Computational & Multiscale Mechanics of Materials



## An inverse Mean-Field-Homogenization-based micro-mechanical model for stochastic multiscale simulations of unidirectional composites

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





### **Objectives**

Multi-scale modelling 2 problems are solved Extraction of a mesoscale Volume Element concurrently Material response Macro-scale The macro-scale problem The meso-scale problem (on a meso-scale Volume Element) **BVP** Length-scales separation  $L_{\text{macro}} >> L_{\text{VE}} >> L_{\text{micro}}$ Ρ, σ, q, ... *F*, *E*, *T*, *∇T*, ... For accuracy: Size of the meso-To be statistically representative: scale volume element smaller than Size of the meso-scale volume the characteristic length of the element larger than the macro-scale loading characteristic length of the micro-

CM<sub>3</sub>

structure



### Objectives

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

- Non-linear responses of composites
  - RVE size is too large
  - Structural response suffers from scatter
  - Requires the use of smaller VEs

For accuracy: Size of the mesoscale volume element smaller than the characteristic length of the macro-scale loading

Meso-scale volume element no longer statistically representative: Stochastic Volume Elements

#### Main objective

To develop an 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 microstructural constituents characterization







Uncertainty quantification of micro-structure & micro-structure generator





2000x and 3000x SEM images



• Fibers detection





- Basic geometric information of fibers' cross sections
  - Fiber radius distribution  $p_R(r)$
- Basic spatial information of fibers
  - The distribution of the nearest-neighbor net distance function  $p_{d_{1st}}(d)$
  - The distribution of the orientation of the undirected line connecting the center points of a fiber to its nearest neighbor  $p_{\vartheta_{1st}}(\theta)$
  - The distribution of the difference between the net distance to the second and the first nearest-neighbor  $p_{\Delta d}(d)$  with  $\Delta d = d_{2nd} - d_{1st}$
  - The distribution of the second nearest-neighbor's location referring to the first nearest-neighbor  $p_{\Delta\vartheta}(\theta)$  with  $\Delta\vartheta = \vartheta_{2nd} \vartheta_{1st}$





Micro-structure stochastic model



- Dependency of the four random variables  $d_{1st}$ ,  $\Delta d$ ,  $\vartheta_{1st}$ ,  $\Delta \vartheta$
- Correlation matrix



|                         | $d_{1st}$ | $\Delta d$ | $\vartheta_{1 { m st}}$ | $\Delta \vartheta$ |
|-------------------------|-----------|------------|-------------------------|--------------------|
| $d_{1st}$               | 1.0       | 0.21       | 0.01                    | 0.02               |
| $\Delta d$              |           | 1.0        | 0.002                   | -0.005             |
| $\vartheta_{1 { m st}}$ |           |            | 1.0                     | 0.02               |
| $\Delta \vartheta$      |           |            |                         | 1.0                |

- Distances correlation matrix
  - $d_{1st}$  and  $\Delta d$  are dependent  $\implies$  they will have to be generated from their empirical copula

|                         | $d_{1st}$ | $\Delta d$ | $\vartheta_{\rm 1st}$ | $\Delta \vartheta$ |
|-------------------------|-----------|------------|-----------------------|--------------------|
| $d_{1st}$               | 1.0       | 0.27       | 0.04                  | 0.08               |
| $\Delta d$              |           | 1.0        | 0.05                  | 0.06               |
| $\vartheta_{1 { m st}}$ |           |            | 1.0                   | 0.05               |
| $\Delta \vartheta$      |           |            |                       | 1.0                |



•  $d_{1st}$  and  $\Delta d$  should be generated using their empirical copula SEM sample Generated sample



## Directly from copula generator

# Statistic result from generated SVE



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



Possibility to generate non-homogenous distributions



### Methodology

• SVEs definition



19 💧

LIÈGE université

- UD Composites with RTM6 epoxy matrix
  - Identified matrix material behaviour
    - Hyperelastic viscoelastic-viscoplastic constitutive model enhanced by
      - a multi-mechanism nonlocal damage model
  - To be used in micro-structural analysis
    - Behaviour in composite is different
    - Introduce a length-scale effect
- Resin model implementation:
  - Requires non-local form [Bažant 1988]
    - Introduction of characteristic length  $l_c$
    - Weighted average:  $\tilde{Z}(x) = \int_{V_c} W(y; x, l_c) Z(y) dy$
  - Implicit form [Peerlings et al. 1998]
    - New degrees of freedom:  $\tilde{Z}$
    - New Helmholtz-type equations:  $\tilde{Z} l_c^2 \Delta \tilde{Z} = Z$
  - Has a length scale effect











#### Resin model

- Material changes represented via internal variables
- Constitutive law P(F; Z(t'))
  - Internal variables  $\mathbf{Z}(t')$
  - Multi-damage strategy  $\mathbf{P} = (\mathbf{1} - D_s)(\mathbf{1} - D_f)\widehat{\mathbf{P}}$
- Non-local damage evolution laws
  - Saturation law

$$\begin{cases} \dot{D}_s = D_s(D_s, \mathbf{F}(t), \chi_s(t); Z(\tau), \tau \in [0 \ t])\dot{\chi}_s \\ \chi_s(t) = \max_{\tau} (\tilde{\gamma}_s(\tau)) \\ \tilde{\gamma}_s - l_s^2 \ \Delta \tilde{\gamma}_s = \gamma_s \end{cases}$$

• Failure law

$$\begin{cases} \dot{D}_f = D_f \left( D_f, \mathbf{F}(t), \chi_f(t); Z(\tau), \tau \in [0 \ t] \right) \dot{\chi}_f \\\\ \chi_f(t) = \max_{\tau} \left( \tilde{\gamma}_f(\tau) \right) \\\\ \tilde{\gamma}_f - l_f^2 \ \Delta \tilde{\gamma}_f = \gamma_f \end{cases}$$





- Resin model: saturated softening ۲
  - Saturated damage evolution

CM<sub>3</sub>

$$\begin{bmatrix} \dot{D}_s = H_s(\chi_s - \chi_{s0})^{\zeta_s}(D_{s\infty} - D_s)\dot{\chi}_s \\ \chi_s = \max_{\tau} (\chi_{s0}, \tilde{\gamma}_s(\tau)) \\ \tilde{\gamma}_s - l_s^2 \Delta \tilde{\gamma}_s = \gamma \end{bmatrix}$$

- \_\_\_\_





- Resin model: saturated softening
  - Several hardening/softening combinations 200
    - Requires composite material tests
      - Length scale effect

$$l_s = 3\mu m \left(1 - \frac{D_s}{D_{s\infty}}\right)$$

Non-local BC at fibre interface

 $\left[\!\left[\dot{\widetilde{\gamma}}_{s}\right]\!\right]=0$ 











- UD Composites with RTM6 epoxy matrix
  - 2D simulations of 25 x 25 µm 40% volume fraction composite SVEs





• Extraction of apparent responses





LIEGE

#### • Window technique

- Extraction of Stochastic Volume Elements
  - $l_{\rm SVE} = 25 \ \mu m$
  - 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

CM3

- Extract apparent homogenized material tensor  $\mathbb{C}_{\mathsf{M}}$ 

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

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



29 👔



• Apparent elastic properties: distribution & Correlation





#### Stochastic Homogenization



SVE realizations





Apparent response

•

•  $l_{SVE} = 25 \, \mu m$ 

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



### Methodology

- Stochastic Mean-Field Homogenization-based model
  - First stage: linear elasticity





#### Stochastic Mean-Field Homogenization

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

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

 $\mathbb{C}_{M} = \mathbb{C}_{M}(I, \mathbb{C}_{0}, \mathbb{C}_{I}, v_{I})$ 

- We use Mori-Tanaka assumption for  $\mathbb{B}^{\varepsilon}(I, \mathbb{C}_0, \mathbb{C}_I)$
- Stochastic MFH

CM3

– 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)



#### Stochastic Mean-Field Homogenization





#### Stochastic Mean-Field Homogenization

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



0.6

0.8

1.0

 $E_x$ 

4.0 <u>le-10</u>

3.5

3.0

Probability 5.0 57 1.5

1.0

0.5

0.0 L 0.4



### Methodology

- Stochastic Mean-Field Homogenization-based model
  - Second stage: damage-enhanced elasto-plasticity





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

 $\boldsymbol{\sigma}_{\mathrm{M}} = \overline{\boldsymbol{\sigma}} = \boldsymbol{v}_{0}\boldsymbol{\sigma}_{0} + \boldsymbol{v}_{\mathrm{I}}\boldsymbol{\sigma}_{\mathrm{I}}$  $\boldsymbol{\varepsilon}_{\mathrm{M}} = \overline{\boldsymbol{\varepsilon}} = \boldsymbol{v}_{0}\boldsymbol{\varepsilon}_{0} + \boldsymbol{v}_{\mathrm{I}}\boldsymbol{\varepsilon}_{\mathrm{I}}$  $\boldsymbol{\varepsilon}_{\mathrm{I}} = \mathbb{B}^{\varepsilon}(\mathrm{I}, \mathbb{C}_{0}, \mathbb{C}_{\mathrm{I}}): \boldsymbol{\varepsilon}_{0}$ 

Non-linear composites







- View to damage Mean-Field-homogenization
  - Incremental forms
    - Strain increments in the same direction

 $\Delta \boldsymbol{\epsilon}_{I} = \mathbb{B}^{\boldsymbol{\epsilon}} \left( \mathsf{I}, \mathbb{C}^{\mathrm{alg}}_{0}, \mathbb{C}^{\mathrm{alg}}_{I} \right) : \Delta \boldsymbol{\epsilon}_{0}$ 

 Because of the damaging process, the fiber phase is elastically unloaded during matrix softening



- Solution
  - We need to define the LCC from another state



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











CM<sub>3</sub>





#### • Damage-enhanced Mean-Field-homogenization

- Virtual elastic unloading from previous state
  - Composite material unloaded to reach the stressfree state
  - Residual stress in components





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

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

Incremental-secant loading

$$\begin{cases} \boldsymbol{\sigma}_{\mathrm{M}} = \overline{\boldsymbol{\sigma}} = v_{0}\boldsymbol{\sigma}_{0} + v_{\mathrm{I}}\boldsymbol{\sigma}_{\mathrm{I}} \\ \boldsymbol{\Delta}\boldsymbol{\varepsilon}_{\mathrm{M}}^{\mathbf{r}} = \overline{\boldsymbol{\Delta}}\overline{\boldsymbol{\varepsilon}} = v_{0}\boldsymbol{\Delta}\boldsymbol{\varepsilon}_{0}^{\mathbf{r}} + v_{\mathrm{I}}\boldsymbol{\Delta}\boldsymbol{\varepsilon}_{\mathrm{I}}^{\mathbf{r}} \\ \boldsymbol{\Delta}\boldsymbol{\varepsilon}_{\mathrm{I}}^{\mathbf{r}} = \mathbb{B}^{\varepsilon} \big( \mathrm{I}, (1 - D_{0})\mathbb{C}_{0}^{\mathrm{S}}, \mathbb{C}_{\mathrm{I}}^{\mathrm{S}} \big) : \boldsymbol{\Delta}\boldsymbol{\varepsilon}_{0}^{\mathbf{r}} \end{cases}$$

Incremental secant operator

$$\Delta \boldsymbol{\sigma}_{\mathrm{M}} = \mathbb{C}_{\mathrm{M}}^{\mathrm{S}} \big( \mathrm{I}, (1 - D_0) \mathbb{C}_0^{\mathrm{S}}, \mathbb{C}_{\mathrm{I}}^{\mathrm{S}}, \boldsymbol{v}_{\mathrm{I}} \big) : \Delta \boldsymbol{\varepsilon}_{\mathrm{M}}^{\mathrm{r}}$$









 $\mathbb{C}_{\mathsf{M}}^{\mathsf{el}}(D) \simeq \widehat{\mathbb{C}}_{\mathsf{M}}^{\mathsf{el}}(\widehat{\mathsf{I}}, (1 - \widehat{D}_0)\widehat{\mathbb{C}}_0^{\mathsf{el}}, \widehat{\mathbb{C}}_{\mathsf{I}}^{\mathsf{el}}, v_{\mathsf{I}}, \theta)$ 

CM3

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





- Stochastic Mean-Field Homogenization-based model
  - Third stage: Failure





 $\mathcal{D}^{end} - \mathcal{D}^{loc}$ 

- Need to recover size objectivity
  - Strength is objective  $\sigma_c$
  - Critical energy release rate is objective  $G_c = \frac{1}{2}$





Non-linear SVE simulations



65 **L** 

#### Mean-Field Homogenization with failure

- Damage-enhanced mean-field homogenization
  - Requires non-local form for the matrix part of homogenized behavior
    - Following implicit form [Peerlings et al. 1998]
      - Apparent matrix plastic strain  $p_0$
      - Non-local apparent matrix plastic strain  $\tilde{p}_0$
      - Matrix damage evolution

 $\Delta D_0 = F_D(\Delta \boldsymbol{\varepsilon_0}, \Delta p_0) \quad \square \quad \Delta D_0 = F_D(\Delta \boldsymbol{\varepsilon_0}, \Delta \tilde{p}_0)$ 

• New Helmholtz-type equations:

$$- \tilde{p}_0 - l_c^2 \nabla \cdot (\nabla \tilde{p}_0) = p_0$$

- Definition of non-local length  $l_c$ 





#### Mean-Field Homogenization with failure

- Damage-enhanced mean-field homogenization
  - Requires non-local form for the matrix homogenized behavior
    - Matrix damage evolution  $\Delta D_0 = F_D(\Delta \epsilon_0, \Delta \tilde{p}_0)$ •
    - New Helmholtz-type equations: •
      - $\tilde{p}_0 l_c^2 \nabla \cdot (\nabla \tilde{p}_0) = p_0$
      - Definition of non-local length  $l_c$

 $R \gg l_c$ 

Evaluation of non-local length

 $l_c$  (µm)

20

5

2

To recover the energy release rate of SVEs

Non-local MFH

material law

 $L \gg l_c$ 

MFH  $G_c$  [N mm<sup>-1</sup>]

1.008

0.363

0.0922





CM3

0.1035

#### Mean-Field Homogenization with failure

- More convenient to fix non-local length
  - For macro-scale Stochastic FEM
  - To increase its length

#### Modify the damage evolution to recover $G_c$

Before localization onset: identified evolution

 $\Delta D_0 = F_D(\Delta \boldsymbol{\varepsilon_0}, \Delta \tilde{p}_0)$ 

After localization onset:

•

•  $\Delta D_0 = \alpha (\tilde{p}_0 + \Delta \tilde{p}_0 - \tilde{p}_{0 \text{ onset}})^{\beta} \Delta \tilde{p}_0$ 





 $R \gg l_c$ 

• Use Stochastic Mean-Field Homogenization as constitutive law





#### Use of stochastic Mean-Field Homogenization



 $\Delta$ 

#### • Generation of random field

- Inverse identification vs. diffusion map -based generator [Soize, Ghanem 2016]





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





### 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

CM3



## Thank you for your attention!

## Special thanks to:







#### References

- L. Wu, V.-D. Nguyen, L. Adam, L. Noels, An inverse micro-mechanical analysis toward the stochastic homogenization of nonlinear random composites, Comp. Meth. in App. Mech. and Engineering (ISSN: 0045-7825) 348, (2019) 97-138, https://doi.org/10.1016/j.cma.2019.01.016
- 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, http://dx.doi.org/10.1016/j.compstruct.2018.01.051
- 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, http://dx.doi.org/10.1016/
- T. Mori, K. Tanaka, Average stress in matrix and average elastic energy of materials with misfitting inclusions, Acta Metall. 21 (5) (1973) 571–574
- L. Wu, L. Noels, L. Adam, I. Doghri, A combined incremental–secant mean–field homogenization scheme with per–phase residual strains for elasto–plastic composites, Int. J. Plast. 51 (2013a) 80–102, http://dx.doi.org/10.1016/j.ijplas.2013.06.006
- L. Wu, L. Noels, L. Adam, I. Doghri, An implicit-gradient-enhanced incremental-secant mean-field homogenization scheme for elasto-plastic composites with damage, Int. J. Solids Struct. (ISSN: 0020-7683) 50 (24) (2013b) 3843–3860, http://dx.doi.org/10.1016/j.ijsolstr.2013.07.022.
- L. Wu, L. Adam, I. Doghri, L. Noels, An incremental-secant mean-field homogenization method with second statistical moments for elasto-visco-plastic composite materials, Mech. Mater. (ISSN: 0167-6636) 114 (2017) 180–200, http://dx.doi.org/10.1016/j.mechmat.2017.08.006.
- V.-D.Nguyen F.Lani T.Pardoen X.P.Morelle L.Noels, A large strain hyperelastic viscoelastic-viscoplastic-damage constitutive model based on a multi-mechanism non-local damage continuum for amorphous glassy polymers. Int. Journal of Sol. and Struct., (ISSN: 0020-7683) 96 (2016) 192-216, https://doi.org/10.1016/j.ijsolstr.2016.06.008
- V.-D. Nguyen, L. Wu, L. Noels, A micro-mechanical model of reinforced polymer failure with length scale effects and predictive capabilities. Validation on carbon fiber reinforced high-crosslinked RTM6 epoxy resin, Mech. Mater. (ISSN: 0167-6636) 133 (2019) 193-213, https://dx.doi.org/10.1016/j.mechmat.2019.02.017