NATIONAL TECHNICAL UNIVERSITY OF ATHENS
SCHOOL OF CIVIL ENGINEERING
INSTITUTE OF STRUCTURAL ANALYSIS &
ANTISEISMIC RESEARCH

MACHINE LEARNING – ASSISTED STOCHASTIC OPTIMIZATION OF STRUCTURES COMPRISED OF NANO-REINFORCED CONCRETE

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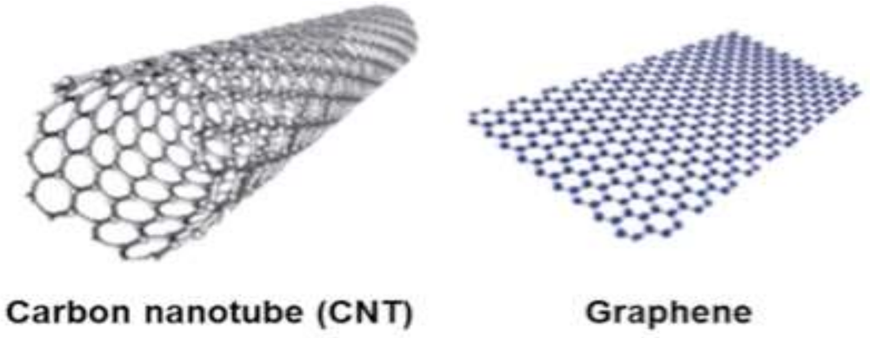
- Carbon nanomaterials exhibit remarkable mechanical, electrical and thermal properties.

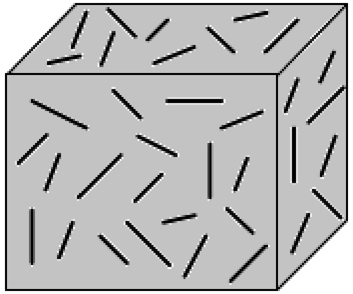
- They constitute ideal fillers for high-performance composites.

- In structural applications, concrete reinforced with carbon nanomaterials, exhibits several desirable properties such as:
  - *High increase in strength*
  - *Crack prevention*
  - *Lightweight reinforcement*
  - *Extremely high-impact strength*
  - *Increased fatigue and corrosion resistance*
  - *Improvement in structural performance, safer structures*



- Concrete reinforced with CNTs exhibits a highly complex behavior.
- This behavior is the result of different physical mechanisms, existing at various length scales.
- A phenomenological constitutive law that takes into account all the interactions between the constituents is difficult to derive.
- We propose a hierarchical modeling approach.

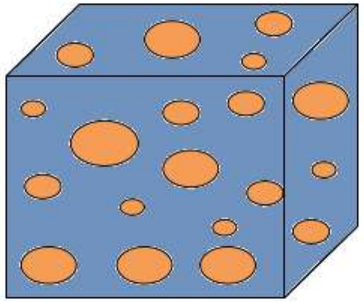
Idea: Decompose the material analysis into multiple scales to account for the different phenomena



1.0^3 μm^3

Nanoscale

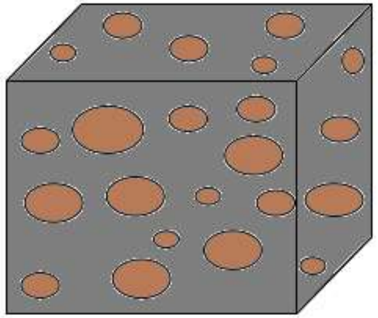
Cement paste + CNTs



40^3 mm^3

Microscale

CNT reinforced cement paste + small aggregates

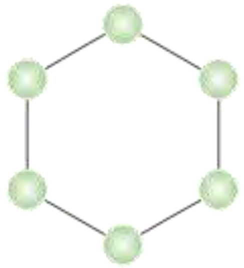


100^3 mm^3

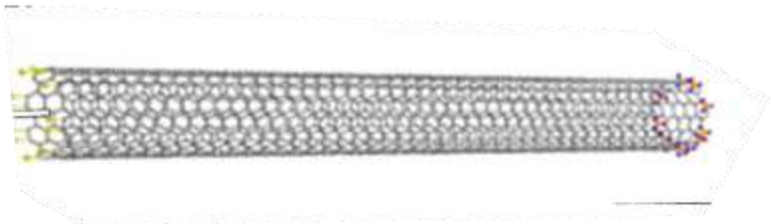
Mesoscale

Reinforced concrete+ large aggregates

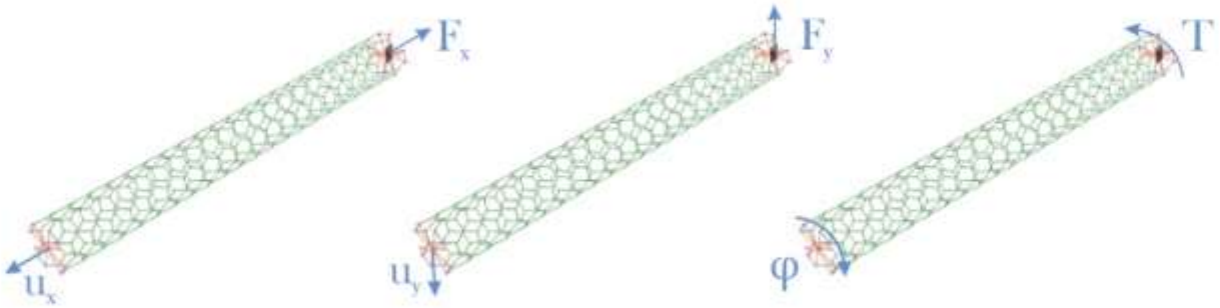
Modeling of a single CNT



Carbon atom C-C bonds modeled as beams (MSM)



CNT simulated as a space frame structure

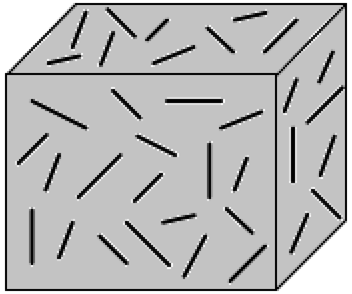


$$(EA)_{eq} = \frac{F_x L_0}{u_x}$$

$$(EI)_{eq} = \frac{F_y L_0^3}{3u_y}$$

$$(GJ)_{eq} = \frac{T}{\varphi} L_0$$

Modeling of nanoscale RVE

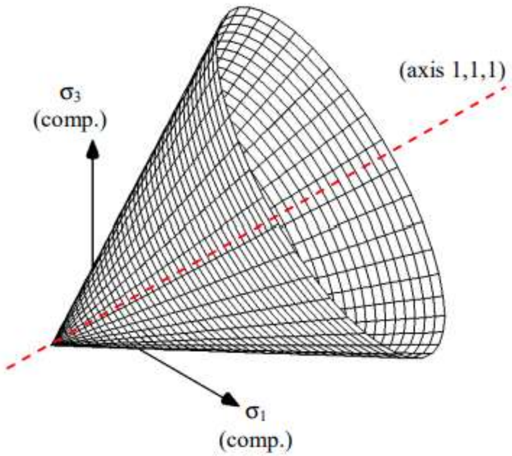


- Use the embedding FE technique

$$\boldsymbol{K}_{nano} = \boldsymbol{K}_{cement} + \boldsymbol{K}_{fibers}$$

- Assume a Drucker-Prager yield criterion

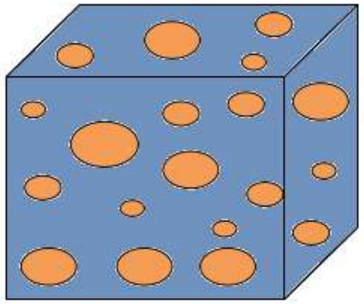
$$(\sigma_1 - \sigma_2)^2 + (\sigma_1 - \sigma_3)^2 + (\sigma_2 - \sigma_3)^2 - 0.88(\mathrm{I}_1 + 23.22)^2 = 0$$



Modeling of microscale RVE

- Embed the small aggregates on a matrix composed of the reinforced cement paste

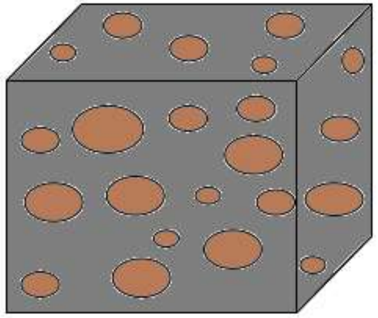
$$\boldsymbol{K}_{micro} = \boldsymbol{K}_{nano} + \boldsymbol{K}_{aggregates}$$



Modeling of mesoscale RVE

- Embed the larger aggregates on a matrix composed of the reinforced composite

$$\boldsymbol{K}_{meso} = \boldsymbol{K}_{micro} + \boldsymbol{K}_{aggregates}$$



Multiscale modeling

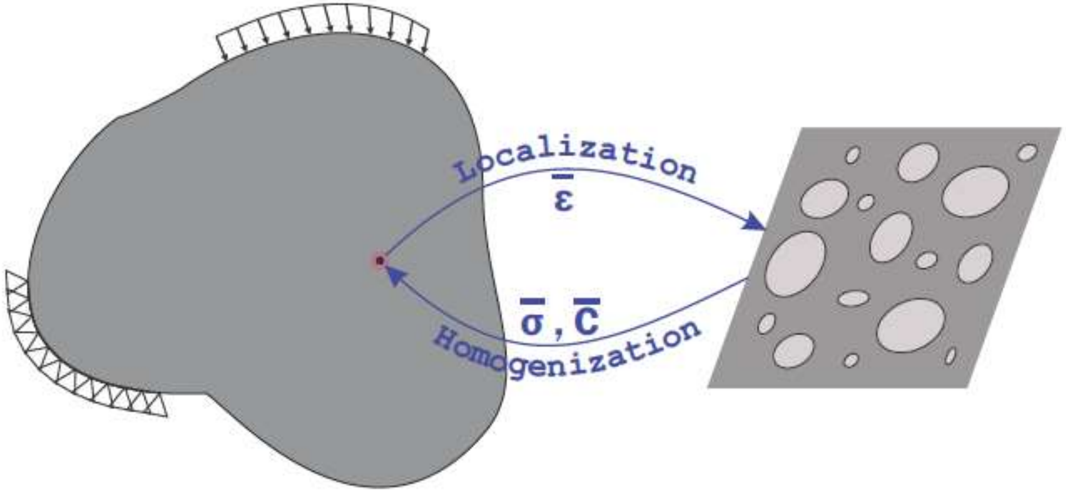
Pass information from lower to upper scales

- Apply BC on RVE according to $\bar{\boldsymbol{\varepsilon}}$ (localization):

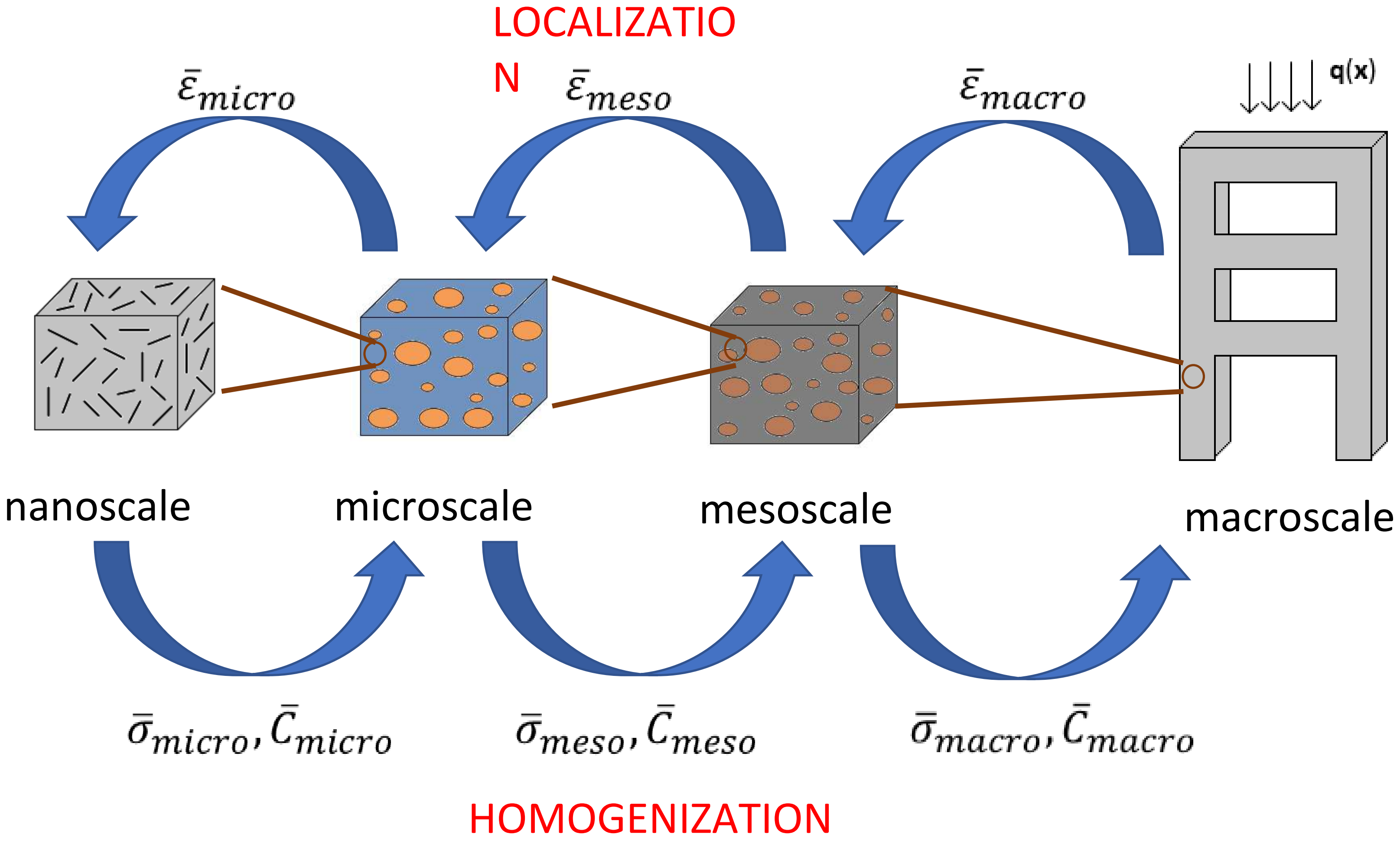
- Discretize and solve RVE

- Return $\bar{\boldsymbol{\sigma}}$ and $\bar{\boldsymbol{C}}$ (homogenization):

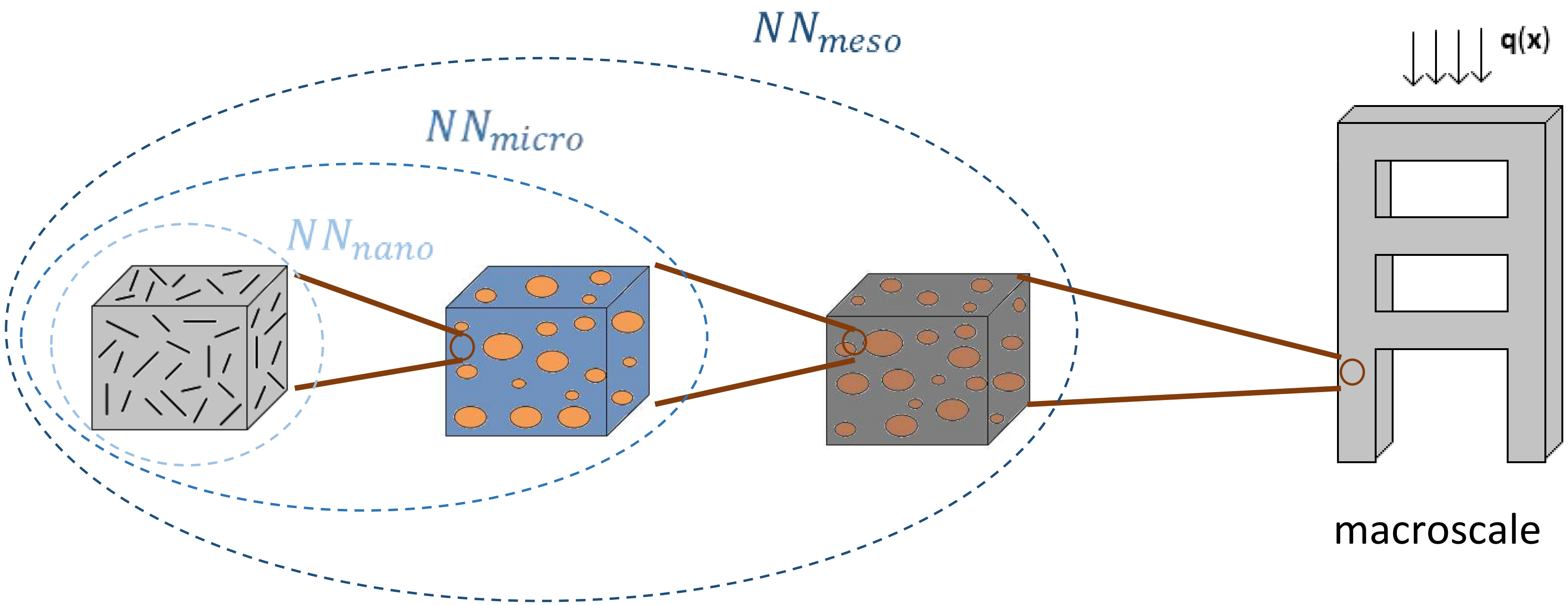
$$\bar{\boldsymbol{\sigma}} = \frac{\mathbf{1}}{\|\boldsymbol{V}\|}\int_{\boldsymbol{V}} \boldsymbol{\sigma} d\boldsymbol{x}\,, \qquad \bar{\boldsymbol{C}} = \partial_{\bar{\boldsymbol{\varepsilon}}}\bar{\boldsymbol{\sigma}}$$



Use the FE^2 multiscale analysis to analyze structures comprised of composite concrete

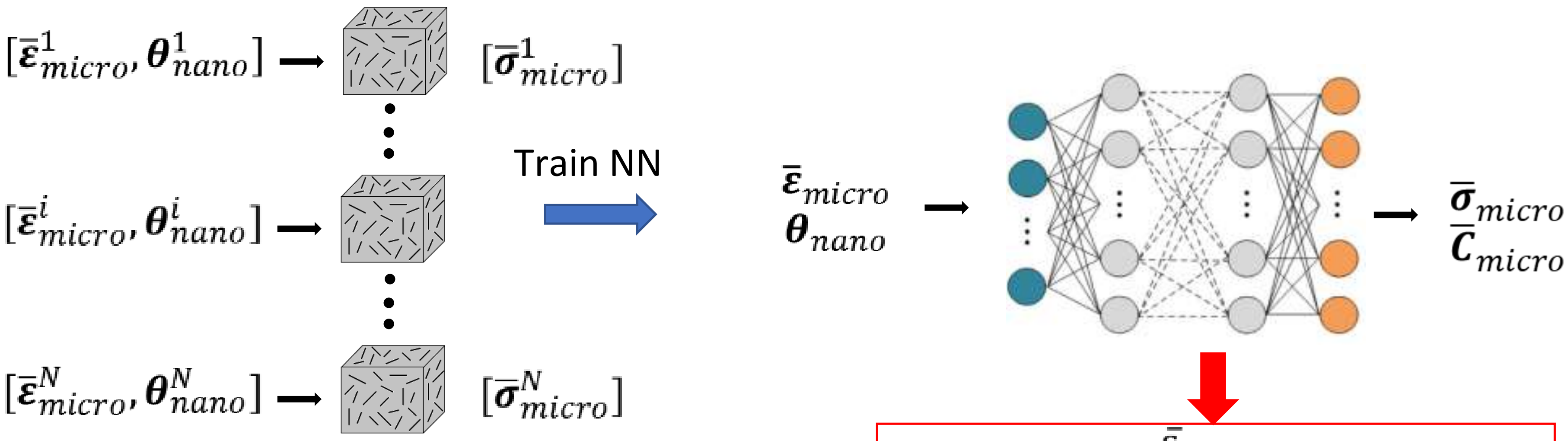


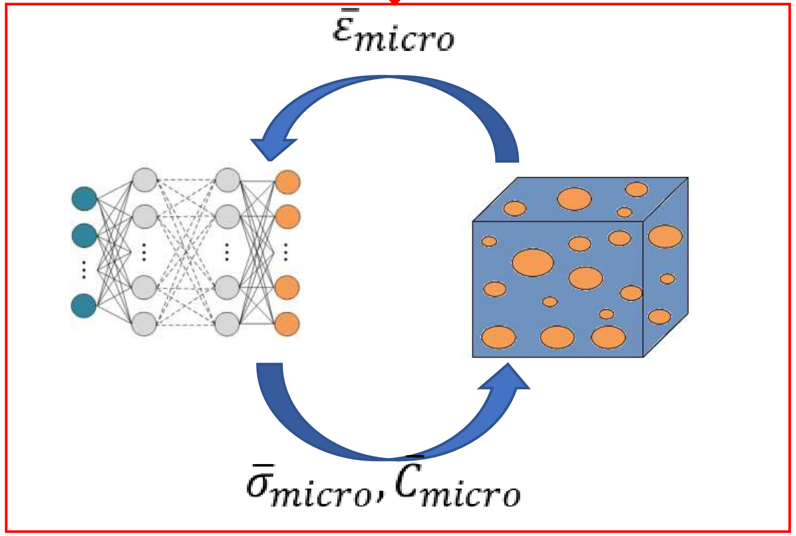
Substitute the triply nested FE2 scheme with one neural network



NN_{meso} → becomes our new concrete material

Offline (training) procedure: Starting from the nanoscale





$\boldsymbol{\theta}_{nano}$ = model input parameters at nanoscale:

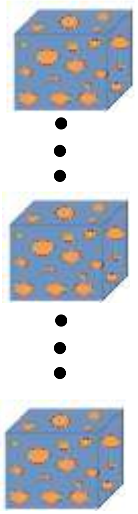
CNT wf%
CNT length, diameter, orientation
cement paste modulus of elasticity,
etc.

Offline (training) procedure: Starting from the nanoscale

$[\bar{\boldsymbol{\varepsilon}}^1_{meso}, \boldsymbol{\theta}^1_{micro}, \boldsymbol{\theta}^1_{nano}] \rightarrow$ $[\bar{\boldsymbol{\sigma}}^1_{meso}]$

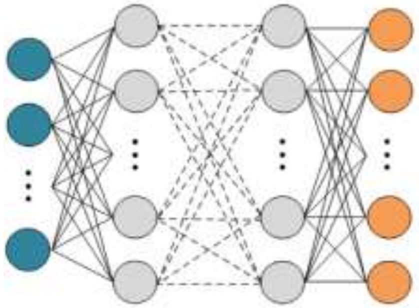
$[\bar{\boldsymbol{\varepsilon}}^i_{meso}, \boldsymbol{\theta}^i_{micro}, \boldsymbol{\theta}^i_{nano}] \rightarrow$

$[\bar{\boldsymbol{\varepsilon}}^N_{meso}, \boldsymbol{\theta}^N_{micro}, \boldsymbol{\theta}^N_{nano}] \rightarrow$ $[\bar{\boldsymbol{\sigma}}^N_{meso}]$

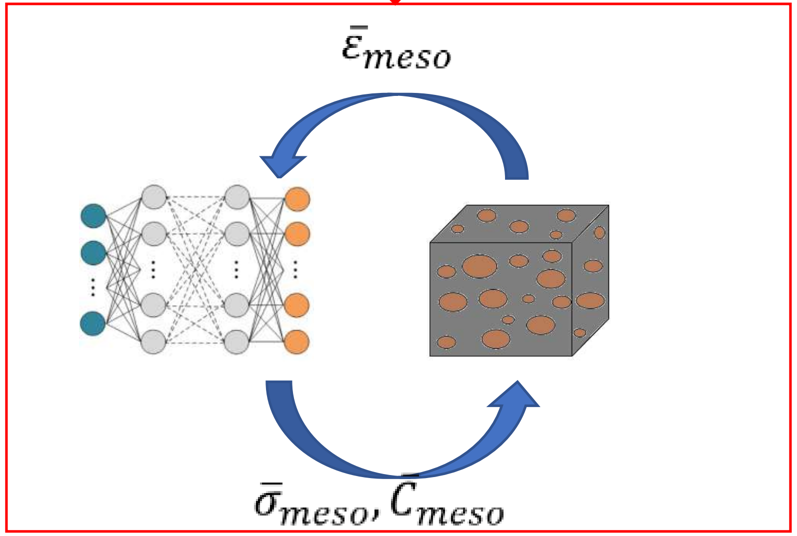


Train NN

$\bar{\boldsymbol{\varepsilon}}_{micro}$
$\boldsymbol{\theta}_{micro}$
$\boldsymbol{\theta}_{nano}$ $\rightarrow$

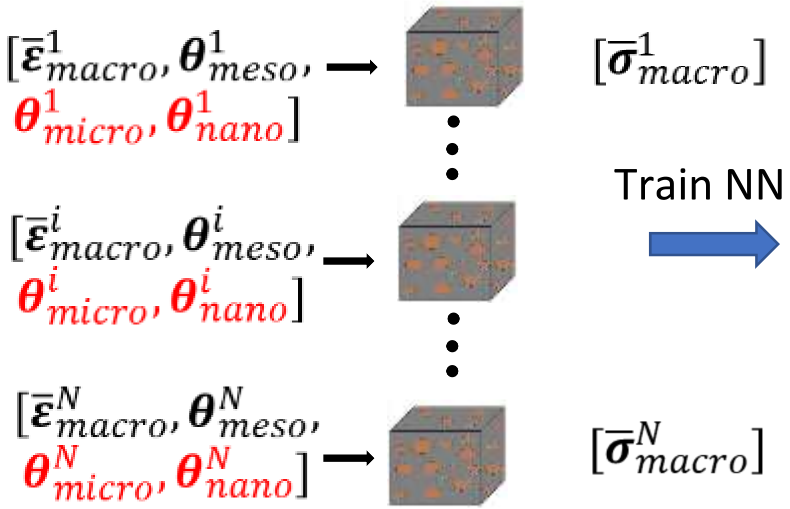


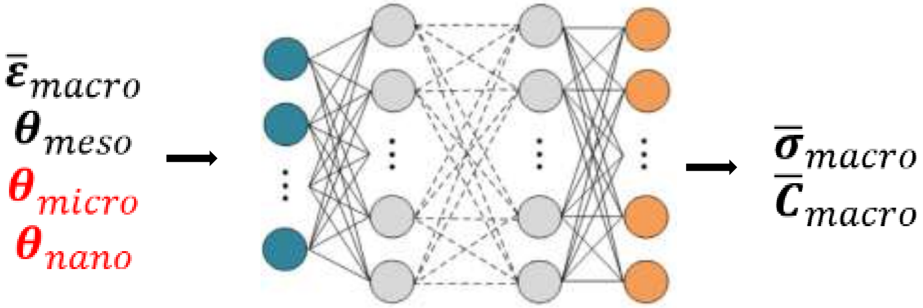
$\rightarrow$ $\bar{\boldsymbol{\sigma}}_{meso}$
$\bar{\boldsymbol{C}}_{meso}$

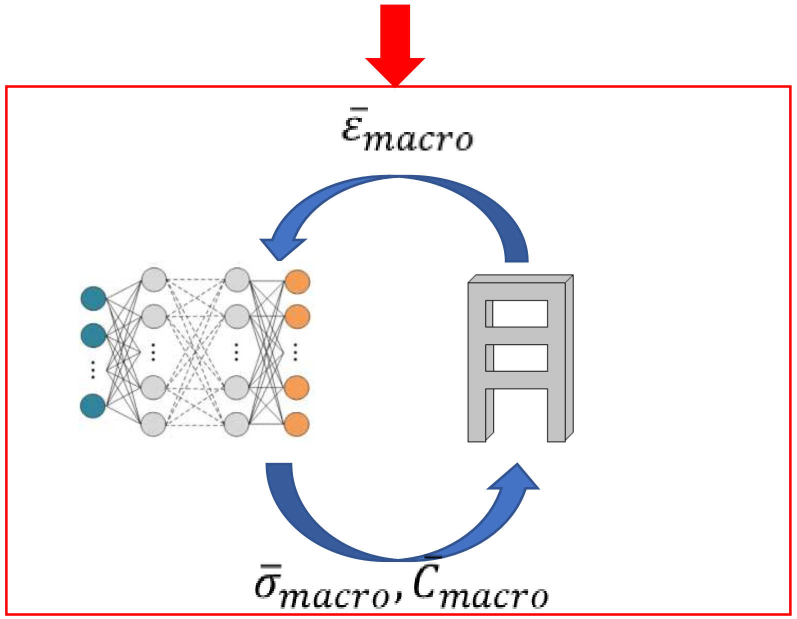


$\boldsymbol{\theta}_{micro}$= model input parameters at microscale:
- aggregates vf%
- aggregates size
- aggregates modulus of elasticity,
- etc.

Offline (training) procedure: Starting from the nanoscale







$\boldsymbol{\theta}_{meso}$= model input parameters at mesoscale:

aggregates vf%
aggregates size
aggregates modulus of elasticity,
etc.

Computational Gain

➢ One analysis of the macroscale problem without the surrogate requires:

(#Gauss points at macroscale) x (mesoscale RVE analyses) x
(#Gauss points at mesoscale RVE) x (microscale RVE analyses) x
(#Gauss points at mesoscale RVE) x (nanoscale RVE analyses)

Vs

.

➢ One analysis of the macroscale problem using the surrogate requires:

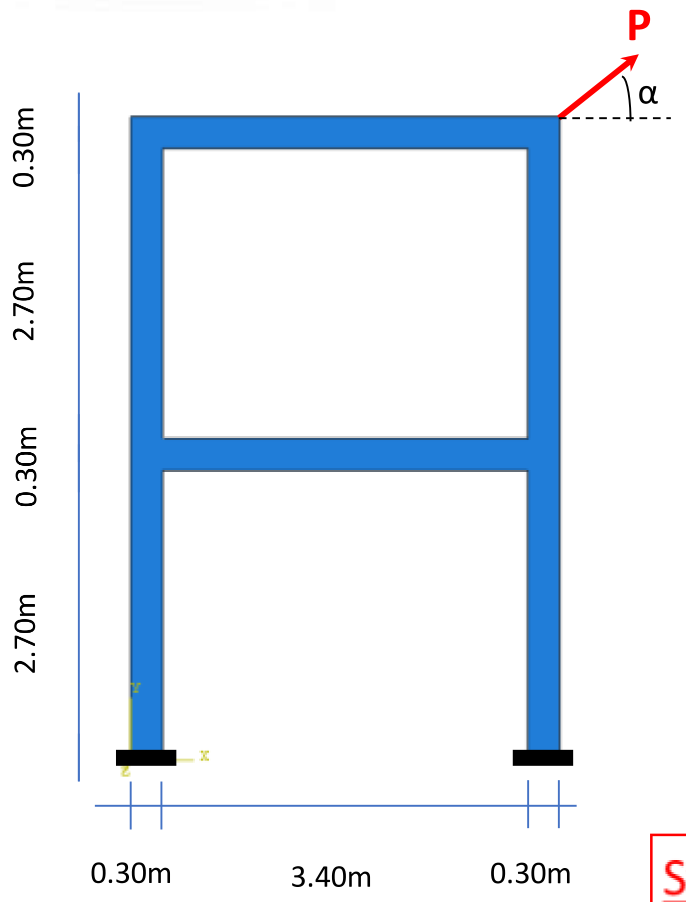
(#Gauss points at macroscale) x (mesoscale Neural Network evaluations)

Drastic cost reduction => Allows us to perform repeated model evaluations

Uncertainty quantification

Optimization

Sensitivity analysis



Problem setting

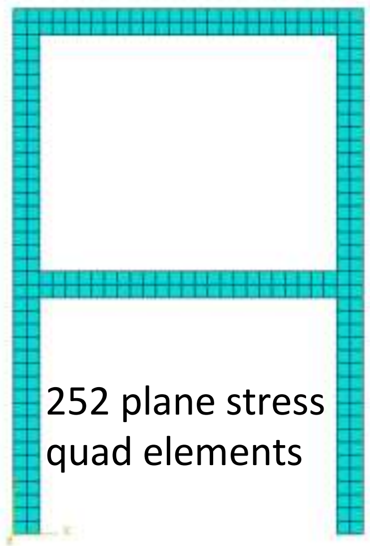
Deterministic parameters:

$$\mathrm{E}_{\mathrm{cement}} = 20\ \mathrm{Gpa}$$
$$wf_{CNTs} = 1\%$$
$$vf_{aggregates,micro} = 40\%$$
$$vf_{aggregates,meso} = 40\%$$
$$P = 100\ kN$$

Stochastic parameters:

$$a \sim N(0, \left(\frac{\pi}{5}\right)^2)$$

FEM discretization:



Design variables: CNT orientation $\{\theta_1, \ldots, \theta_{252}\}$ at each quad element

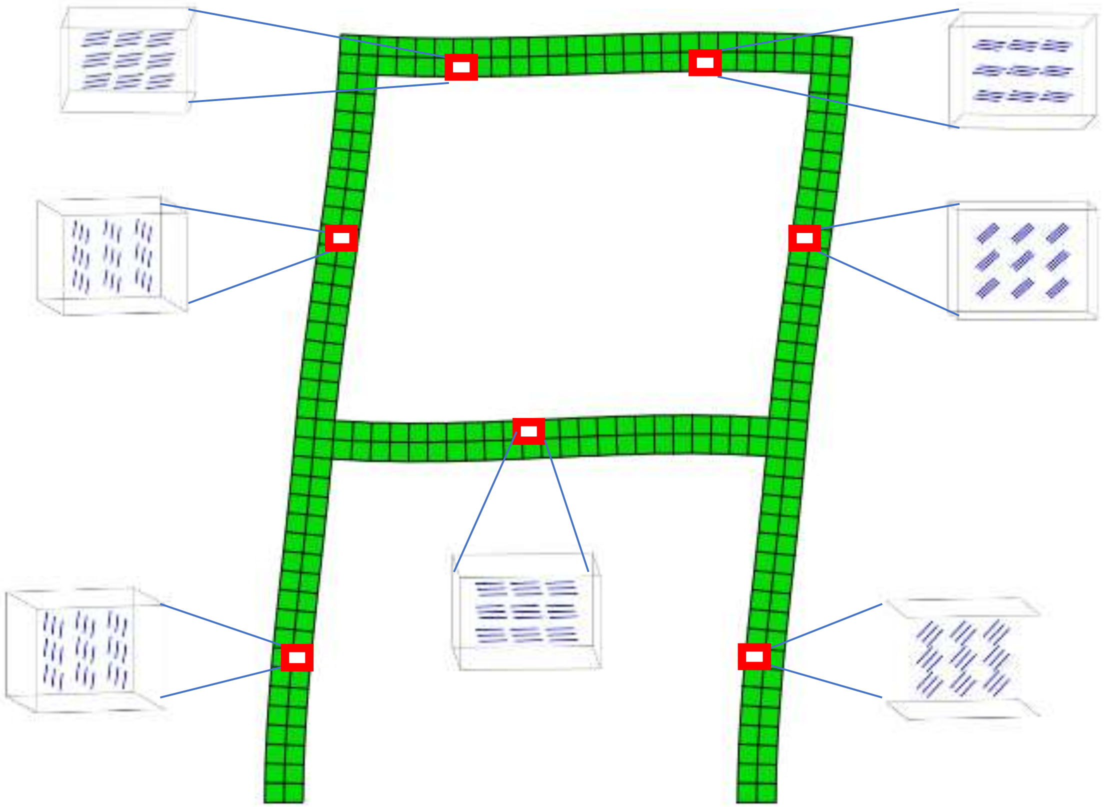
Stochastic Optimization Problem:

$$argmin_{\{\theta_1,\ldots,\theta_{252}\}\in[0,2\pi)}\ \mathcal{E}[||\boldsymbol{U}||] + Std[||\boldsymbol{U}||]$$

Results

<u>Stochastic Optimization Problem</u>:

$$argmin_{\{\theta_1,\ldots,\theta_{252}\}\in[0,2\pi)}\ \mathcal{E}[\|\boldsymbol{U}\|]+Std[\|\boldsymbol{U}\|]$$



Genetic Algorithm: population size 1000
50 generations
crossover fraction 0.6

100 Monte Carlo Simulations for each candidate solution

➢ A total of $5 \cdot 10^6$ deterministic analyses

$$\frac{\mathcal{E}[\|\boldsymbol{U}\|]+Std[\|\boldsymbol{U}\|]}{(\mathcal{E}[\|\boldsymbol{U}\|]+Std[\|\boldsymbol{U}\|])^{unreinforced}}=86\%$$

- A multiscale model has been proposed for CNT-reinforced concrete.
- It is capable of taking into account all physical mechanisms, arising at different scales of the problem.
- The immense computational requirements of this complex model have been effectively tackled using artificial neural networks.

Thank you for your attention