Efficient surrogate models for microstructured materials based on interaction-based material networks

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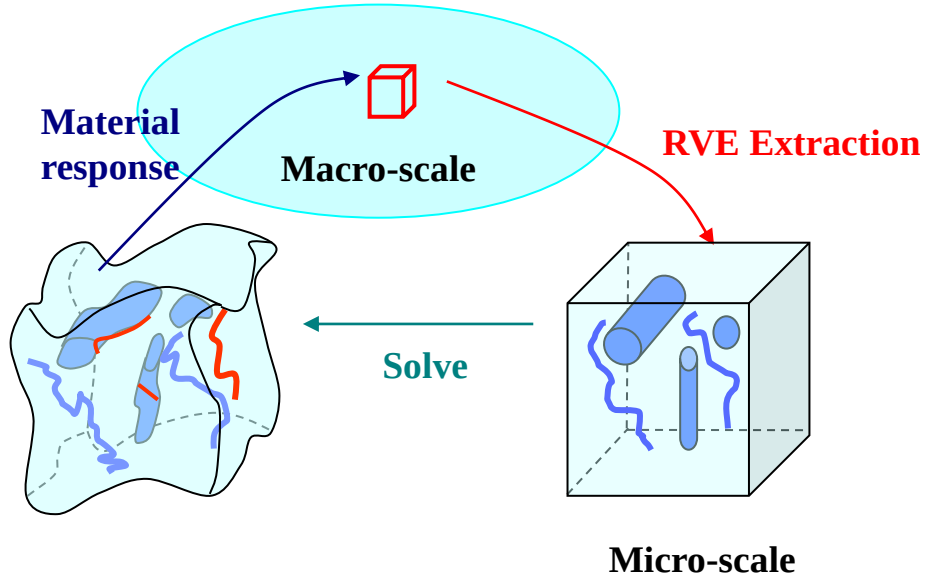
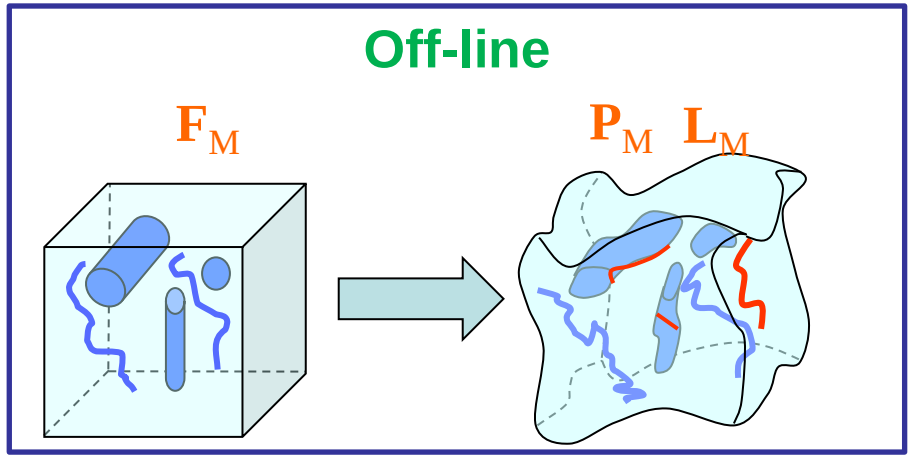
Introduction

- Computational homogenization (**FE^2**)
  - Microstructured materials
  - Two problems are solved concurrently:
    - Macro-scale: seen as a continuum
    - Micro-scale: Representative Volume Element (**RVE**)
- Advantage
  - Account directly for the micro–structural parameters (microstructure, constitutive behavior) with high accuracy.
- Drawback
  - Computational time & memory:
- Solution
  - Surrogate model of the microscopic BVP

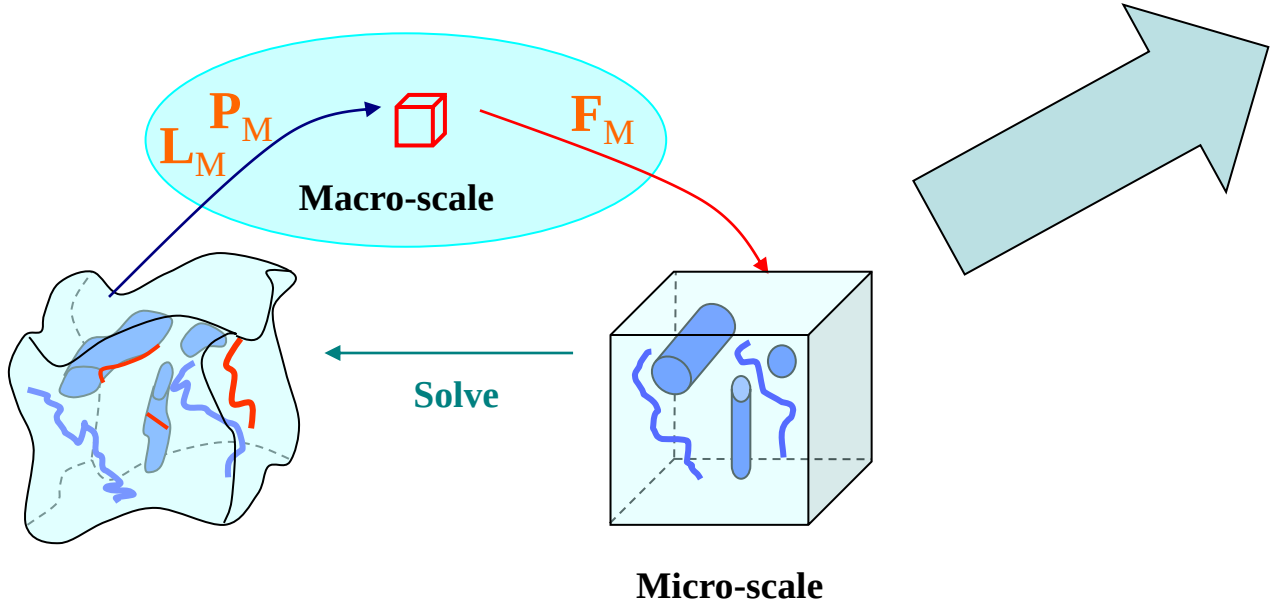


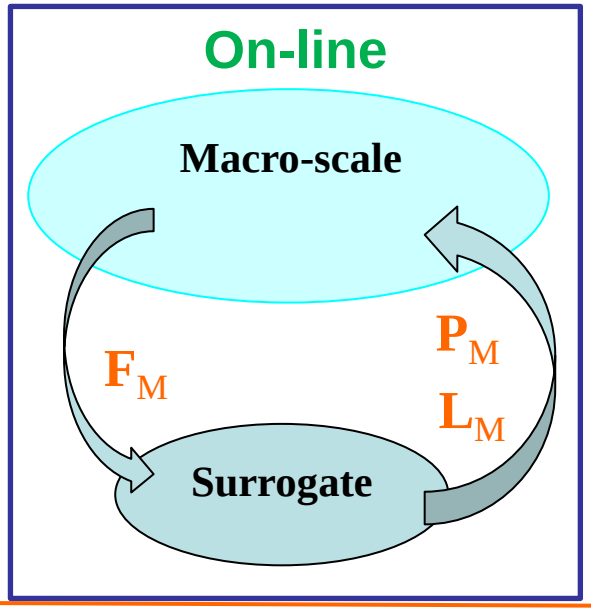
Introduction

- Surrogate model of the microscopic BVP
  - Define a surrogate model
  - Off-line:
    - Construct off-line data-base (using RVE simulations)
    - Train surrogate model
  - On-line:
    - Use the trained surrogate model during analyses



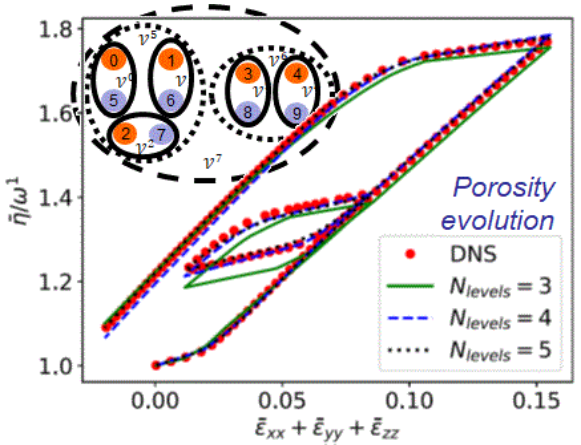
Trained





Deep material networks

- Based on thermodynamic consistency
- Possesses extrapolation capabilities in
  - Strain (history): $\mathbf{F}_{\mathrm{M}}$
  - Material parameters: $\boldsymbol{\gamma}_{\mathrm{m}}$

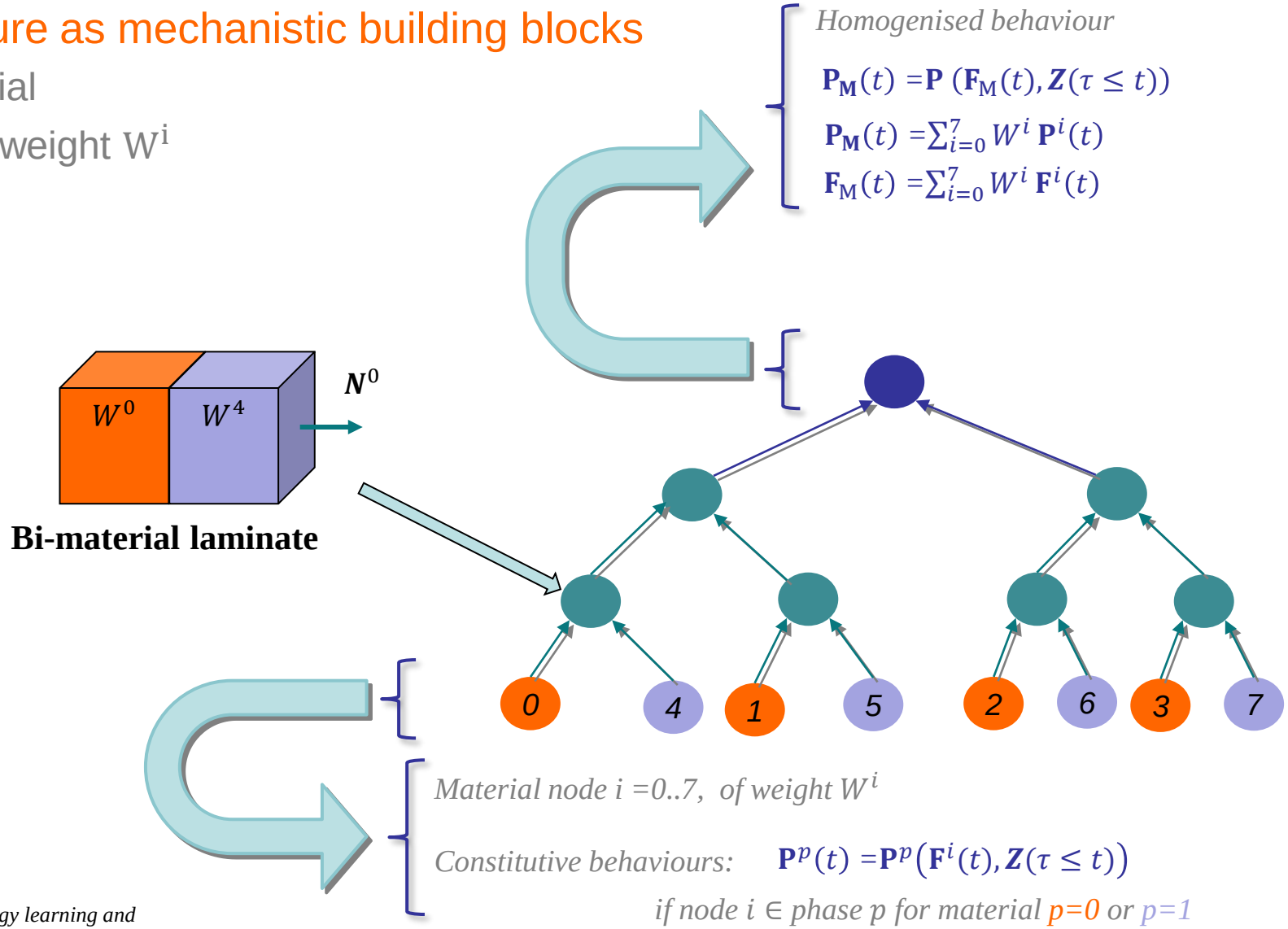


- Emerging methodology
  - Seminal work
    - Liu, Wu, Koishi, (2019). A deep material network for multiscale topology learning and accelerated nonlinear modeling of heterogeneous materials. CMAME
  - Reformulation and use as surrogate for arbitrary material law
    - Gajek, Schneider, Böhlke, (2021). An FE–DMN method for the multiscale analysis of short fiber reinforced plastic components. CMAME
    - Nguyen V.-D., Noels, L. (2022). Interaction-based material network: A general framework for (porous) microstructured materials. CMAME

Deep material networks

- Bi-material laminate architecture as mechanistic building blocks
  - Example for a 2-phase material
  - Material node i =0,...,N-1, of weight W^i

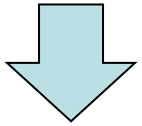
$$\sum_i W^i = 1$$



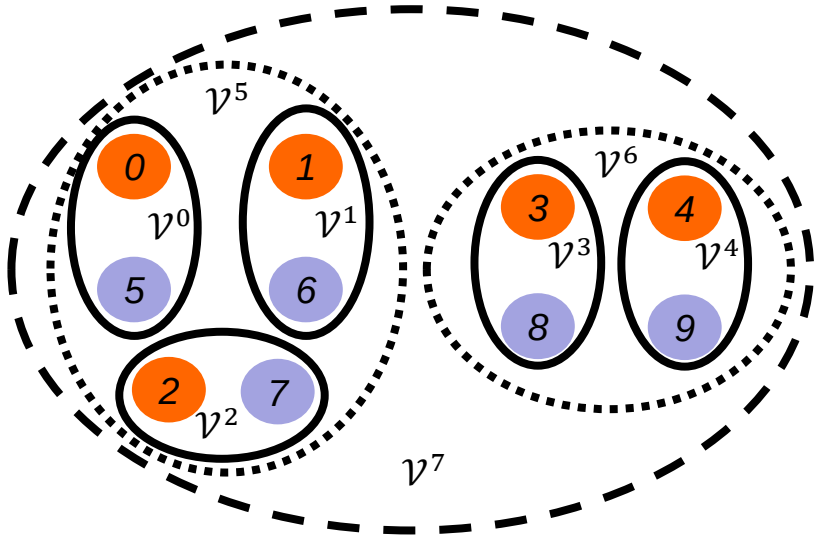
Z. Liu, C. Wu, M. Koishi, A deep material network for multiscale topology learning and accelerated nonlinear modeling of heterogeneous materials

Deep material networks

- Our contributions
  - The solution is provided under a closed form, which is equivalent to the weak form in the finite element method
  - Material networks are revisited with interactions



  - Interaction-based material network:
    - A network of **interaction mechanisms**
    - General framework for (porous) microstructured materials



Material nodes are linked through **interactions**

- *Nguyen, V. D., & Noels, L. (2022). Micromechanics-based material networks revisited from the interaction viewpoint; robust and efficient implementation for multi-phase composites. European Journal of Mechanics - A/Solids.*
- *Nguyen V.-D., Noels, L. (2022). Interaction-based material network: A general framework for (porous) microstructured materials. CMAME*

Interaction-based material networks – interactions & closed form solution

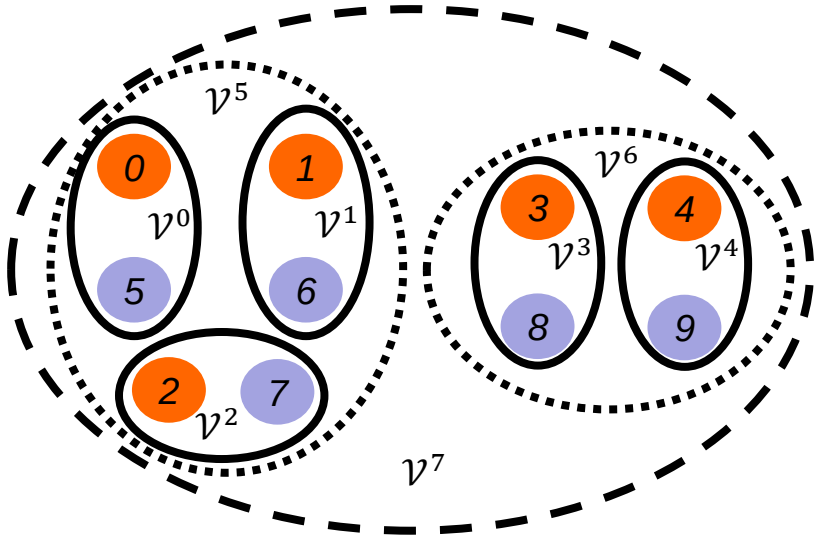
- Link homogenised deformation gradient to nodes
  - Interaction $k = 0..M-1$

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

*Contribution of node i in **interaction** k (parameter?)*

Degrees of freedom of interaction k defining the strain fluctuation

*Direction of **interaction** k (parameter)*



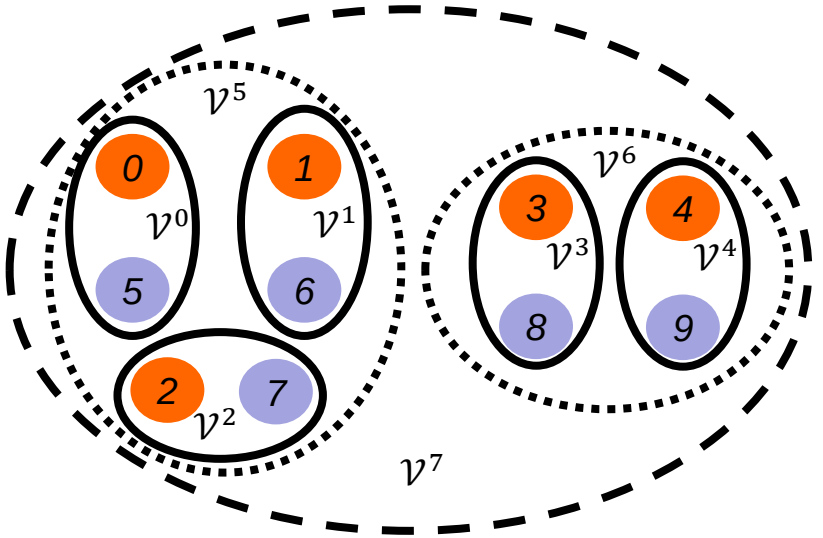
A material network

- **10 material nodes**
- **8 interactions**

Interaction-based material networks – interactions & closed form solution

- Link homogenised deformation gradient to nodes
  - Interaction $k = 0..M-1$

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



- Constraints from strain averaging

$$\mathbf{F}_\mathrm{M} = \sum_i W^i \mathbf{F}^i \;\Rightarrow\; \sum_k \left(\sum_i W^i \alpha^{i,k} \right) \boldsymbol{a}^k \otimes \boldsymbol{G}^k = 0 \;\Rightarrow\; \underbrace{\sum_i W^i \alpha^{i,k} = 0}$$

*Constraint to be satisfied in **interaction** k*

- Weak form from Hill-Mandel

$$\mathbf{P}_\mathrm{M} : \delta\mathbf{F}_\mathrm{M} = \sum_i W^i\, \mathbf{P}^i : \delta\mathbf{F}^i \;\Rightarrow\; \left[\sum_k \left(\sum_i W^i \mathbf{P}^i \alpha^{i,k} \right) \cdot \boldsymbol{G}^k \right] \cdot\, \delta\boldsymbol{a}^k = 0 \;\Rightarrow\; \sum_k \left(\sum_i W^i \mathbf{P}^i \alpha^{i,k} \right) \cdot \boldsymbol{G}^k = \mathbf{0}$$

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

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

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

- Homogenized stress from stress averaging

$$\boldsymbol{P}_\mathrm{M} = \sum_i W^i \boldsymbol{P}^i$$

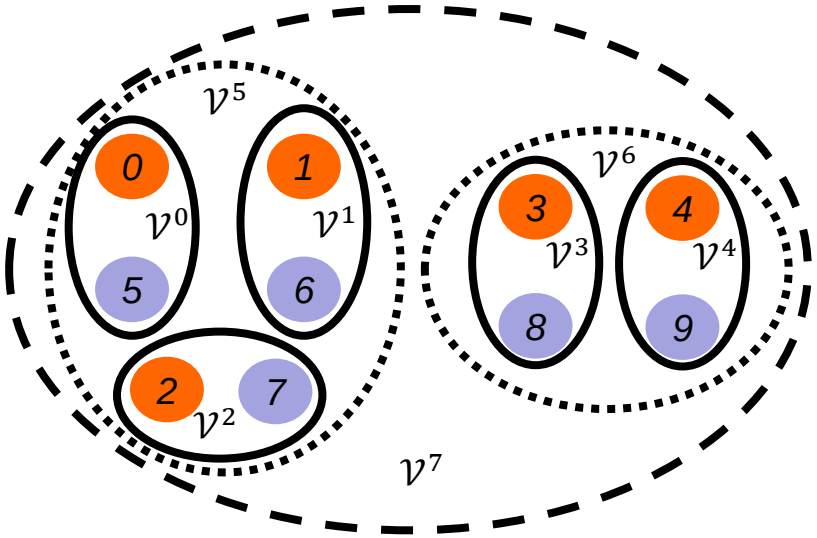
Interaction-based material network – interactions

- How to define an interaction?
  - For an interaction k

$$\sum_i W^i \alpha^{i,k} = 0$$

  - Each interaction includes several nodes
    - $\alpha^{i,k} = 0$ if node i does not participate the interaction k

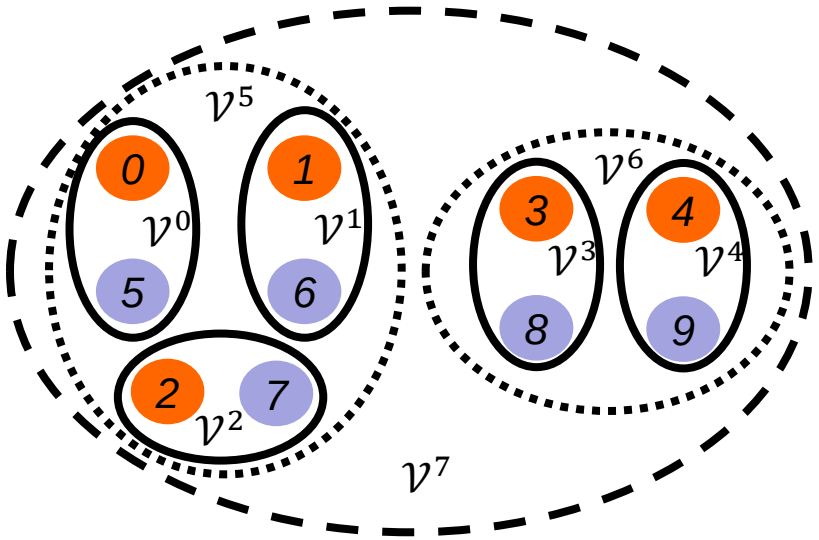
- Network architecture
  - A set of material nodes
  - A set of network interactions

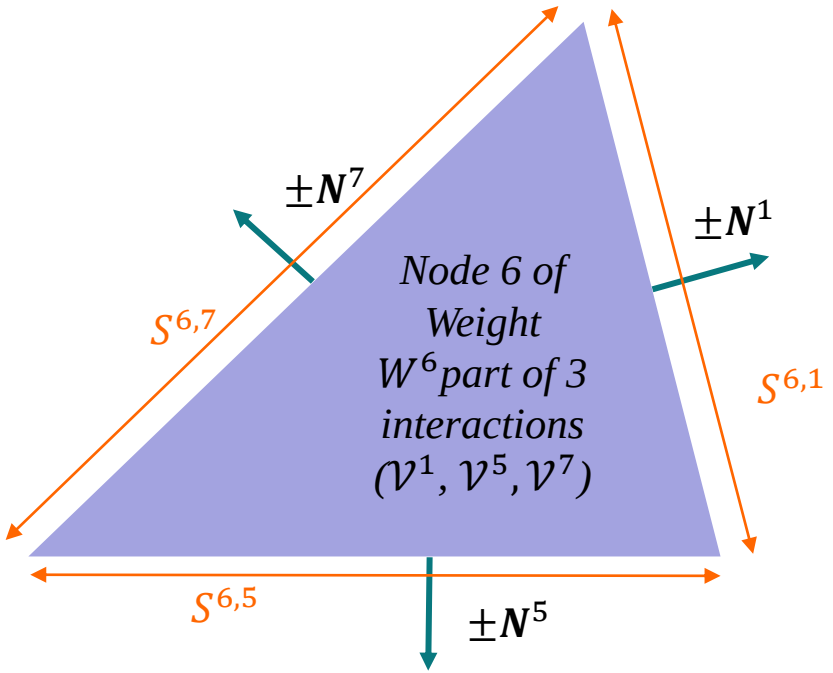


A material network
- **10 material nodes**
- **8 interactions**

Interaction-based material networks – interactions

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





  - Fluctuation field: $\mathbf{w} = \mathbf{x} - \mathbf{F}_M \cdot \boldsymbol{X}$
    - Integration by parts on a polyhedron of volume V^i associated to node i

$$\mathbf{F}_M + \frac{1}{V^i}\int_{V^i} \mathbf{w} \otimes \nabla_0 \, dV = \mathbf{F}^i \quad \Rightarrow \quad \mathbf{F}_M + \sum_{j:i\in\mathcal{V}^j} \frac{S^{i,j}}{V^i} \mathbf{w} \otimes (\pm \mathbf{N}^j) = \mathbf{F}^i$$

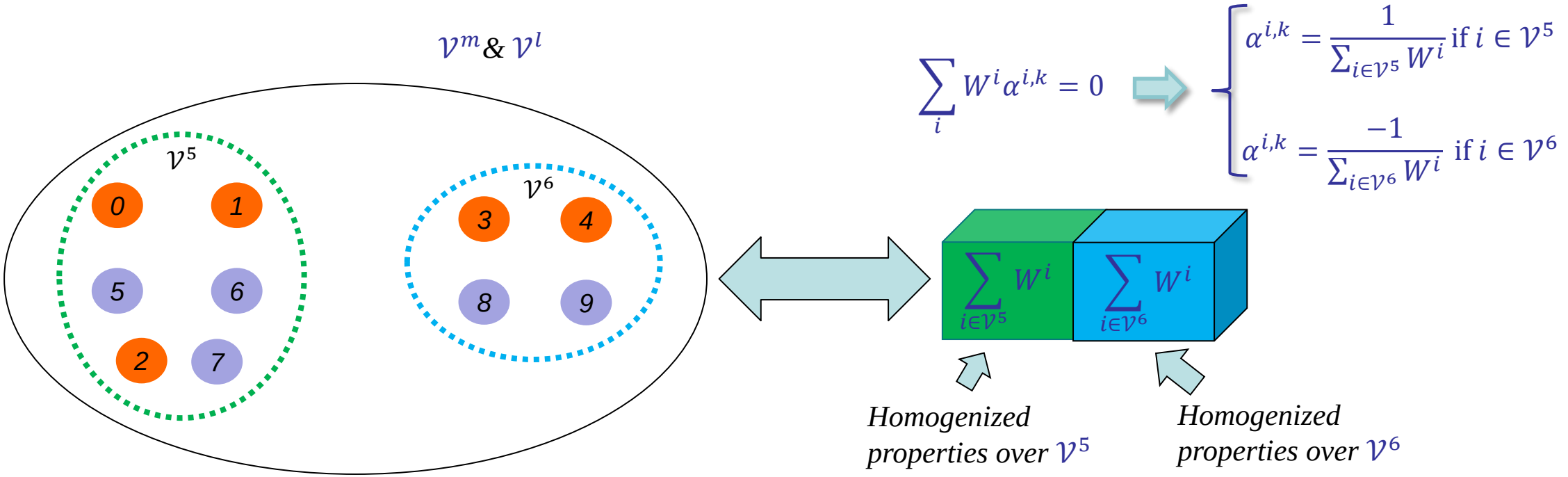
    - To be compared with the interactions

$$\mathbf{F}_M + \sum_{k=0}^{M-1} \alpha^{i,k} \, \boldsymbol{a}^k \otimes \boldsymbol{G}^k = \mathbf{F}^i$$

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

Interaction-based material network – interactions

- Mechanistic building blocks: we can recover laminate building blocks
  - Between two groups of nodes



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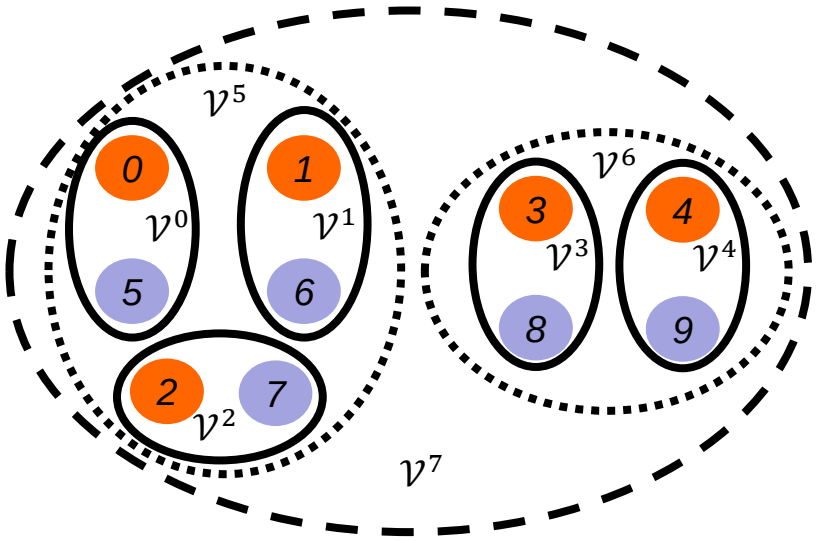
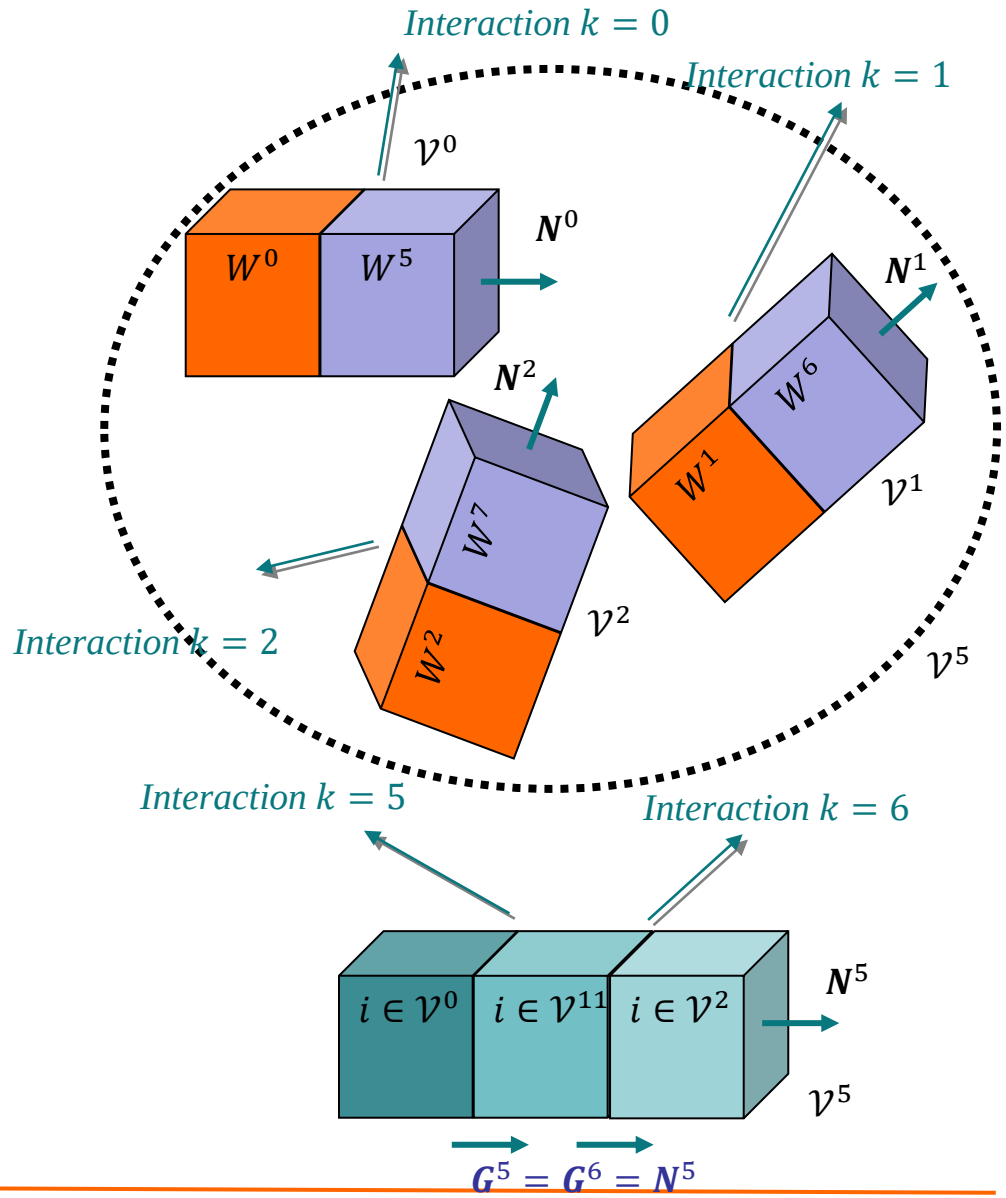
Interaction-based material network – interactions

- Mechanistic building blocks: Laminate





Trainable parameters:

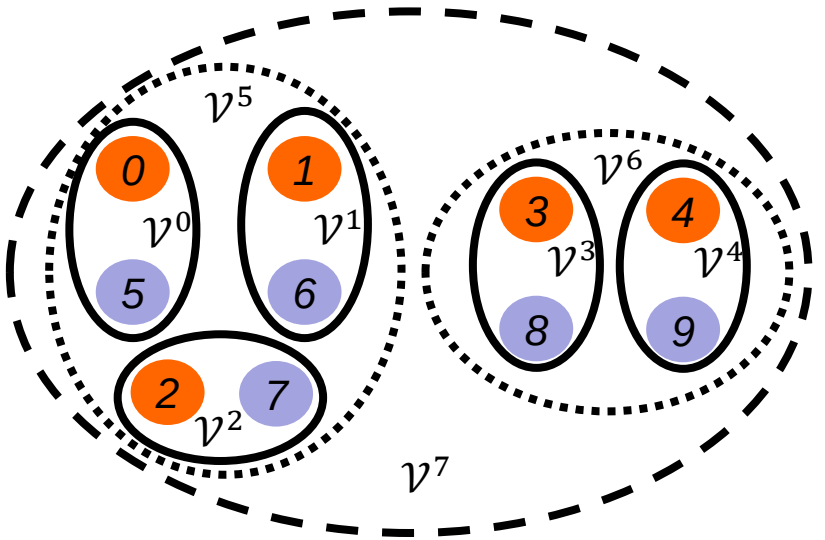
- *Weights:* $W^i, i = 0..9$
- *Direction for an interaction* $\boldsymbol{G}^k \Rightarrow \boldsymbol{N}^j, j = 0..7$

Interaction-based material network – interactions

- Mechanistic building blocks: Full interaction
  - Interaction $\mathcal{V}^j$ as a full interaction
    - Mechanism j is a full interaction if satisfying

$$\sum_i W^i \alpha^{i,k} = 0$$

    - $\alpha^{i,k}\ \forall i,k$ are considered as fitting parameters



  - More trainable parameters than laminate-based interactions

Trainable parameters

$$\mathcal{L} = [W_i, \alpha_{ij}, \mathbf{G}_j \text{ with } i = 0, \ldots, N-1, j = 0, \ldots, M-1]$$

satisfying $\sum_{i=0}^{N-1} W_i \alpha_{ij} = 0\ \forall j$

Represent RVE geometry

Interaction-based material network – offline training

- Linear elastic training
  - The tangent at zero strain is considered:

$$\mathbf{L}_{\mathrm{M}} = \frac{\partial \mathbf{P}_{\mathrm{M}}}{\partial \mathbf{F}_{\mathrm{M}}} \text{ at } \mathbf{F}_{\mathrm{M}} = \mathbf{I}$$

$$\mathbf{L}_{\mathrm{M}} = \mathbf{L}_{\mathrm{M}}(\mathbf{L}_0, \dots, \mathbf{L}_{P-1};\ \mathcal{L})$$

Elastic tangent tensors of P underlying phases

Trainable parameters

  - Offline data
    - RVE & microscopic boundary condition
    - Elastic tangent tensors of P underlying phases randomly generated
    - Homogenized tangent obtained by computational micromechanics
  - A loss function is defined
  - Gradient-descent optimizer to minimize this loss function

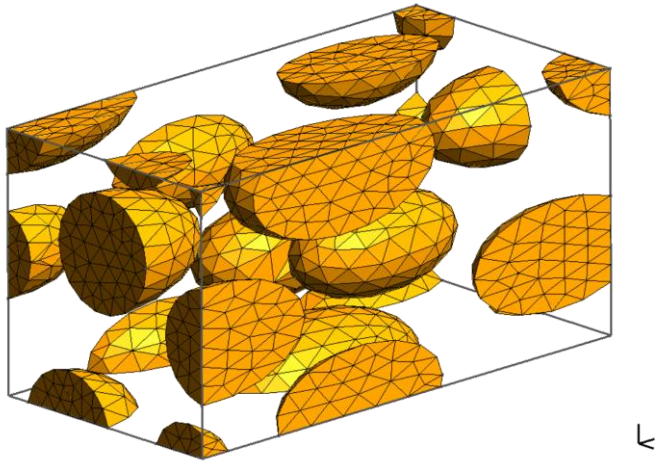
- Nonlinear training
  - Consider history path dependent

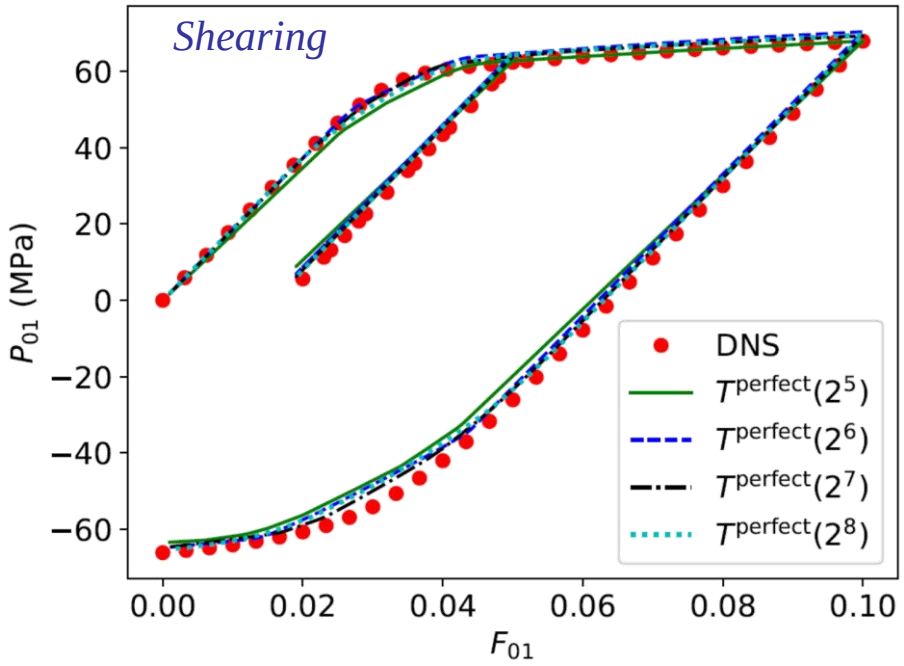
$$\mathbf{P}_{\mathrm{M}}(t) = \mathbf{P}_{\mathrm{M}}\left(\mathbf{F}_{\mathrm{M}}(\tau), \tau \le t;\ \mathcal{L}\right)$$

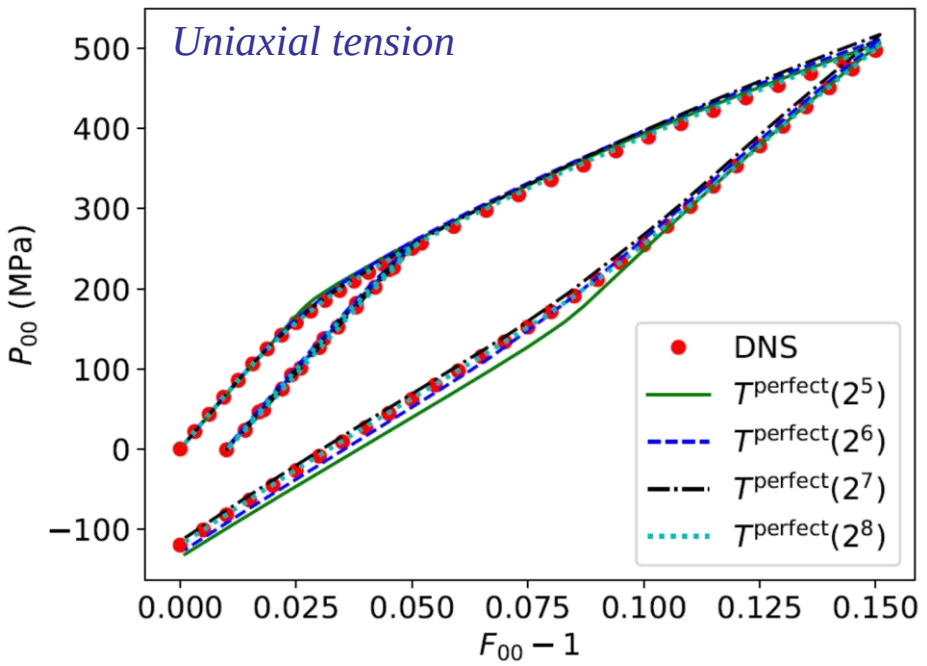
  - Offline data
    - RVE & microscopic boundary condition
    - Inputs : strain paths $\mathbf{F}_{\mathrm{M}}(\tau), \tau \le t$
    - Output: stress path $\mathbf{P}_{\mathrm{M}}(\tau), \tau \le t$ obtained by computational micromechanics
  - A loss function is defined
  - Gradient-descent optimizer to minimize this loss function

Interaction-based material network as surrogate model

- Online stage on a particle-reinforced composite
  - Properties
    - Elastic inclusions & elasto-plastic matrix
  - Laminate-based interactions
  - Linear elastic training



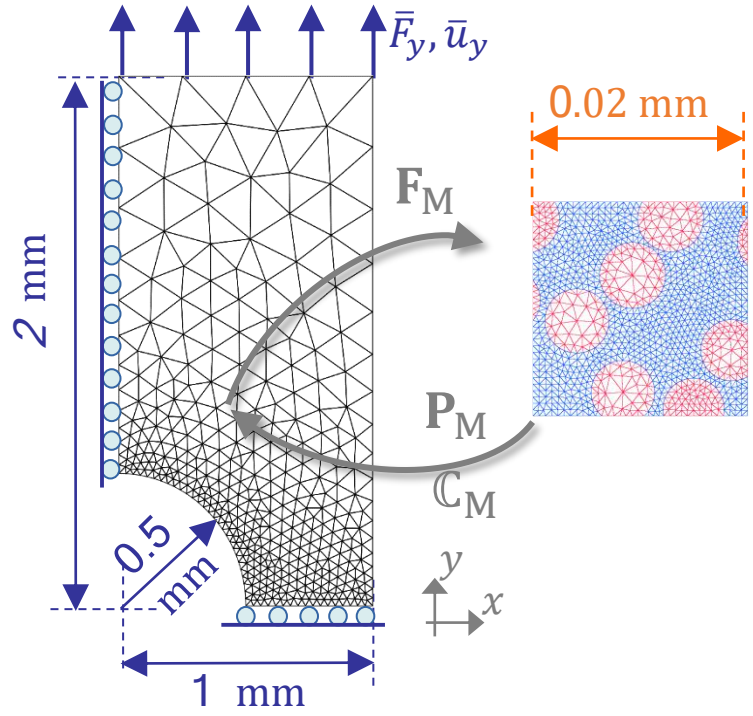


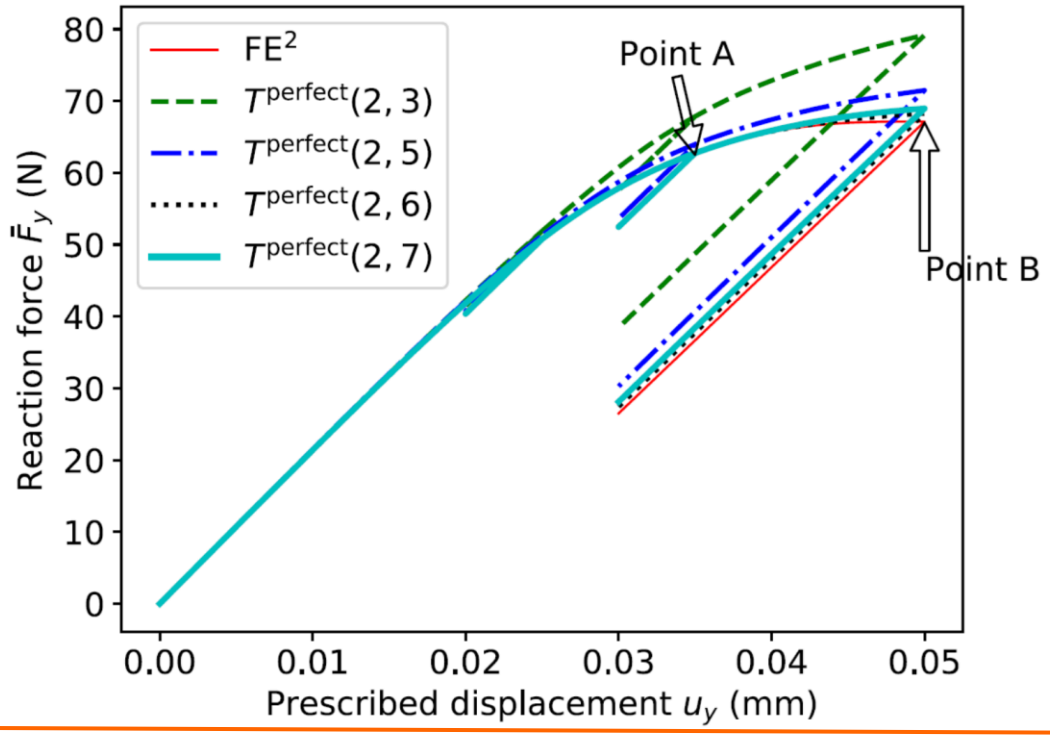


Interaction-based material network as surrogate model

- Multiscale simulation
  - Elasto-plastic composite RVE
  - Comparison FE^2 vs. Material network-surrogate
  - Laminate-based interactions
  - Linear elastic training

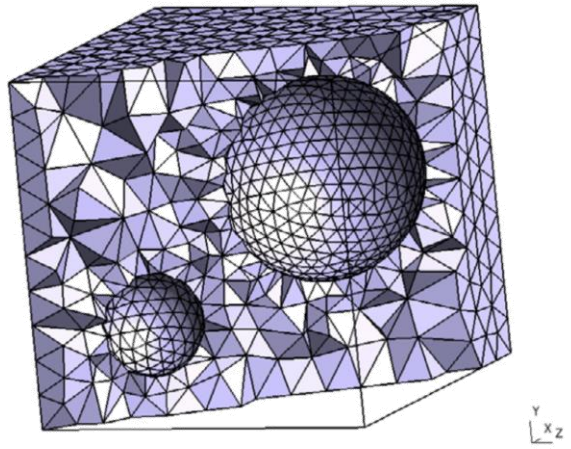
Off-line	FE^2	FE-DMN
Data generation	-	10 min.-cpu
Training	-	2 min.-cpu
On-line	**FE^2**	**FE-DMN**
Simulation	18000 h-cpu	½ to 34 h-cpu

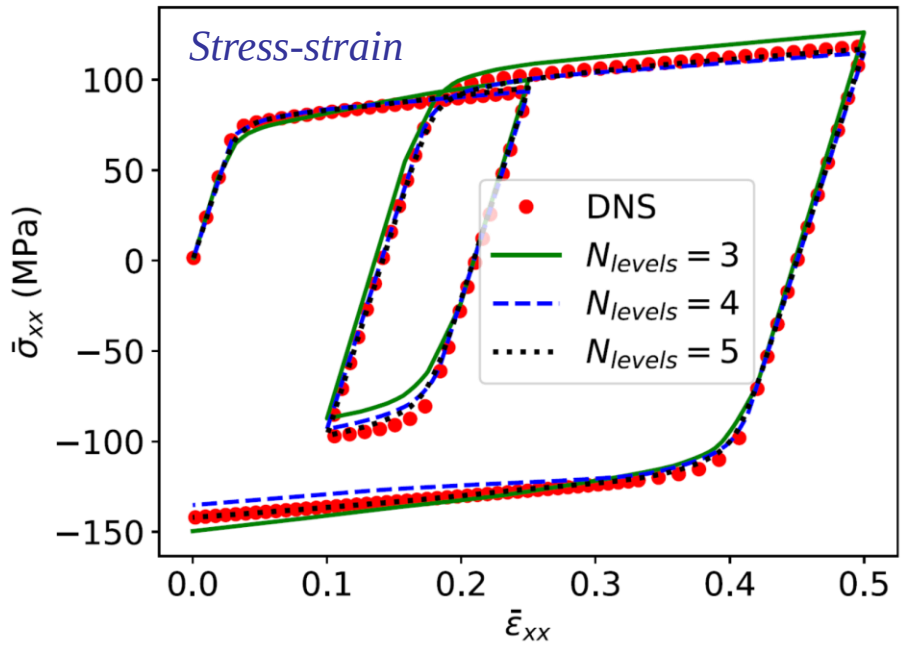


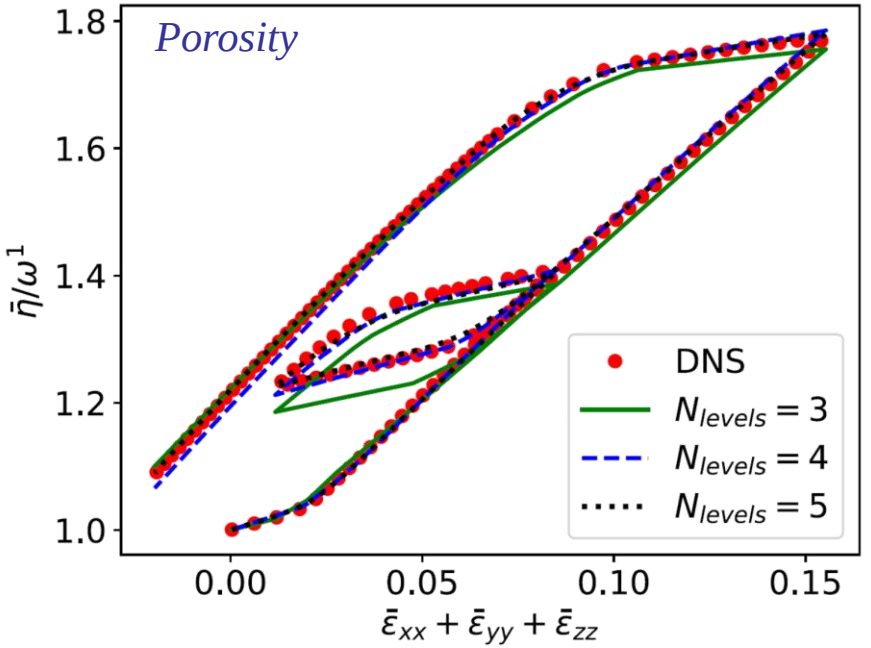


Interaction-based material network as surrogate model

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

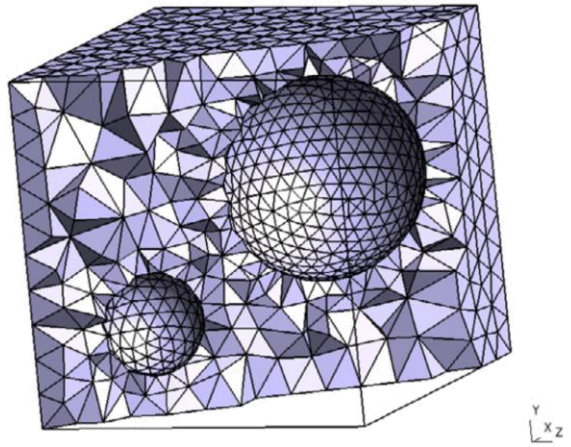


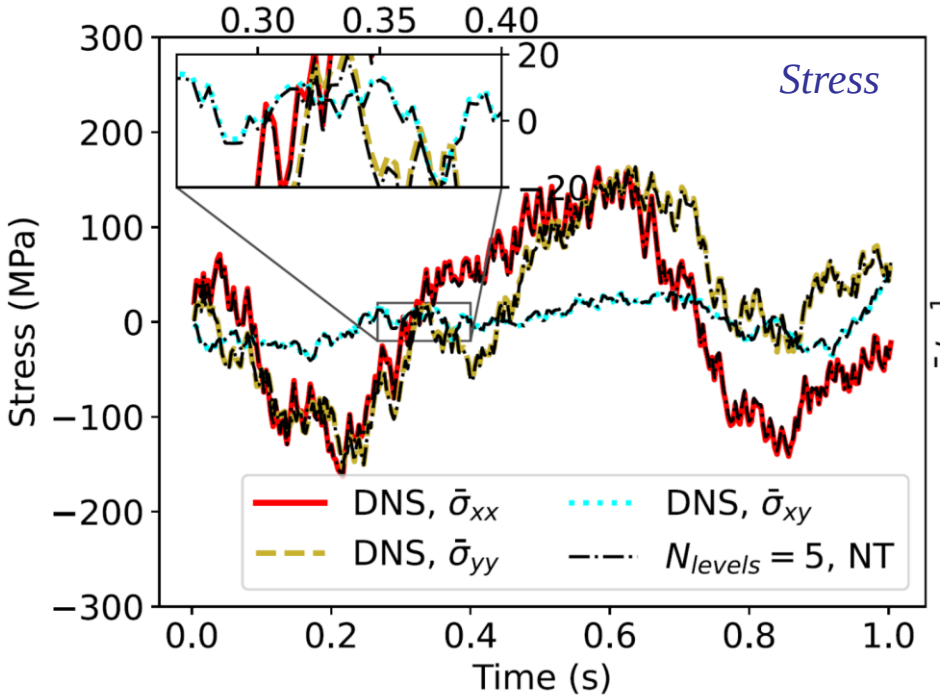


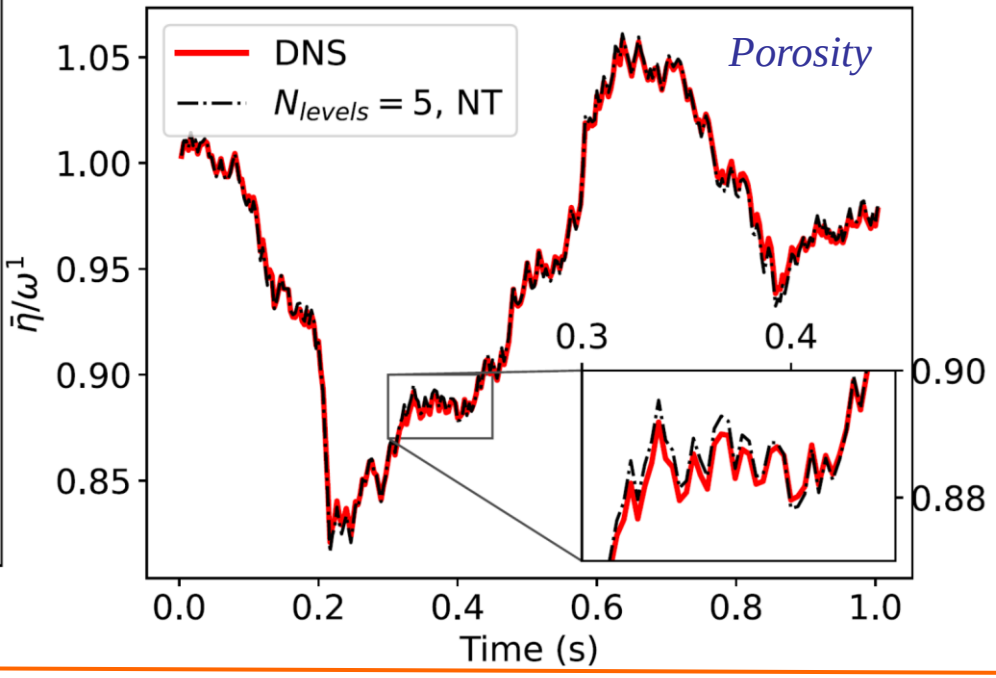


Interaction-based material network as surrogate model

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

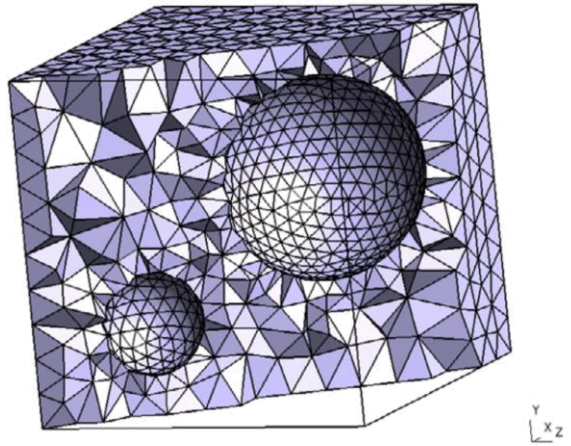


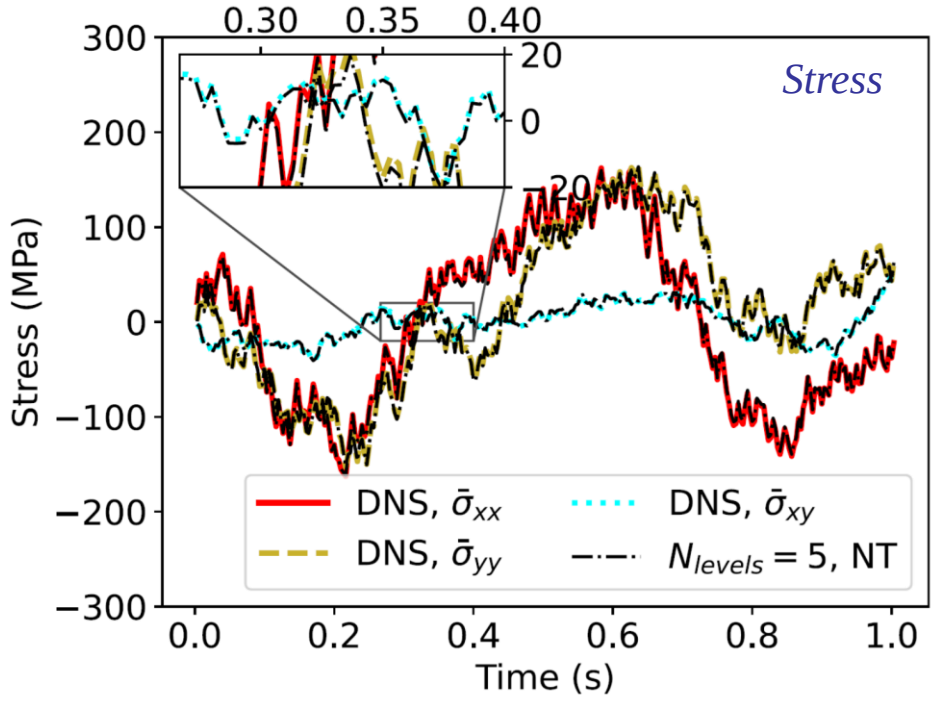


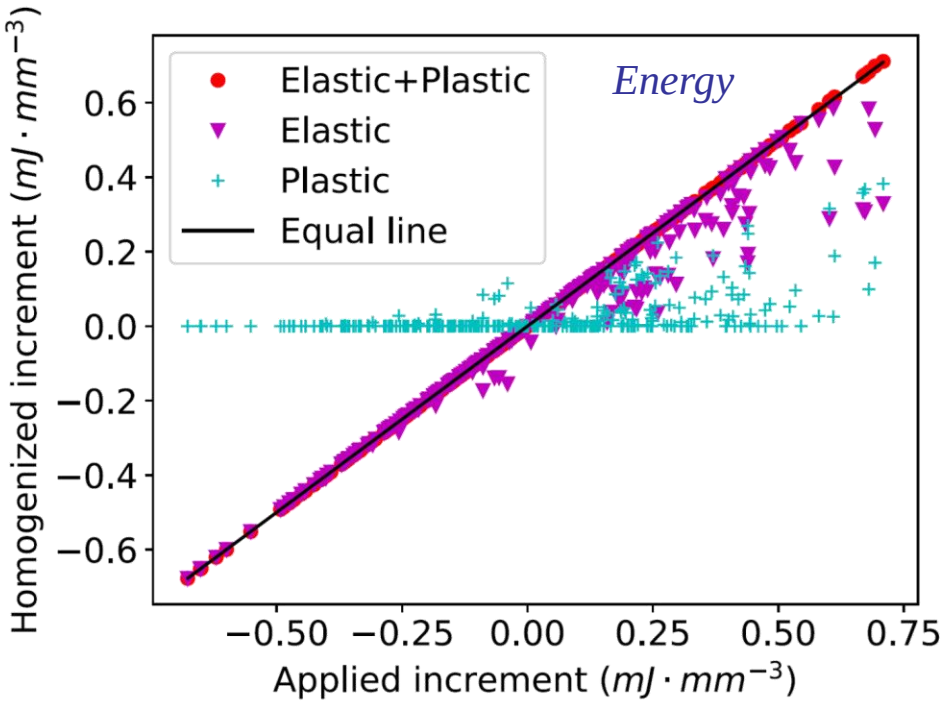


Interaction-based material network as surrogate model

- Online stage on a porous material
  - Properties
    - Elasto-plastic matrix
    - Small strain
  - Full interactions as mechanistic building blocks
  - Non-linear training
  - Thermodynamically consistent

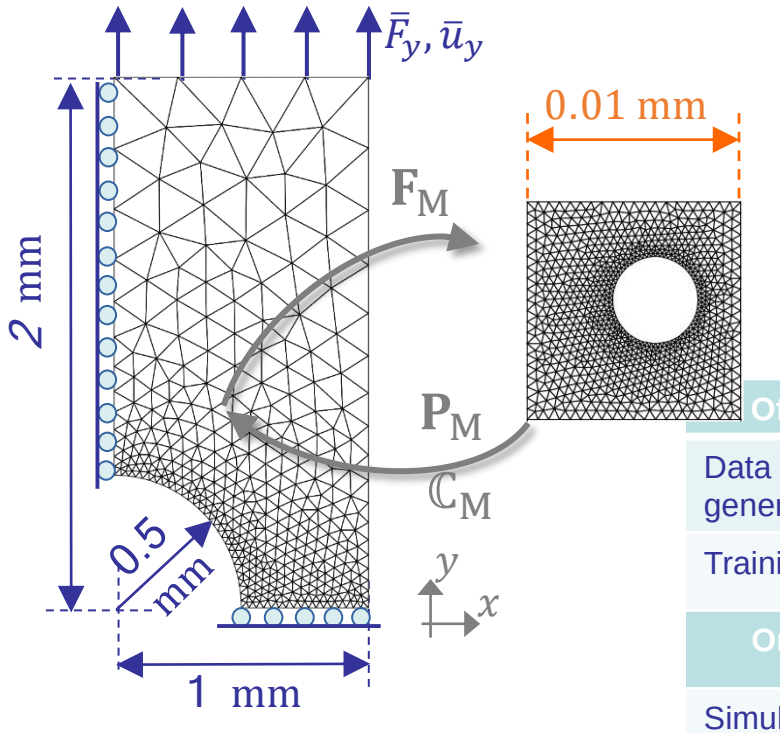




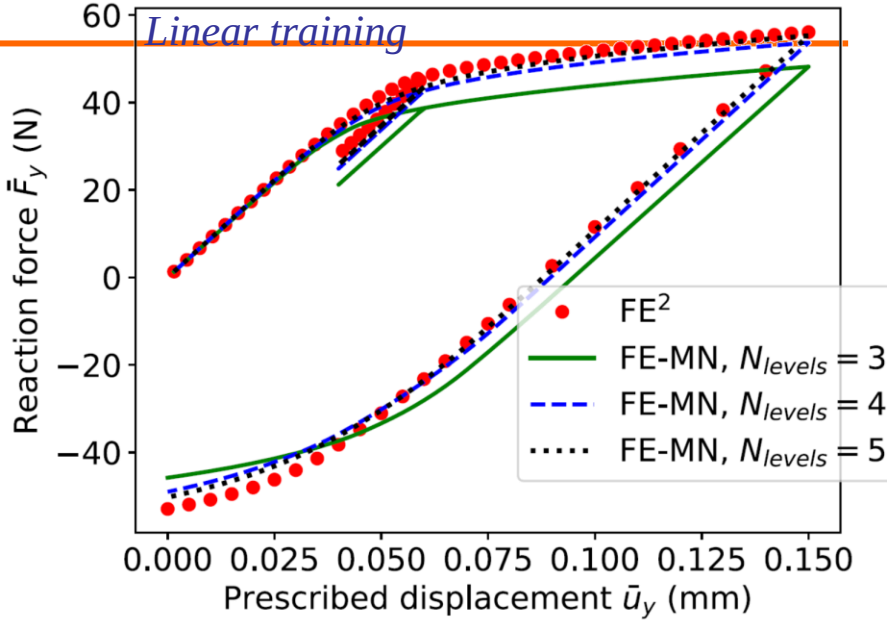


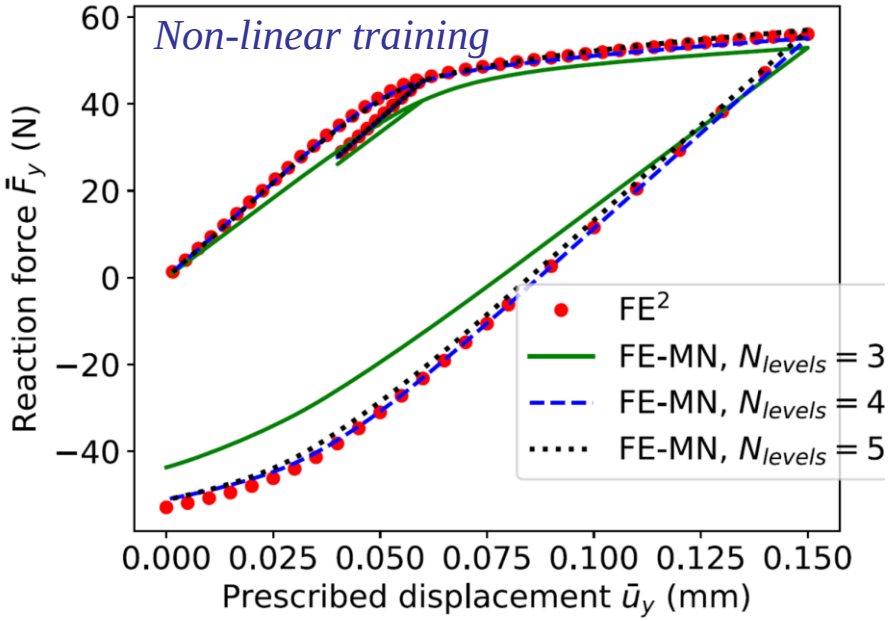
Interaction-based material network as surrogate model

- Multiscale simulation
  - Comparison FE^2 vs. Material network-surrogate
  - Full interactions as mechanistic building blocks



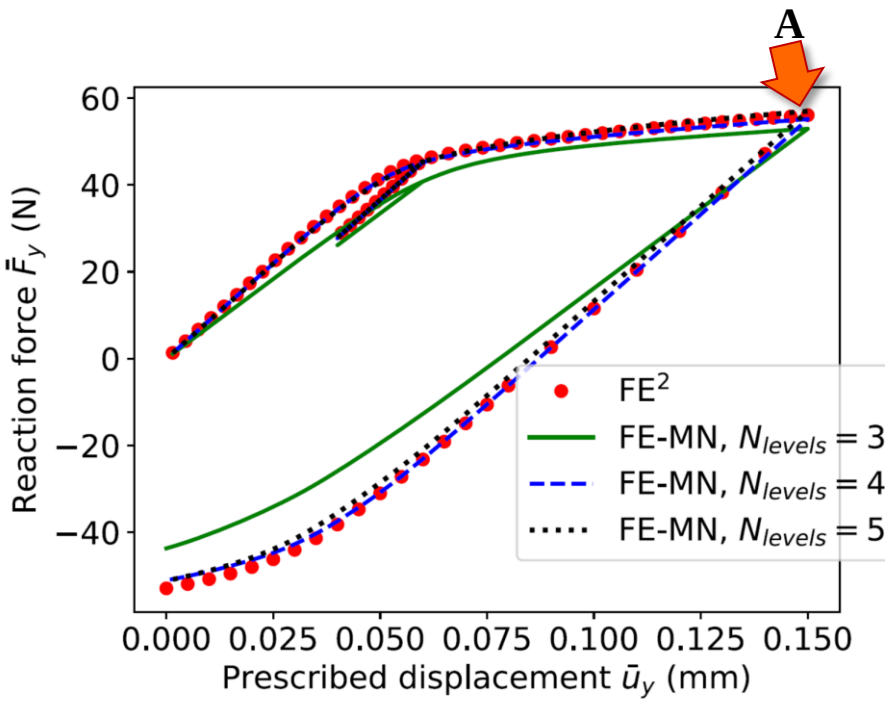
Off-line	FE^2	FE-DMN
Data generation	-	0.04 (linear) – 3.5 (non-linear) hour.-cpu
Training	-	0.16-20 hours.-cpu
On-line	**FE^2**	**FE-DMN**
Simulation	7200 h-cpu	0.1 to 1 h-cpu

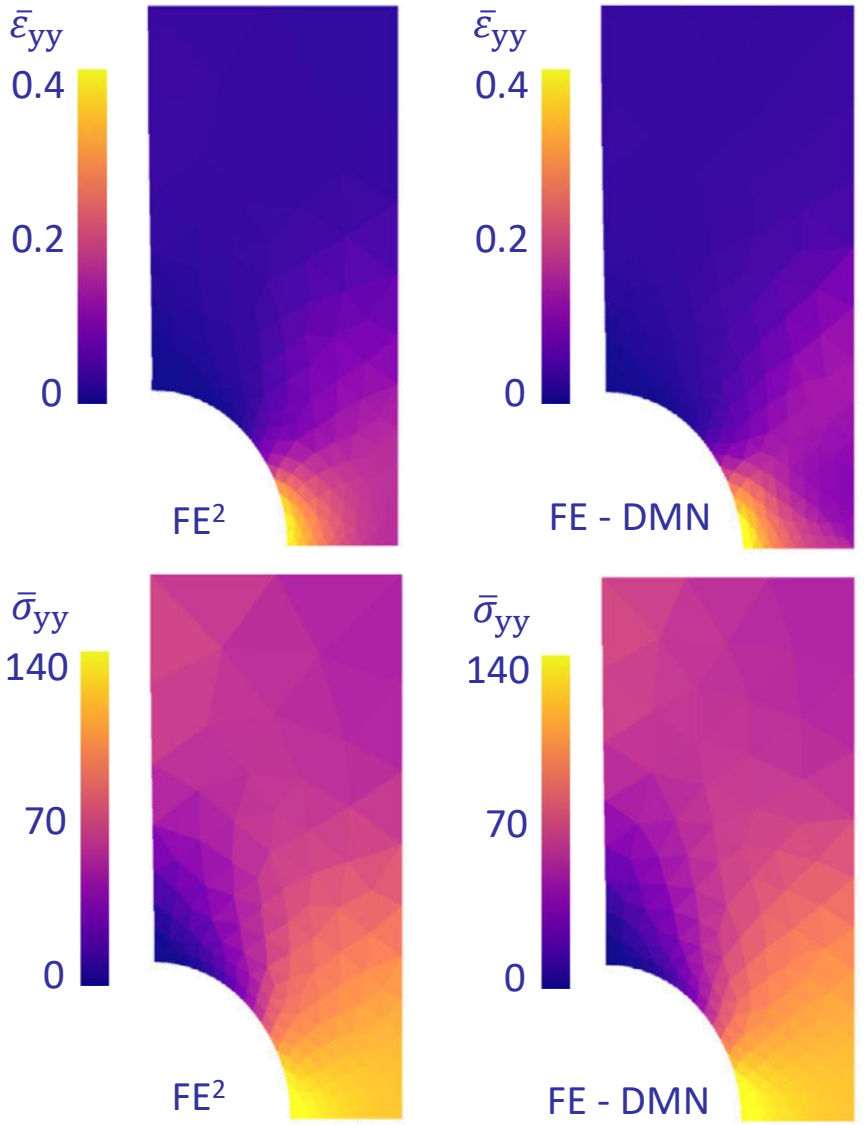




Interaction-based material network as surrogate model

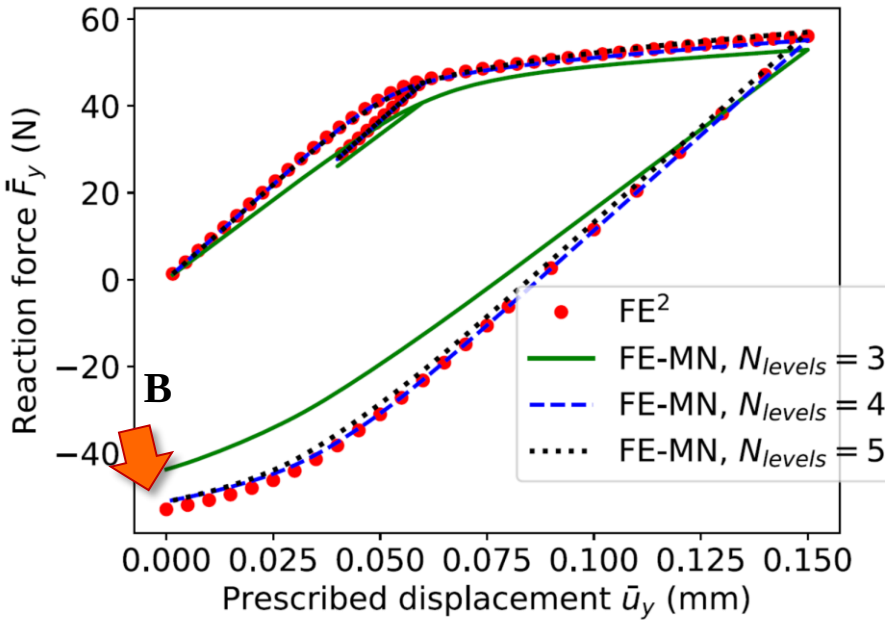
- Multiscale simulation
  - Stress-strain distribution at point **A**
  - For 2^5 material nodes
  - Full interactions as mechanistic building blocks
  - Non-linear training

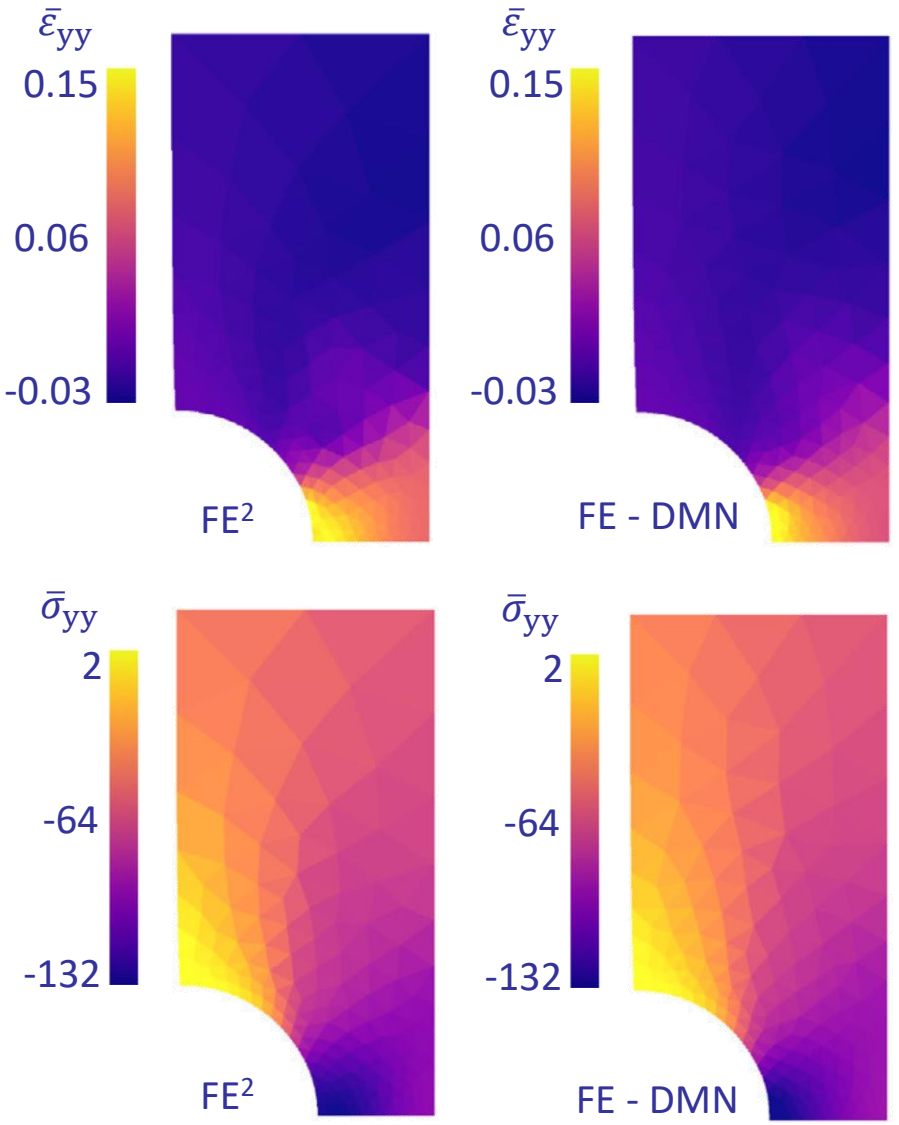




Interaction-based material network as surrogate model

- Multiscale simulation
  - Stress-strain distribution at point **B**
  - For 2^5 material nodes
  - Full interactions as mechanistic building blocks
  - Non-linear training





Conclusions and perspectives

- Interaction-based material network
  - a general framework to build surrogate models for micro-structured materials
  - Satisfy all requirements of a truly microscopic boundary value problem including the stress and strain averaging principles and the Hill–Mandel energetically consistent condition
  - Efficient training procedures
  - Trained material networks with the ones of the direct numerical simulations in both contexts of virtual testing and multiscale simulations.

Thank you for your attention

- *Nguyen, V. D., & Noels, L. (2022). Micromechanics-based material networks revisited from the interaction viewpoint; robust and efficient implementation for multi-phase composites. European Journal of Mechanics - A/Solids.*
- *Nguyen V.-D., Noels, L. (2022). Interaction-based material network: A general framework for (porous) microstructured materials. CMAME*
- *Data of " V. D. Nguyen and L. Noels. "Interaction-based material network: a general framework for (porous) microstructured materials." Computer Methods in Applied Mechanics and Engineering", https://doi.org/10.5281/zenodo.5568832*
- *Data of " V. D. Nguyen and L. Noels. "Micromechanics-based material networks revisited from the interaction viewpoint; robust and efficient implementation for multi-phase composites." European Journal of Mechanics. A, Solids 91 (January 2022): 104384. ", https://doi.org/10.5281/zenodo.4743654*