MODELISATION ET HOMOGENEISATION DE POLYMERES THERMOPLASTIQUES RENFORCES

I. Doghri

Université catholique de Louvain, Belgique

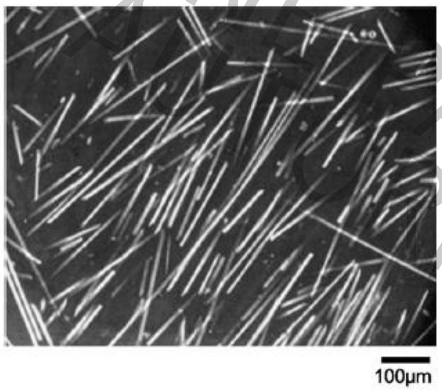
Remerciements: A. Krairi (U.C. Louvain), e-Xstream engineering, Brose, Solvay

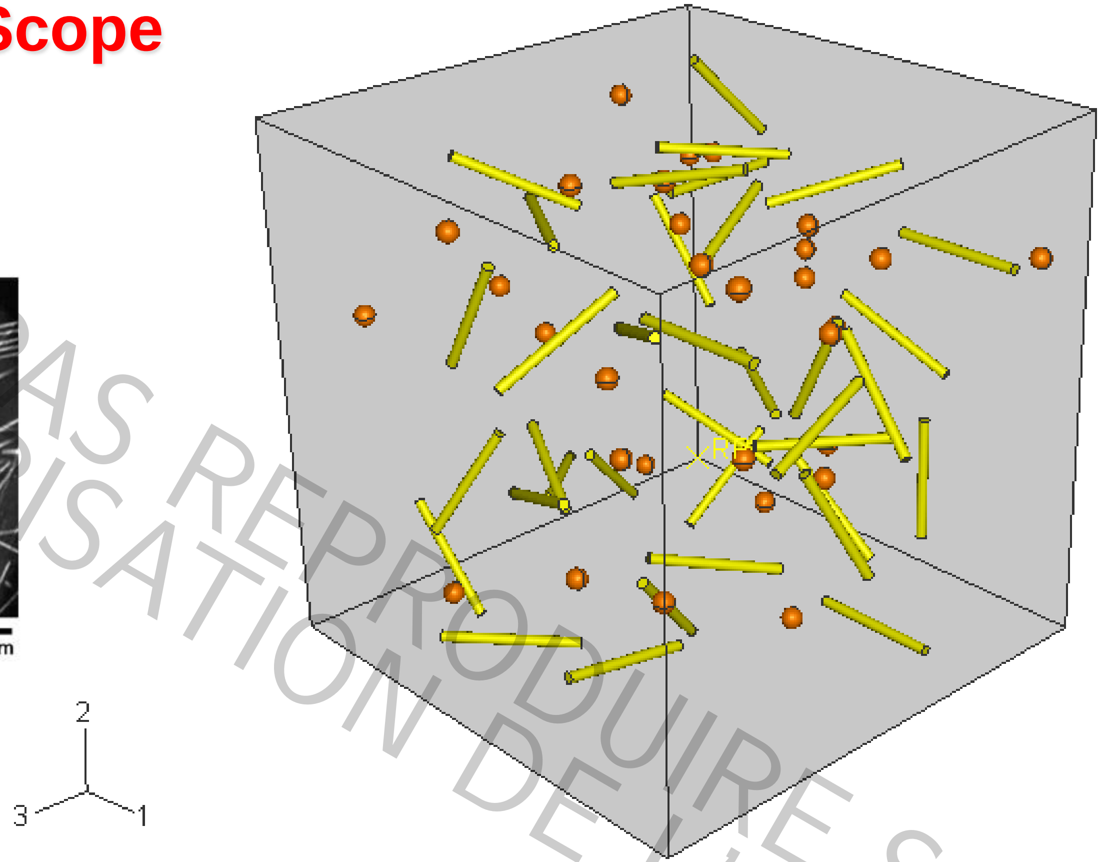
Colloque MECAMAT, Aussois, 23 janvier 2014

- **Multi-scale modeling and mean-field homogenization (MFH)**
- **A thermodynamically-based constitutive model for homogeneous thermoplastic polymers**
- **MFH for inelastic composites**
- **Applicability to bio composites**

Multi-scale modeling
and
mean-field homogenization (MFH)

Introduction: Scope

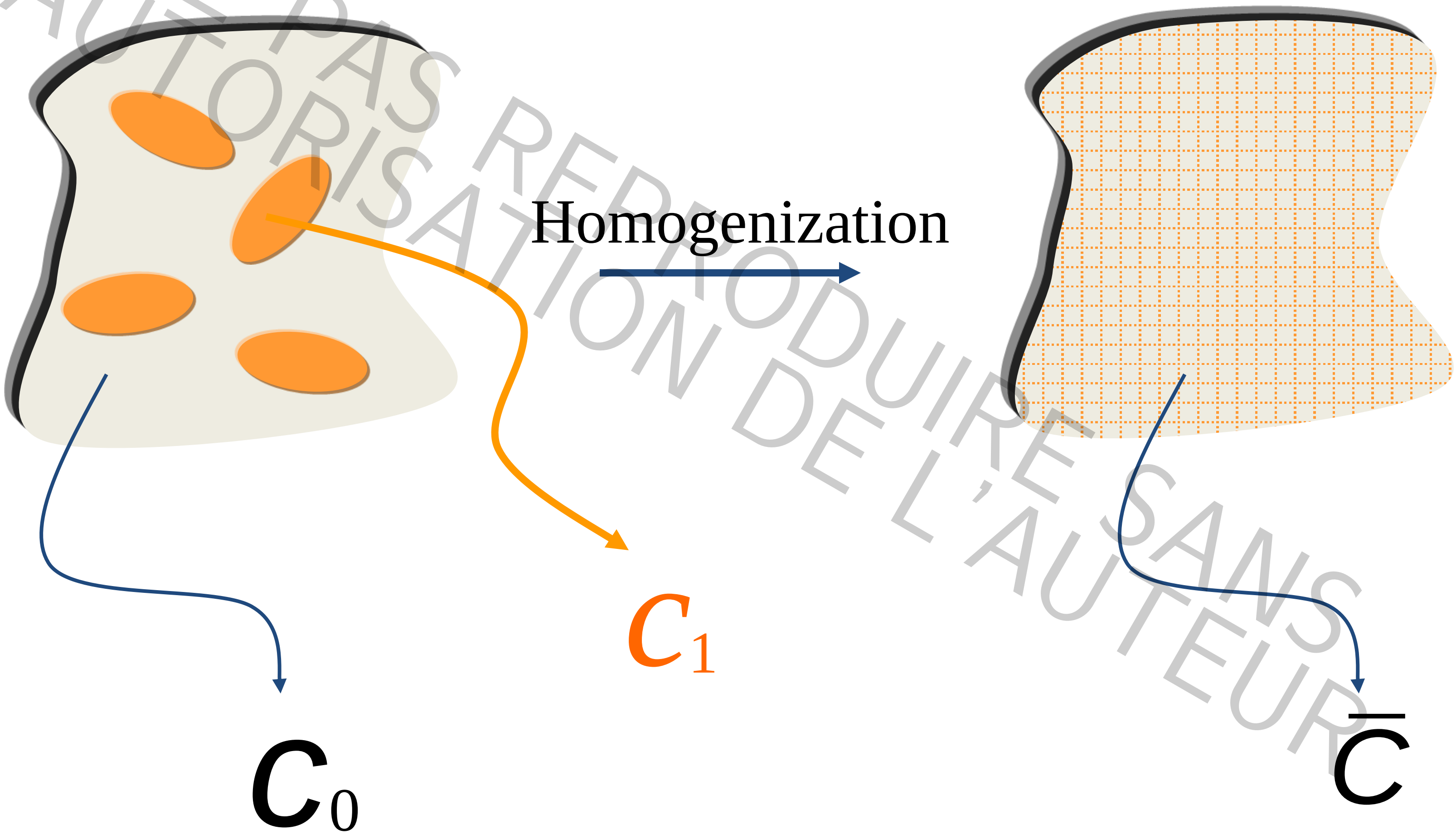




- Composite: matrix phase and multiple *inclusions* (particles, short fibers, platelets, cavities). Many applications in polymer, metal, rubber, concrete matrix composites; in biomaterials, etc.

- *Objective:* predict *interaction* between *microstructure* and *macroscopic* (or overall or effective) properties, in a *cost-effective manner*, usable in practice.

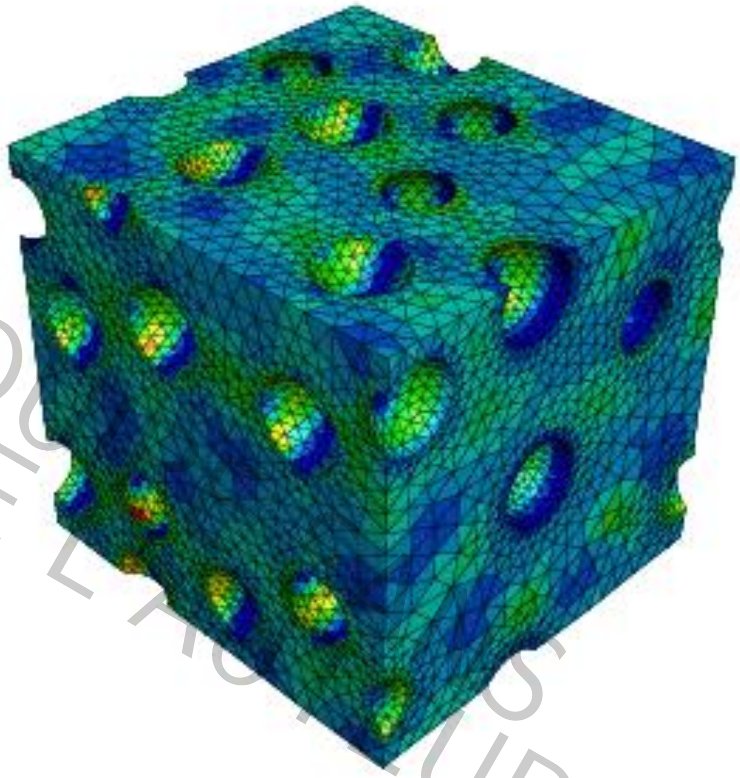
Homogenization, scale-transition methods



Direct FE computation of RVE

Example (Brassart, Delannay & Doghri, 2008):

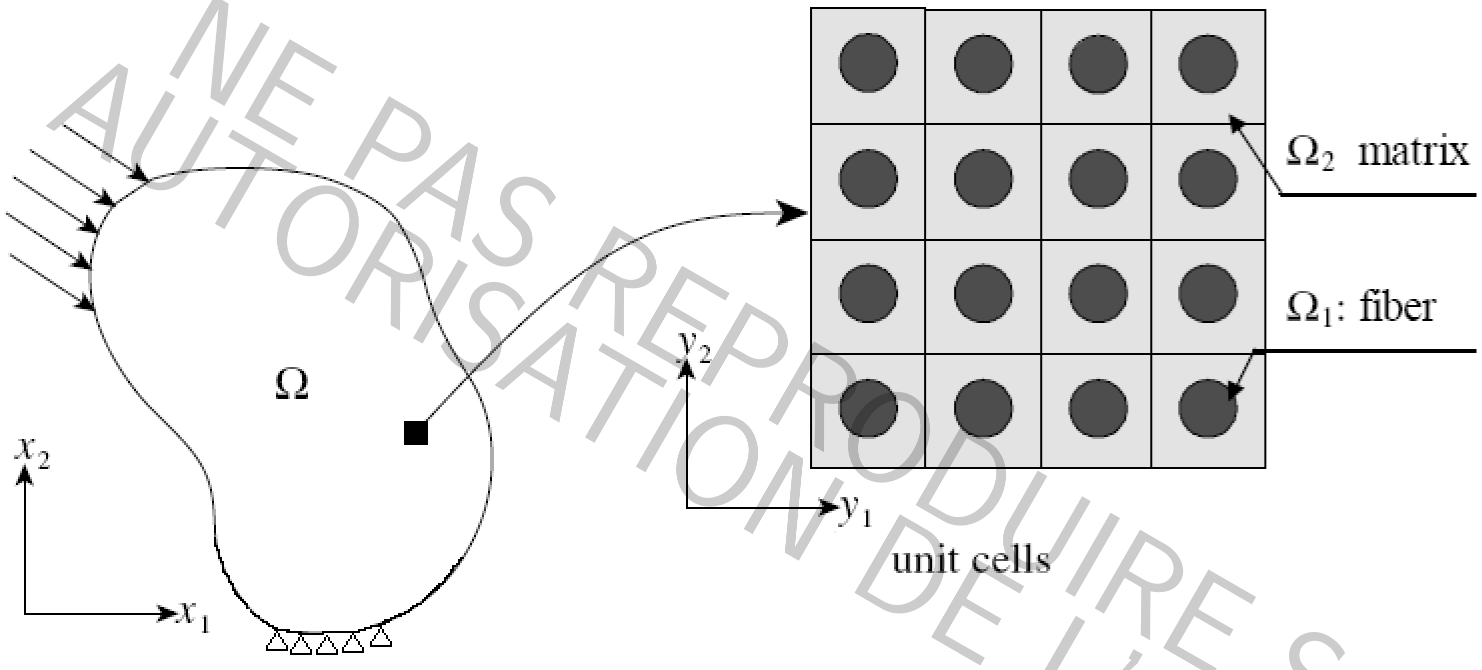
- RVE with 35 particles
- Periodic mesh and microstructure
- Particle volume fraction: up to 35%
- Typical model: 130,000 ABAQUS quadratic elements C3D10M, and 185,000 nodes



Advantages: general; accurate at macro and micro levels

Drawbacks: meshing difficulties for realistic microstructures; large CPU time for nonlinear problems.

Asymptotic homogenization
[E. Sanchez-Palencia, G. Duvaut, F. Léné, R. Peerlings, …]



Ideas: periodic microstructures, x: macro coordinates, y: micro unit cell coordinates, small parameter δ, asymptotic expansion of displacement field:

$$u_i^{\delta}(\mathbf{x}) = u_i^{(0)}(\mathbf{x},\mathbf{y}) + \delta u_i^{(1)}(\mathbf{x},\mathbf{y}) + \delta^2 u_i^{(2)}(\mathbf{x},\mathbf{y}) + .. \quad ; \quad \frac{\mathbf{x}}{\delta} = \mathbf{y}$$

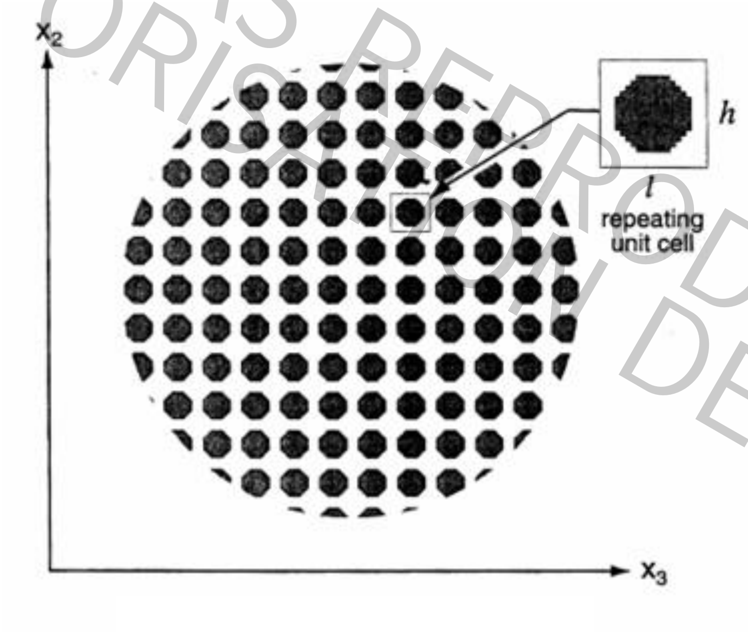
Advantages: mathematically elegant; very accurate.

Drawbacks: limited to linear elasticity or weakly nonlinear problems; needs FE.

Method of cells and subcells

[Dvorak *et al*., Pindera *et al*., Moulinec & Suquet, Chaboche & Kruch, …]

Ideas: discretize the microstructure into simple cells: 2D pixels or 3D voxels. Each cell can subdivided into subcells. Assume uniform strain in each subcell (e.g. Pindera *et al*.) or use Fourier Transforms (e.g. Moulinec and Suquet) or…



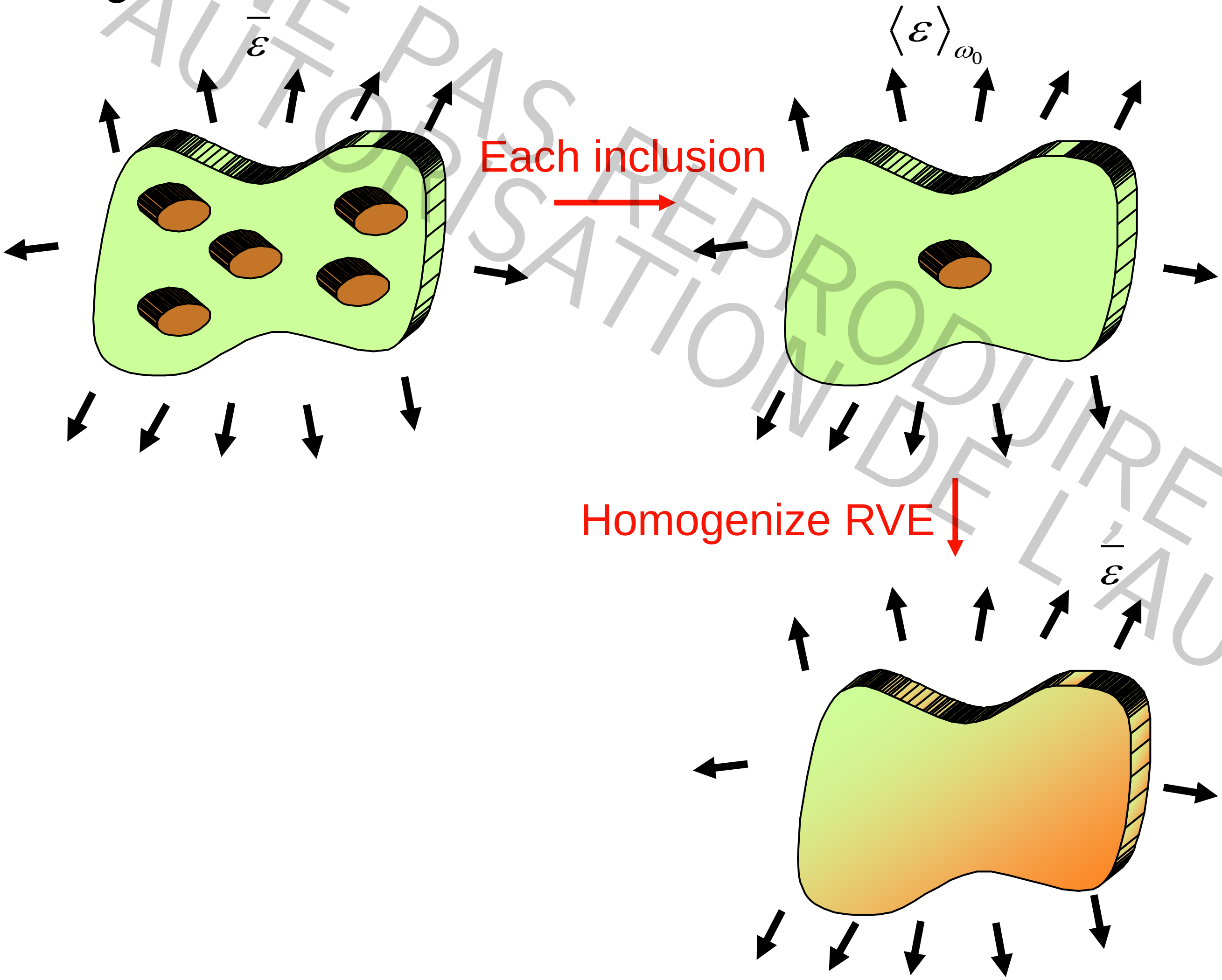
Doubly periodic array of fibers [Pindera and Bednarcyk (1999)]

Advantage: easy "meshing": simple regular grid.

Drawback: real geometry of microstructure is not respected, unless a large number of cells is used (CPU cost becomes then comparable to FE).

Mean-field homogenization.
Example: the Mori-Tanaka model (1973)

Interpretation (Benveniste, 1987): Each inclusion as if in *real matrix* but seeing *average matrix strains* as the far field.



Single ellipsoidal inclusion in an *infinite body* (Eshelby, 1957).

Example: short Glass fiber/Polyamide. Aligned case

[Doghri, Brassart, Adam, Gérard, *IJP*, 2011]

320000 second-order tetrahedra (C3D10M in ABAQUS)

Figure 1: Typical microstructure for the FE simulations comprising 166 aligned fibers in direction 1. The volume fraction of inclusions and their aspect ratio are respectively 15.7% and $\alpha = 15$.

Direct method: full finite element simulation

400000 second-order tetrahedra

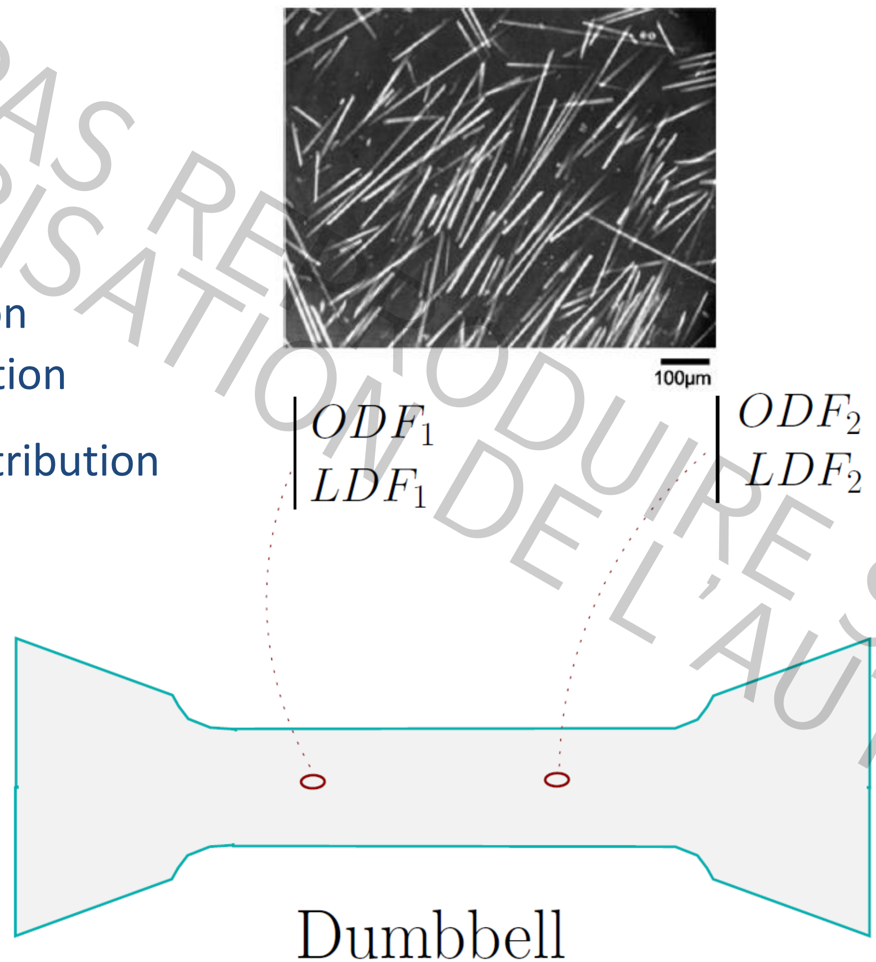
Figure 2: Typical microstructure for the FE simulations comprising 245 randomly oriented fibers in the 1-2 plane. The volume fraction of inclusions and their aspect ratio are respectively 15.7% and $\alpha = 15$.

(+) Accurate, detailed micro-fields.

(-) Difficult, expensive, not for practical engineering use.

Distributed orientations and aspect ratios.
Example: short Glass fiber reinforced thermoplastics

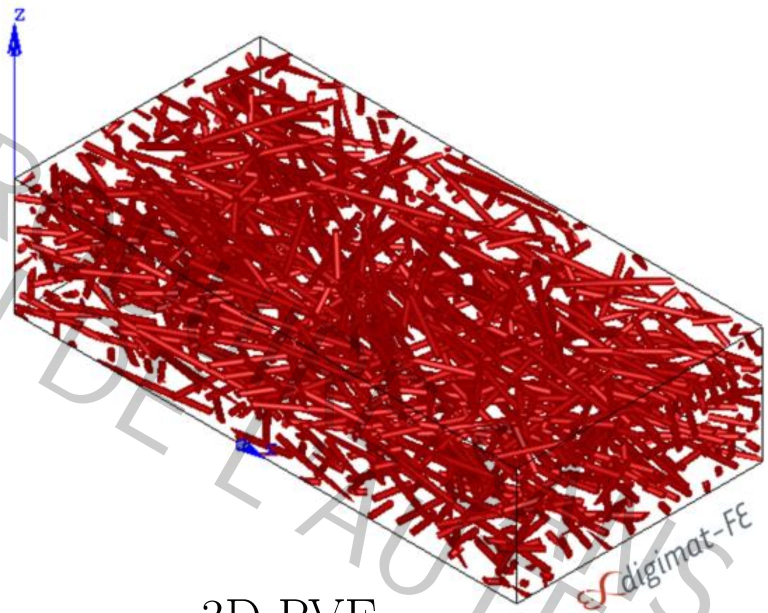
- ODF: Orientation Distribution Function
- LDF: Length Distribution Function



Composite behavior

Mechanical behavior depends strongly on the microstructure

- Matrix and fiber behaviors.
- Fiber volume fraction.
- Fiber orientation distribution.
- Fiber length.
- Moisture level.



3D RVE

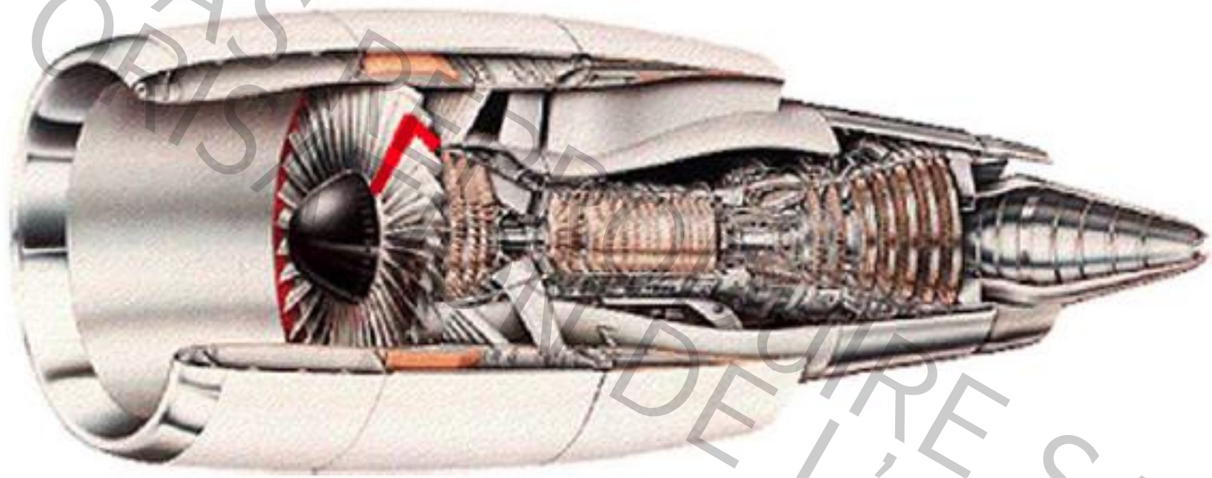


Fig. 6. View of a jet engine. Each turbine blade is supposed to be made of a Ti matrix reinforced with short SiC fibers.

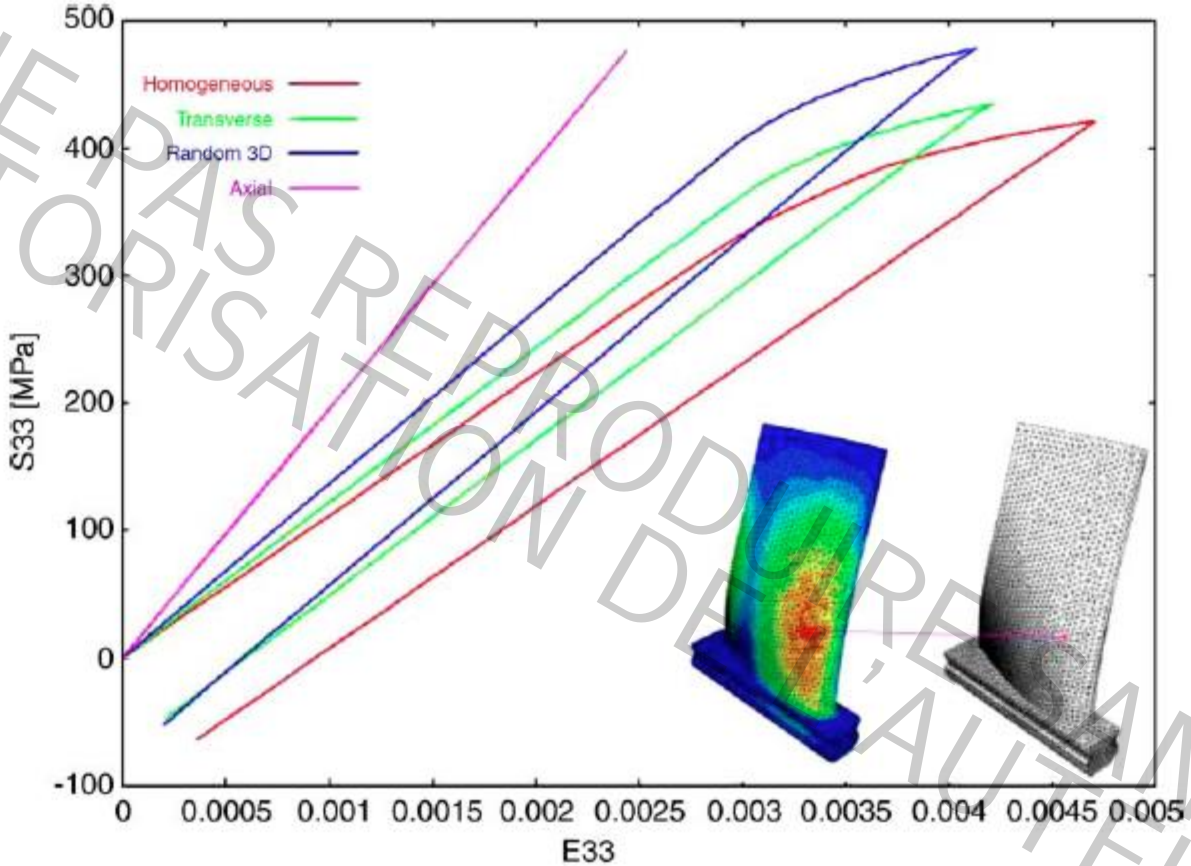


Fig. 7. Two-scale simulation of a turbine blade. FE analysis at the macro scale and homogenization at the microlevel for each macro integration point. Axial stress (MPa) versus axial strain at the most stressed point for the homogeneous and reinforced matrix.

A thermodynamically-based constitutive model for homogeneous thermoplastic polymers coupling viscoelasticity, viscoplasticity and ductile damage

(Krairi and Doghri, Int. J. Plasticity, submitted, 2014)

Total strain decomposition

$$\varepsilon = \varepsilon^{ve} + \varepsilon^{vp}$$

Helmholtz free energy function

$$\psi = \psi^{ve} + \psi^{h}$$

VE-D part of free energy function

$$\rho\psi^{ve}(t) = \frac{1}{2}(1 - D(t)) \int_{-\infty}^{t} \int_{-\infty}^{t} \frac{\partial\varepsilon^{ve}(\tau)}{\partial\tau} : C^{ve}(2t - \tau - \eta) : \frac{\partial\varepsilon^{ve}(\eta)}{\partial\eta} d\tau d\eta$$

Hardening part of free energy

$$\rho\psi^{h}(t) = \frac{1}{2}\alpha(t) : \alpha(t) + \int_{0}^{r(t)} R(\xi) d\xi$$

Clausius-Duhem: non-negative dissipation

$$\phi = \boldsymbol{\sigma} : \frac{d\varepsilon}{dt} - \rho\frac{d\psi}{dt} \geq 0$$

Summary of VE-VP-D model

$$
\left\{
\begin{aligned}
\boldsymbol{\varepsilon} &= \boldsymbol{\varepsilon}^{ve} + \boldsymbol{\varepsilon}^{vp} \\
\boldsymbol{\sigma}(t) &= (1 - D(t)) \int_{-\infty}^{t} \boldsymbol{C}^{ve}(t-\eta) : \frac{\partial \boldsymbol{\varepsilon}^{ve}(\eta)}{\partial \eta} d\eta, \\
\dot{\boldsymbol{\varepsilon}}^{vp} &= \frac{3}{2} \frac{(\tilde{\boldsymbol{s}} - \boldsymbol{X})}{(\tilde{\boldsymbol{\sigma}} - \boldsymbol{X})_{eq}} \dot{p}, \\
\dot{\boldsymbol{X}} &= (1 - D)(a \dot{\boldsymbol{\varepsilon}}^{vp} - b \boldsymbol{X} \dot{p}), \\
\dot{r} &= (1 - D)\dot{p} = g_v((\tilde{\boldsymbol{\sigma}} - \boldsymbol{X})_{eq}, r) \geq 0, \text{ if } f > 0 \text{ otherwise} : \dot{r} = 0 \\
\dot{D} &= \left(\frac{Y}{S}\right)^{s} \dot{p} \geq 0 \text{ if } p > p_D \text{ until } D = D_c \rightarrow \text{crack initiation} \\
Y &= \frac{\tilde{\boldsymbol{s}}_\infty : \tilde{\boldsymbol{s}}_\infty}{4G_\infty} + \frac{(\tilde{\sigma}_{H_\infty})^2}{2K_\infty} + \sum_{i=1}^{I} \frac{\tilde{\boldsymbol{s}}_i : \tilde{\boldsymbol{s}}_i}{4G_i} + \sum_{j=1}^{J} \frac{(\tilde{\sigma}_{H_j})^2}{2K_j}
\end{aligned}
\right.
$$

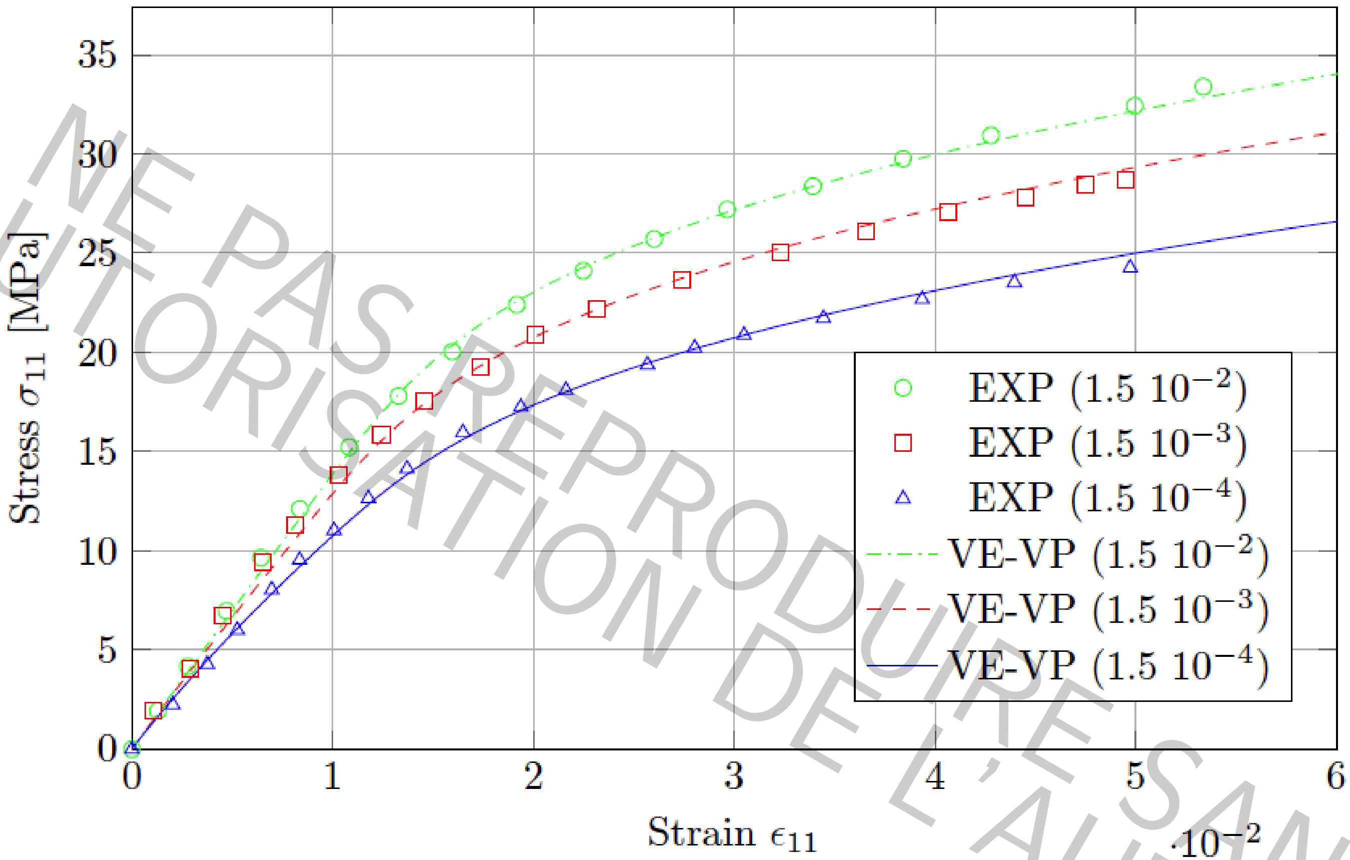
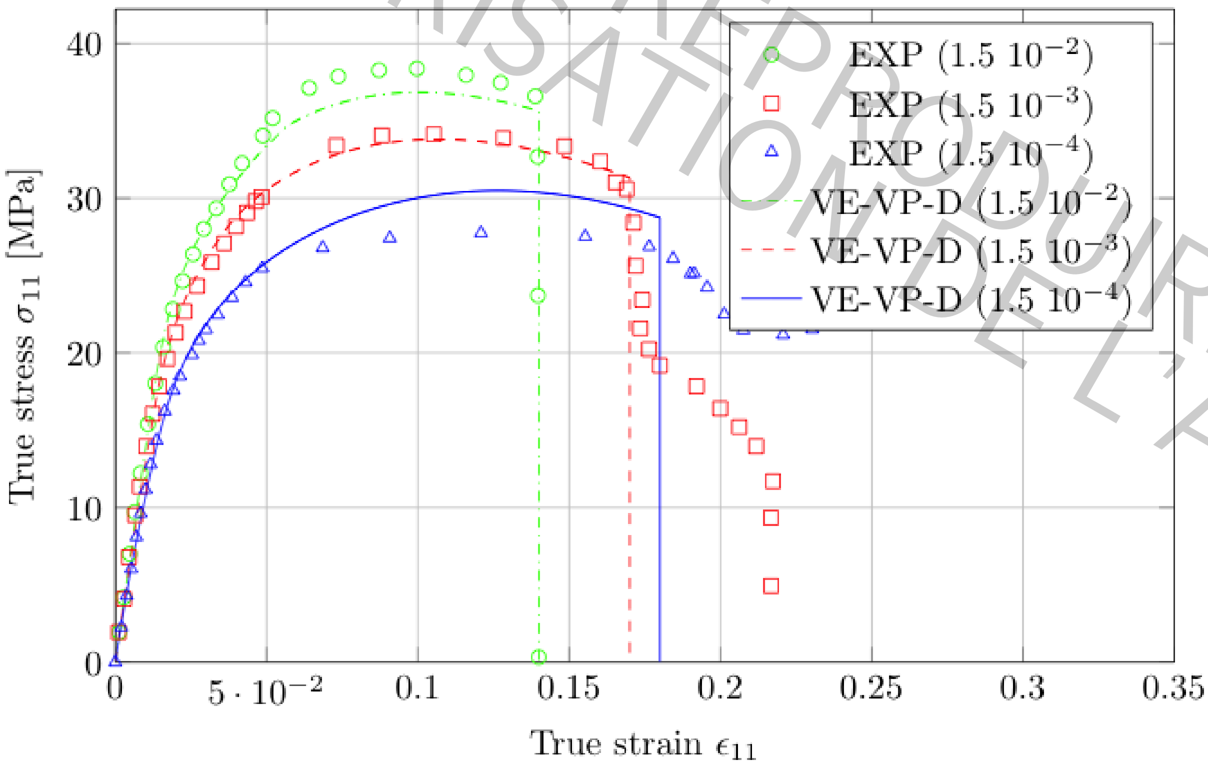
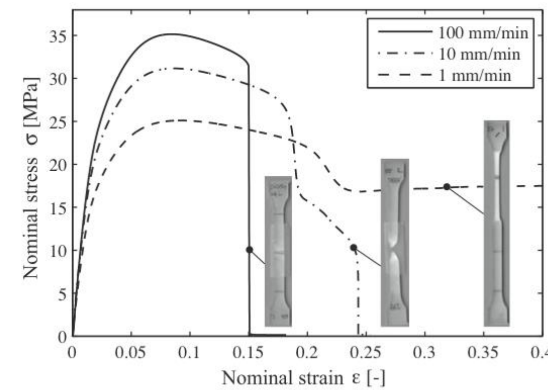


Figure 4: Prediction of the Polypropylene response under tensile loading with different strain rates. Fitted material parameters are listed in table 1. Dots stands for experimental results Kästner et al. (2012) and solid lines for numerical simulations with VE-VP model.

Prediction of failure of polypropylene under monotonic tensile loading using **VE-VP-D model**.

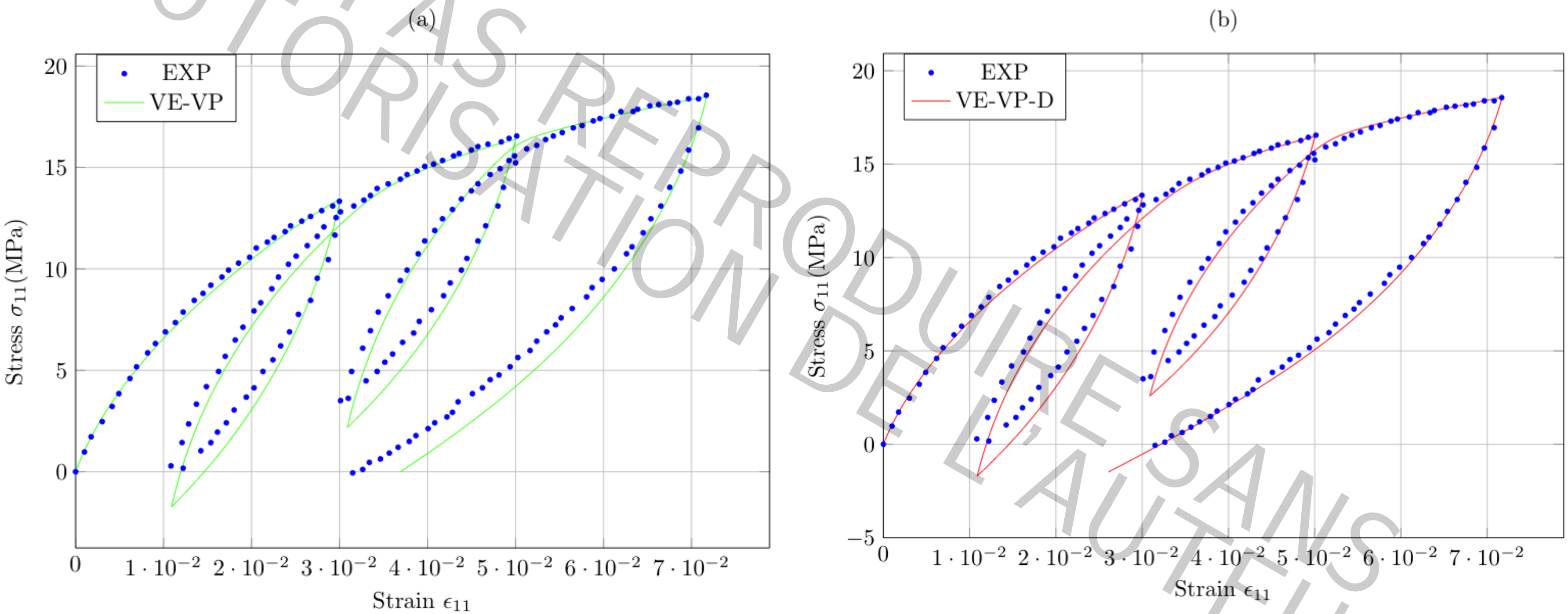




Prediction of uniaxial response of polypropylene under monotonic loading and different strain rates

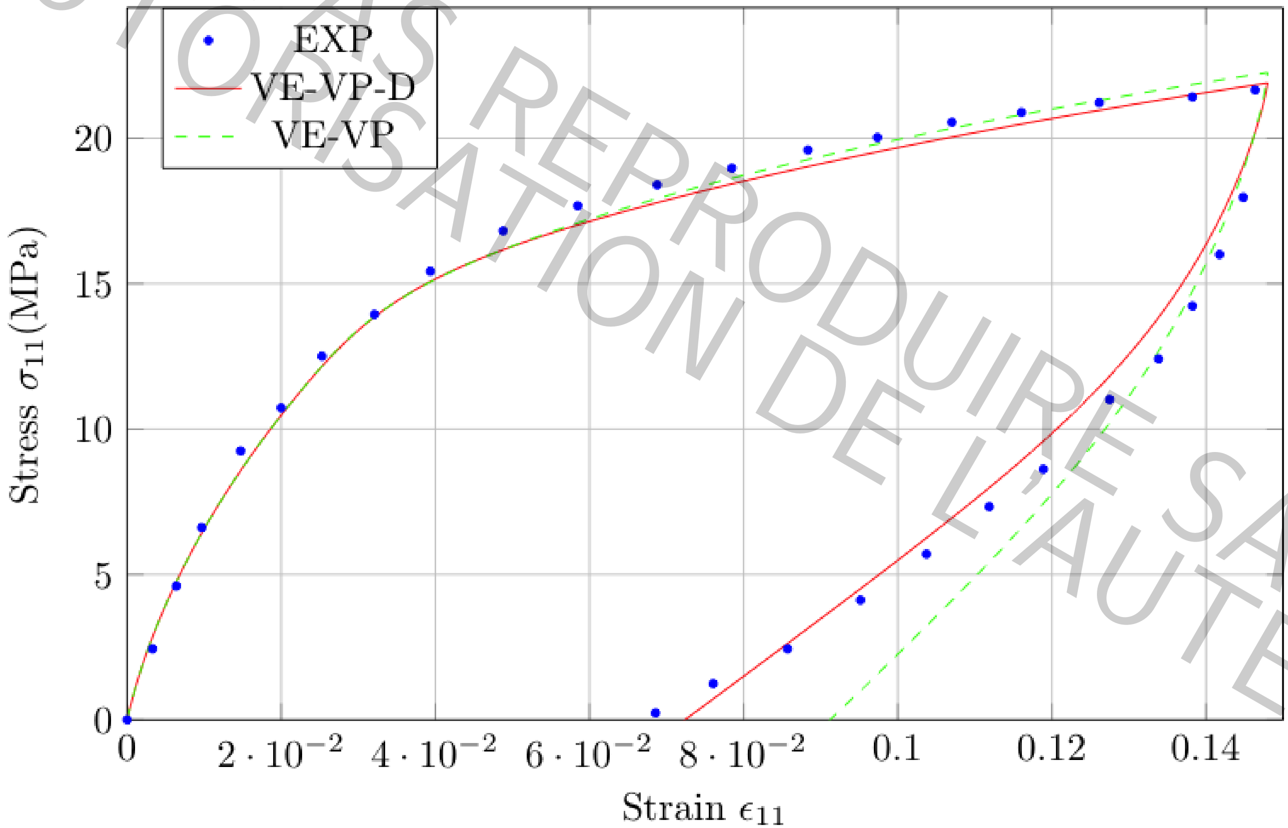
<u>Reference of experimental results</u> : M.Kästner et al./Mechanics of materials 52(2012)40-57

Prediction of behaviour of HDPE under cyclic loading using VE-VP-D model



Reference of experimental results on HDPE : Zhang et al./Polymer Engineering & Science (1997), 414--420

Prediction of behaviour of HDPE under cyclic loading using VE-VP-D model



Reference of experimental results on HDPE : Zhang et al./Polymer Engineering & Science (1997), 414--420

MFH for inelastic composites

Nonlinear mean-field homogenization

- Based on definition of a *Linear Comparison Material* (LCC).

- **First approach**:

  - *direct linearization* of micro nonlinear constitutive models
  - LCC definition based on first moments of strain field per phase (volume averages), or on first and second moments (variance).

- **Second approach:**

  - *variational formulation*
  - *LCC definition is an outcome of the variational formulation*

Direct linearization of the local response

- **secant**:

$$\boldsymbol{\sigma} = \boldsymbol{C}^{\text{sec}} : \boldsymbol{\varepsilon}$$

(Berveiller and Zaoui 1979, Tandon and Weng 1988)

- **tangent/affine**

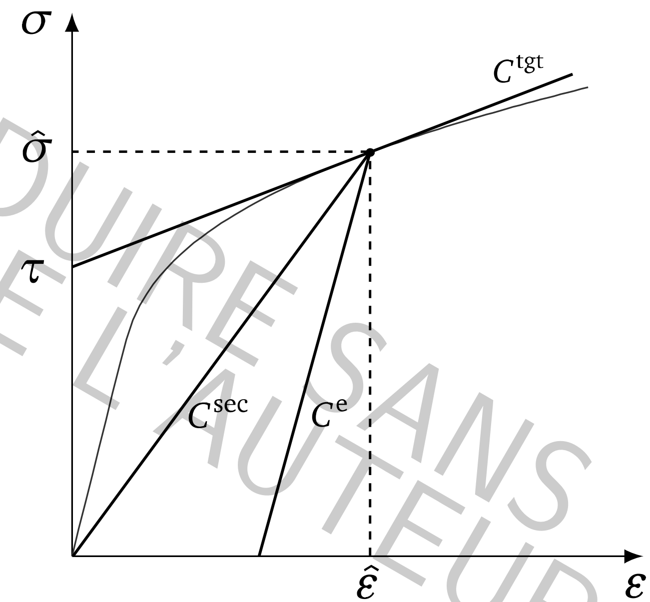
$$\boldsymbol{\sigma} = \boldsymbol{C}^{\text{tgt}} : \boldsymbol{\varepsilon} + \boldsymbol{\tau}$$

(Molinari et al. 1987, Masson et al. 2000)

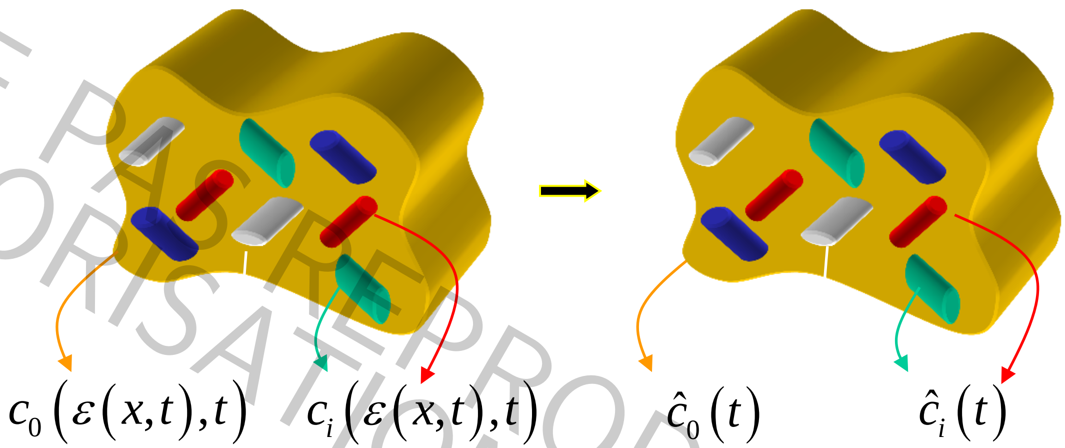
- **incremental tangent**

$$\dot{\boldsymbol{\sigma}} = \boldsymbol{C}^{\text{tgt}} : \dot{\boldsymbol{\varepsilon}}$$

(Hill 1965, Hutchinson 1970, Doghri and Ouaar 2003)



Direct linearization approach
Second issue: comparison materials



- Instantaneous stiffness operator (tangent or algorithmic or secant): not uniform per phase, depends on position ***x*** and time *t*.

- Workaround: fictitious comparison materials, uniform tangent operator per phase, depending only on time *t*.

- First-order homogenization: comparison materials computed from average strain field per phase.
- Second-moment and variational formulations: include variance of per-phase strain and stress fields

Incrementally affine linearization method

(Doghri, Adam, Bilger, IJP, 2010; Miled, Doghri, Brassart, Delannay, IJSS, 2013)

- General viscoplastic model, set of internal variables ***V*** (scalars, tensors)

$$\dot{\epsilon}^{vp}(t) = \tilde{\epsilon}(\boldsymbol{\sigma}(t), \boldsymbol{V}(t)), \quad \dot{\boldsymbol{V}}(t) = \tilde{\boldsymbol{V}}(\boldsymbol{\sigma}(t), \boldsymbol{V}(t))$$

- Linearization of evolution equations of internal variables:

$$\dot{\epsilon}^{vp}(t) \approx \dot{\epsilon}^{vp}(\tau) + \tilde{\epsilon}_{,\boldsymbol{\sigma}}(\tau) : (\boldsymbol{\sigma}(t) - \boldsymbol{\sigma}(\tau)) + \tilde{\epsilon}_{,\boldsymbol{V}}(\tau) \bullet (\boldsymbol{V}(t) - \boldsymbol{V}(\tau))$$

$$\dot{\boldsymbol{V}}(t) \approx \dot{\boldsymbol{V}}(\tau) + \tilde{\boldsymbol{V}}_{,\boldsymbol{\sigma}}(\tau) : (\boldsymbol{\sigma}(t) - \boldsymbol{\sigma}(\tau)) + \tilde{\boldsymbol{V}}_{,\boldsymbol{V}}(\tau) \bullet (\boldsymbol{V}(t) - \boldsymbol{V}(\tau))$$

Choices : $\tau = t_{n+1}$ and $t = t_n$.

- Backward Euler time discretization (fully implicit).

- **Final result:**

$$\Delta\boldsymbol{\sigma} = \boldsymbol{c}^{alg}(t_{n+1}) : (\Delta\epsilon - \Delta\epsilon^{af})$$

$\boldsymbol{c}^{alg}$: algorithmic tangent operator, $\Delta\epsilon^{af}$: affine strain increment.

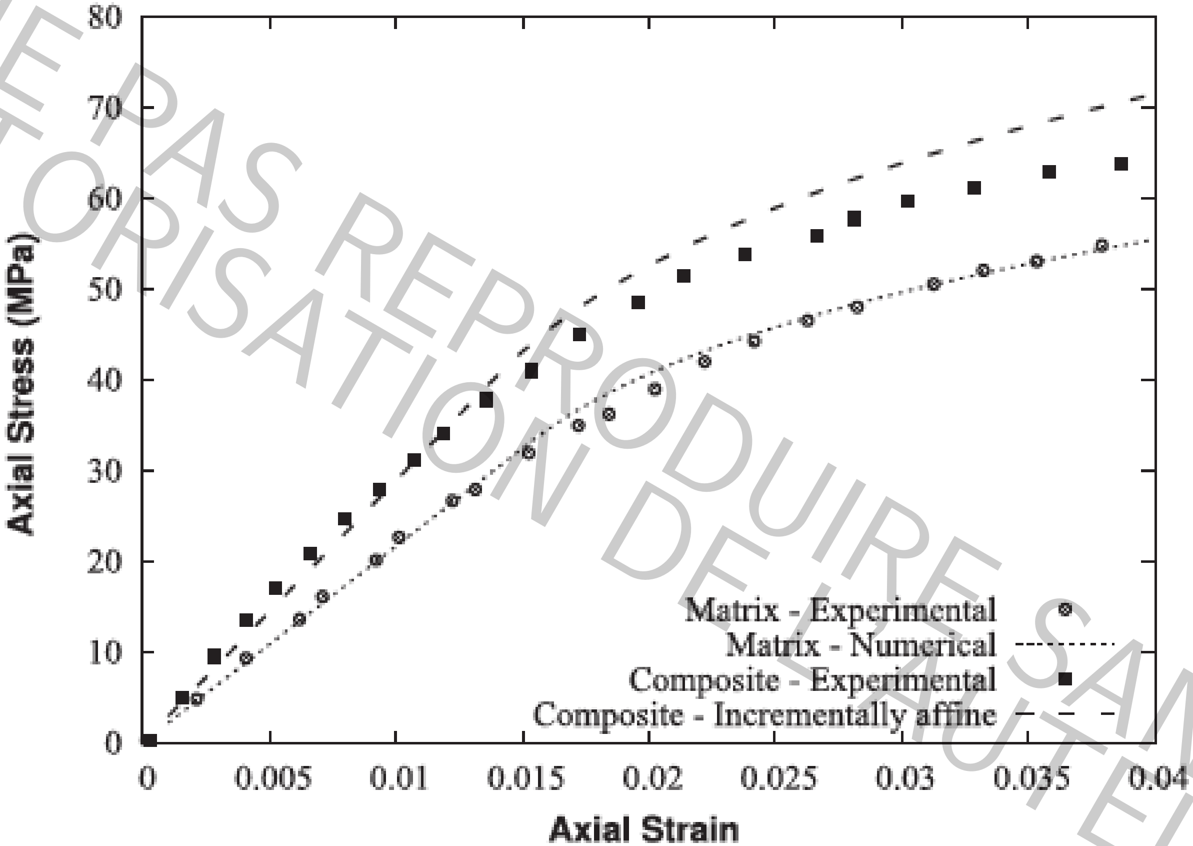


Fig. 14. Polycarbonate matrix reinforced with 10% of short glass fibers (with an aspect ratio of the order of 100) under uniaxial tension test at the strain rate of $0.0011\ s^{-1}$. Experimental data from Drozdov et al. (2003).

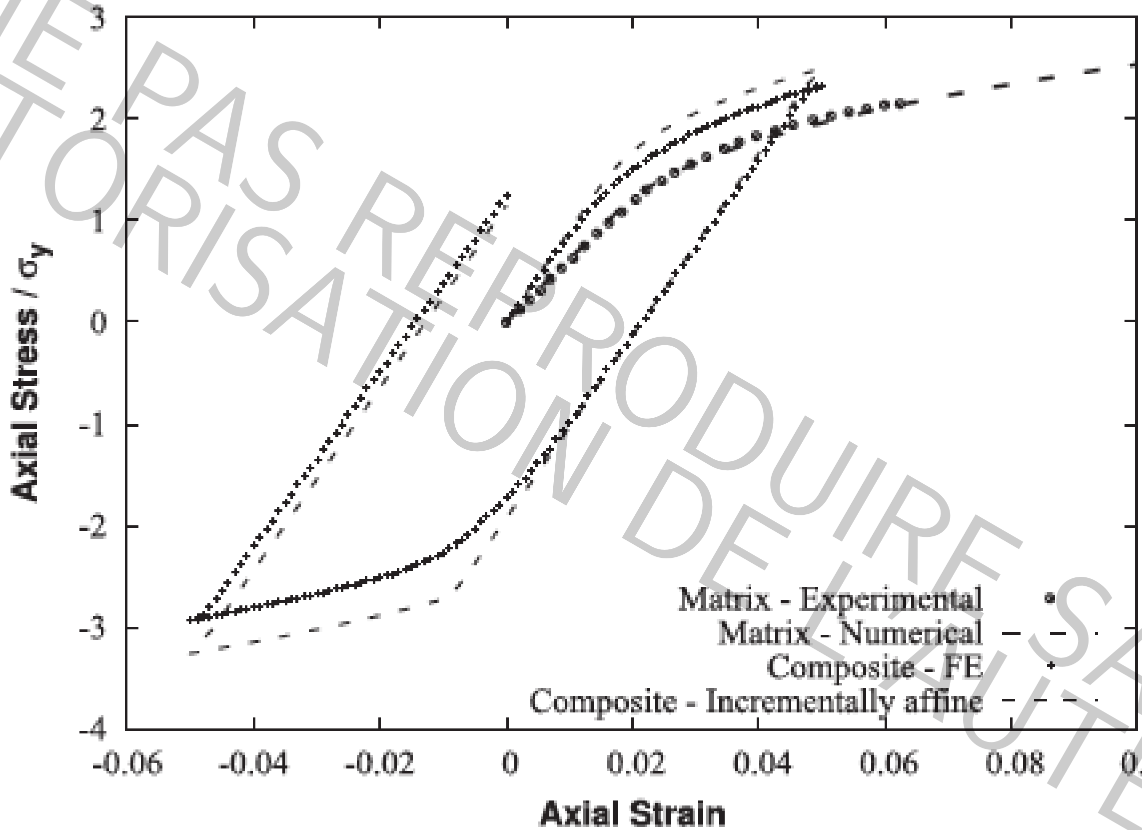


Fig. 3. Polycarbonate matrix reinforced with elastic spherical particles. Uniaxial cyclic loading at the strain rate of 0.005 s^{-1} for a volume fraction of inclusions equal to 15%.

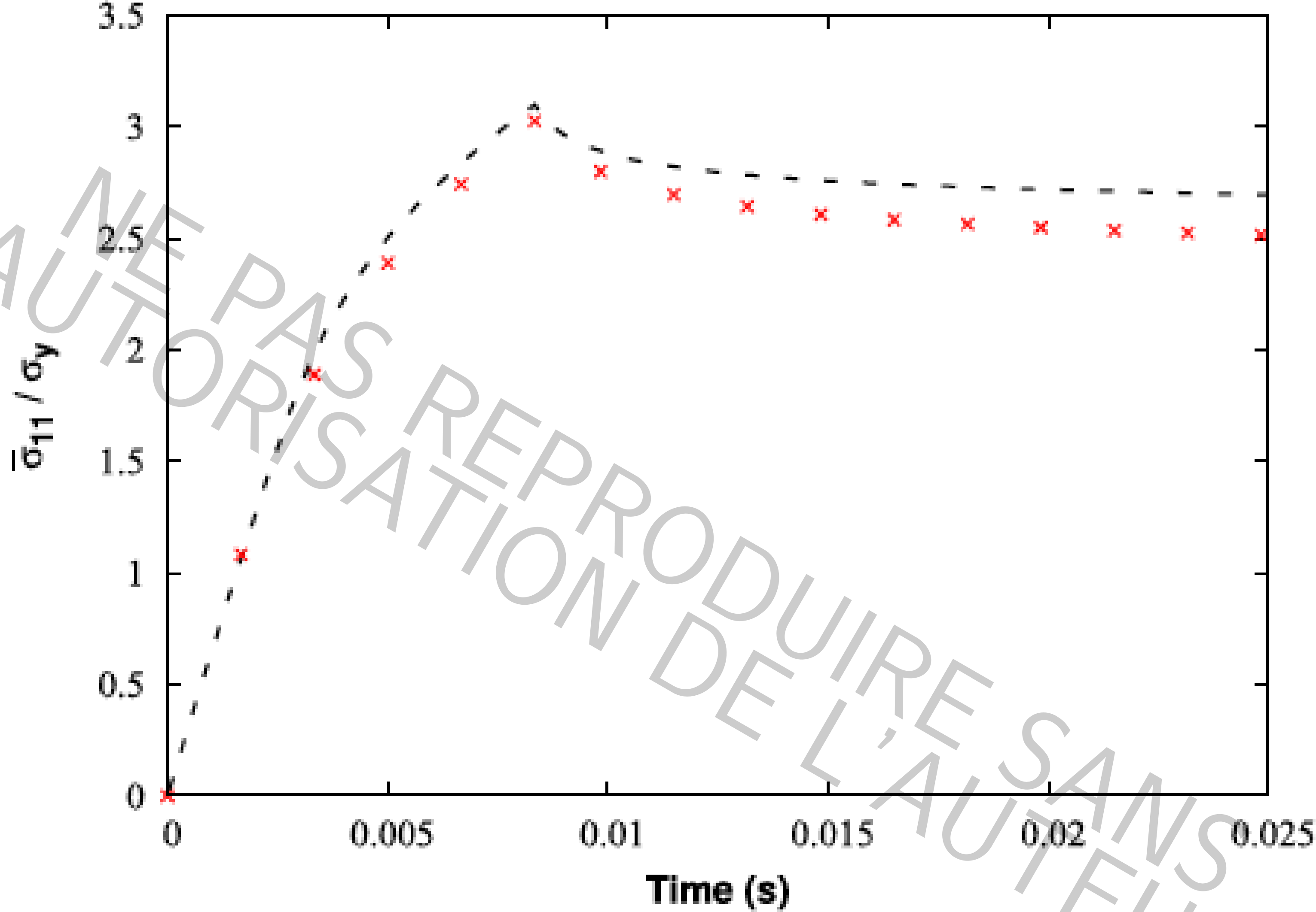


Fig. 8. Finite-element (symbols) and incrementally affine homogenization (dashed line) results for a volume fraction of inclusions of 15%. Two-stage uniaxial load: (1) strain rate of 6 s^{-1} up to time $t = 0.00833$ s, (2) relaxation. Fitted matrix material parameters are listed in Table 1.

Applicability to bio composites

For mechanical modeling, main differences between natural and Glass or Carbon fibers:

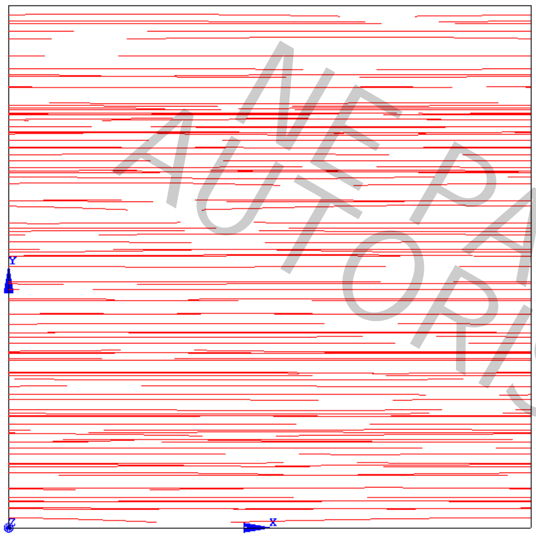
- Important variability of some material properties,
- Larger spread of fibers’ geometry distribution,
- Fibers not well dispersed in the volume (clustering),
- More curved fibers.

Impossible d'afficher l'image.

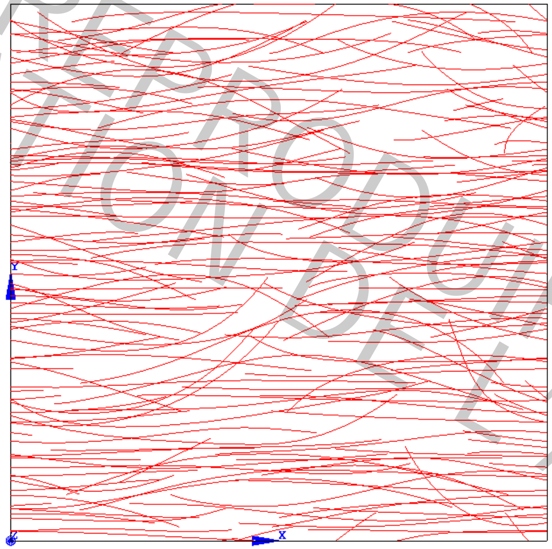
Impossible d'afficher l'image.

Fiber curvature

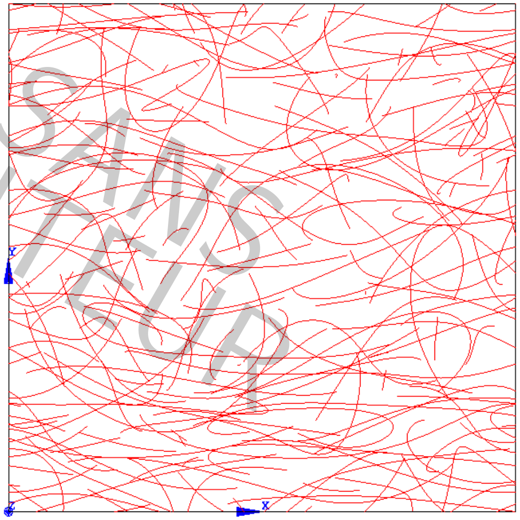
- Additional parameter to characterize fiber tortuosity
- Random process



Very low tortuosity

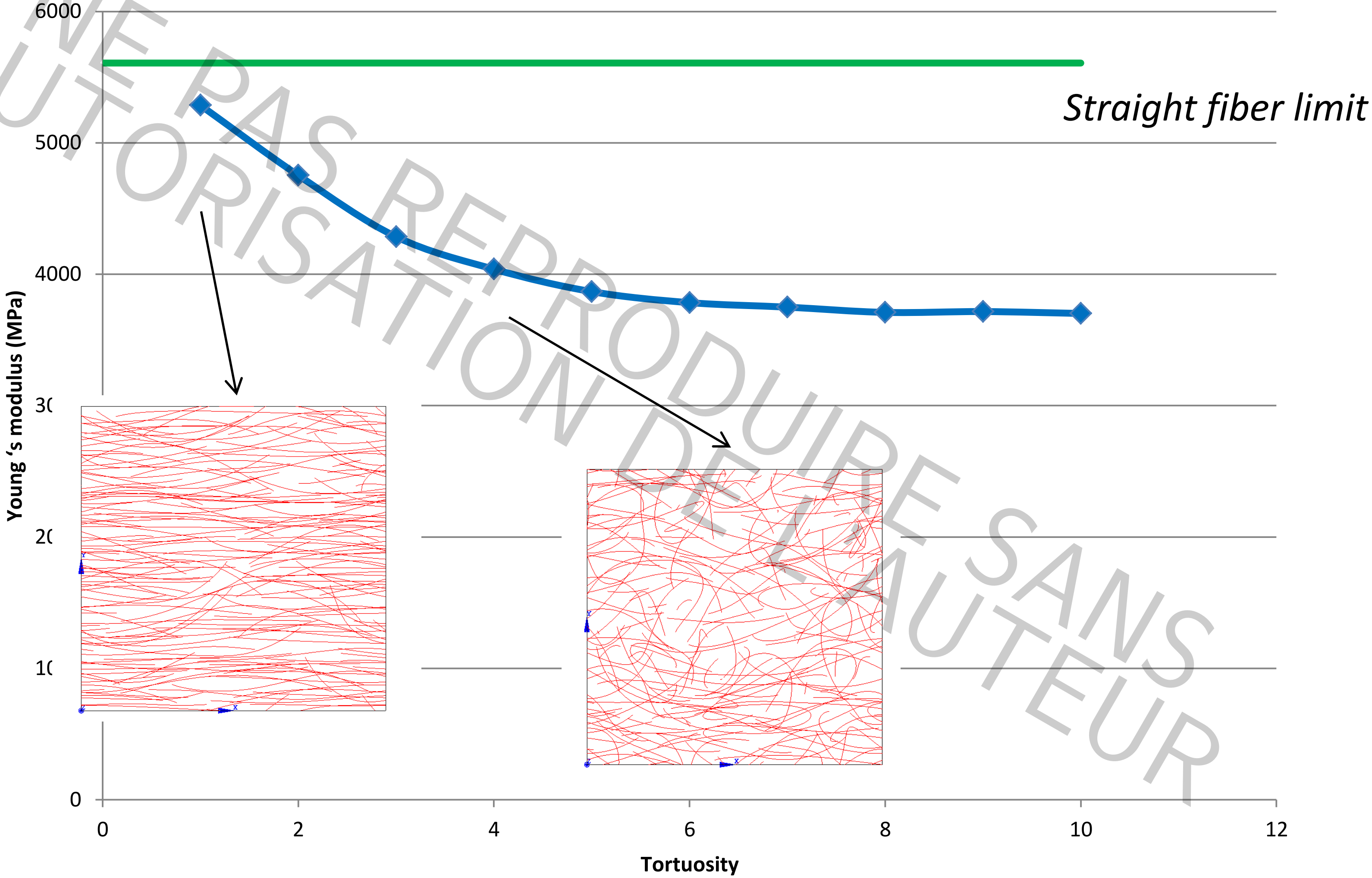


Medium tortuosity



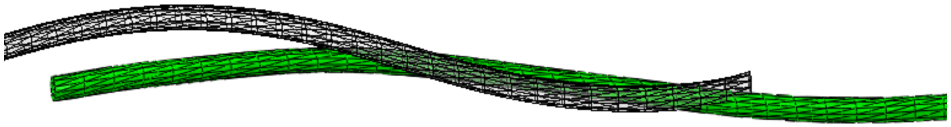
High tortuosity

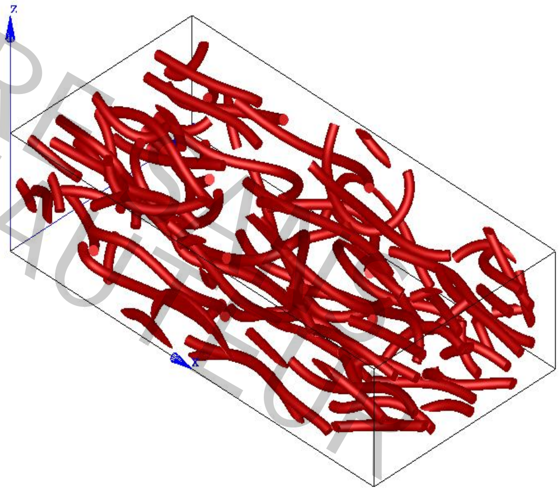
Fiber curvature : Effect on elastic stiffness



Mimicking fiber waviness in Digimat-MF

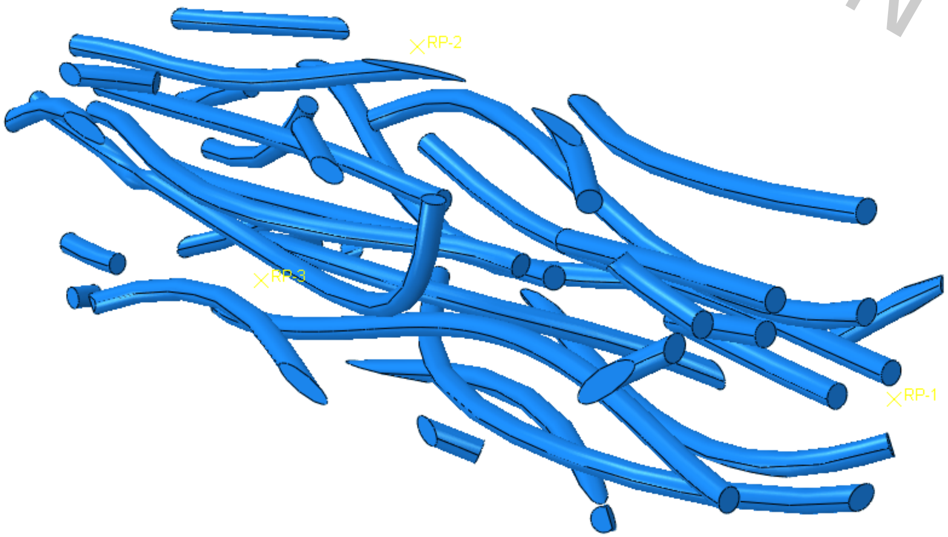
- Using :
  - Orientation tensor
    - Addition/replacement of the predicted straight/short fiber orientation tensor by a long/curved fiber equivalent
  - Equivalent aspect ratio
  - Nonlinear elastic stiffness including material and structural stiffness

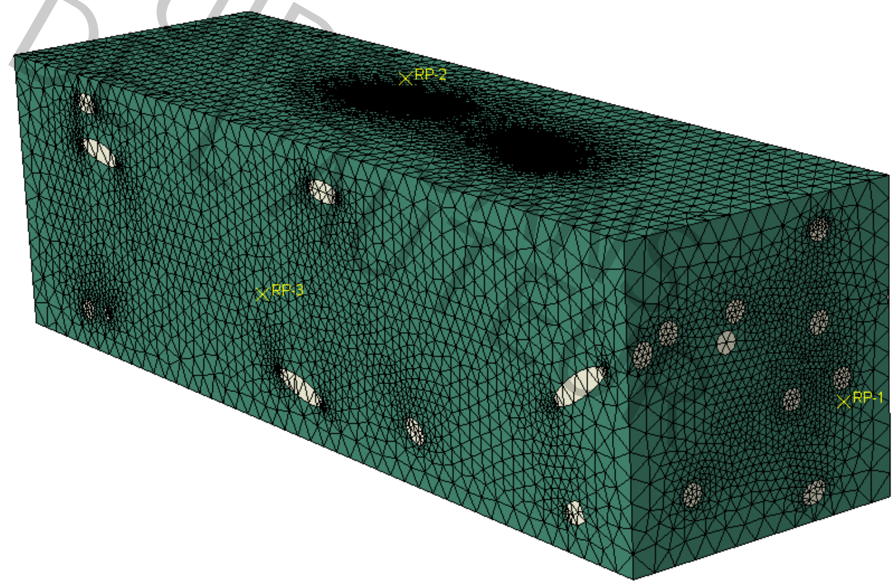




Influence of fiber waviness using Digimat-FE

- Microstructure :
  - 5% VF (+- 13% weight fraction)
  - 15 fibers
  - Periodic
  - AR = 40 (AR = curvilinear length / diameter)
- Mesh
  - 465 173 second order tetrahedral elements
  - Mesh quality indicator : 1390 elements with warning (0.298814%)

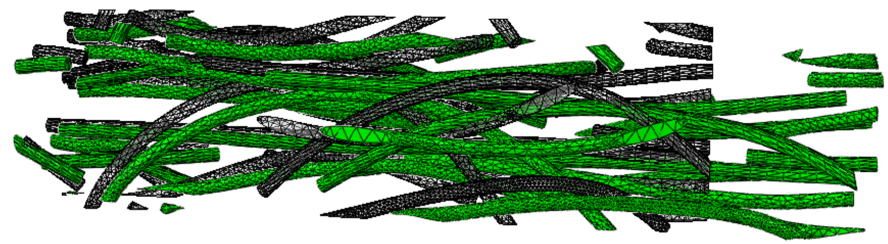


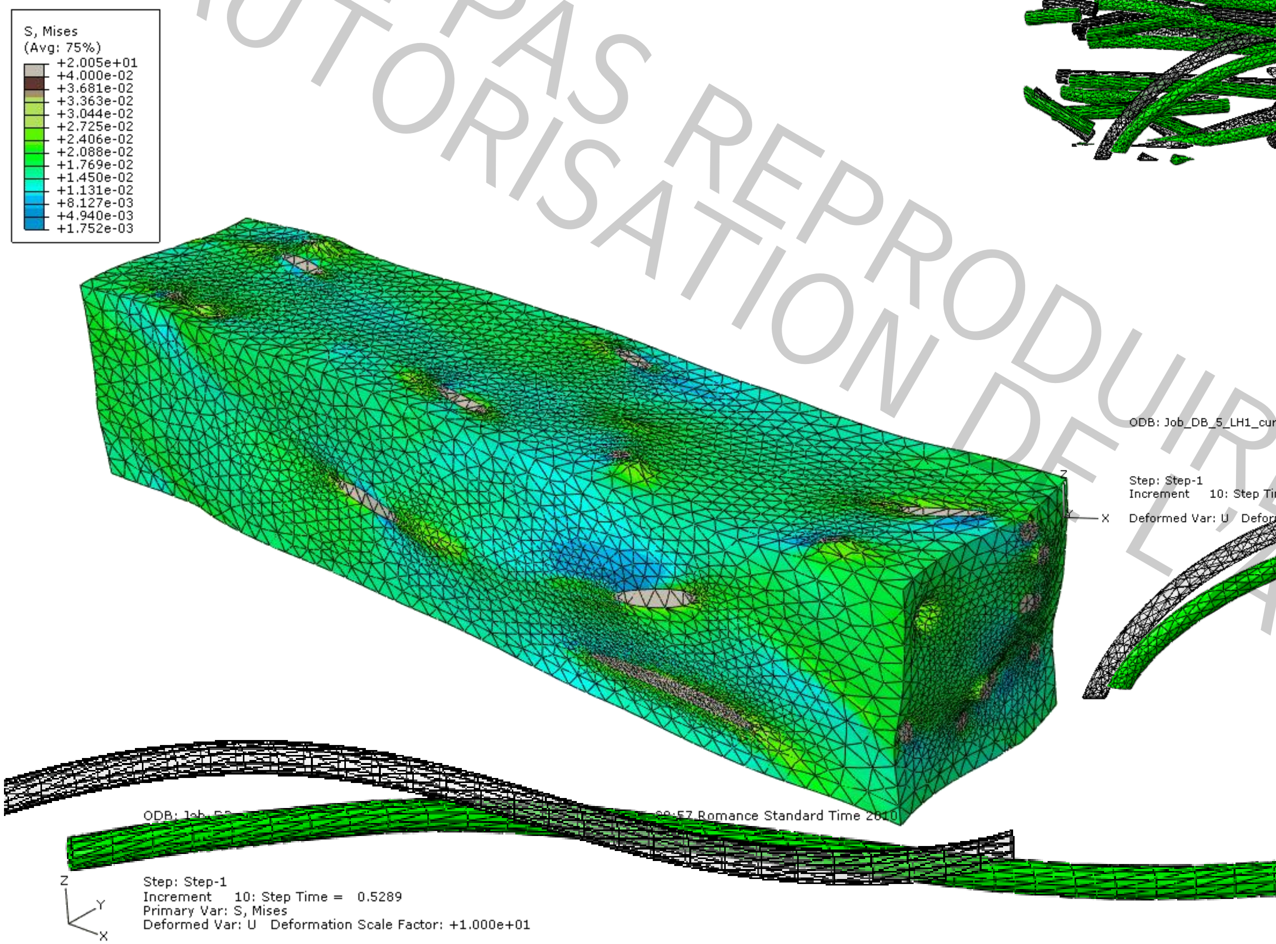


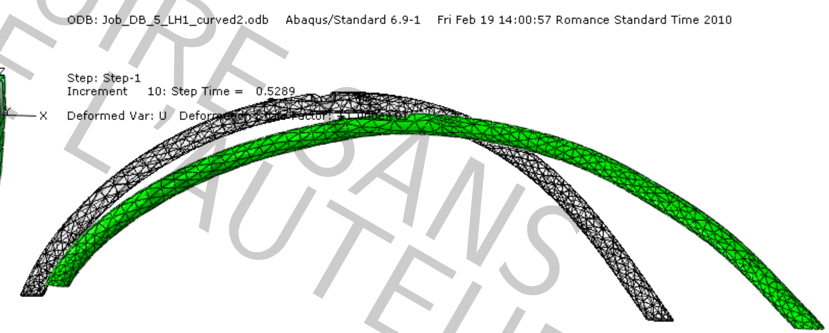
Influence of fiber waviness using Digimat-FE

Macro strain E_xx = 2.12%

Scale factor = 10







Bent fibers straighten under uniaxial strain

Conclusions

Multi-scale modeling

- Enables to predict the influence of the micro-structure on the macroscopic properties. For composite materials, two main methods:

Direct numerical simulation of microstructures, e.g. by finite elements:

- Very accurate, gives details micro fields
- Very expensive, especially for nonlinear problems
- Great verification tool for simpler and cheaper methods

Mean-field homogenization (MFH):

- Easiest to use and cheapest scale-transition approach.
- Nonlinear MFH: active reserach field

A thermodynamically based VE-VP-D model for homogeneous polymers

Applicability of MFH for bio composites