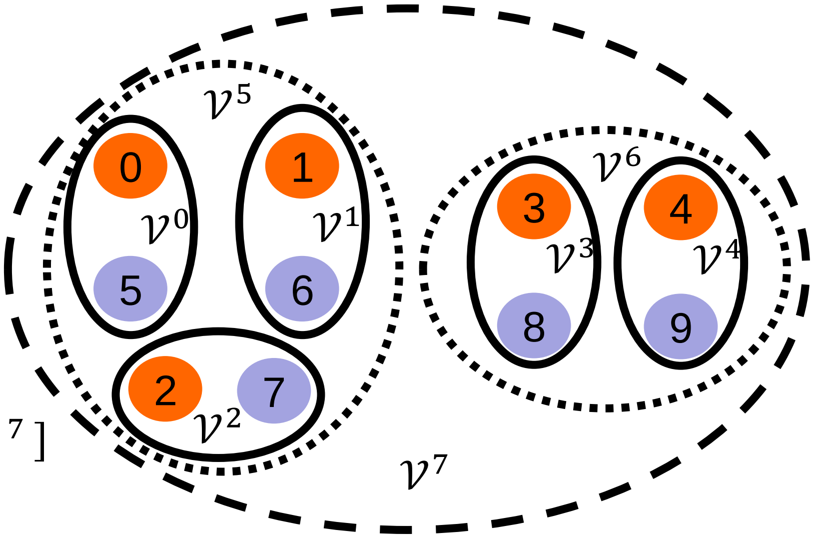
    - To be compared with the interactions $\overline{\boldsymbol{F}} + \sum_{j:i\in\mathcal{V}^j} \alpha^{i,j} \boldsymbol{a}^j \otimes \boldsymbol{N}^j = \boldsymbol{F}^i$, $j = 0..M-1$

⇒
- $\alpha^{i,j}$ is the weighted surface of a polyhedron face (parameter to be identified)
- $\boldsymbol{N}^j$ is the inward or outward normal of the polyhedron face (parameter to be identified)
- $\boldsymbol{a}^j$ is the fluctuation field (degree of freedom for online simulations)

Deep Material Networks from the interactions viewpoint

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

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



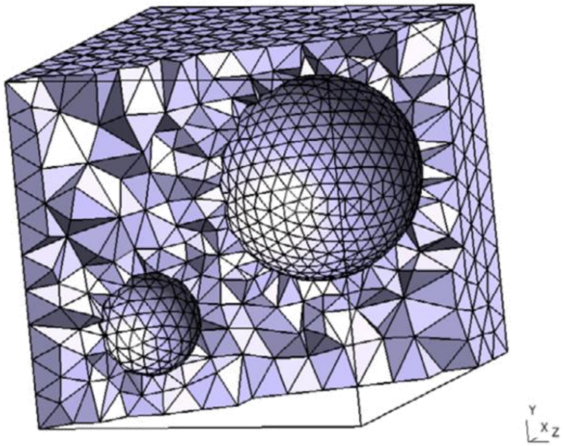
  - Using elastic data
    - Random properties on RVE ⇨ $\hat{\mathbb{C}}(\boldsymbol{\gamma})$

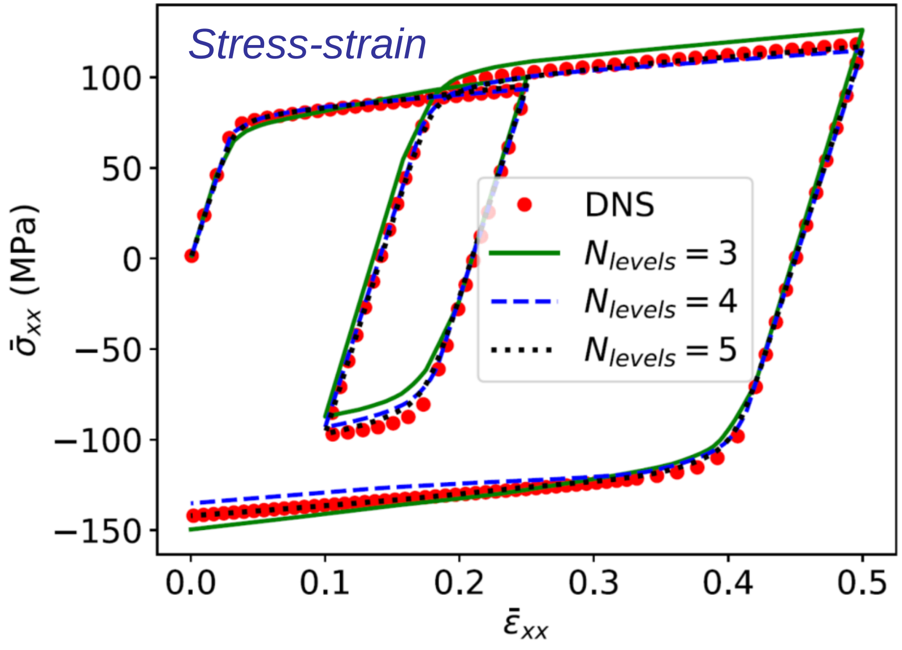
$$\boldsymbol{\gamma} = [E_0,\ \nu_0, E_1,\ \nu_1 \dots E_p,\ \nu_p\ ]$$

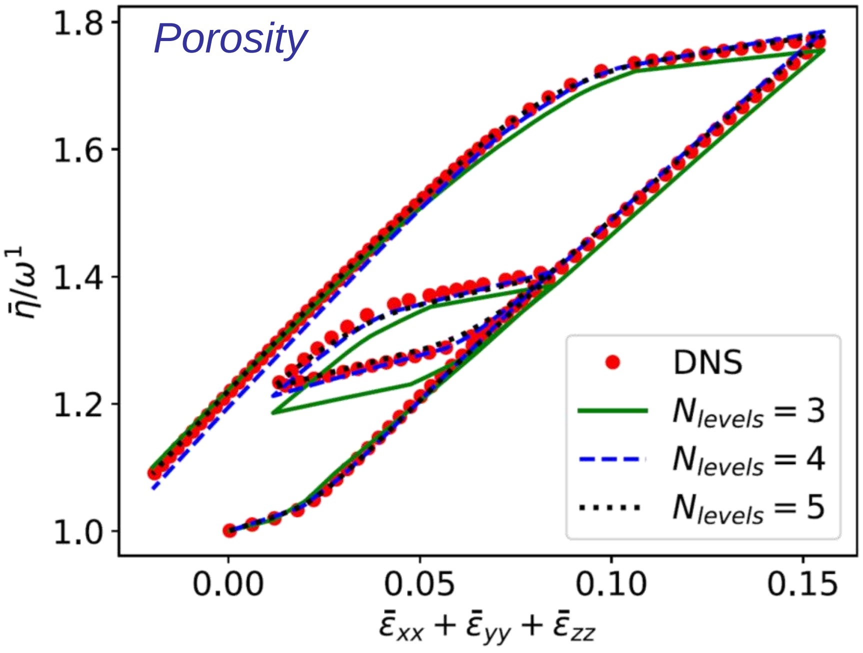
    - Cost functions to minimise $L(\hat{\mathbb{C}},\ \mathbb{C}(\boldsymbol{\chi})) = \frac{1}{n}\sum_{s=1}^{n}\frac{\|\hat{\mathbb{C}}(\boldsymbol{\gamma}_s) - \bar{\mathbb{C}}\ (\boldsymbol{\chi}|\boldsymbol{\gamma}_s)\|}{\|\hat{\mathbb{C}}(\boldsymbol{\gamma}_s)\|}$
  - Using non-linear response
  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

Deep Material Networks from the interactions viewpoint

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

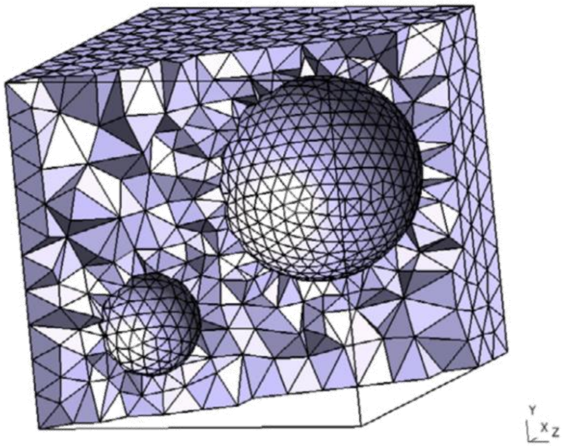


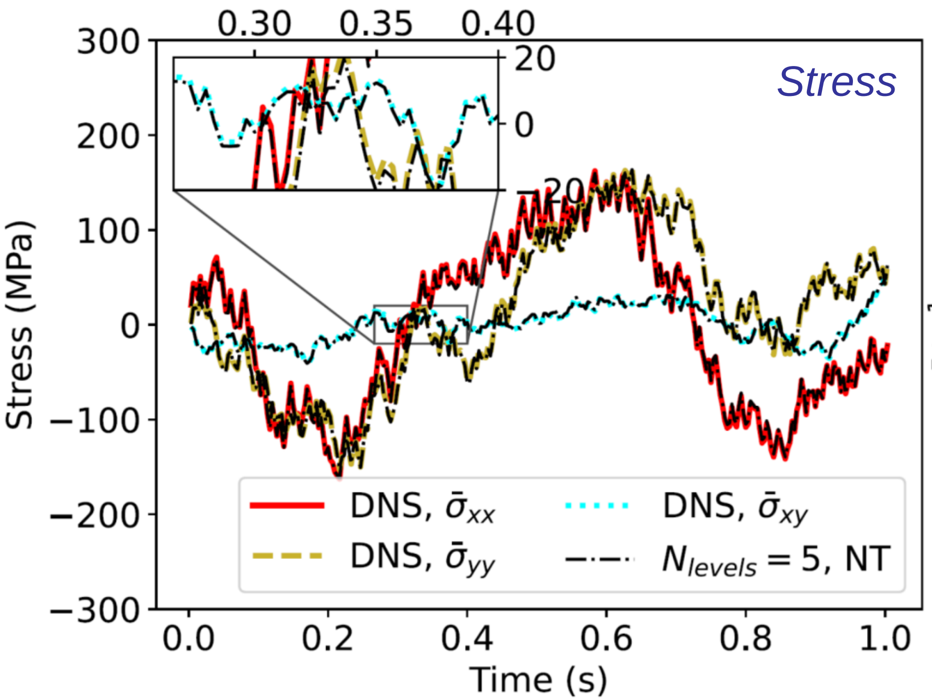


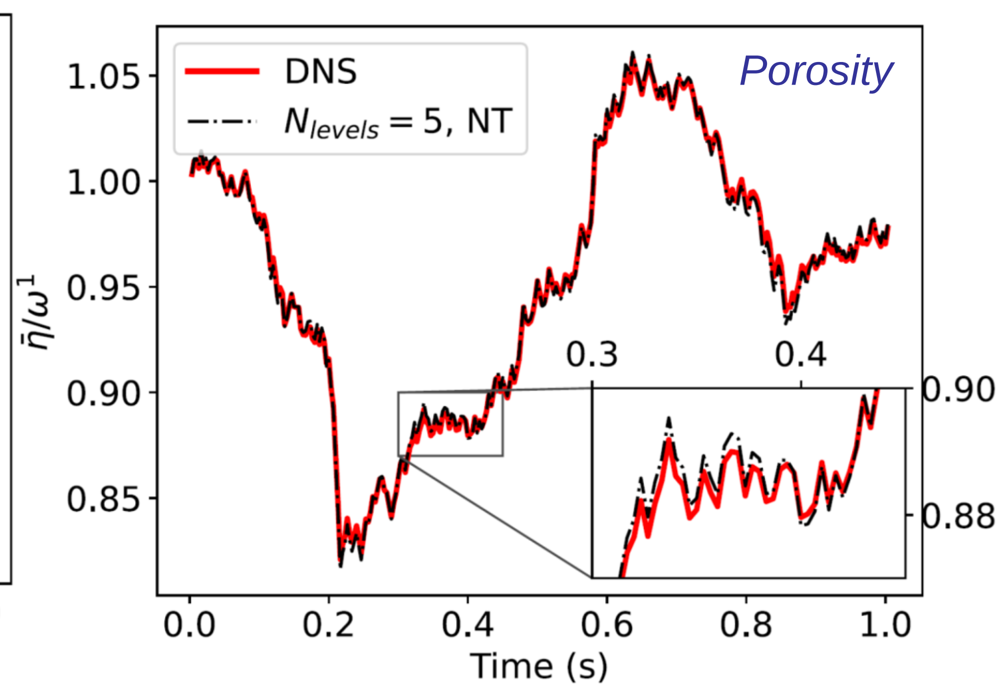


Deep Material Networks from the interactions viewpoint

- Online stage on a porous material
  - Properties
    - Elasto-plastic matrix
    - Small strain
  - Non-linear training with Material 1, on-line Material 2
  - Random loading

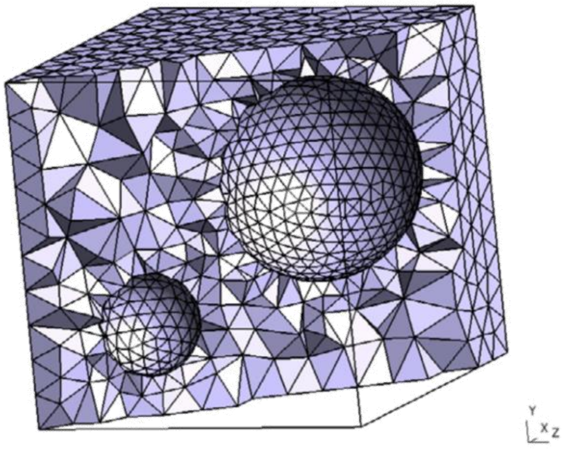


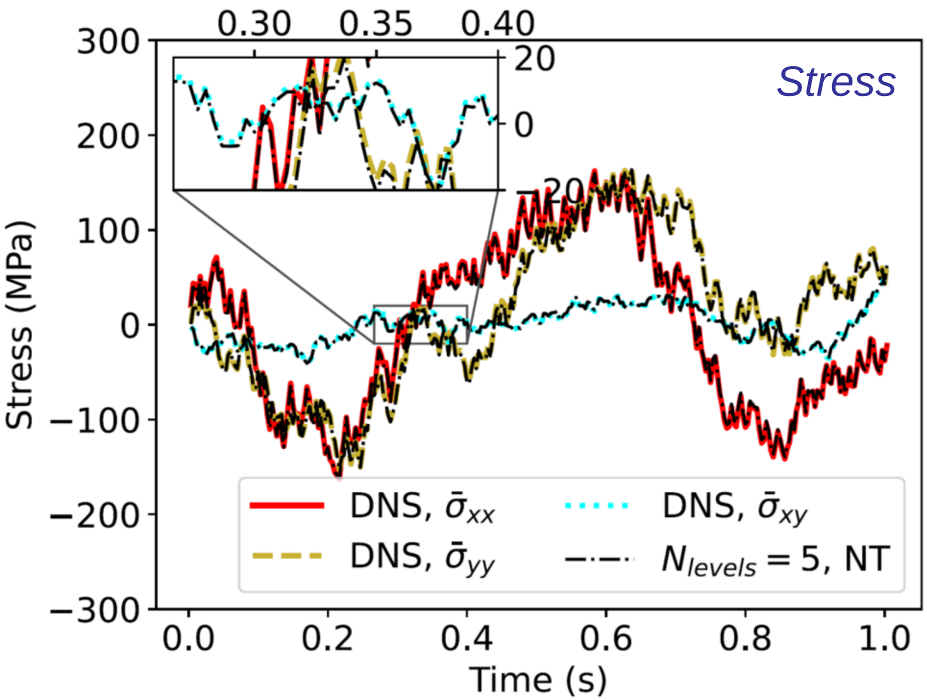


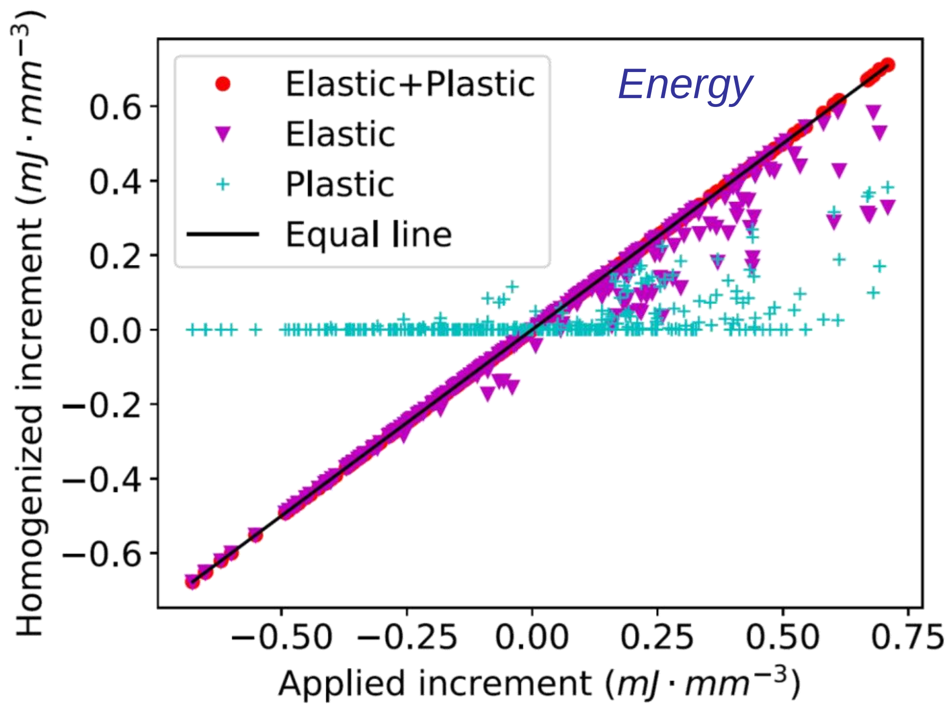


Deep Material Networks from the interactions viewpoint

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



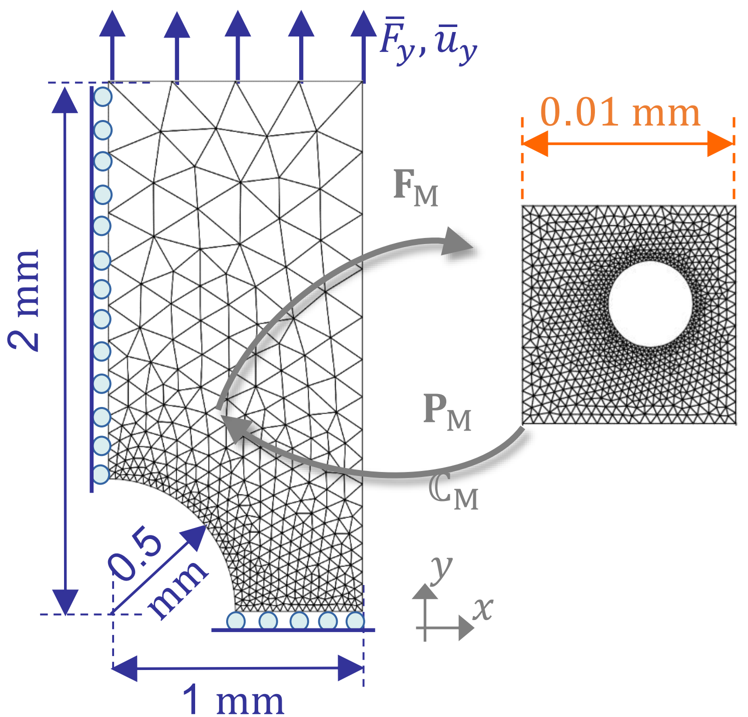


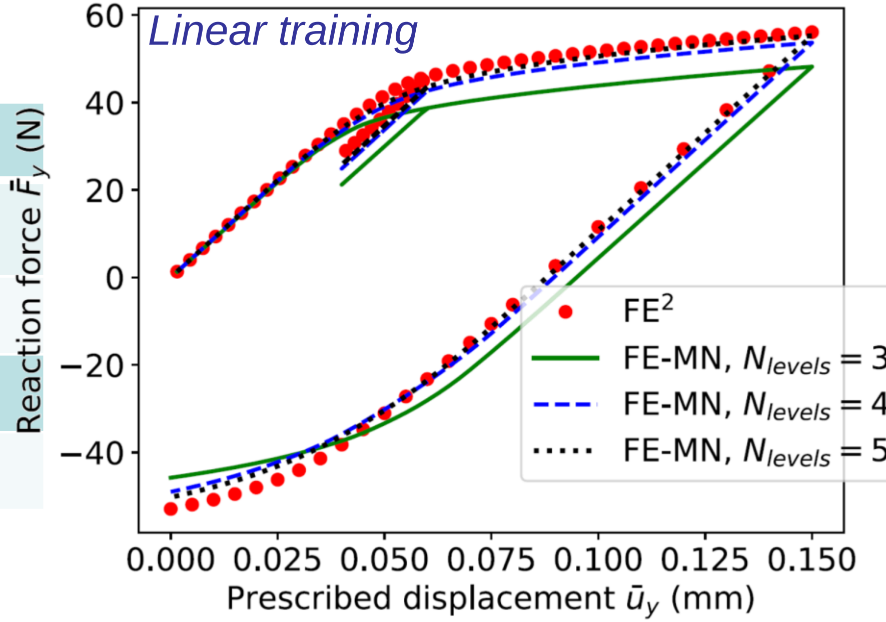


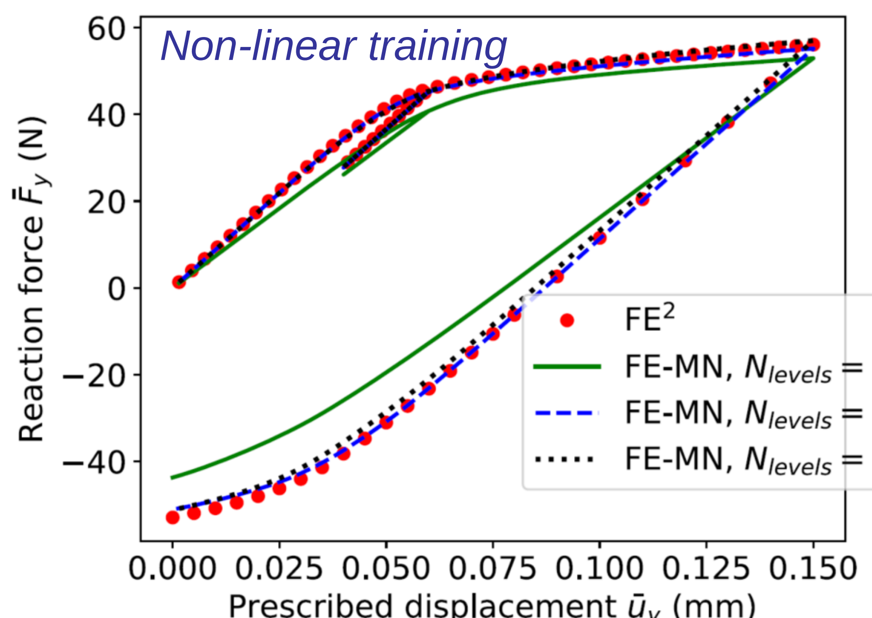
Deep Material Networks from the interactions viewpoint

- Multiscale simulation

Off-line	FE²	FE-DMN
Data generation	-	0.04 (linear) – 3.5 (non-linear) hour.-cpu
Training	-	0.16-20 hours.-cpu
On-line	**FE²**	**FE-DMN**
Simulation	7200 h-cpu	0.1 to 1 h-cpu

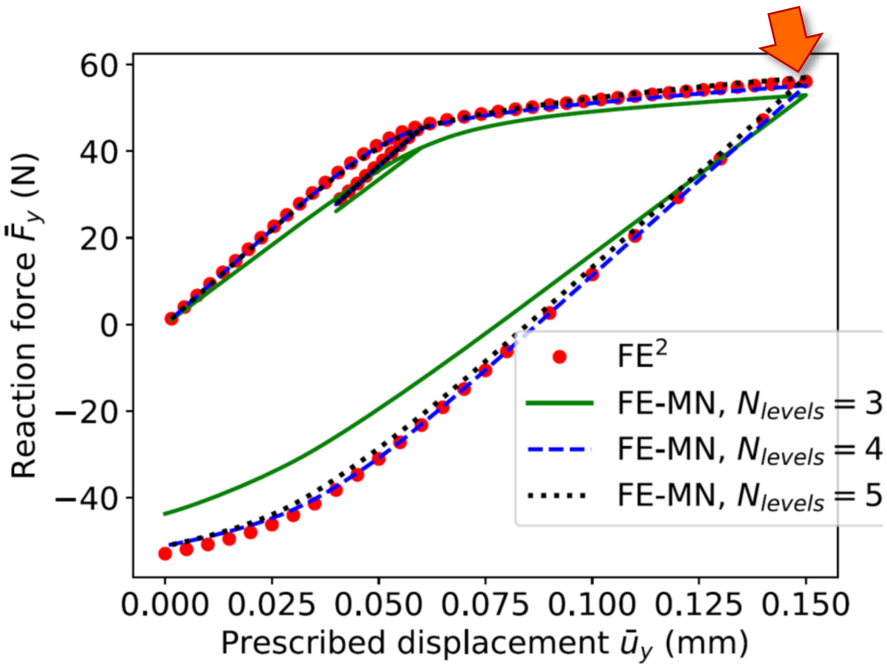


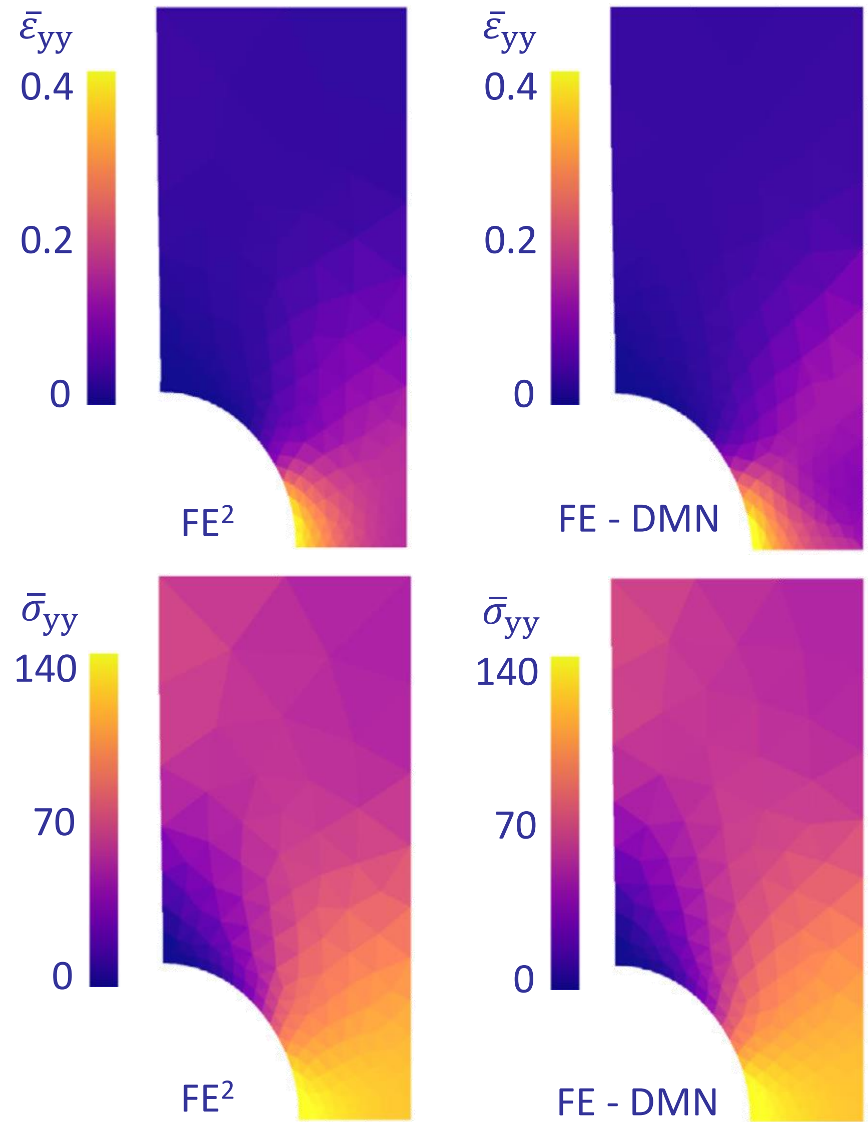




Deep Material Networks from the interactions viewpoint

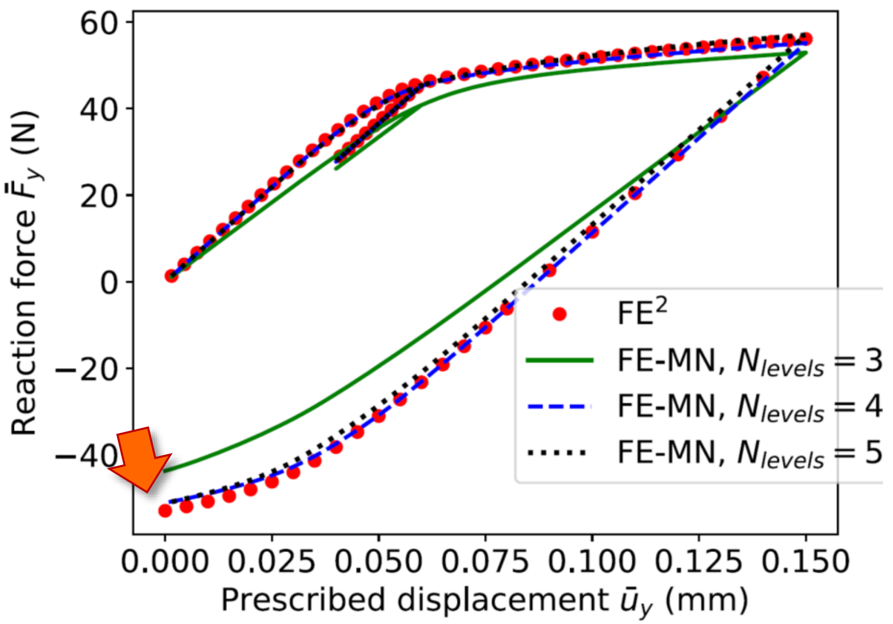
- Multiscale simulation
  - Stress-strain distribution at point A
  - For 2^5 material nodes
  - Non-linear training

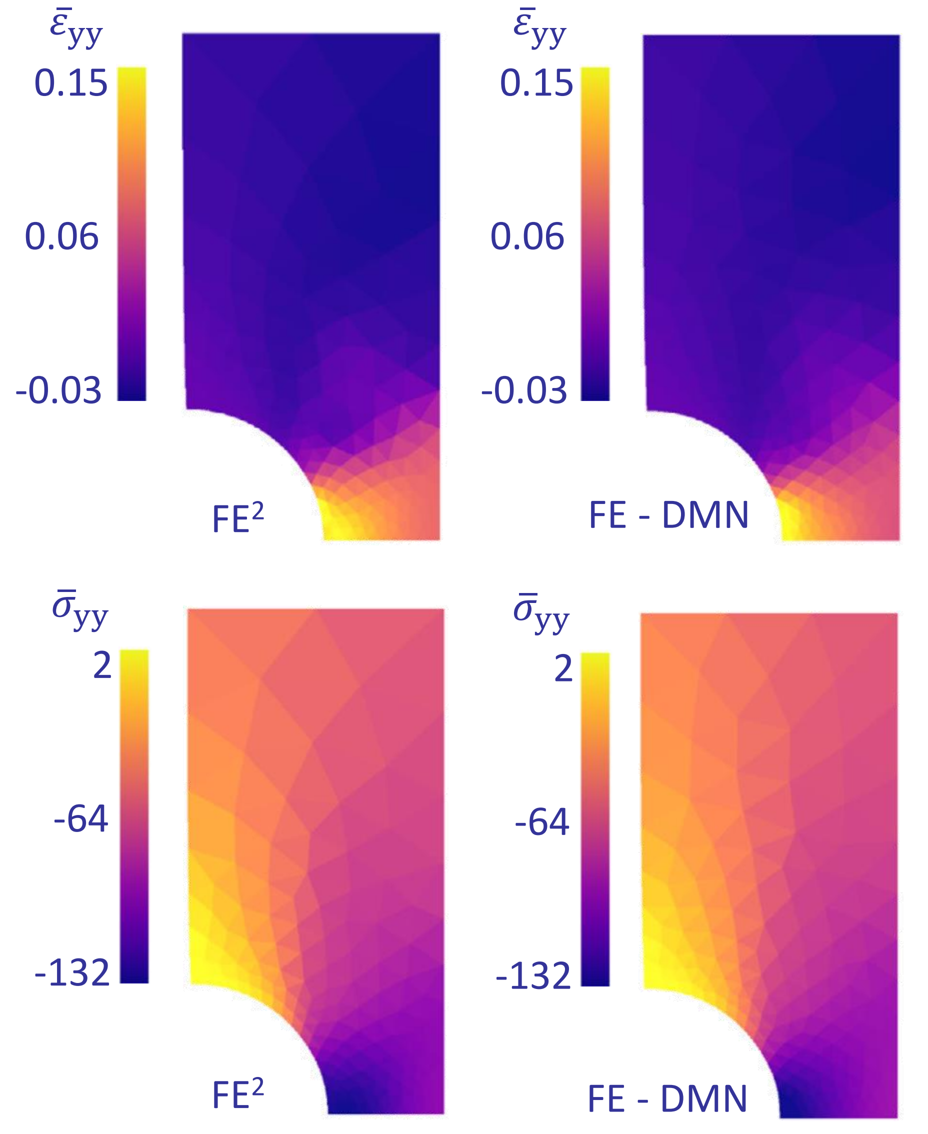




Deep Material Networks from the interactions viewpoint

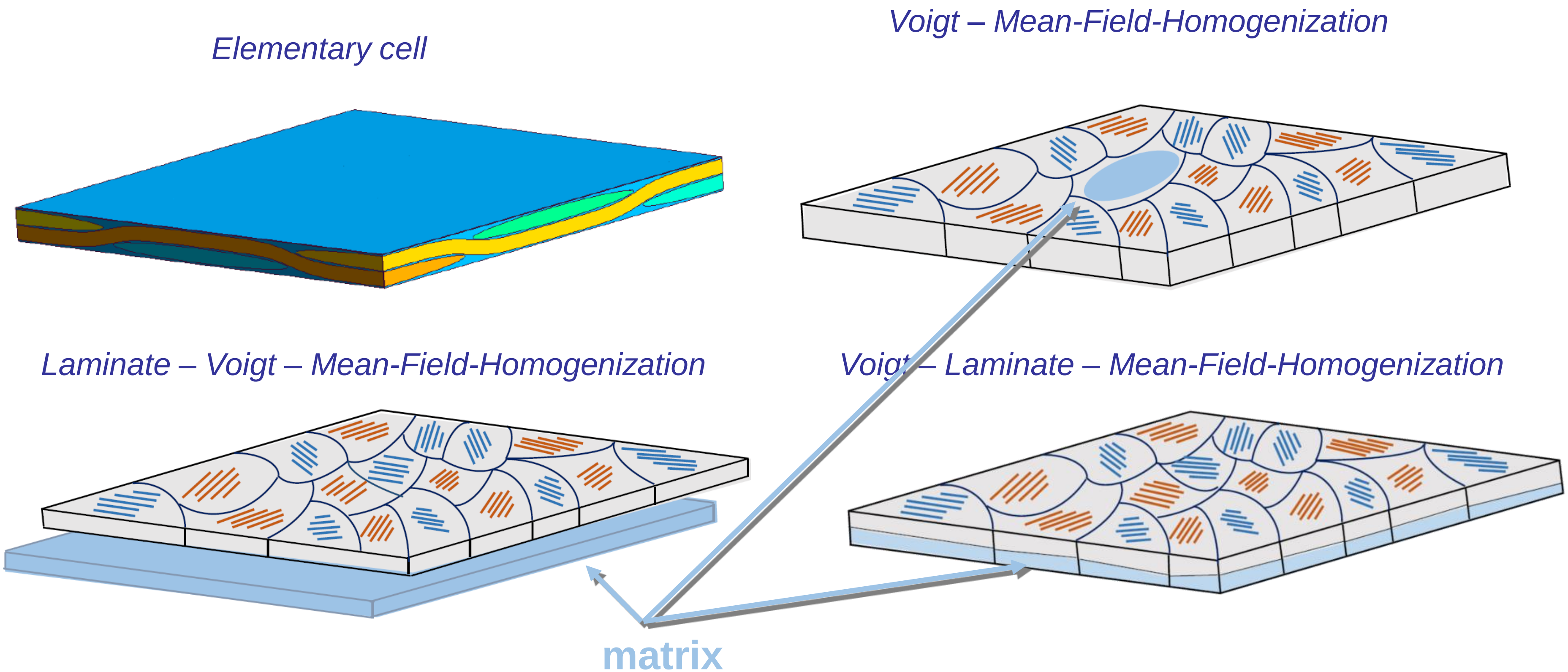
- Multiscale simulation
  - Stress-strain distribution at point B
  - For 2^5 material nodes
  - Non-linear training





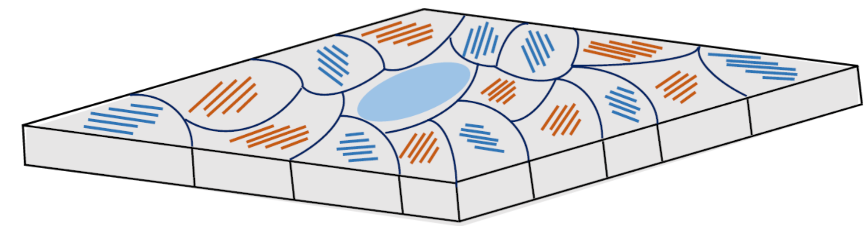
Mean-Field-Based Deep Material Networks for woven composites

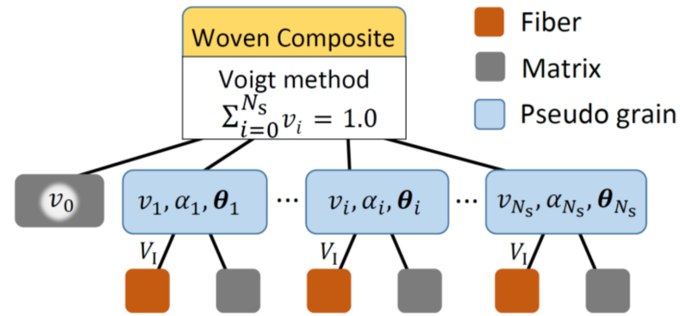
- Definition of 3 Reduced-order-models
- Using simple micro-mechanistic grains
  - MFH (short fibre-reinforced matrix)
  - Voigt mixture
  - Laminate theory



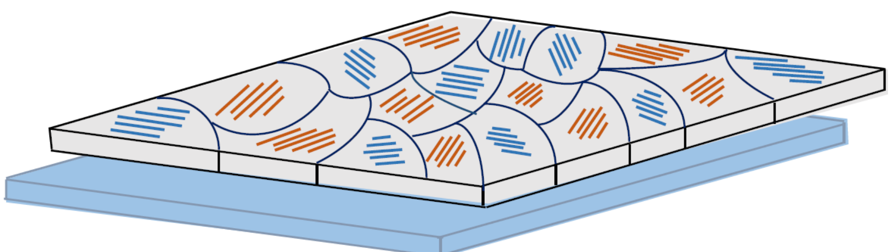
Mean-Field-Based Deep Material Networks for woven composites

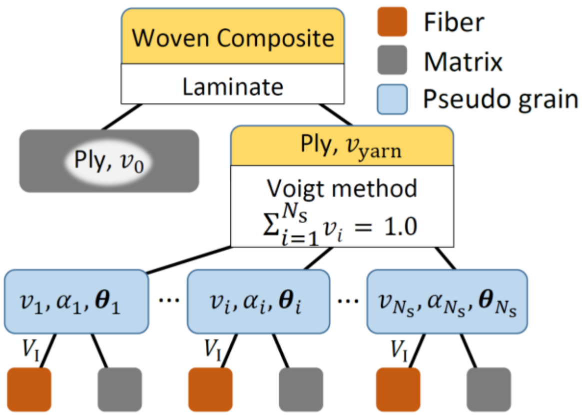
- Definition of material networks



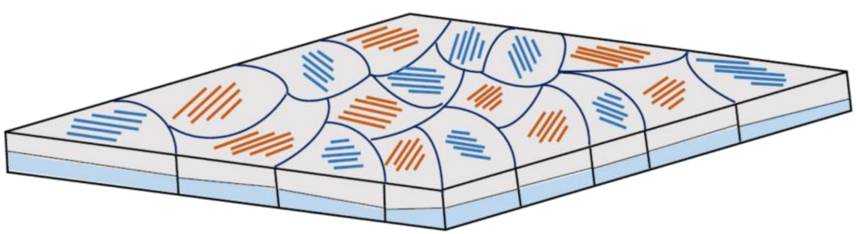


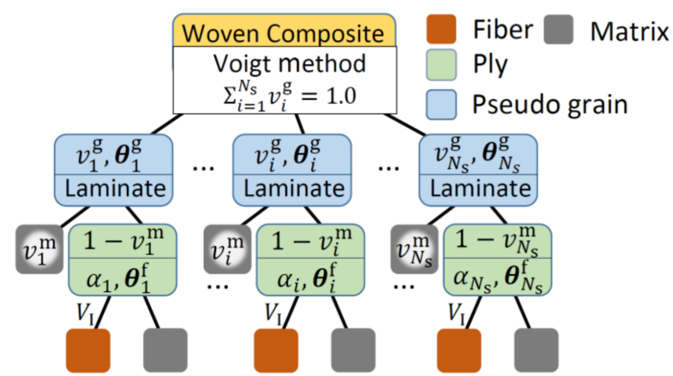
$$\chi^{\mathrm{VM}} = \left\{ v_i,\, \boldsymbol{\theta}_i,\, \alpha_i \mid i = 1, \ldots, N_S;\ \sum_{i=1}^{N_S} v_i = 1.0 - v_0 \right\}$$





$$\chi^{\mathrm{LVM}} = \left\{ v_i,\, \boldsymbol{\theta}_i,\, \alpha_i \mid i = 1, \ldots, N_S;\ \sum_{i=1}^{N_S} v_i = 1.0 \right\}$$





$$\chi^{\mathrm{VLM}} = \left\{ v_i^{\mathrm{g}},\, \boldsymbol{\theta}_i^{\mathrm{g}},\, v_i^{\mathrm{m}},\, \boldsymbol{\theta}_i^{\mathrm{f}},\, \alpha_i \mid i = 1, \ldots, N_S;\ \sum_{i=1}^{N_S} v_i^{\mathrm{g}} = 1.0;\ \sum_{i=1}^{N_S} v_i^{\mathrm{g}} v_i^{\mathrm{m}} = v_0 \right\}$$

- Identification of topological parameters from direct simulations
  - Parameters:

$$\chi^{\mathrm{VM}} = \left\{ v_i,\, \boldsymbol{\theta}_i,\, \alpha_i \mid i = 1, \dots, N_S;\ \sum_{i=1}^{N_S} v_i = 1.0 - v_0 \right\}$$

$$\chi^{\mathrm{LVM}} = \left\{ v_i,\, \boldsymbol{\theta}_i,\, \alpha_i \mid i = 1, \dots, N_S;\ \sum_{i=1}^{N_S} v_i = 1.0 \right\}$$

$$\chi^{\mathrm{VLM}} = \left\{ v_i^{\mathrm{g}},\, \boldsymbol{\theta}_i^{\mathrm{g}},\, v_i^{\mathrm{m}},\, \boldsymbol{\theta}_i^{\mathrm{f}},\, \alpha_i \mid i = 1, \dots, N_S;\ \sum_{i=1}^{N_S} v_i^{\mathrm{g}} = 1.0;\ \sum_{i=1}^{N_S} v_i^{\mathrm{g}} v_i^{\mathrm{m}} = v_0 \right\}$$

Constraints

  - Using elastic data
    - Random properties on RVE

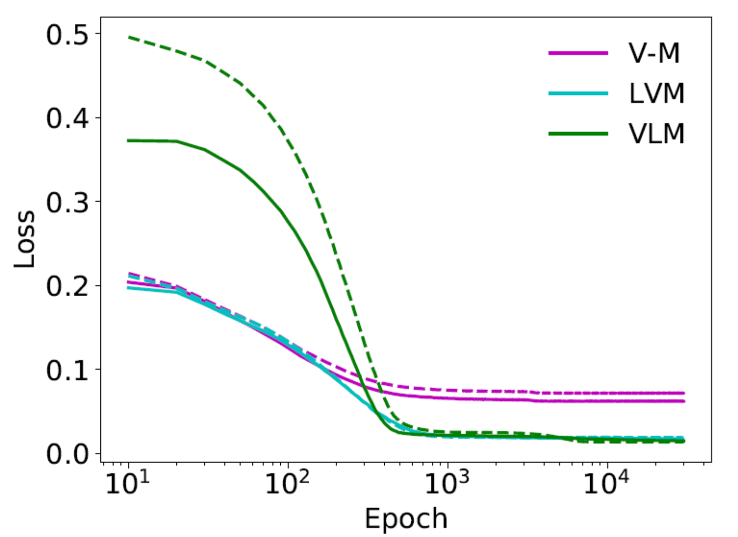
$$\boldsymbol{\gamma} = \left[E_0,\, \nu_0,\, E_{\mathrm{I}}^{\mathrm{T}},\, E_{\mathrm{I}}^{\mathrm{L}},\, \nu_{\mathrm{I}}^{\mathrm{LT}},\, \nu_{\mathrm{I}}^{\mathrm{TT}},\, G_{\mathrm{I}}^{\mathrm{LT}},\, V_{\mathrm{I}}\right]$$

→ Direct simulations on RVE

    - Cost functions to minimise

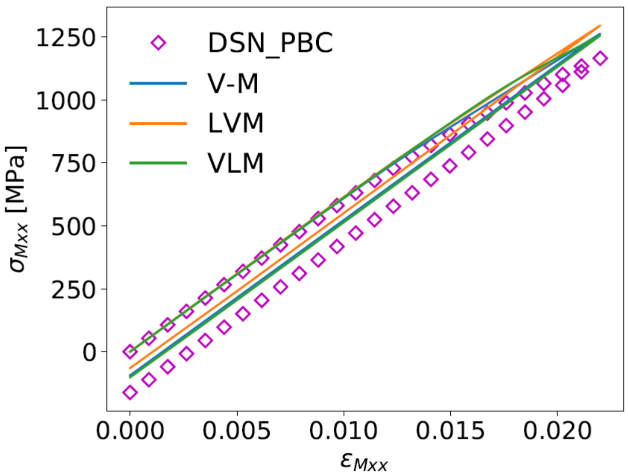
$$L(\hat{\mathbb{C}}, \mathbb{C}(\boldsymbol{\chi})) = \frac{1}{n}\sum_{s=1}^{n} \frac{\|\hat{\mathbb{C}}(\boldsymbol{\gamma}_s) - \mathbb{C}(\boldsymbol{\chi}|\boldsymbol{\gamma}_s)\|}{\|\hat{\mathbb{C}}(\boldsymbol{\gamma}_s)\|} + \frac{\lambda}{2} G(\boldsymbol{\chi})$$

    - « stochastic gradient descent (SGD) » algorithm

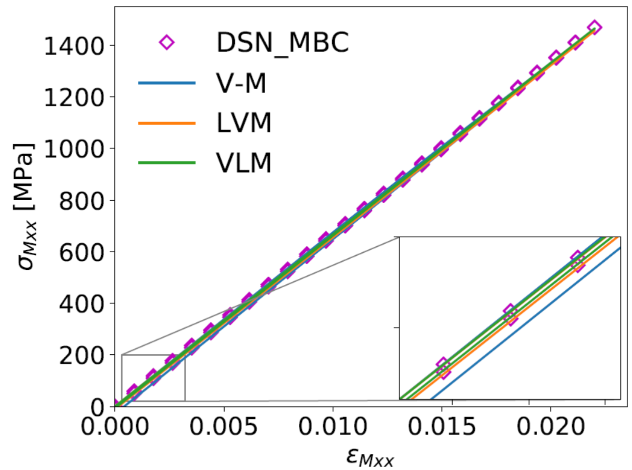


- Elasto-plastic matrix case

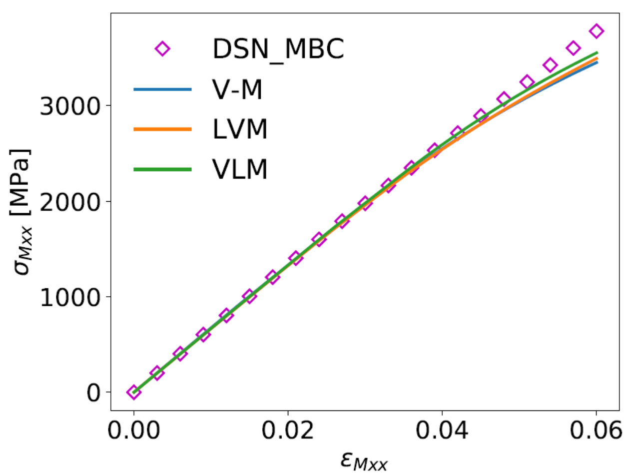
PBC tension cyclique



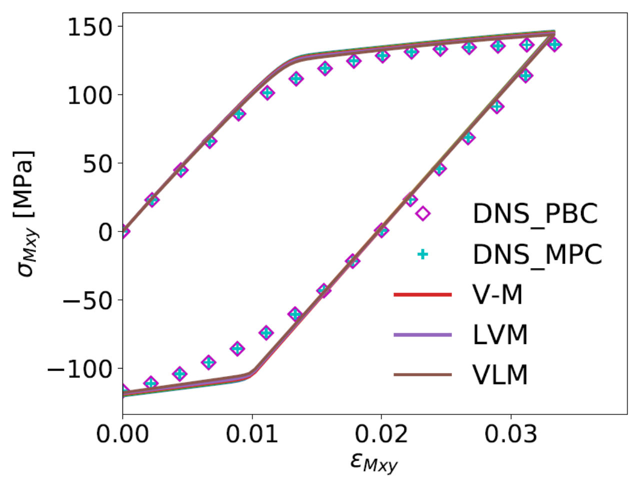
MBC tension cyclique



MBC tension



Cisaillement



Mean-Field-Based Deep Material Networks for woven composites

- Publications (doi)
  - 10.1016/j.cma.2021.114300
    - Open data
  - 10.1016/j.euromechsol.2021.104384
    - Open data
  - 10.1016/j.compstruct.2021.114058
    - Open data