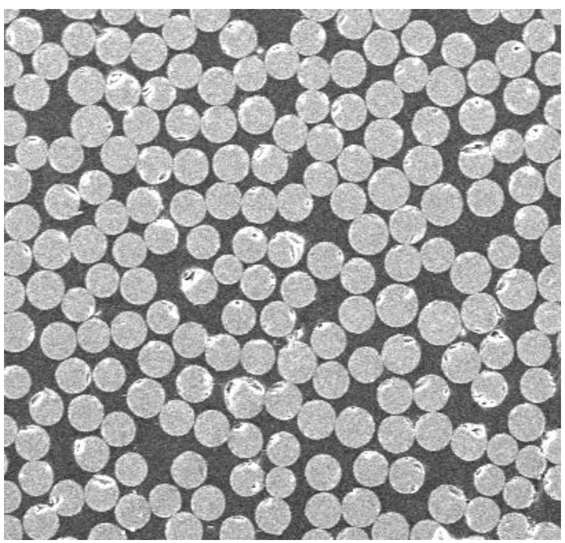
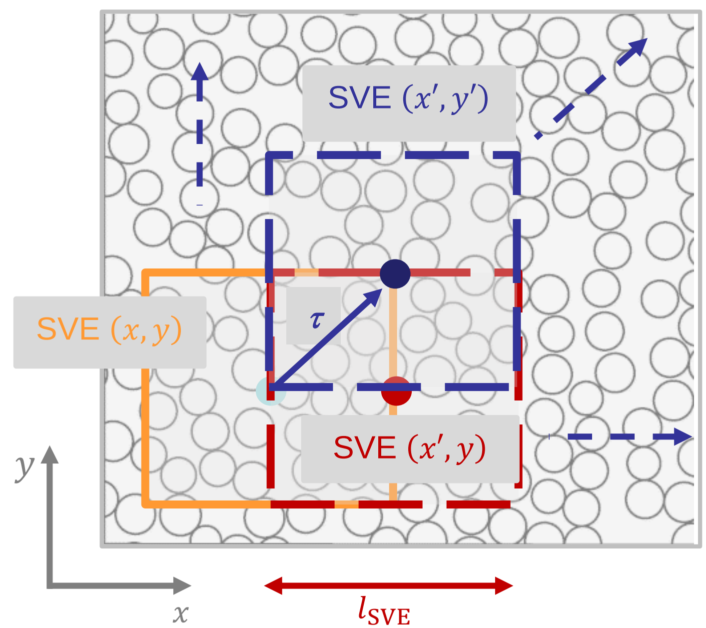
A stochastic Mean-Field-Homogenization-based micro-mechanical model of unidirectional composites

L. Wu, J. M. Calleja, V.-D. Nguyen, L. Noels





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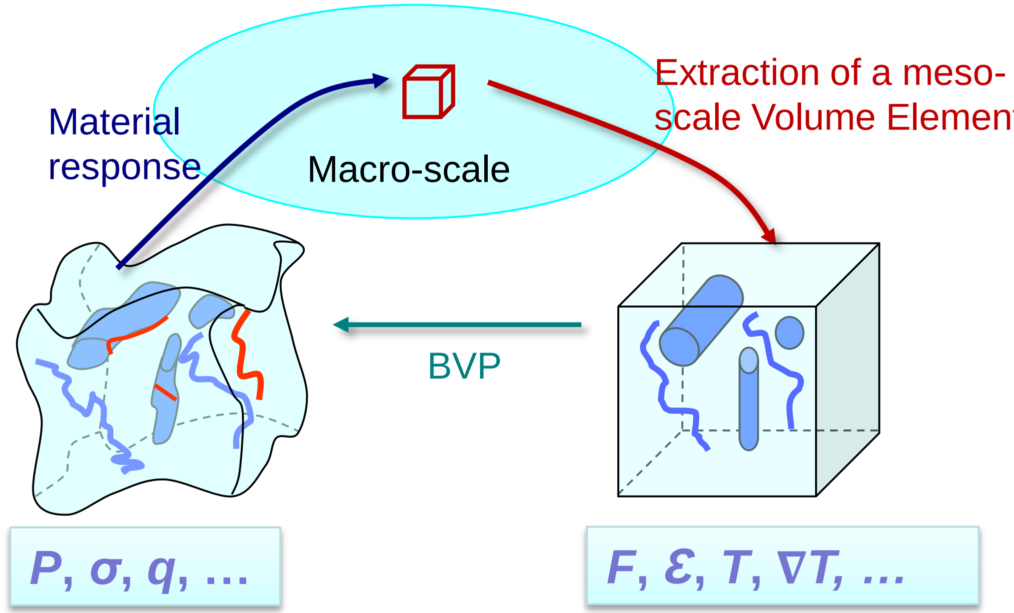
Objectives

- Multi-scale modelling
  - 2 problems are solved concurrently
    - The macro-scale problem
    - The meso-scale problem (on a meso-scale Volume Element)
  - Length-scales separation

    $L_{macro} >> L_{VE} >> L_{micro}$



BVP on a meso-scale Volume Element

Direct FE simulation vs. Semi-analytical method

- All the details of SVE

- General information e.g. volume fraction of inclusions,

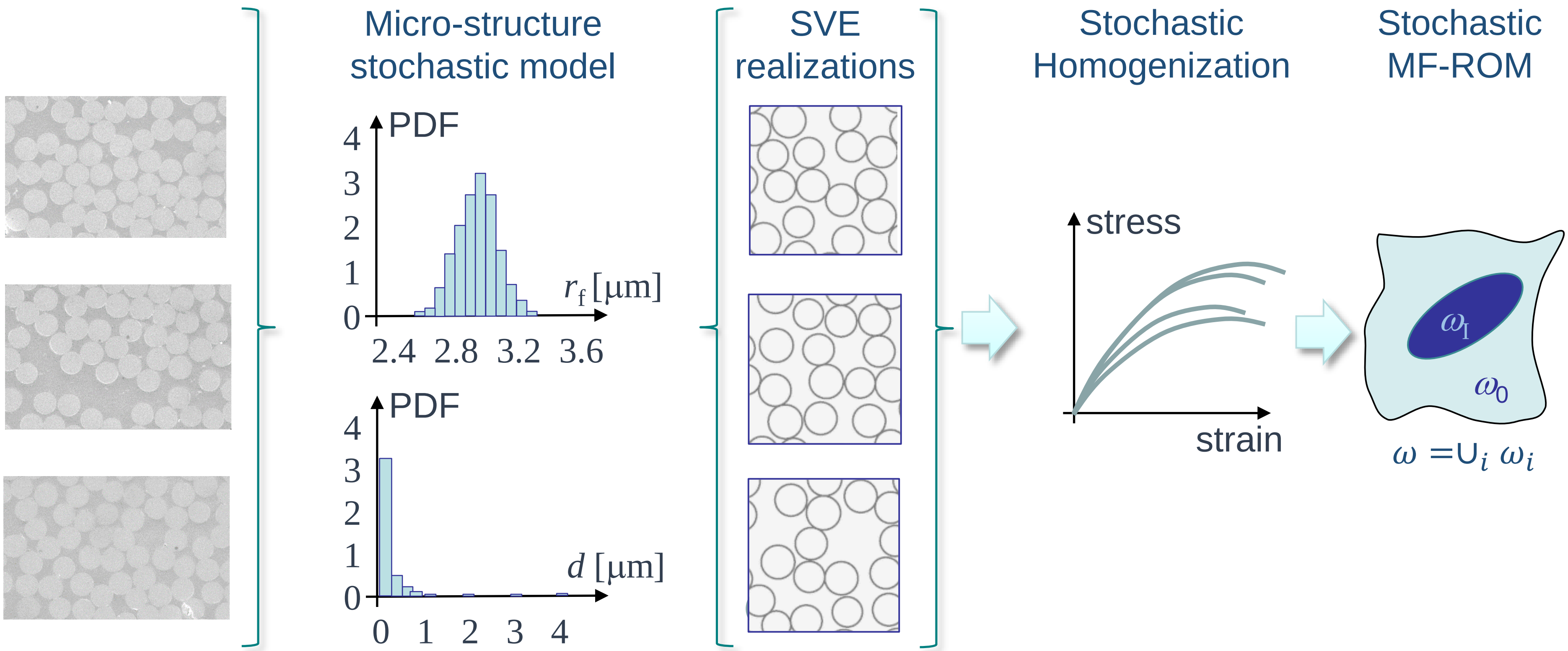
- Failure of composite materials:
  - Statistical representativity is lost

    $L_{macro} >> L_{VE} \sim L_{micro}$

- Main objective: To develop an efficient integrated stochastic multiscale approach to predict failure of composites

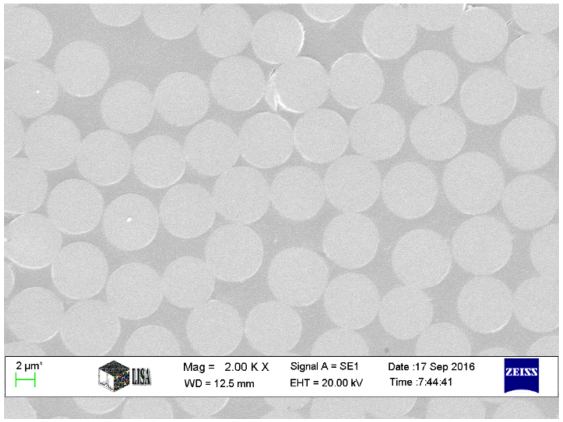
Methodology

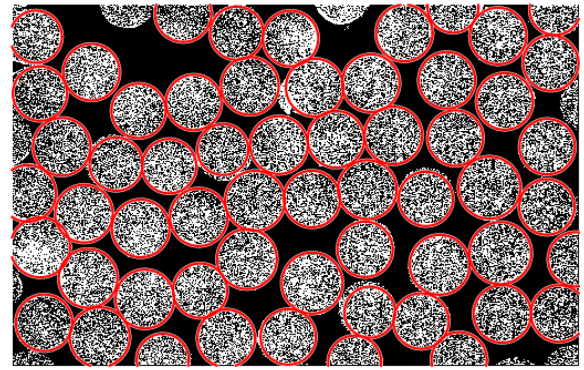
- Proposed methodology
  - To develop a stochastic Mean Field Homogenization method able to predict the probabilistic distribution of material response at an intermediate scale from micro-structural constituents characterization

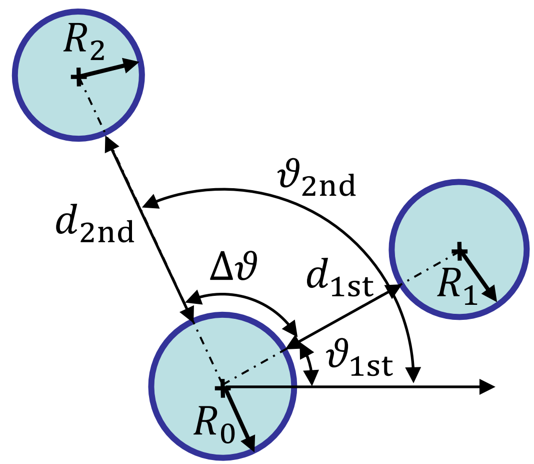


Experimental measurements

- Uncertainty quantification of micro-structure & micro-structure generator
  - 2000x and 3000x SEM images, fibers detection





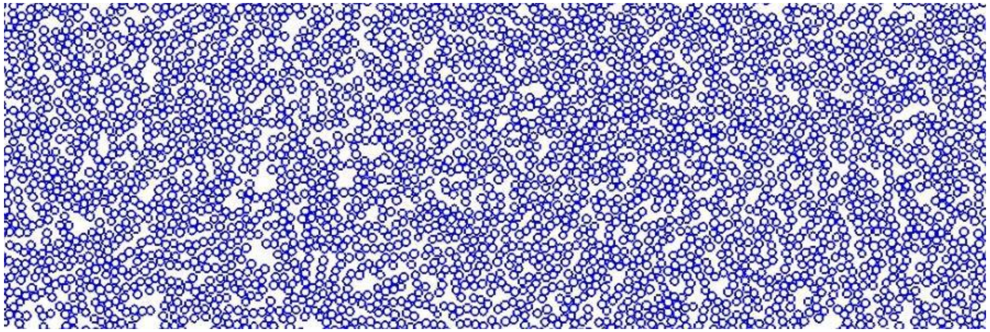


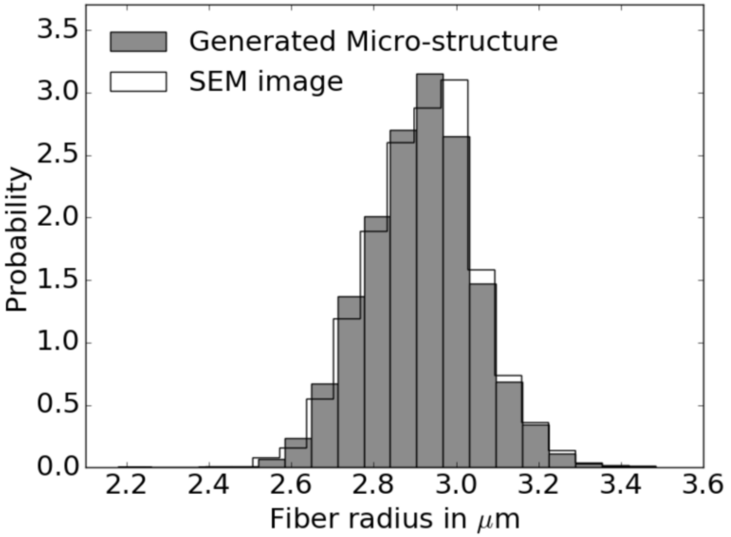
  - Basic geometric information
  - Distributions Random variables:
    - $p_R(r)$,
    - $p_{d_{1\text{st}}}(d)$,
    - $p_{\vartheta_{1\text{st}}}(\theta)$,
    - $p_{\Delta d}(d)$ with $\Delta d = d_{2\text{nd}} - d_{1\text{st}}$
    - $p_{\Delta\vartheta}(\theta)$ with $\Delta\vartheta = \vartheta_{2\text{nd}} - \vartheta_{1\text{st}}$

* L. Wu, C.N. Chung, Z. Major, L. Adam, L. Noels, From SEM images to elastic responses: A stochastic multiscale analysis of UD fiber reinforced composites, Compos. Struct. (ISSN: 0263-8223) 189 (2018a) 206–227

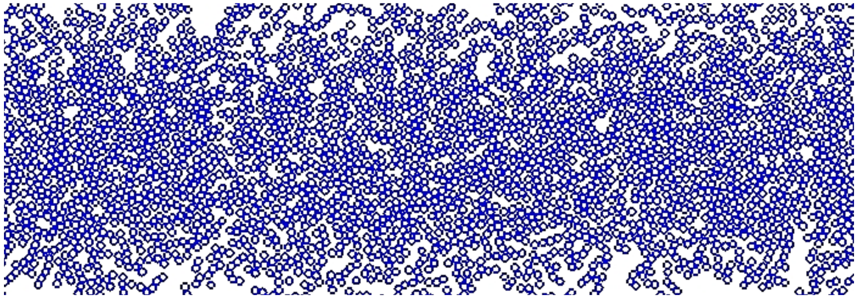
Micro-structure stochastic model

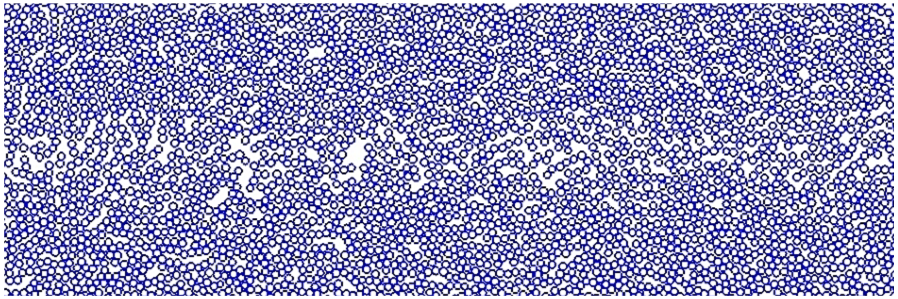
- Numerical micro-structures are generated by a fiber additive process
  - Arbitrary size
  - Arbitrary number





  - Possibility to generate non-homogenous distributions





Stochastic homogenization on the SVEs

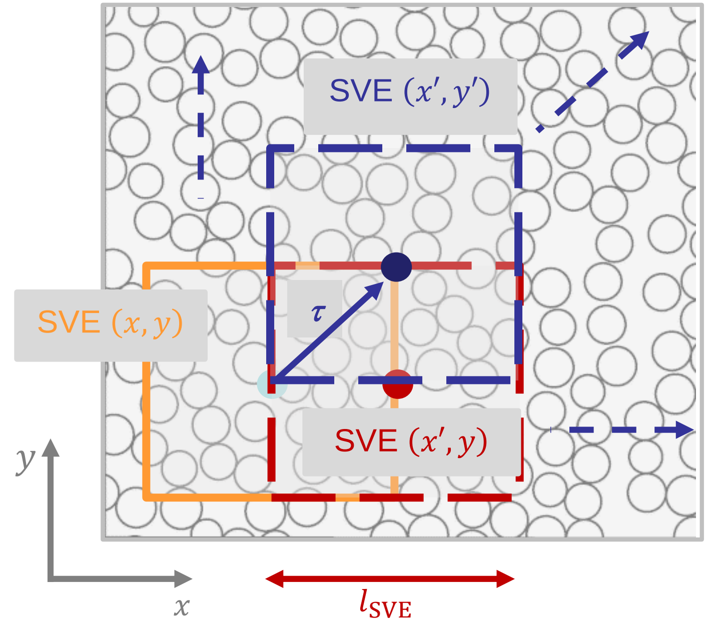
- Window technique
  - Extraction of Stochastic Volume Elements
    - $l_{\text{SVE}} = 25\ \mu m$
    - Correlation

$$R_{\mathbf{rs}}(\boldsymbol{\tau}) = \frac{\mathbb{E}\left[\left(r(\boldsymbol{x}) - \mathbb{E}(r)\right)\left(s(\boldsymbol{x}+\boldsymbol{\tau}) - \mathbb{E}(s)\right)\right]}{\sqrt{\mathbb{E}\left[\left(r - \mathbb{E}(r)\right)^2\right]}\sqrt{\mathbb{E}\left[\left(s - \mathbb{E}(s)\right)^2\right]}}$$

  - For each SVE
    - Extract apparent homogenized material tensor $\mathbb{C}_{\text{M}}$

$$\begin{cases} \boldsymbol{\varepsilon}_{\text{M}} = \dfrac{1}{V(\omega)} \displaystyle\int_{\omega} \boldsymbol{\varepsilon}_{\text{m}} d\omega \\ \boldsymbol{\sigma}_{\text{M}} = \dfrac{1}{V(\omega)} \displaystyle\int_{\omega} \boldsymbol{\sigma}_{\text{m}} d\omega \\ \mathbb{C}_{\text{M}} = \dfrac{\partial \boldsymbol{\sigma}_{\text{M}}}{\partial \boldsymbol{u}_{\text{M}} \otimes \boldsymbol{\nabla}_{\text{M}}} \end{cases}$$

    - Consistent boundary conditions:
      - Periodic (PBC)
      - Minimum kinematics (SUBC)
      - Kinematic (KUBC)

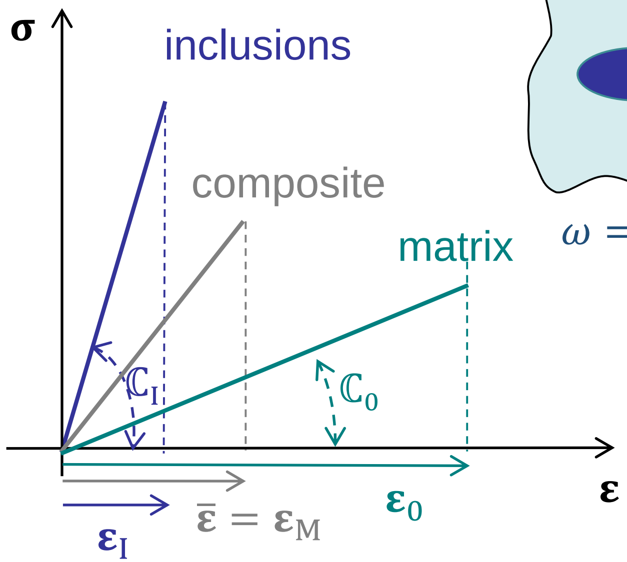


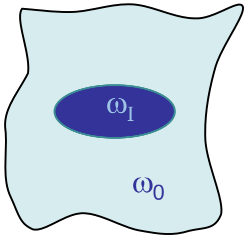
Stochastic Mean-Field Homogenization

- Mean-Field-Homogenization (MFH)
  - Linear composites

$$\begin{cases} \boldsymbol{\sigma}_{\mathrm{M}} = \bar{\boldsymbol{\sigma}} = v_0 \boldsymbol{\sigma}_0 + v_{\mathrm{I}} \boldsymbol{\sigma}_{\mathrm{I}} \\ \boldsymbol{\varepsilon}_{\mathrm{M}} = \bar{\boldsymbol{\varepsilon}} = v_0 \boldsymbol{\varepsilon}_0 + v_{\mathrm{I}} \boldsymbol{\varepsilon}_{\mathrm{I}} \\ \boldsymbol{\varepsilon}_{\mathrm{I}} = \mathbb{B}^{\varepsilon}(\mathrm{I}, \mathbb{C}_0, \mathbb{C}_{\mathrm{I}}) : \boldsymbol{\varepsilon}_0 \end{cases}$$

$$\Rightarrow \mathbb{C}_{\mathrm{M}} = \mathbb{C}_{\mathrm{M}}(\mathrm{I}, \mathbb{C}_0, \mathbb{C}_{\mathrm{I}}, v_{\mathrm{I}})$$





$\omega = \cup_i \omega_i$

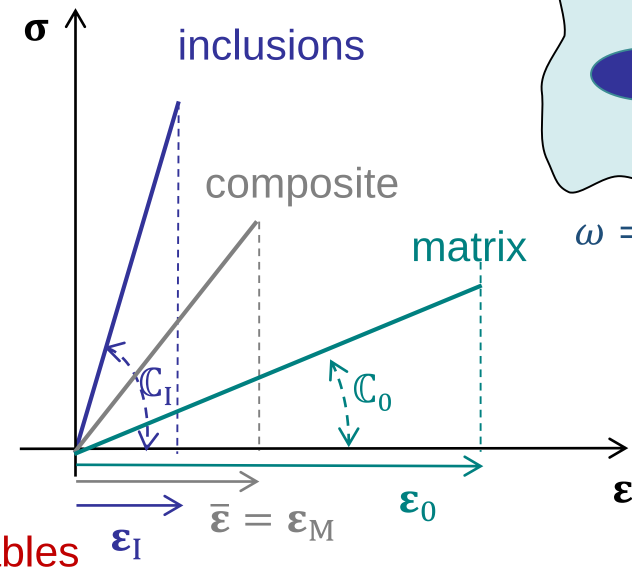
  - We use Mori-Tanaka assumption for $\mathbb{B}^{\varepsilon}(\mathrm{I}, \mathbb{C}_0, \mathbb{C}_{\mathrm{I}})$
- Stochastic MFH
  - How to define randomness?

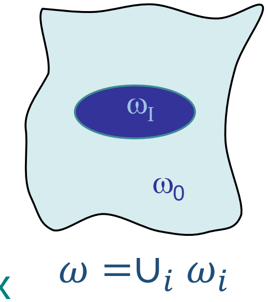
L. Wu, V.-D. Nguyen, L. Adam, L. Noels, An inverse micro-mechanical analysis toward the stochastic homogenization of nonlinear random composites (2019)

- Mean-Field-Homogenization (MFH)
  - Linear composites

$$\begin{cases} \boldsymbol{\sigma}_{\mathrm{M}} = \bar{\boldsymbol{\sigma}} = v_0 \boldsymbol{\sigma}_0 + v_{\mathrm{I}} \boldsymbol{\sigma}_{\mathrm{I}} \\ \boldsymbol{\varepsilon}_{\mathrm{M}} = \bar{\boldsymbol{\varepsilon}} = v_0 \boldsymbol{\varepsilon}_0 + v_{\mathrm{I}} \boldsymbol{\varepsilon}_{\mathrm{I}} \\ \boldsymbol{\varepsilon}_{\mathrm{I}} = \mathbb{B}^{\varepsilon}(\mathrm{I}, \mathbb{C}_0, \mathbb{C}_{\mathrm{I}}) : \boldsymbol{\varepsilon}_0 \end{cases}$$

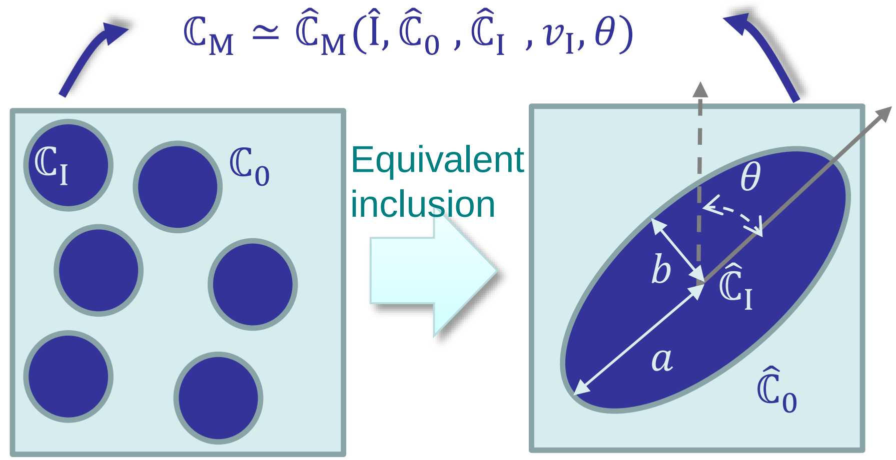
$\Rightarrow$ $\hat{\mathbb{C}}_{\mathrm{M}} = \hat{\mathbb{C}}_{\mathrm{M}}(\mathrm{I}, \mathbb{C}_0, \mathbb{C}_{\mathrm{I}}, v_{\mathrm{I}})$ → Defined as random variables





- Consider an equivalent system
  - For each SVE realization i:
    - $\Rightarrow$ $\mathbb{C}_{\mathrm{M}}$ and v_{I} known
  - Anisotropy from $\mathbb{C}_{\mathrm{M}}^{i}$
    - $\Rightarrow$ θ is evaluated
  - Fiber behavior uniform
    - $\Rightarrow$ $\hat{\mathbb{C}}_{\mathrm{I}}$ for one SVE

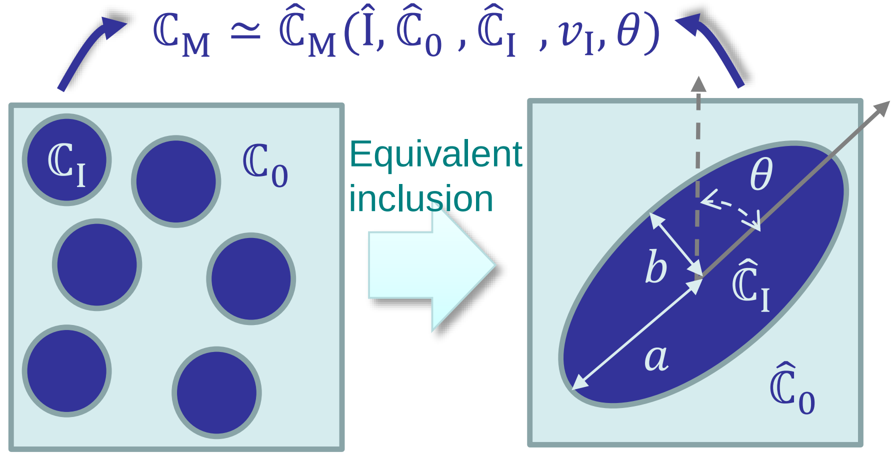
$$\mathbb{C}_{\mathrm{M}} \simeq \hat{\mathbb{C}}_{\mathrm{M}}(\hat{\mathrm{I}}, \hat{\mathbb{C}}_0, \hat{\mathbb{C}}_{\mathrm{I}}, v_{\mathrm{I}}, \theta)$$

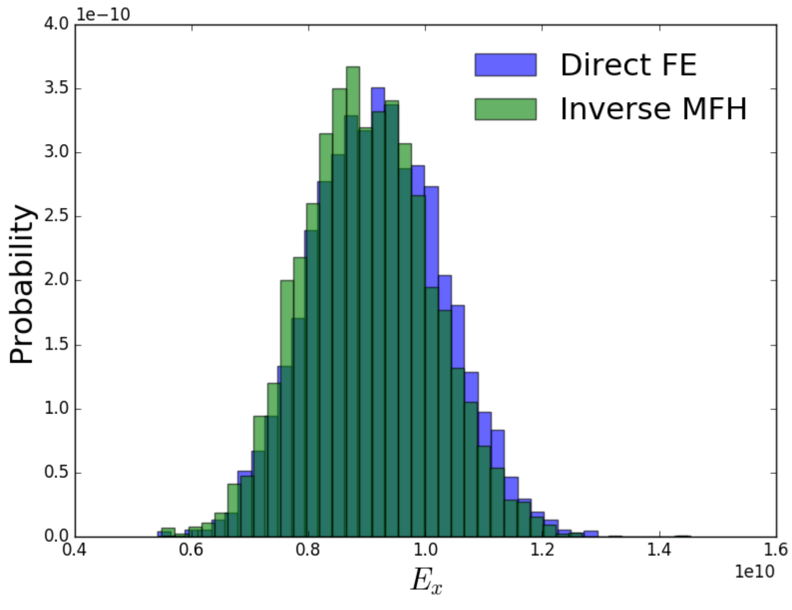


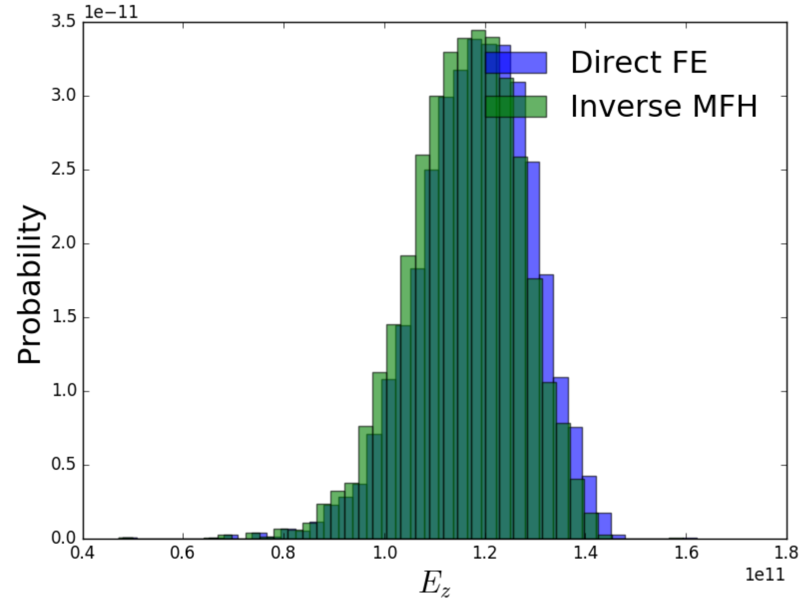
  - Remaining optimization problem: $\min_{\frac{a}{b}, \hat{E}_0, \hat{\nu}_0} \left\| \mathbb{C}_{\mathrm{M}} - \hat{\mathbb{C}}_{\mathrm{M}}\left(\frac{a}{b}, \hat{E}_0, \hat{\nu}_0; v_{\mathrm{I}}, \theta, \hat{\mathbb{C}}_{\mathrm{I}}\right) \right\|$

Stochastic Mean-Field Homogenization

- Inverse stochastic identification
  - Comparison of homogenized properties from SVE realizations and stochastic MFH







* L. Wu, C. Nghia Chung, Z. Major, L. Adam, L. Noels, A micro-mechanics-based inverse study for stochastic order reduction of elastic UD-fiber reinforced composites analyzes, Internat. J. Numer. Methods Engrg. (ISSN: 0263-8223) 115 (2018b) 1430–1456

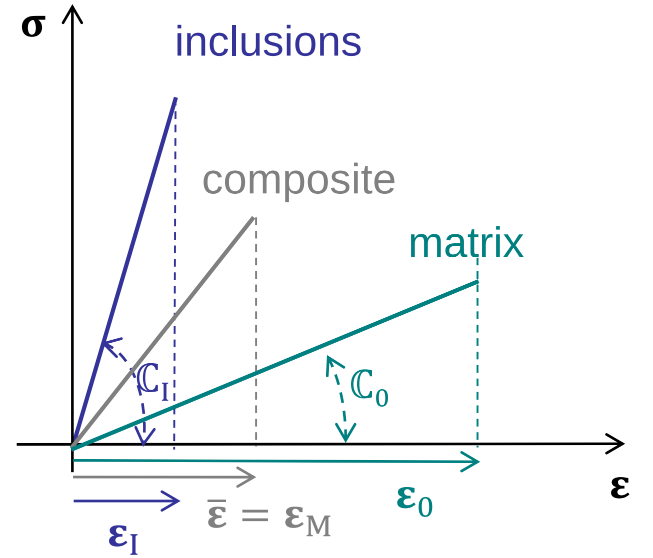
- Non-linear Mean-Field-homogenization
  - Linear composites

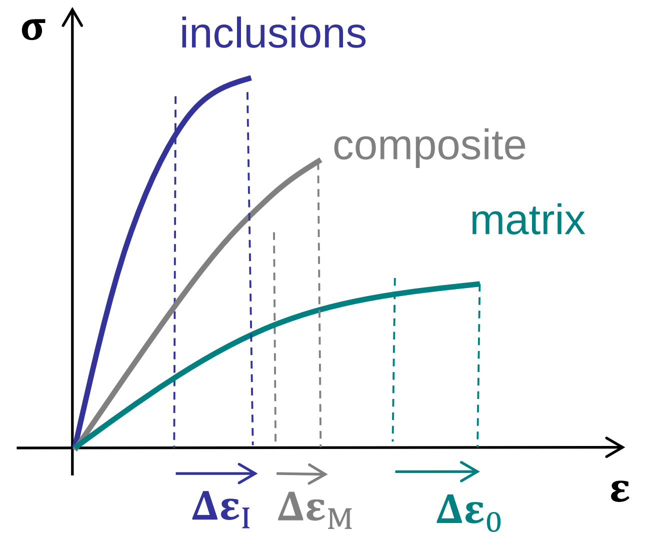
$$\begin{cases} \boldsymbol{\sigma}_\mathrm{M} = \bar{\boldsymbol{\sigma}} = v_0 \boldsymbol{\sigma}_0 + v_\mathrm{I} \boldsymbol{\sigma}_\mathrm{I} \\ \boldsymbol{\varepsilon}_\mathrm{M} = \bar{\boldsymbol{\varepsilon}} = v_0 \boldsymbol{\varepsilon}_0 + v_\mathrm{I} \boldsymbol{\varepsilon}_\mathrm{I} \\ \boldsymbol{\varepsilon}_\mathrm{I} = \mathbb{B}^\varepsilon(\mathrm{I}, \mathbb{C}_0, \mathbb{C}_\mathrm{I}) : \boldsymbol{\varepsilon}_0 \end{cases}$$

  - Non-linear composites

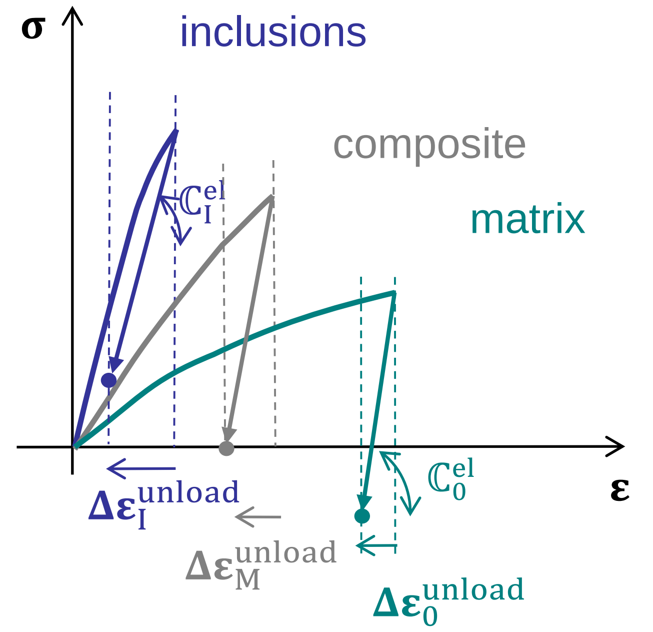
$$\begin{cases} \boldsymbol{\sigma}_\mathrm{M} = \bar{\boldsymbol{\sigma}} = v_0 \boldsymbol{\sigma}_0 + v_\mathrm{I} \boldsymbol{\sigma}_\mathrm{I} \\ \Delta\boldsymbol{\varepsilon}_\mathrm{M} = \overline{\Delta\boldsymbol{\varepsilon}} = v_0 \Delta\boldsymbol{\varepsilon}_0 + v_\mathrm{I} \Delta\boldsymbol{\varepsilon}_\mathrm{I} \\ \Delta\boldsymbol{\varepsilon}_\mathrm{I} = \mathbb{B}^\varepsilon(\mathrm{I}, \mathbb{C}_0^\mathrm{LCC}, \mathbb{C}_I^\mathrm{LCC}) : \Delta\boldsymbol{\varepsilon}_0 \end{cases}$$

Define a linear comparison composite material





- Incremental-secant Mean-Field-homogenization
  - Virtual elastic unloading from previous state
    - Composite material unloaded to reach the stress-free state
    - Residual stress in components



- Incremental-secant Mean-Field-homogenization
  - Virtual elastic unloading from previous state
    - Composite material unloaded to reach the stress-free state
    - Residual stress in components
  - Define Linear Comparison Composite
    - From unloaded state

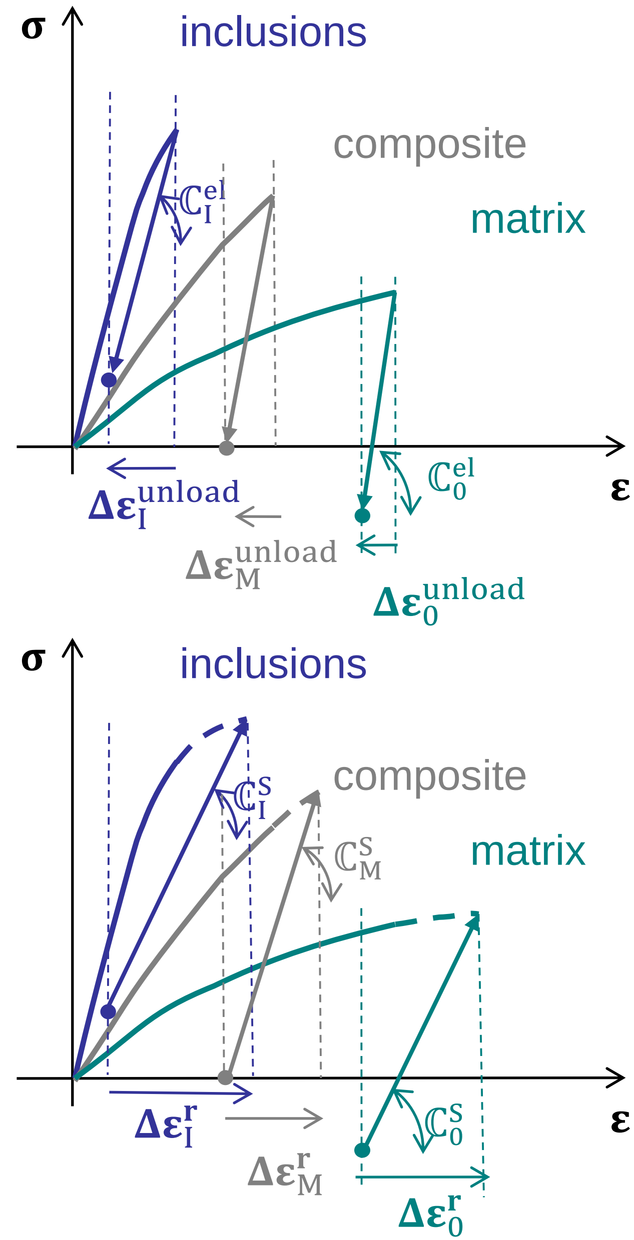
$$\Delta\boldsymbol{\varepsilon}^{\mathbf{r}}_{\mathrm{I}/0} = \Delta\boldsymbol{\varepsilon}_{\mathrm{I}/0} + \Delta\boldsymbol{\varepsilon}^{\mathrm{unload}}_{\mathrm{I}/0}$$

    - Incremental-secant loading

$$\begin{cases} \boldsymbol{\sigma}_{\mathrm{M}} = \bar{\boldsymbol{\sigma}} = v_0\boldsymbol{\sigma}_0 + v_{\mathrm{I}}\boldsymbol{\sigma}_{\mathrm{I}} \\ \Delta\boldsymbol{\varepsilon}^{\mathbf{r}}_{\mathrm{M}} = \overline{\Delta\boldsymbol{\varepsilon}} = v_0\Delta\boldsymbol{\varepsilon}^{\mathbf{r}}_0 + v_{\mathrm{I}}\Delta\boldsymbol{\varepsilon}^{\mathbf{r}}_{\mathrm{I}} \\ \Delta\boldsymbol{\varepsilon}^{\mathbf{r}}_{\mathrm{I}} = \mathbb{B}^{\varepsilon}\left(\mathrm{I}, \mathbb{C}^{\mathrm{S}}_0, \mathbb{C}^{\mathrm{S}}_{\mathrm{I}}\right) : \Delta\boldsymbol{\varepsilon}^{\mathbf{r}}_0 \end{cases}$$

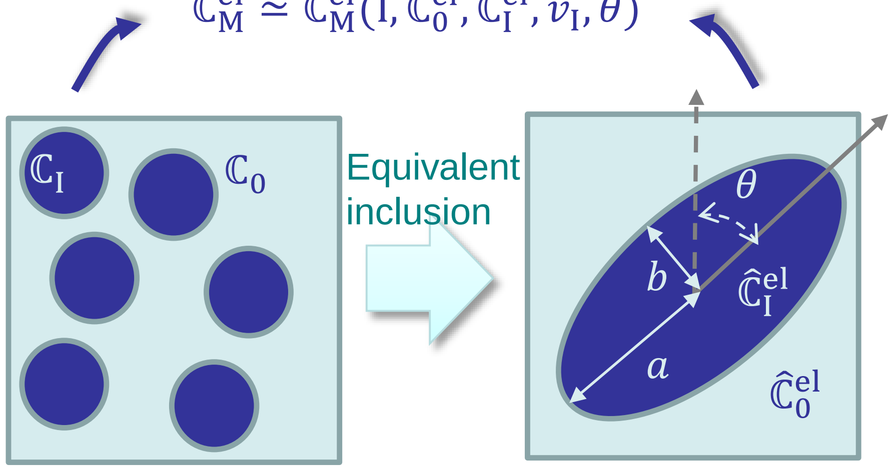
    - Incremental secant operator

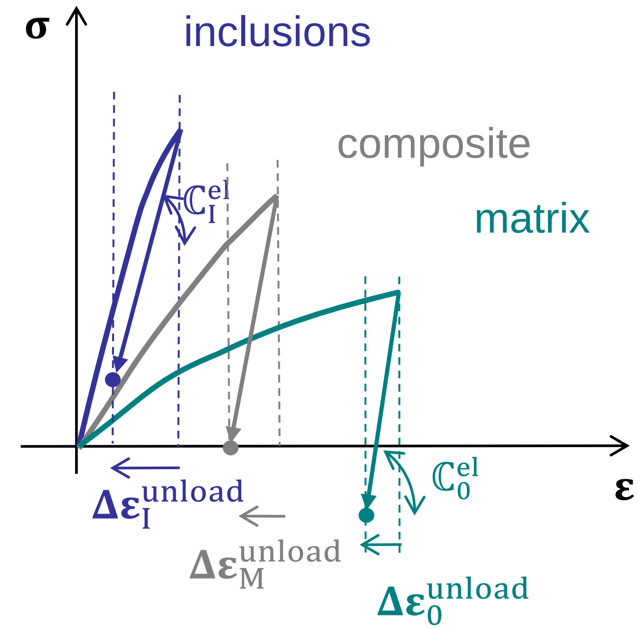
$$\Rightarrow \Delta\boldsymbol{\sigma}_{\mathrm{M}} = \mathbb{C}^{\mathrm{S}}_{\mathrm{M}}\left(\mathrm{I}, \mathbb{C}^{\mathrm{S}}_0, \mathbb{C}^{\mathrm{S}}_{\mathrm{I}}, v_{\mathrm{I}}\right) : \Delta\boldsymbol{\varepsilon}^{\mathbf{r}}_{\mathrm{M}}$$



- Non-linear inverse identification
  - First step from elastic response

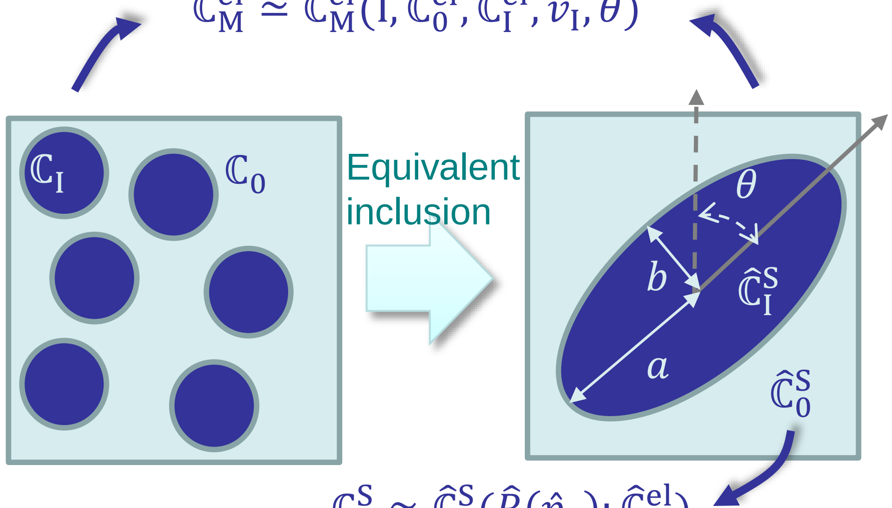
$$\mathbb{C}_{\mathrm{M}}^{\mathrm{el}} \simeq \hat{\mathbb{C}}_{\mathrm{M}}^{\mathrm{el}}(\hat{\mathrm{I}}, \hat{\mathbb{C}}_{0}^{\mathrm{el}}, \hat{\mathbb{C}}_{\mathrm{I}}^{\mathrm{el}}, v_{\mathrm{I}}, \theta)$$



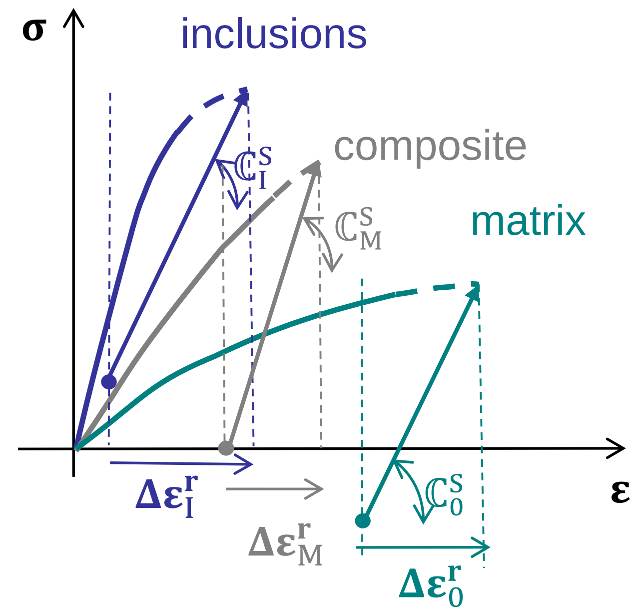


- Non-linear inverse identification
  - First step from elastic response

$$\mathbb{C}_{\mathrm{M}}^{\mathrm{el}} \simeq \hat{\mathbb{C}}_{\mathrm{M}}^{\mathrm{el}}(\hat{\mathrm{I}}, \hat{\mathbb{C}}_{0}^{\mathrm{el}}, \hat{\mathbb{C}}_{\mathrm{I}}^{\mathrm{el}}, v_{\mathrm{I}}, \theta)$$



$$\mathbb{C}_{0}^{\mathrm{S}} \simeq \hat{\mathbb{C}}_{0}^{\mathrm{S}}(\hat{R}(\hat{p}_0); \hat{\mathbb{C}}_{0}^{\mathrm{el}})$$

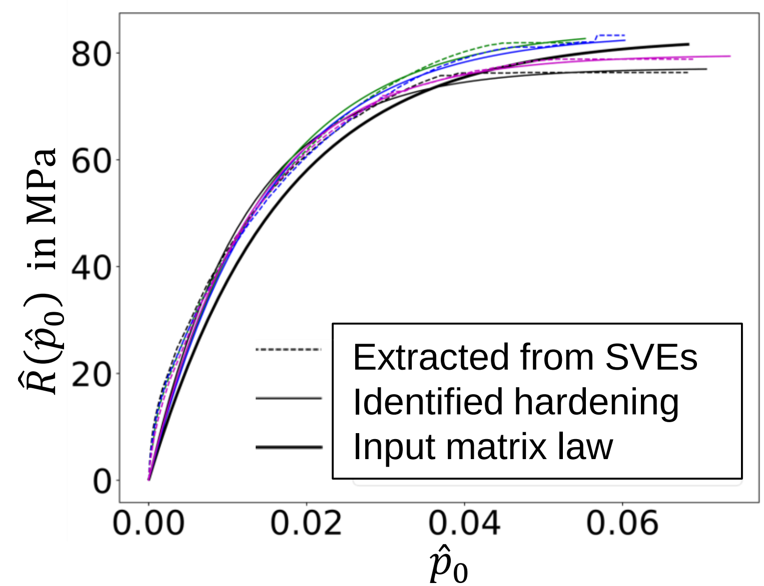


  - Second step from the LCC
    - New optimization problem

$$\Delta\boldsymbol{\sigma}_{\mathrm{M}} \simeq \hat{\mathbb{C}}_{\mathrm{M}}^{\mathrm{S}}\left(\hat{\mathrm{I}}, \hat{\mathbb{C}}_{0}^{\mathrm{S}}, \mathbb{C}_{\mathrm{I}}^{\mathrm{S}}, v_{\mathrm{I}}, \theta\right) : \Delta\boldsymbol{\varepsilon}_{\mathrm{M}}^{\mathrm{r}}$$

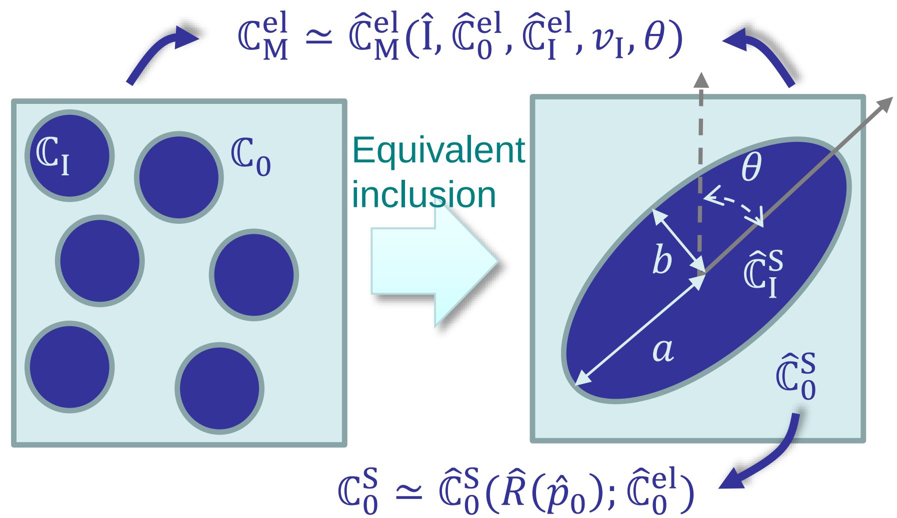
    - Extract the equivalent hardening $\hat{R}(\hat{p}_0)$ from the incremental secant tensor

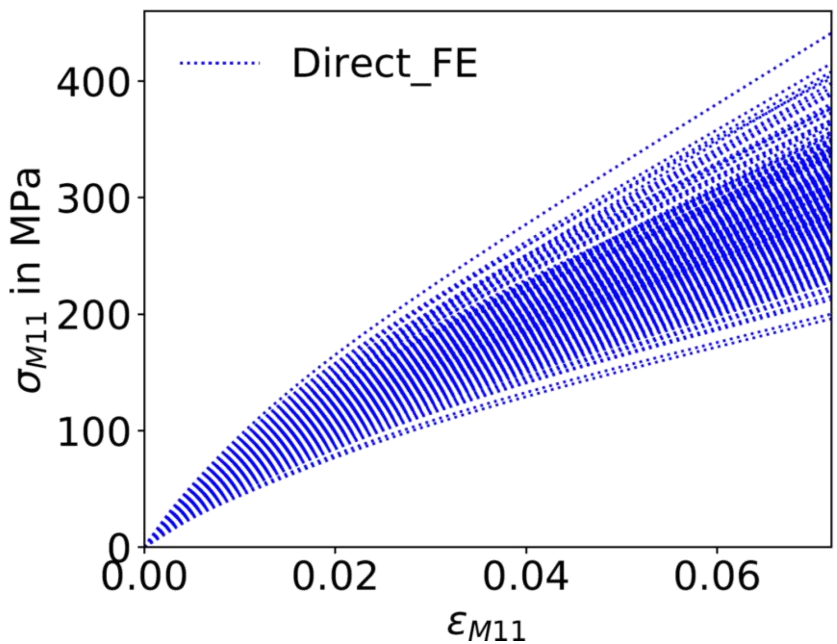
$$\mathbb{C}_{0}^{\mathrm{S}} \simeq \hat{\mathbb{C}}_{0}^{\mathrm{S}}(\hat{R}(\hat{p}_0); \hat{\mathbb{C}}_{0}^{\mathrm{el}})$$

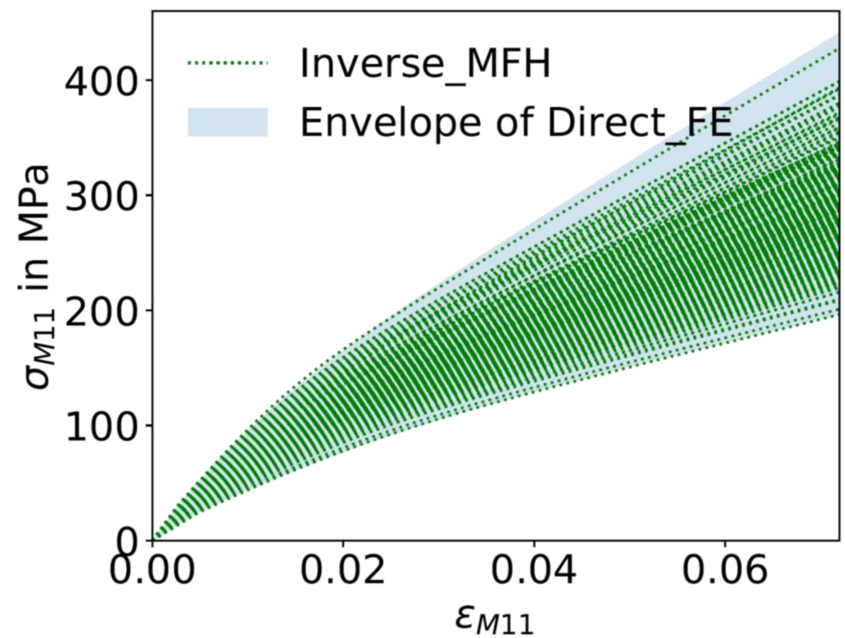


Non-linear stochastic Mean-Field Homogenization

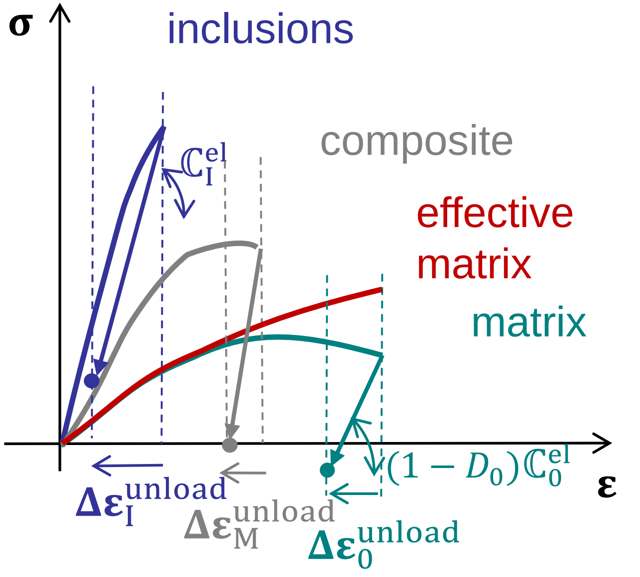
- Non-linear inverse identification
  - Comparison SVE vs. MFH



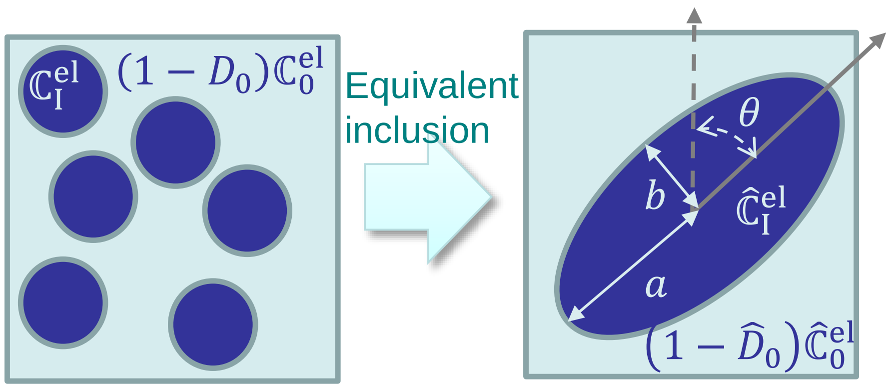


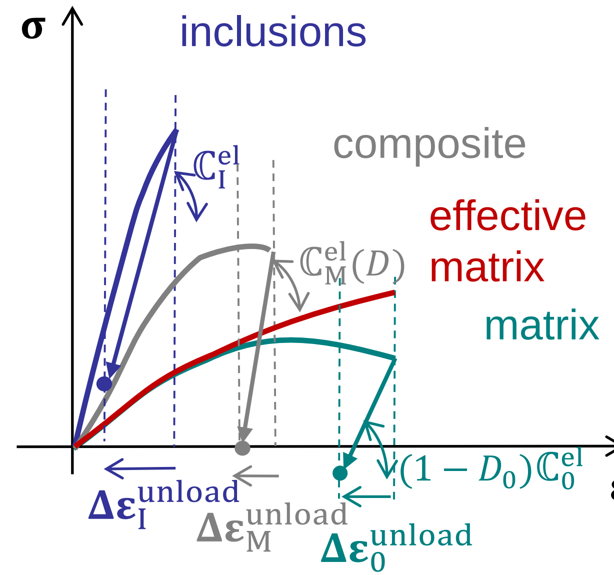


- Damage-enhanced Mean-Field-homogenization
  - Virtual elastic unloading from previous state
    - Composite material unloaded to reach the stress-free state
    - Residual stress in components



- Damage-enhanced inverse identification
  - Elastic unloading



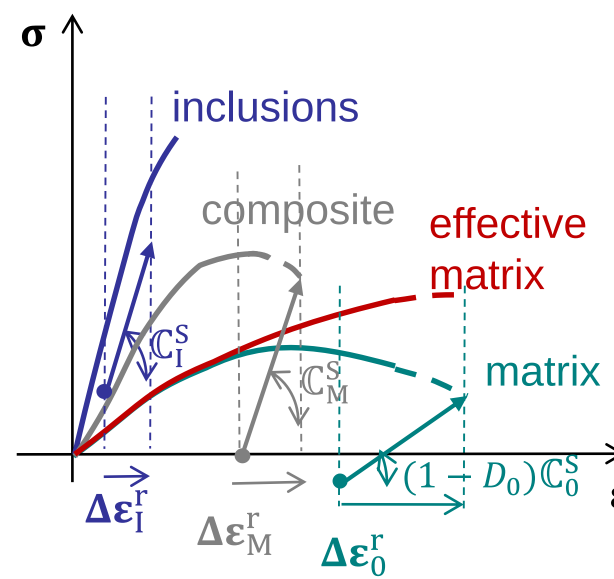


    - Identify damage evolution $\hat{D}_0$

$$\mathbb{C}^{\mathrm{el}}_{\mathrm{M}}(D) \simeq \hat{\mathbb{C}}^{\mathrm{el}}_{\mathrm{M}}\left(\hat{\mathrm{I}}, \left(1-\hat{D}_0\right)\hat{\mathbb{C}}^{\mathrm{el}}_0, \hat{\mathbb{C}}^{\mathrm{el}}_{\mathrm{I}}, v_{\mathrm{I}}, \theta\right)$$

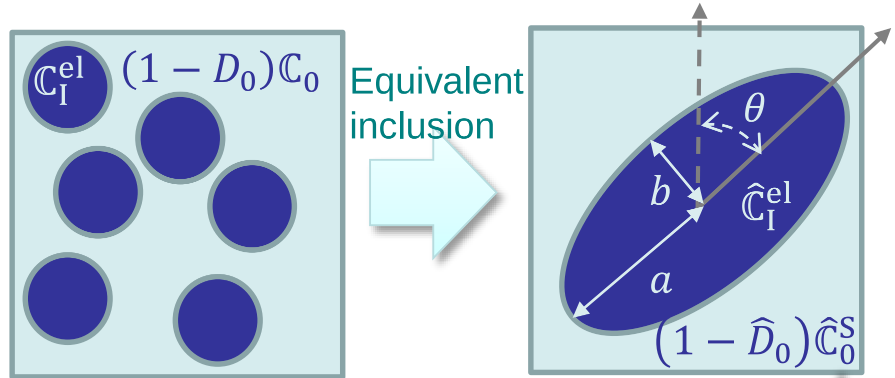
  - Reloading with the LCC
    - $\Delta\boldsymbol{\sigma}_{\mathrm{M}} = \mathbb{C}^{S}_{\mathrm{M}}\left(\mathrm{I}, (1-D_0)\mathbb{C}^{S}_0, \mathbb{C}^{S}_{\mathrm{I}}, v_{\mathrm{I}}\right): \Delta\boldsymbol{\varepsilon}^{\mathrm{r}}_{\mathrm{M}}$
    - Extract the equivalent hardening $\hat{R}(\hat{p}_0)$ & damage evolution $\hat{\mathrm{D}}_0(\hat{p}_0)$ from incremental secant tensor:

$$(1-\mathrm{D}_0)\mathbb{C}^{S}_0 \simeq \left(1-\hat{\mathrm{D}}_0(\hat{p}_0)\right)\hat{\mathbb{C}}^{S}_0\left(\hat{R}(\hat{p}_0); \hat{\mathbb{C}}^{\mathrm{el}}_0\right)$$

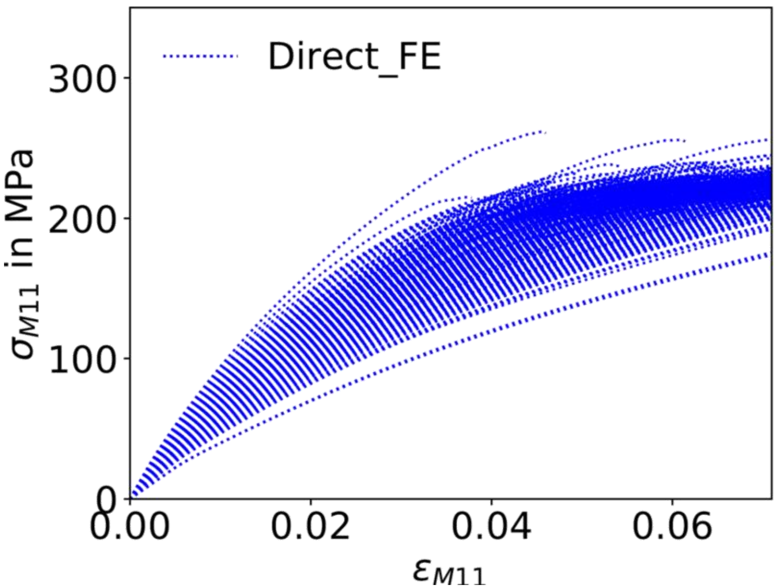


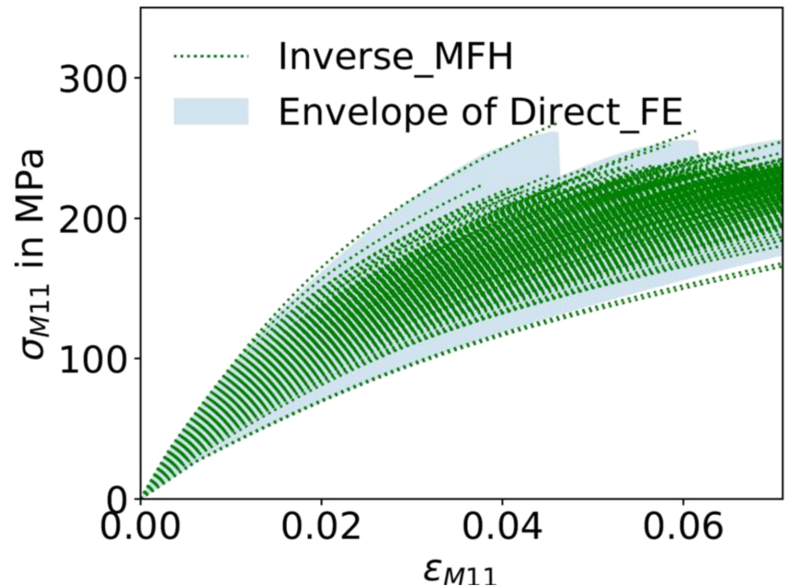
Non-linear stochastic Mean-Field Homogenization

- Damage-enhanced inverse identification
  - Similar process as for elasto-plasticity



$$(1-\mathrm{D}_0)\mathbb{C}_0^S \simeq \left(1-\hat{\mathrm{D}}_0(\hat{p}_0)\right)\hat{\mathbb{C}}_0^S\left(\hat{R}(\hat{p}_0);\hat{\mathbb{C}}_0^{\mathrm{el}}\right)$$





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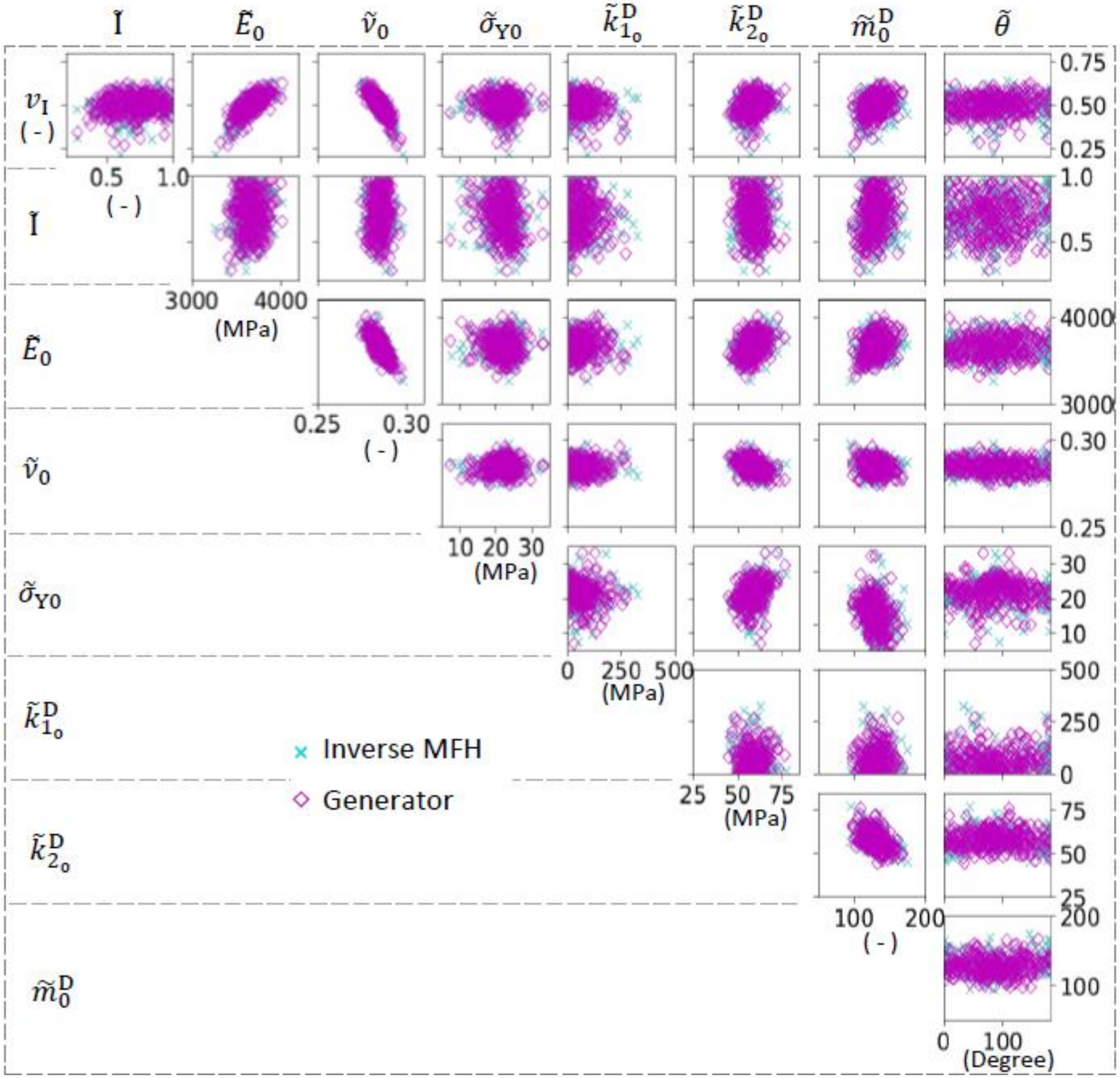
Use of stochastic Mean-Field Homogenization

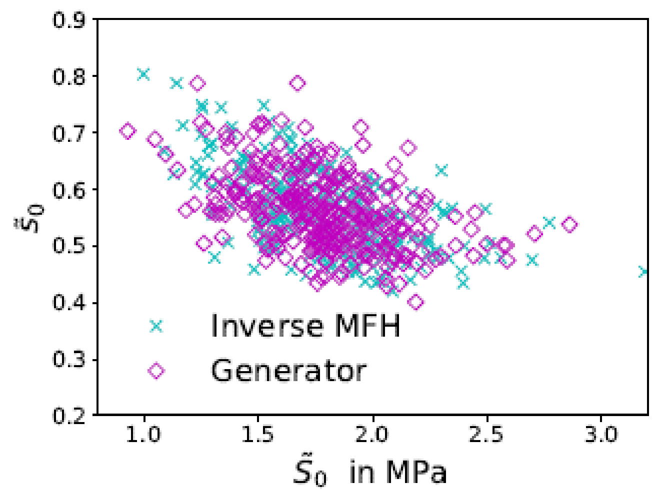
- Generation of random field
  - Inverse identification vs. diffusion map –based generator [Soize, Ghanem 2016]



$$\tilde{R}_0(\tilde{p}_0) = k_{1_0}\tilde{p}_0 + k_{2_0}\left(1 - e^{-m_0\tilde{p}_0}\right)$$

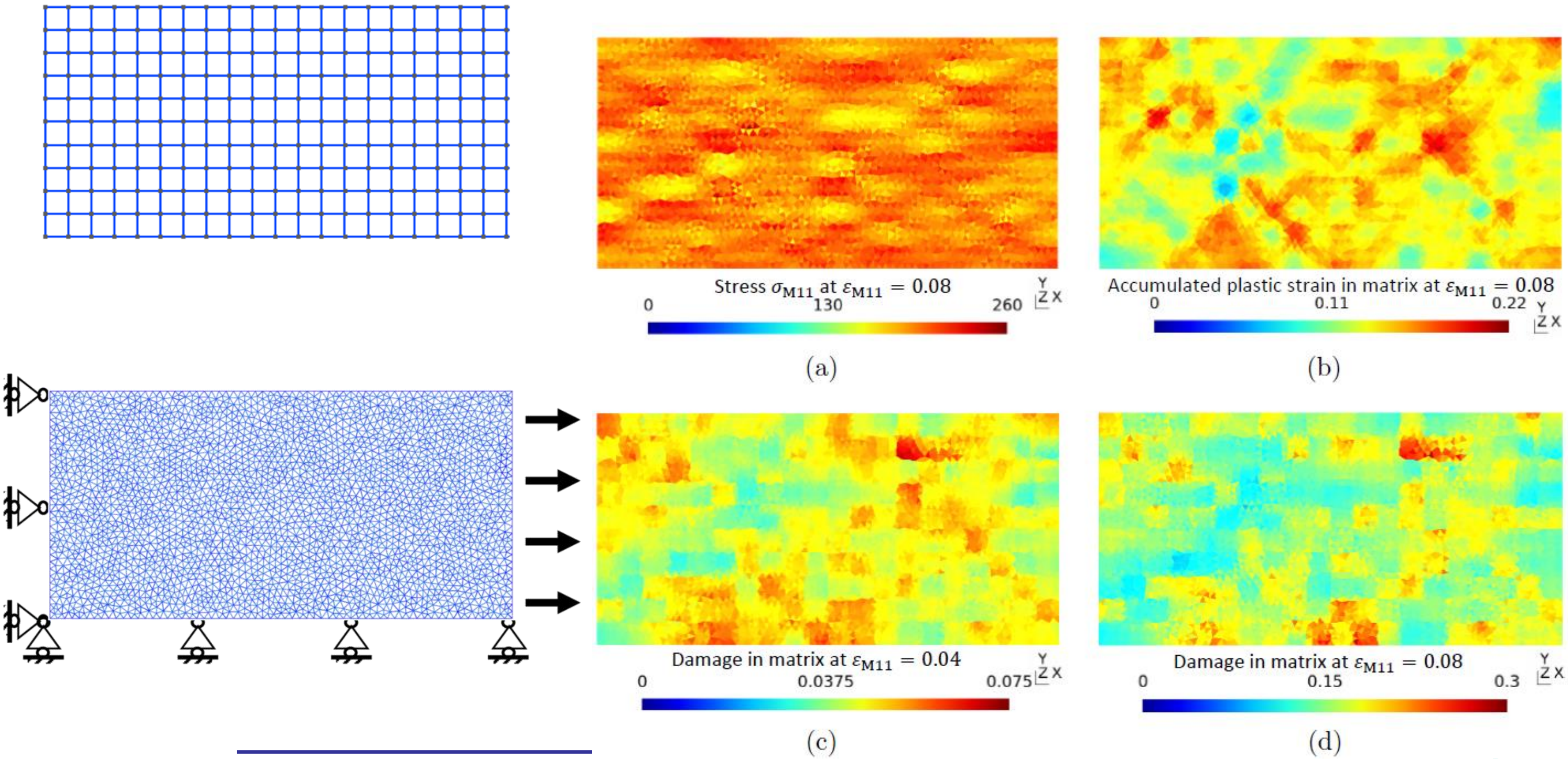
$$\dot{\tilde{D}}_0 = \begin{cases} 0, & \text{if } \tilde{p}_0 \leqslant p_{C_0} \,; \\ \left(\frac{Y}{\tilde{S}_0}\right)^{s_0}\dot{\tilde{p}}_0, & \text{if } \tilde{p}_0 > p_{C_0} \,, \end{cases}$$

Damage model Parameters



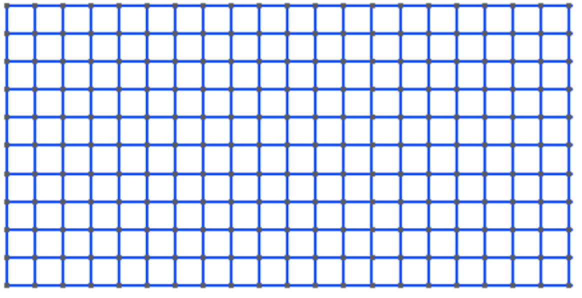
Use of stochastic Mean-Field Homogenization

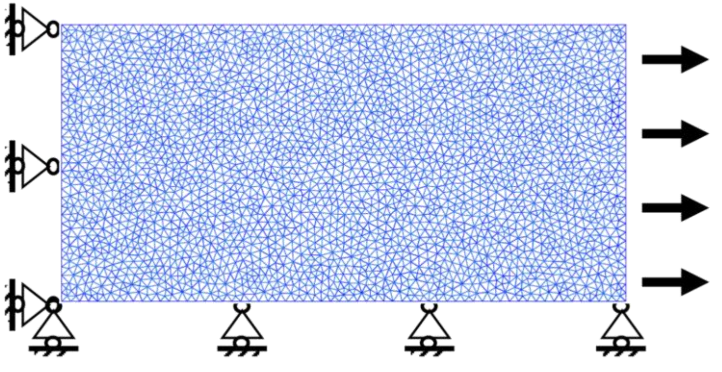
- One single ply loading realization
  - Random field and finite elements discretization
  - Non-uniform homogenized stress distributions
  - Creates damage localization

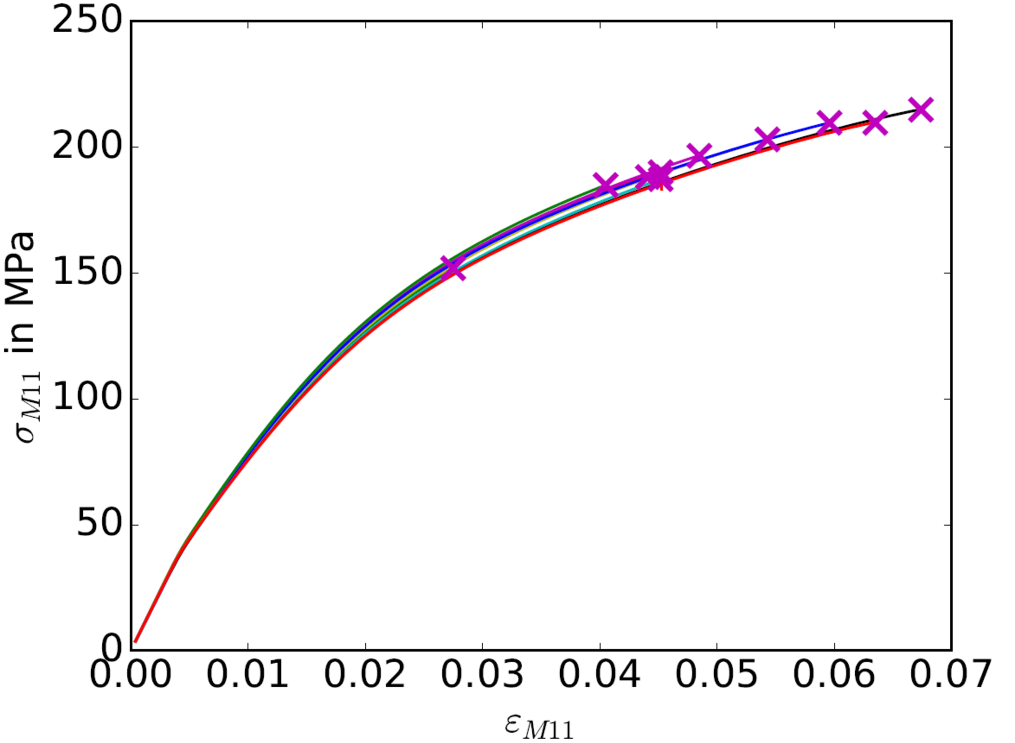


Use of stochastic Mean-Field Homogenization

- Ply loading realizations
  - Preliminary results (softening part not implemented)

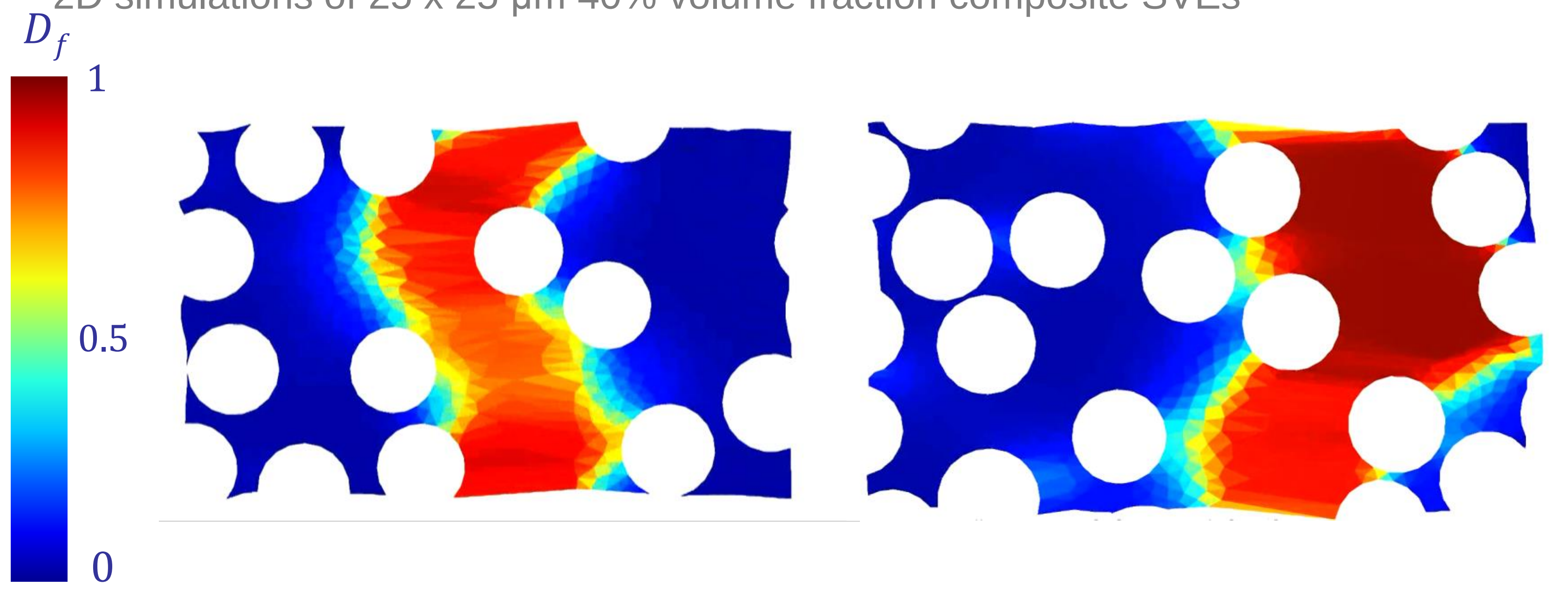






Micro-structural model of fiber-reinforced highly crosslinked epoxy

- UD Composites with RTM6 epoxy matrix
  - Identified matrix material behaviour
    - Hyperelastic viscoelastic-viscoplastic constitutive model enhanced by a multi-mechanism nonlocal damage model
    - Hardening: $\tilde{R}(p) = \sigma_y + h\,(1 - e^{-h_{exp}\tilde{p}})$
    - Softening: $D_s = (H_s(p - p_{init})^{\alpha})$
    - Failure: $\Phi_f = \gamma - a\exp(-bT) - c = 0$ & $\dot{D}_f = H_f\,(\chi_f)^{\zeta_f}(1 - D_f)^{\zeta_d}\dot{\chi}_f$
  - 2D simulations of 25 x 25 µm 40% volume fraction composite SVEs



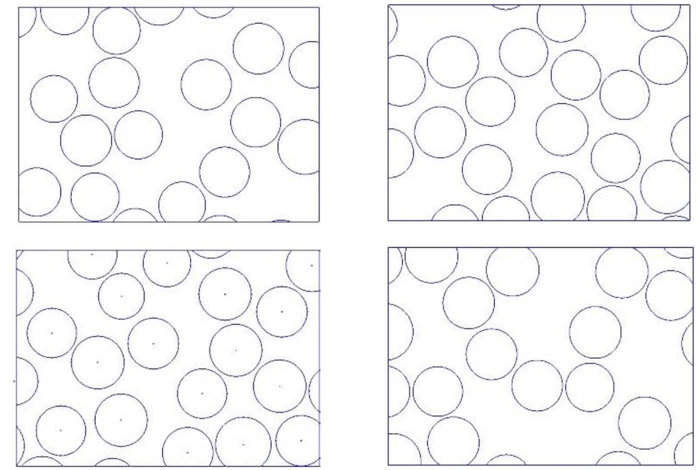
Stochastic homogenization on the SVEs

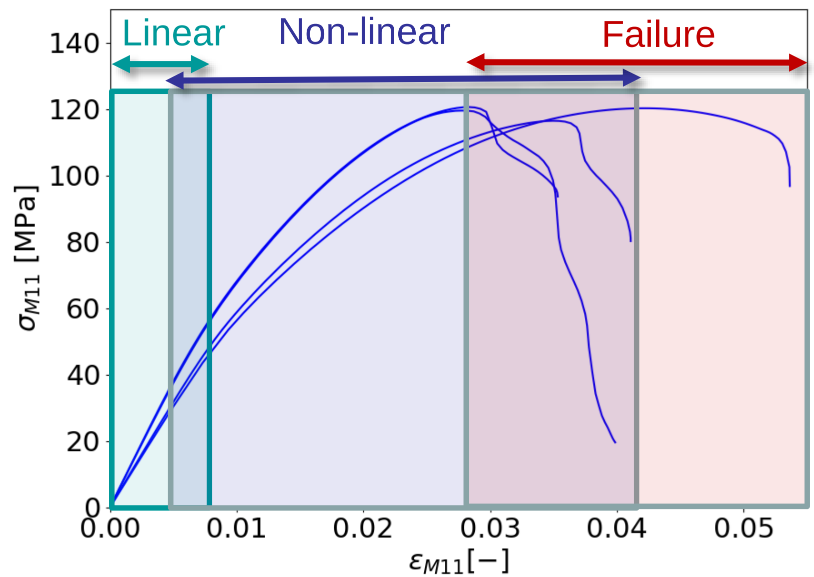
- Apparent response
  - Independent Stochastic Volume Elements
    - $l_{\mathrm{SVE}} = 25\ \mu m$
  - Stochastic homogenization
    - Extract apparent responses

$$
\begin{cases}
\boldsymbol{\varepsilon}_{\mathrm{M}} = \dfrac{1}{V(\omega)} \displaystyle\int_{\omega} \boldsymbol{\varepsilon}_{\mathrm{m}} d\omega \\
\boldsymbol{\sigma}_{\mathrm{M}} = \dfrac{1}{V(\omega)} \displaystyle\int_{\omega} \boldsymbol{\sigma}_{\mathrm{m}} d\omega \\
\mathbb{C}_{\mathrm{M}} = \dfrac{\partial \boldsymbol{\sigma}_{\mathrm{M}}}{\partial \boldsymbol{u}_{\mathrm{M}} \otimes \boldsymbol{\nabla}_{\mathrm{M}}}
\end{cases}
$$

  - 3 stages
    - Linear response
    - (Damage-enhanced) elasto-plasticity
    - Failure (loss of size objectivity)

SVE realizations

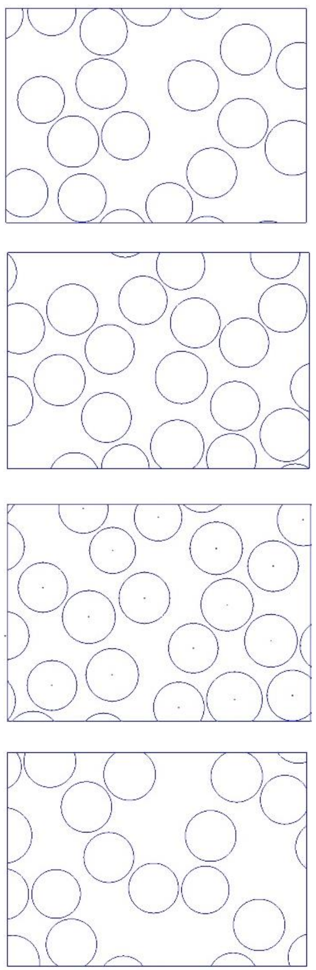


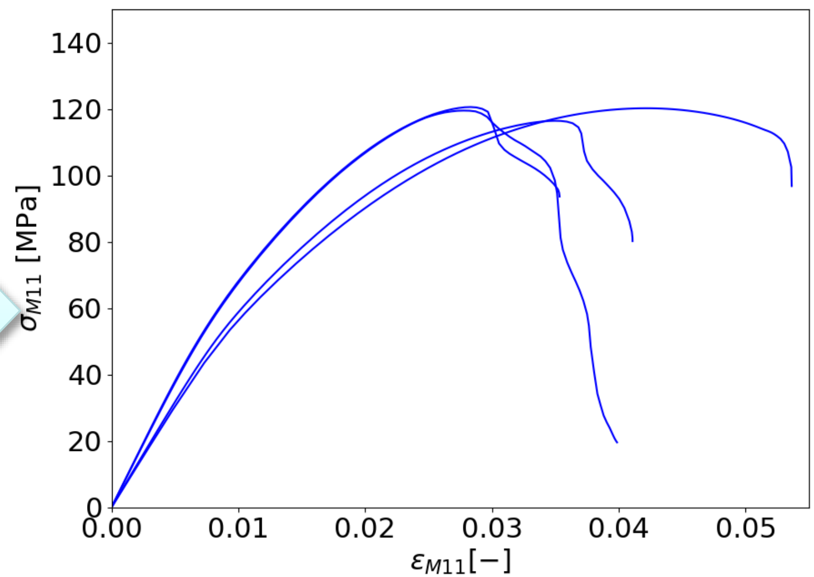


Stochastic Homogenization

Mean-Field Homogenization with failure

- Non-linear SVE simulations





G_c [N/mm]

0.0408

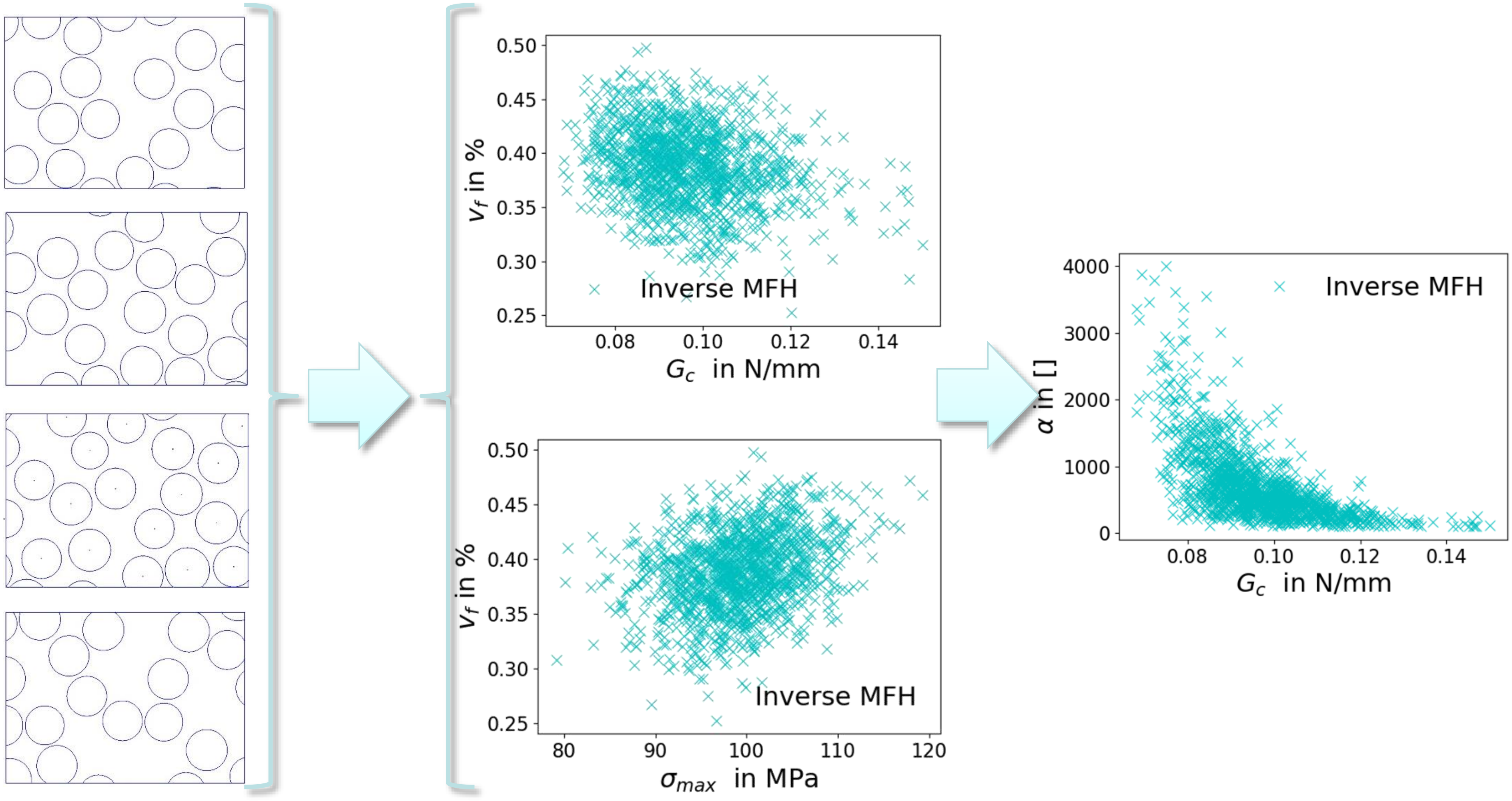
0.0780

0.0654

0.1019

Mean-Field Homogenization with failure

- Extracted failure characteristics



Conclusions

- Stochastic micro-structures
  - Geometrical features from statistical measurements
  - Micro-structure geometry generator
  - Experimentally calibrated/validated epoxy model with length scale effect

- Inverse MFH identification
  - MFH is used as a micro-mechanics based model
  - Parameters identified from SVE simulations
  - Localization behaviour identified using objective fields

- Stochastic Finite elements
  - Stochastic MFH is used as material law
  - Random fields (MFH parameters) generated using data-driven approach
  - First ply simulations

Thank you for your attention!

Special thanks to:

Wallonie

VISCOS

fnrs

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