Interaction-based material networks for efficiently estimating the homogenized behavior of microstructured materials

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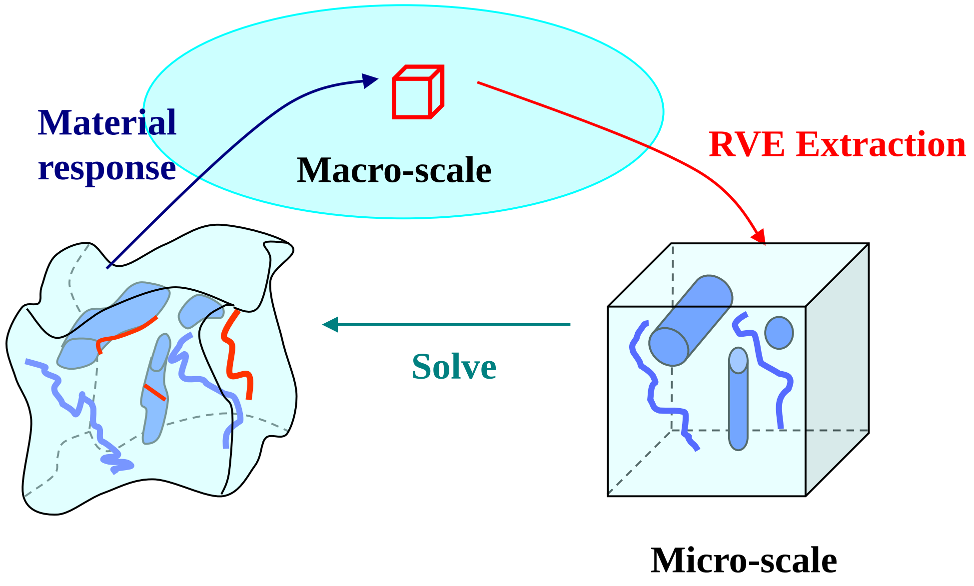
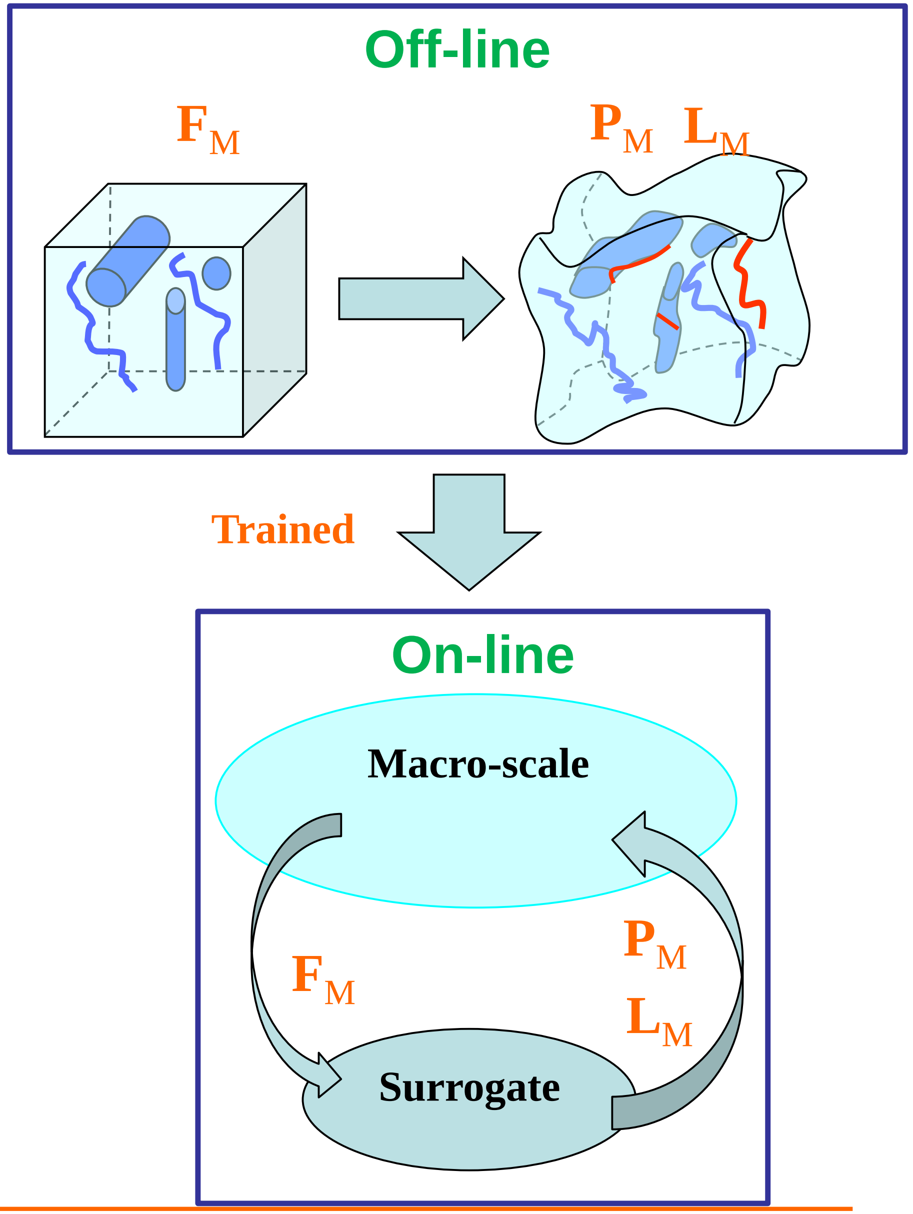
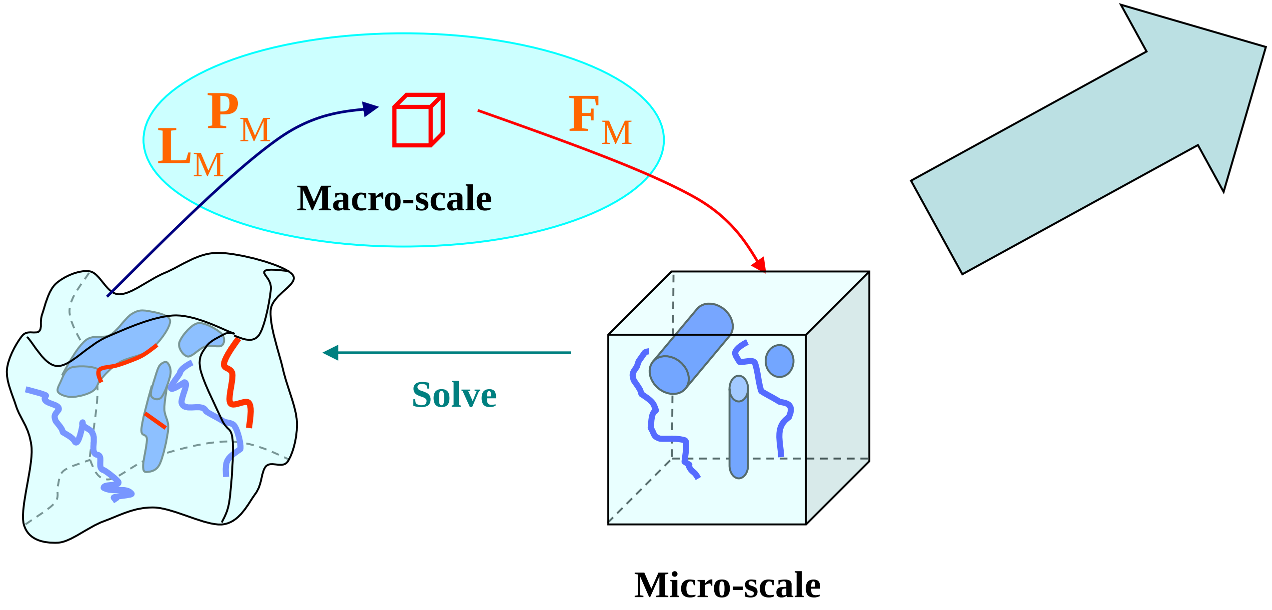
- Computational homogenization (**FE^2**)
  - Microstructured materials
  - Two problems are solved concurrently
    - Macro-scale: seen as a continuum
    - Micro-scale: Representative Volume Element (**RVE**)
      - cell, grains, inclusions…
- Advantage
  - Account for directly micro–structural parameters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



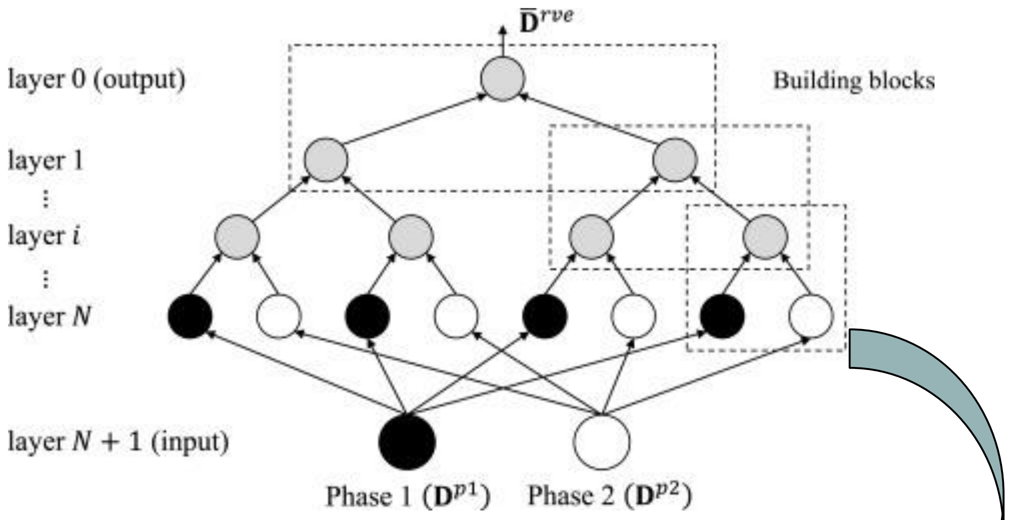
- Surrogate model of the microscopic BVP
  - Define a surrogate model
  - Off-line:
    - Construct off-line data-base (using RVE simulations)
    - Train surrogate model
  - On-line:
    - Use the trained surrogate model during analyses

Interaction-based material network



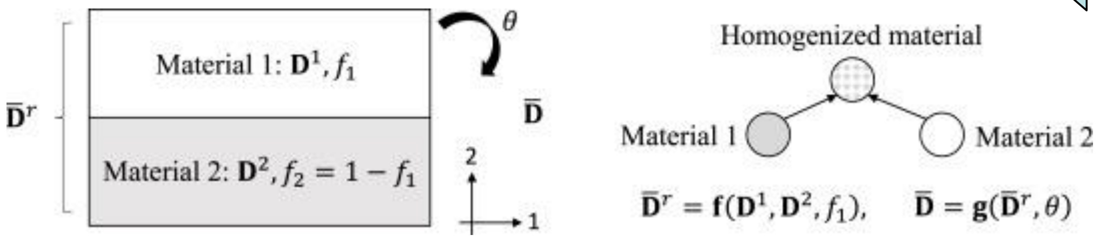


- Deep material networks (DMN)
  - Proposed by Liu et al. (2019)
  - Hierarchical laminate building blocks
  - Applicable for different kind of microstructures
    - Multiphase composites, polycrystalline materials, etc.



- Limitations
  - The solution is not provided under a closed form
  - The original DMN is still limited for porous microstructures

Revisit the DMN with interactions

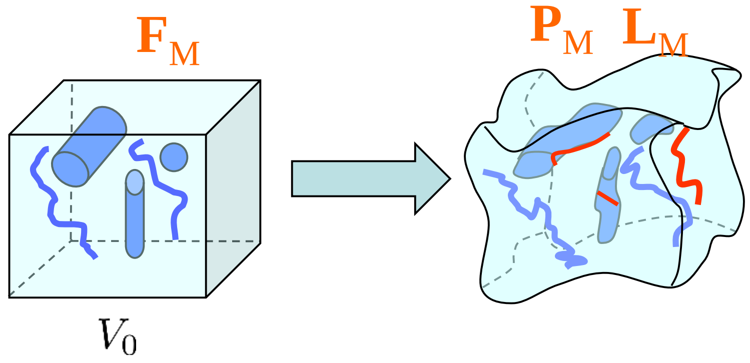


Interaction-based material network:

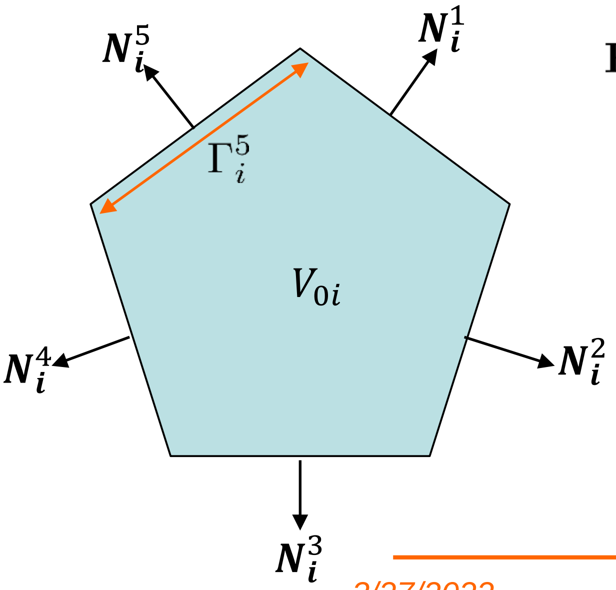
- A network of **interaction mechanisms**
- General framework for (porous) microstructured materials

Liu, Z., Wu, C.T. and Koishi, M., 2019. *Computer Methods in Applied Mechanics and Engineering*, *345*, pp.1138-1168.

- **FE² full-field model**



- Virtual polyhedral decomposition $V_0 = \cup_i V_{0i}$
  - Weights $W_i = \dfrac{V_{0i}}{V_0}$ with $i = 0, ;\ldots, N-1$
  - Each polyhedral sub-volume V_{0i}



$$\mathbf{F}_i = \frac{1}{V_{0i}} \int_{V_{0i}} \mathbf{F}\, dV = \mathbf{F}_M + \frac{1}{V_{0i}} \int_{\partial V_{0i}} \mathbf{w} \otimes \boldsymbol{N}\, dA$$

$$\Rightarrow \quad \mathbf{F}_i = \mathbf{F}_M + \sum_k \frac{\Gamma_i^k}{V_{0i}} \bar{\mathbf{w}}_i^k \otimes \mathbf{N}_i^k$$

$\mathbf{w} = \mathbf{x} - \mathbf{F}_M \cdot \mathbf{X}$: fluctuation field

$\bar{\mathbf{w}}_j^k$: average fluctation on Γ_j^k

Averaging strain

$$\mathbf{F}_M = \frac{1}{V_0} \int_{V_0} \mathbf{F}\, dV$$

Averaging stress

$$\mathbf{P}_M = \frac{1}{V_0} \int_{V_0} \mathbf{P}\, dV$$

Hill-Mandel condition

$$\mathbf{P}_M : \delta\mathbf{F}_M = \frac{1}{V_0} \int_{V_0} \mathbf{P} : \delta\mathbf{F}\, dV$$

$$\Downarrow \quad \mathbf{P}_i = \frac{1}{V_{0i}} \int_{V_{0i}} \mathbf{P}\, dV$$

Averaging strain

$$\mathbf{F}_M = \sum_{i=0}^{N-1} W_i \mathbf{F}_i$$

Averaging stress

$$\mathbf{P}_M = \sum_{i=0}^{N-1} W_i \mathbf{P}_i$$

Hill-Mandel condition

$$\mathbf{P}_M : \delta\mathbf{F}_M = \sum_{i=0}^{N-1} W_i \mathbf{P}_i : \delta\mathbf{F}_i$$

- Virtual polyhedral connectivity
  - Each polyhedral sub-volume: $\mathbf{F}_i = \mathbf{F}_M + \sum_k \frac{\Gamma_i^k}{V_{0i}} \bar{\mathbf{w}}_i^k \otimes \mathbf{N}_i^k$
  - Define M interaction mechanisms: $[(\mathbf{a}_j, \mathbf{G}_j) \text{ for } j = 0, \ldots, M-1]$

$$\Rightarrow \quad \mathbf{F}_i = \mathbf{F}_M + \sum_j \alpha_{ij} \mathbf{a}_j \otimes \mathbf{G}_j$$

Contribution of node i in mechanism j (α_{ij})

Degrees of freedom of mechanism j definition the strain fluctuation ($\mathbf{a}_j$)

Direction of mechanism j ($\mathbf{G}_j$)

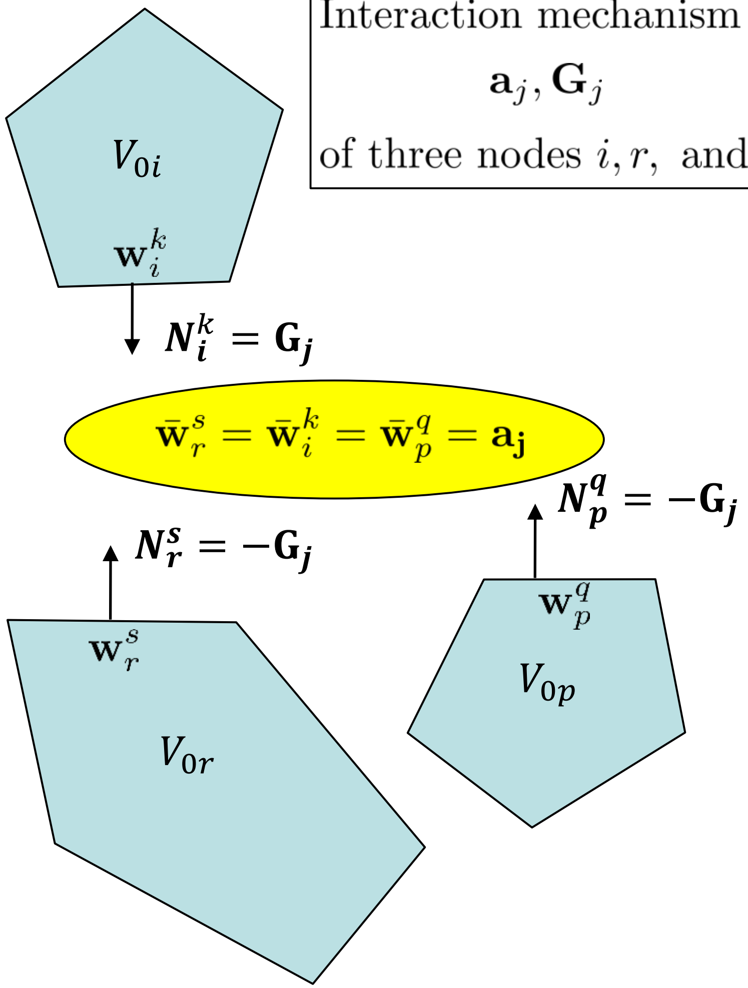
  - Constraints from strain averaging

$$\mathbf{F}_M = \sum_{i=0}^{N-1} W_i \mathbf{F}_i \;\forall [(\mathbf{a}_j, \mathbf{G}_j) \text{ for } j = 0, \ldots, M-1] \Rightarrow \sum_{i=0}^{N-1} W_i \alpha_{ij} = 0 \;\forall j = 0, \ldots, M-1$$

  - Weak form from Hill-Mandel

$$\mathbf{P}_M : \delta\mathbf{F}_M = \sum_{i=0}^{N-1} W_i \mathbf{P}_i : \delta\mathbf{F}_i \Rightarrow \sum_{j=0}^{M-1} \left[\left(\sum_{i=0}^{N-1} W_i \mathbf{P}_i \alpha_{ij} \right) \cdot \mathbf{G}_j \right] \cdot \delta\mathbf{a}_j = 0$$

Interaction mechanism j: $\mathbf{a}_j, \mathbf{G}_j$ of three nodes $i, r,$ and p



Nguyen &Noels 2022, CMAME

$W_i, \alpha_{ij}, \mathbf{G}_j$ with $i = 0, \ldots, N-1, j = 0, \ldots, M-1$ are known (by training) $\Rightarrow$ **equations to find** $[\mathbf{a}_j \text{ for } j = 0, \ldots, M-1]$

Interaction-based material network - summary

$\mathbf{F}_M(t)$

Constitutive behaviors for each phase $\mathbf{P}_i(t) = \mathbf{\Sigma}^{p_i}(\mathbf{F}_i(t), \mathbf{Z}_i(t))$

Interaction-based material network

Represent RVE geometry

Trainable parameters

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

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

Homogenized behavior $\mathbf{P}_M = \sum_{i=0}^{N-1} W_i \mathbf{P}_i$

$$\mathbf{P}_M = \sum_i W_i \mathbf{\Sigma}^{p_i}\left(\mathbf{F}_M + \sum_j \alpha_{ij} \mathbf{a_j} \otimes \mathbf{G}_j, \mathbf{Z}_i\right) := \mathbf{P}_M(\mathbf{F}_M, \mathbf{Z}_M; \mathcal{L})$$

$$\mathbf{L}_M = \frac{\partial \mathbf{P}_M}{\partial \mathbf{F}_M}$$

Interaction-based material network - training

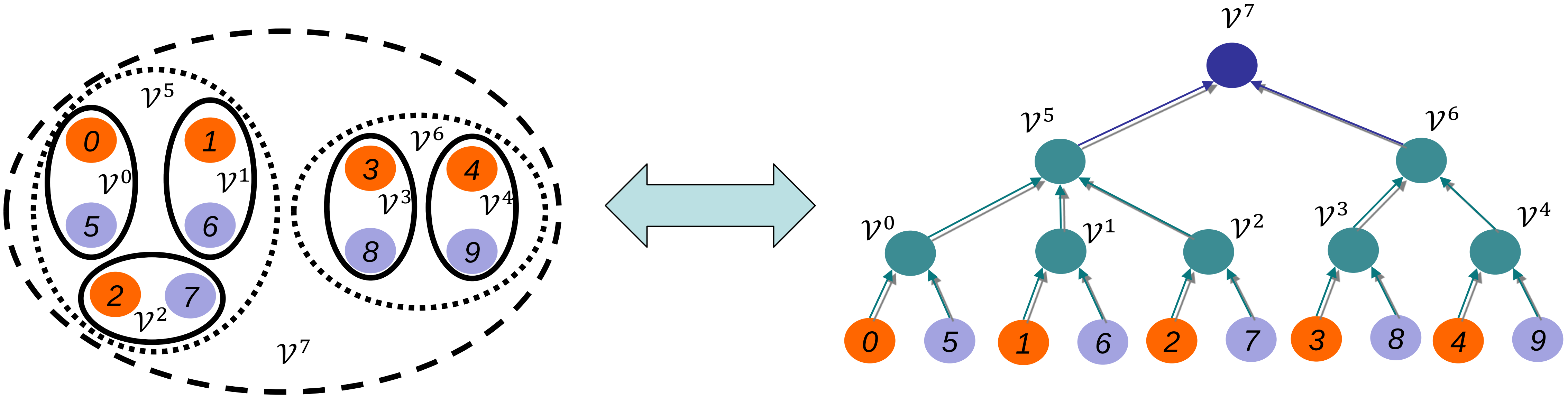
- Linear elastic training
  - The tangent at zero strain is considered: $\mathbf{L}_M = \frac{\partial \mathbf{P}_M}{\partial \mathbf{F}_M}$ at $\mathbf{F}_M = \mathbf{I}$
  - At zero strain, the elastic homogenized tensor predicted by the material can be expressed as a function of the elastic tangent tensors of P underlying phases $\mathbf{L}_0, \ldots, \mathbf{L}_{P-1}$ and fitting parameters $\mathcal{L}$

    $$\Rightarrow \quad \mathbf{L}_M = \mathbf{L}_M \left(\mathbf{L}_0, \ldots, \mathbf{L}_{P-1}, \mathcal{L}\right)$$

  - Offline data provided by elastic simulations
    - RVE & microscopic boundary condition
    - Inputs: $\mathbf{L}_0^k, \ldots, \mathbf{L}_{P-1}^k$ with $k = 0, \ldots, N_s - 1$ which can be artificially randomly generated
    - Outputs: $\mathbf{L}_M^k$ with $k = 0, \ldots, N_s - 1$ computed by computational micromechanics
  - A loss function is defined to characterize the accuracy of the prediction of the material network.
  - Gradient-descent optimizer to minimize this loss function

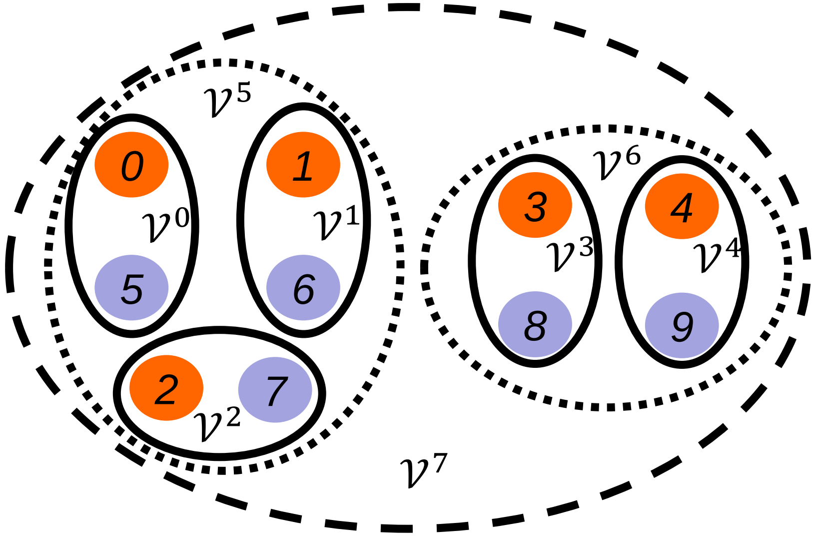
- Nonlinear training
  - Consider history dependent $\Rightarrow \quad \mathbf{P}_M(t) = \mathbf{P}_M\left(\mathbf{F}_M(\tau) \text{ for } \tau \in [0, t]; \mathcal{L}\right)$
  - Offline data provide by paths
    - RVE & microscopic boundary condition
    - Inputs: strain paths $\left[\mathbf{F}_M(t)\right]_k$ with $k = 0, \ldots, N_s - 1$ which can be artificially randomly generated
    - Output: stress paths $\left[\mathbf{P}_M(t)\right]_k$ with $k = 0, \ldots, N_s - 1$ is computed by computational micromechanics
  - A loss function is defined to characterize the accuracy of the prediction of the material network.
  - Gradient-descent optimizer to minimize this loss function

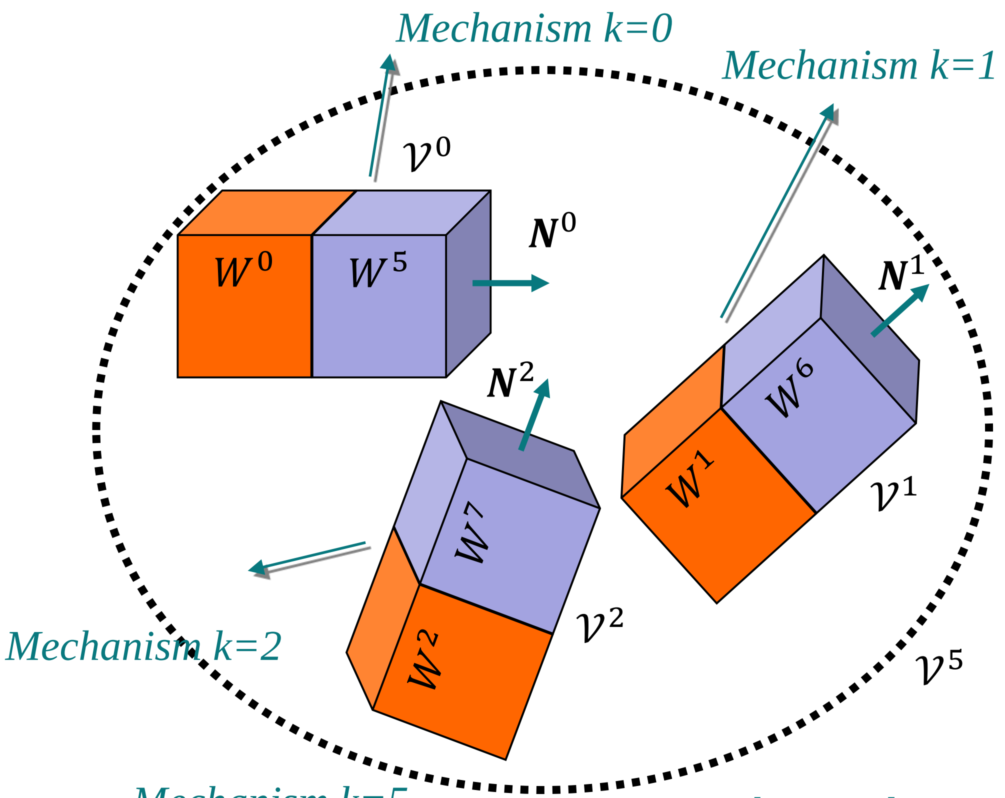
- Trainable parameters: $\mathcal{L} = [W_i, \alpha_{ij}, \mathbf{G}_j \text{ with } i = 0, \ldots, N-1, j = 0, \ldots, M-1]$
  - satisfying $$\sum_{i=0}^{N-1} W_i \alpha_{ij} = 0 \ \forall j$$
- How to define architecture?
  - Each interaction includes several nodes → $\alpha_{ij} = 0 \text{ if node } i \text{ does not participate interation } j$
  - Hierarchical architecture



Example for a 2-phase material with 10 material nodes & 8 interactions

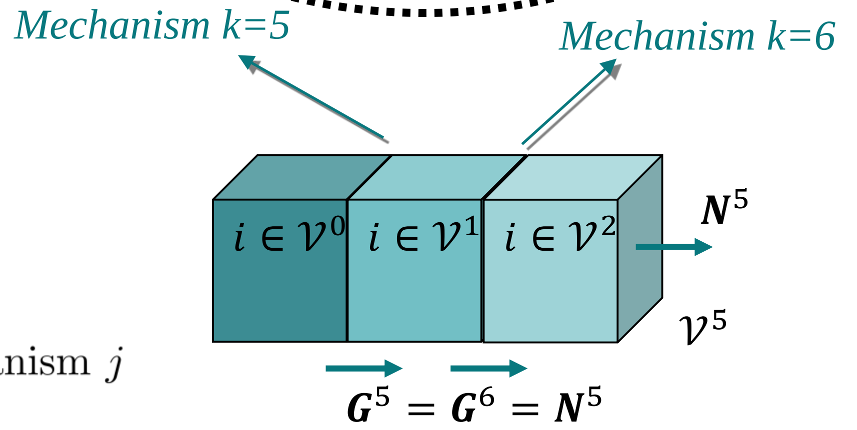
- Mechanistic building blocks: Laminate
  - Interaction $\mathcal{V}^j$ as a laminate



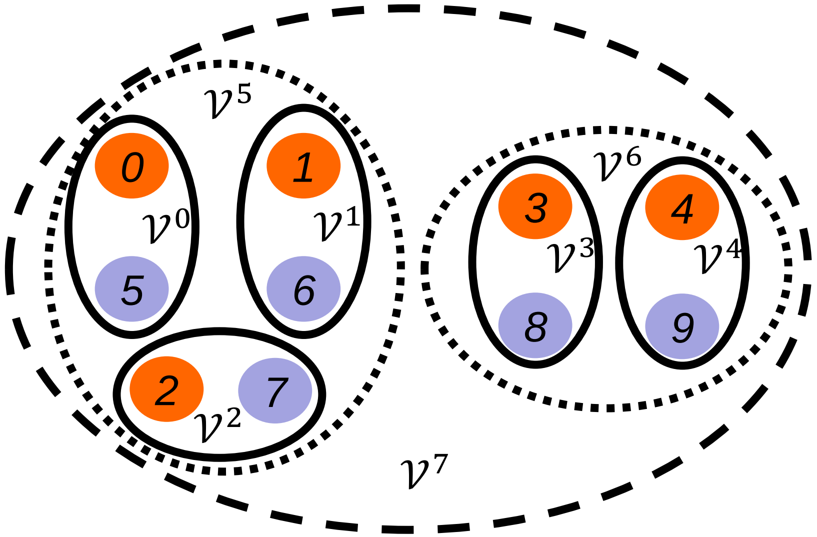


  - Tuning parameters
    - Weight: W_i with $i = 0, \ldots, 9$
    - Unique direction for an interaction $\mathcal{V}^j$: $\mathbf{G}_j$ ⇨ $\mathbf{N}_j$ with $j = 0, \ldots, 7$
    - Constraints:

$$\sum_{i=0}^{N-1} W_i \alpha_{ij} = 0 \ \forall j$$ ⇨ α_{ij} from node weights in mechanism j



- Mechanistic building blocks: Full interaction



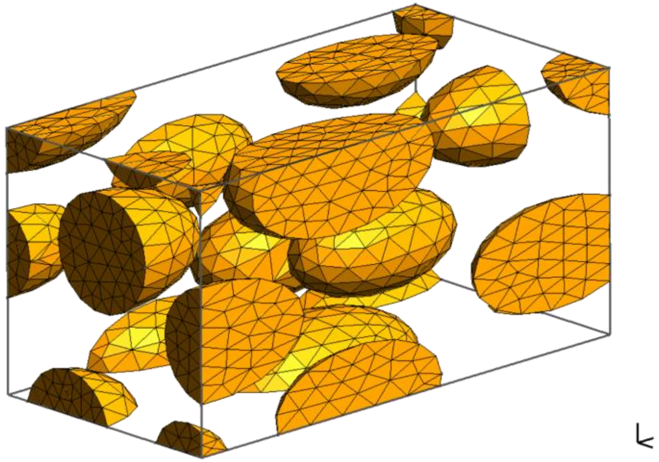
  - Interaction $\mathcal{V}^j$ as a full interaction
    - Mechanism j is a full interaction if satisfying

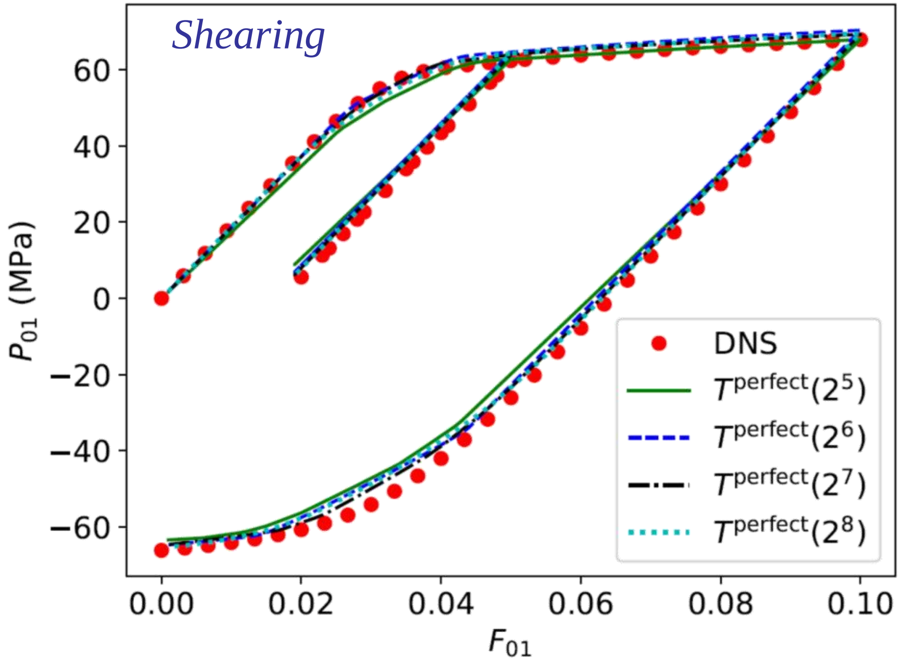
$$\sum_{i=0}^{N-1} W_i \alpha_{ij} = 0$$

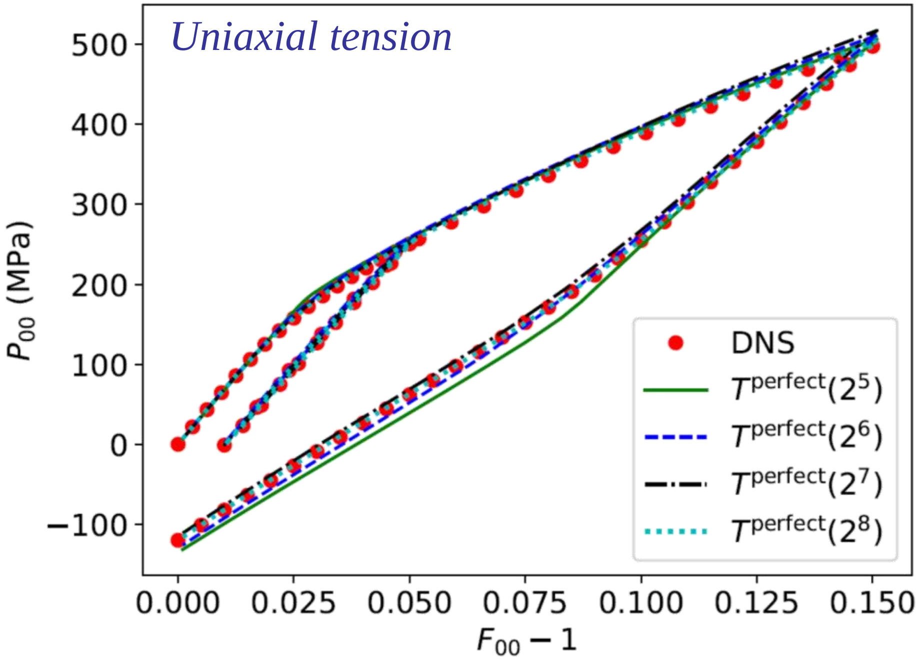
  - Tuning parameters
    - Weight: W_i with $i = 0, \dots, 9$
    - Unique direction for an interaction $\mathcal{V}^j$: $\mathbf{G}_j$ ⇨ $\mathbf{N}_j$ with $j = 0, \dots, 7$
    - Coefficients: α_{ij} with $i \in \mathcal{V}^j$ and $j = 0, \dots, 7$
    - Constraints: $\sum_{i=0}^{N-1} W_i \alpha_{ij} = 0 \ \forall j$ are enforced during training iterations

Interaction-based material network as surrogate model

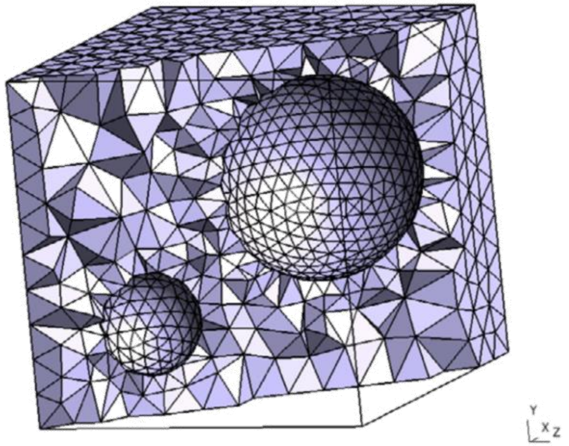
- Online stage on a particle-reinforced composite
  - Properties
    - Elastic inclusions
    - Elasto-plastic matrix
  - Laminate as mechanistic building blocks
  - Linear elastic training

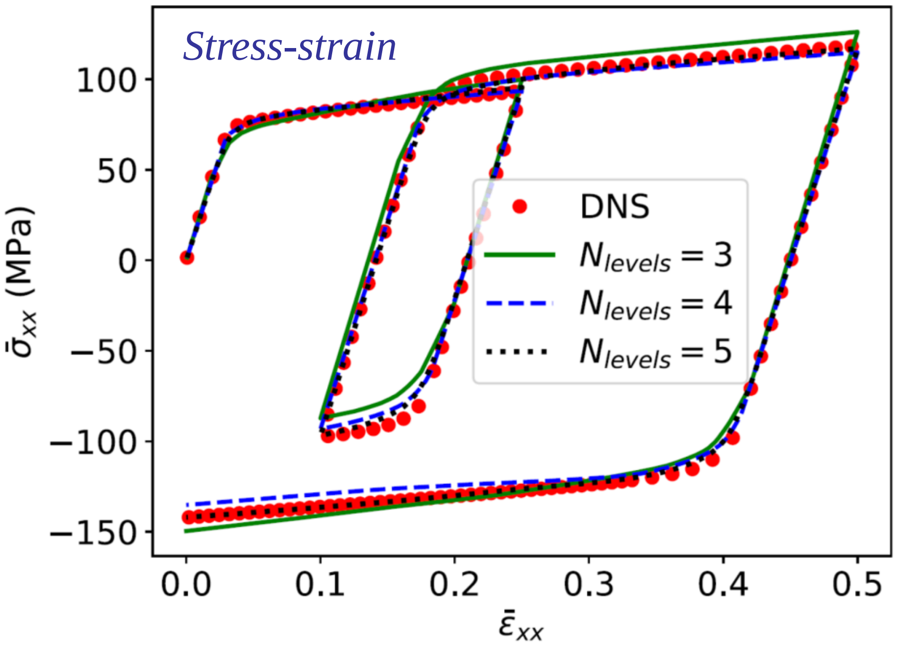


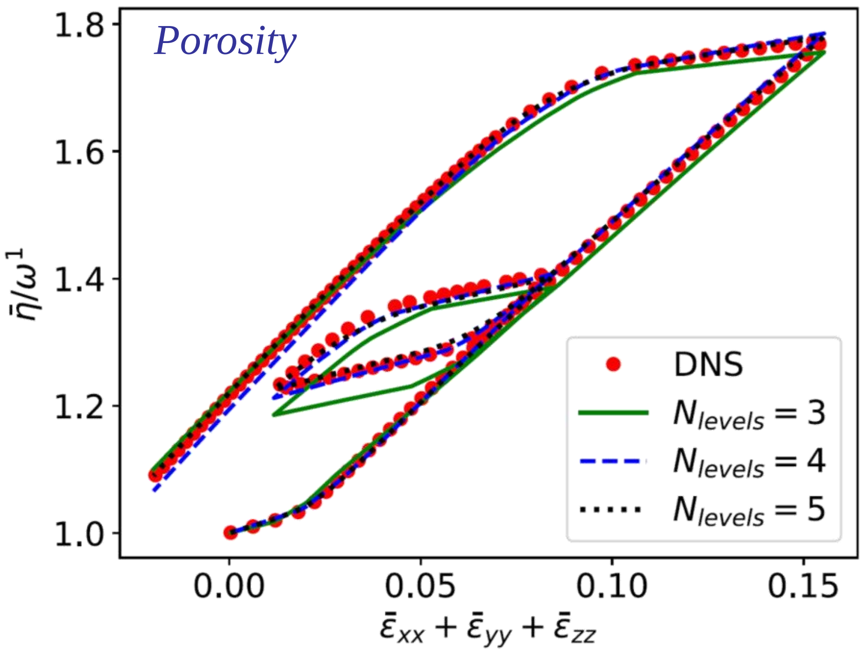




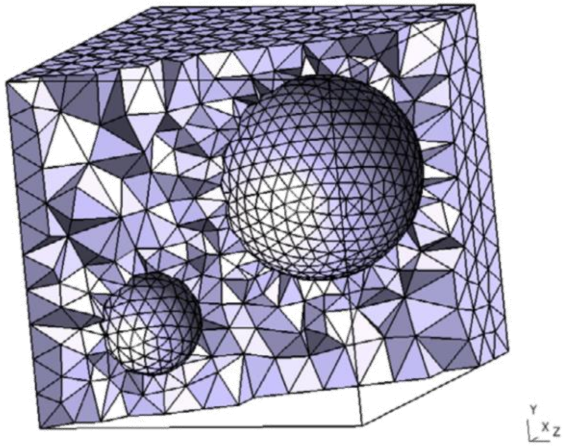
- Online stage on a porous material
  - Properties
    - Elasto-plastic matrix
    - Small strain
  - Full interactions as mechanistic building blocks
  - Non-linear training
  - Uniaxial tension

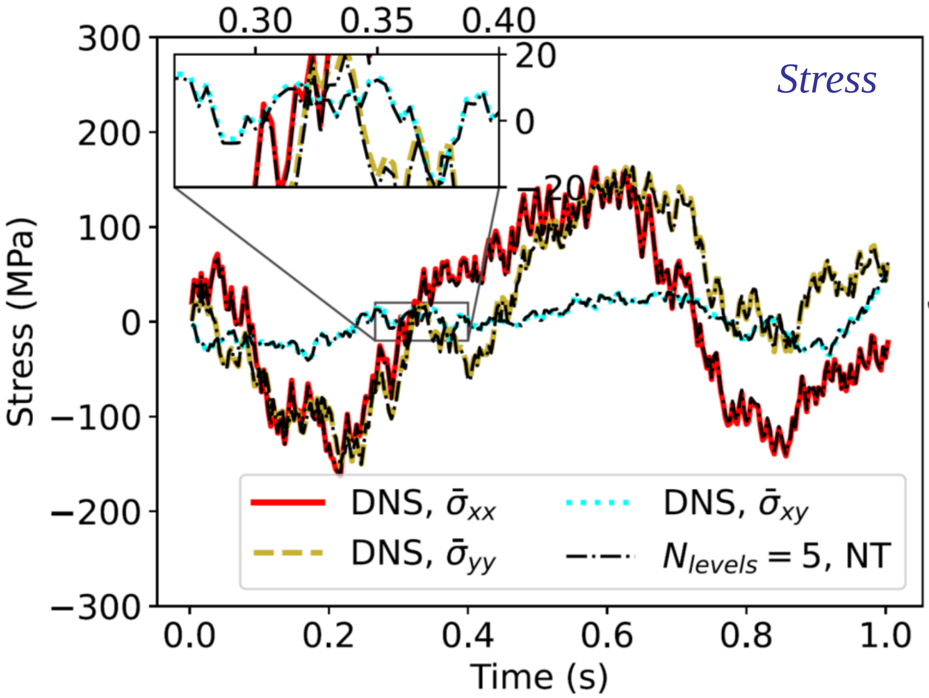


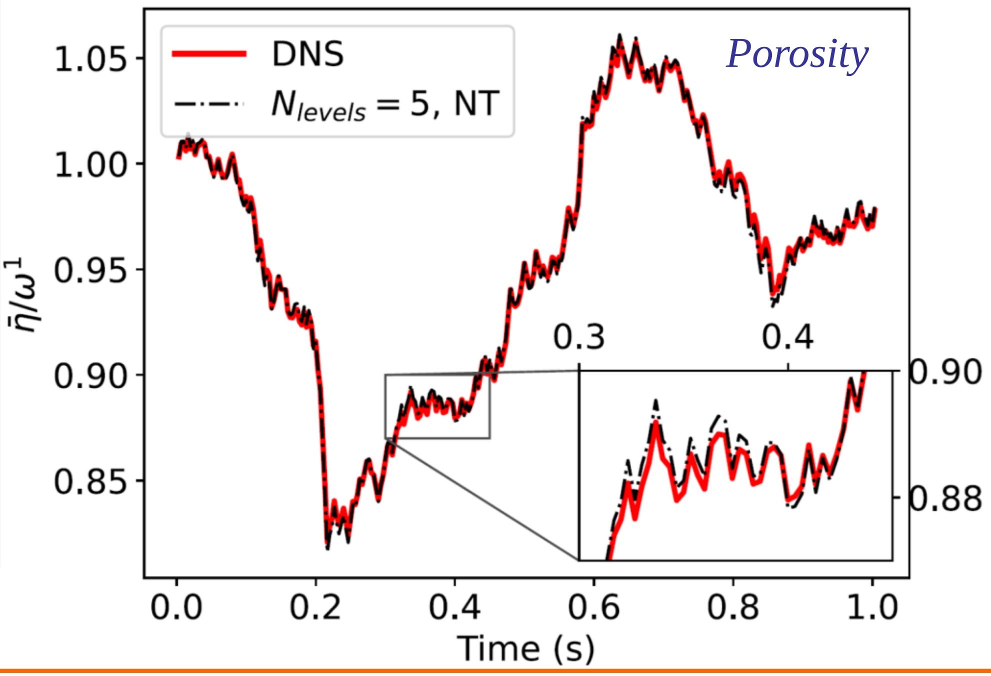




- Online stage on a porous material
  - Properties
    - Elasto-plastic matrix
    - Small strain
  - Full interactions as mechanistic building blocks
  - Non-linear training with Material 1, on-line material 2
  - Random loading

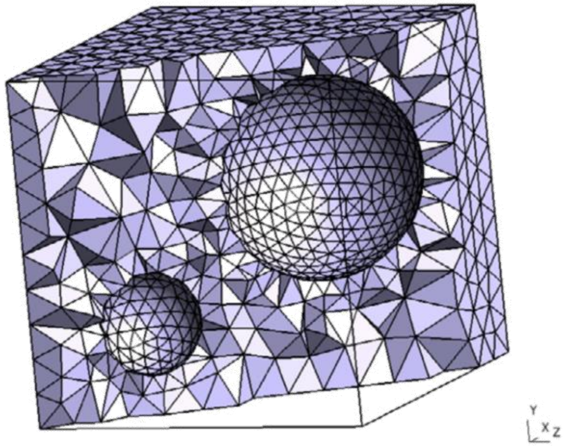


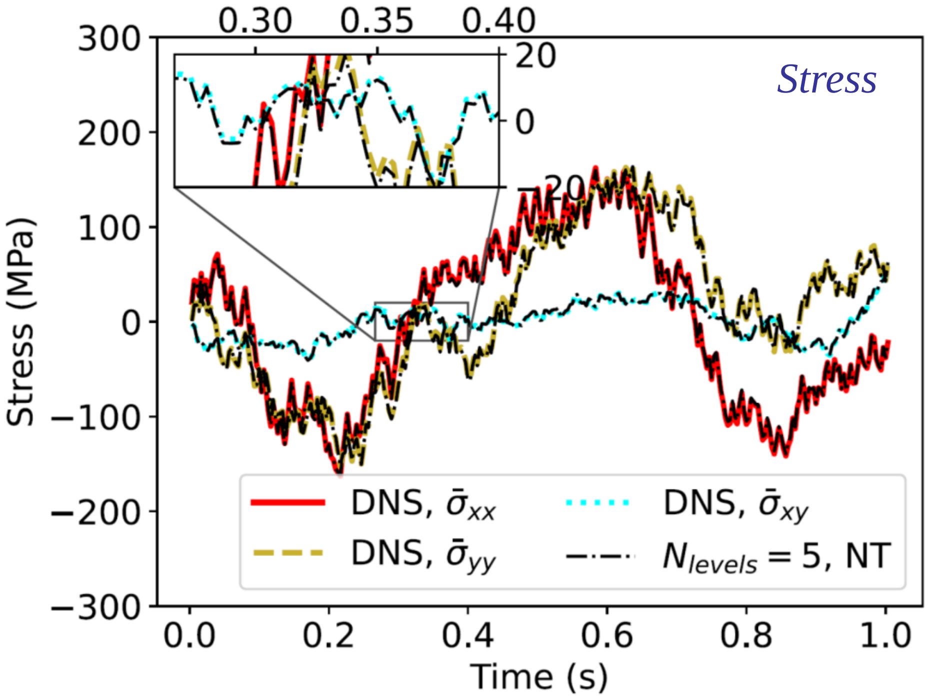


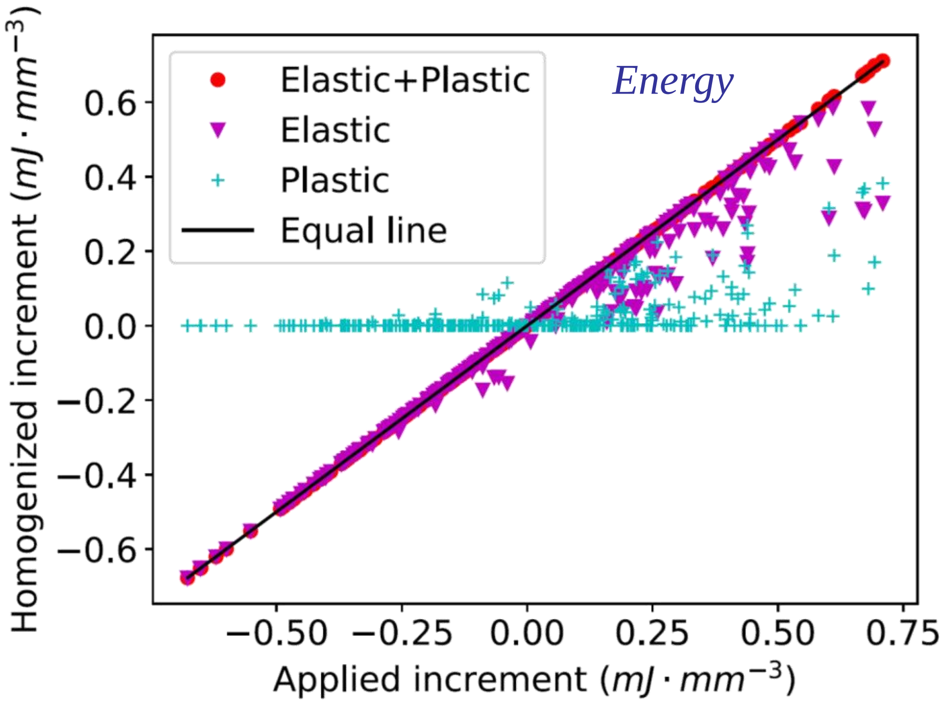


Interaction-based material network as surrogate model

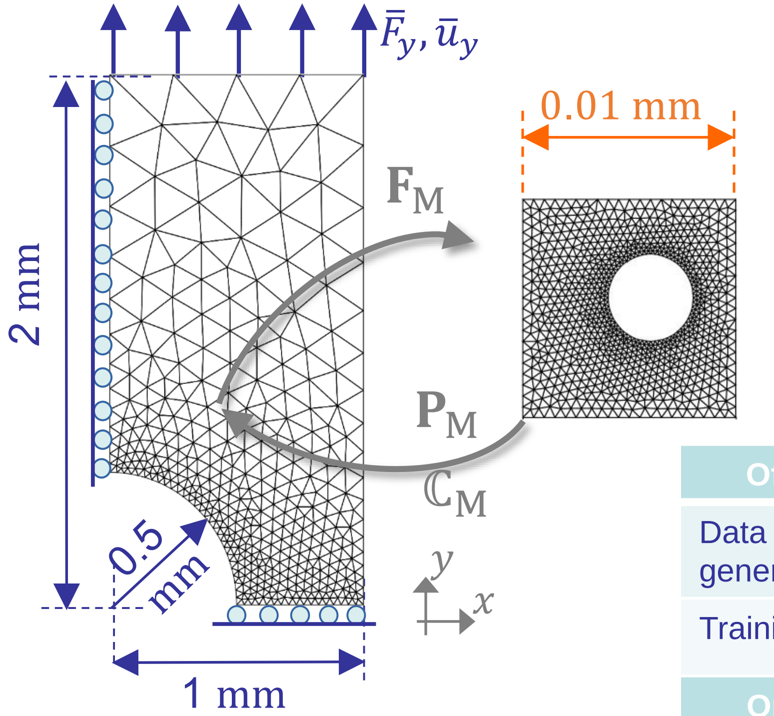
- Online stage on a porous material
  - Properties
    - Elasto-plastic matrix
    - Small strain
  - Full interactions as mechanistic building blocks
  - Non-linear training
  - Thermodynamically consistent



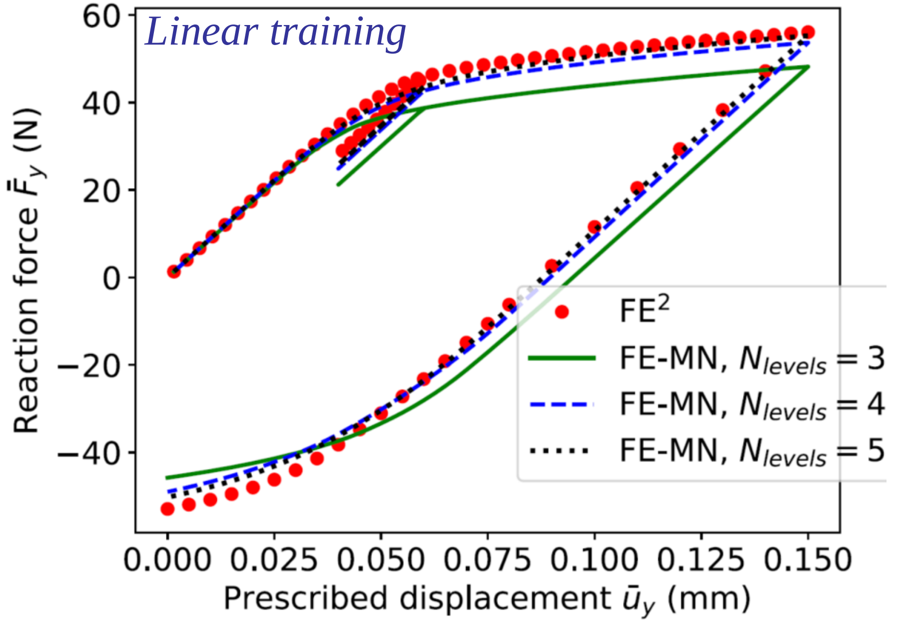


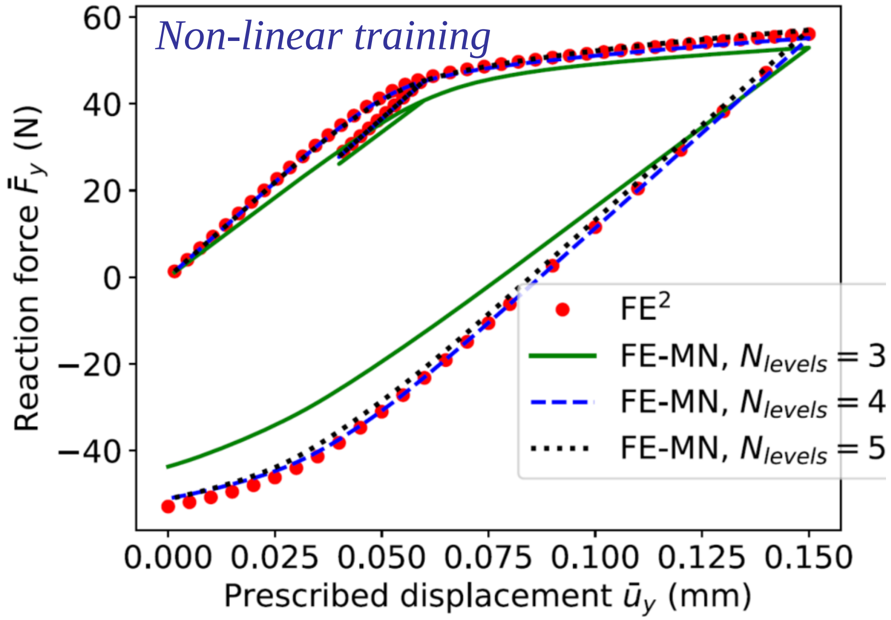


- Multiscale simulation
  - Comparison FE^2 vs. Material network-surrogate
  - Full interactions as mechanistic building blocks
  - Non-linear training



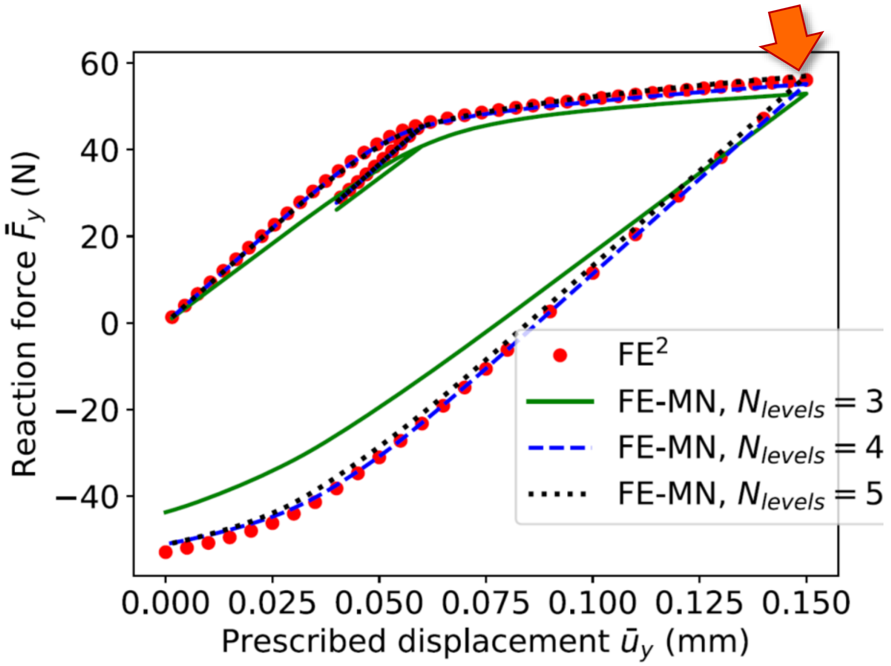
Off-line	FE^2	FE-DMN
Data generation	-	0.04 (linear) – 3.5 (non-linear) hour.-cpu
Training	-	0.16-20 hours.-cpu
On-line	**FE^2**	**FE-DMN**
Simulation	7200 h-cpu	0.1 to 1 h-cpu

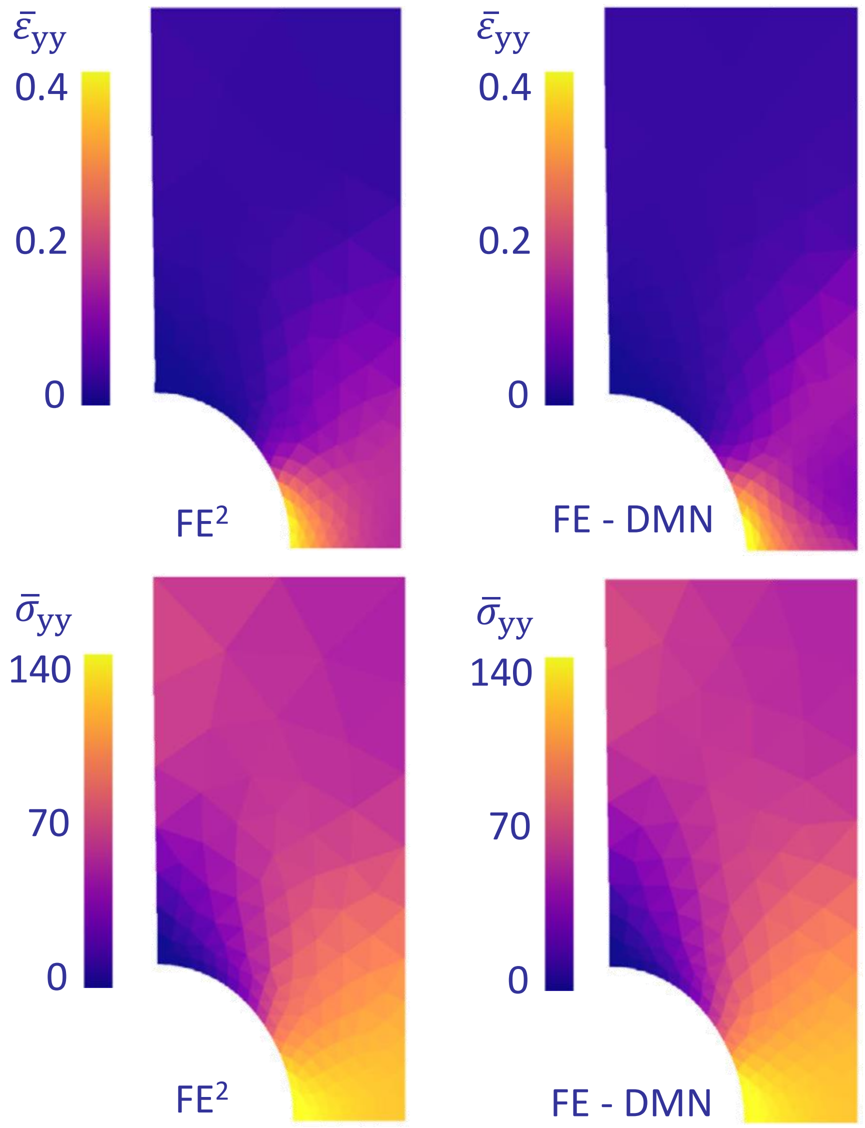




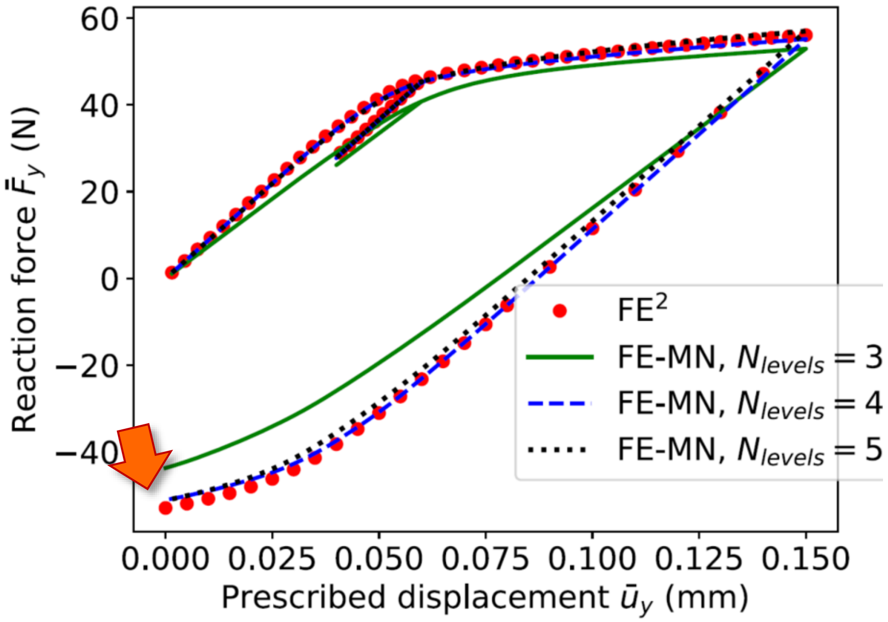
Interaction-based material network as surrogate model

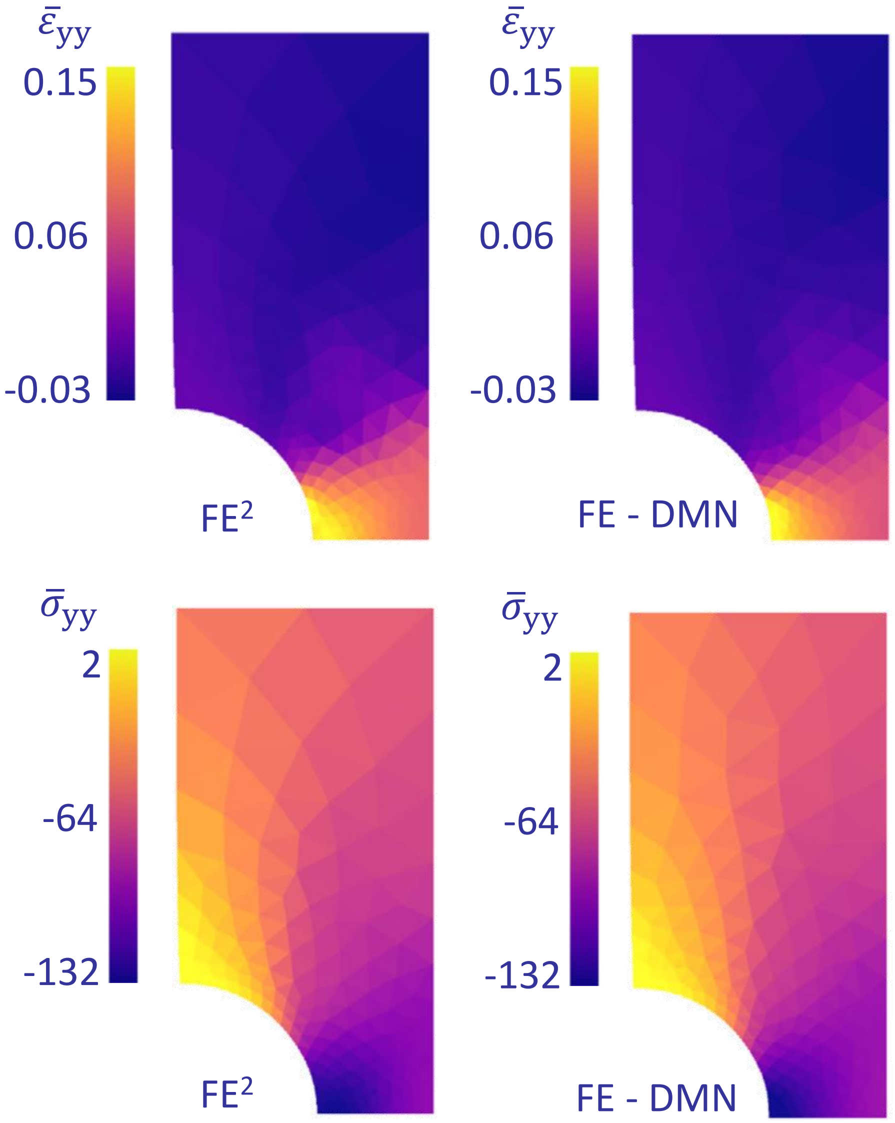
- Multiscale simulation
  - Stress-strain distribution at point A
  - For 2^5 material nodes
  - Full interactions as mechanistic building blocks
  - Non-linear training





- 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.
- Future works
  - Interaction-based material network for dame and fracture

Thank you for your attention