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**Modélisation multi-échelle non-linéaire par homogénéisation périodique et analyses par  $FE^2$ : application aux composites à matrice elastoviscoplastique endommageable**

*Non-linear multi-scale modelling through periodic homogenization and  $FE^2$  analyses: application for composites with elastoviscoplastic damageable matrix*

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## Résumé

Dans ce papier, une technique de modélisation multi-échelle ( $FE^2$ ) basée sur le principe d'homogénéisation périodique a été développée pour décrire le comportement des structures composites 3D avec un comportement elastoviscoplastique des endommageable. L'approche proposée permet de simuler le comportement macroscopique non linéaire d'un composite à microstructure périodique à partir d'un calcul EF sur sa cellule unitaire, elle-même alimentée par les lois de comportement de chacun de ses constituants. La méthode introduit ainsi le concept de méta modèle. Le principal avantage de cette méthode est de s'affranchir totalement des limitations sur les lois de comportement locales, ainsi que les lois constitutives à l'échelle macroscopique ne sont pas nécessaire. La mise en œuvre numérique de cette stratégie a été réalisée dans ABAQUS Implicit. Enfin l'approche a été validée sur macro-structure 3D sur laquelle, une cellule unitaire est affectée à chaque point d'intégration.

## Abstract

In this paper, a two-level Finite Element method ( $FE^2$ ), based on periodic homogenization, has been introduced to describe the behavior of 3D composite structures with elastoviscoplastic behavior and ductile damage. In the present approach, the unknown constitutive relationship at the macroscale is obtained by solving a local finite element problem at the microscale (unit cell). The main advantage of the proposed strategy is that the  $FE^2$  method does not require an analytical form for the constitutive law at the macroscale. It can integrate any kind of microstructure with any type of non-linear behavior of the reinforcement (fibers and/or particles) embedded in the matrix. The numerical implementation of this model has been achieved with parallel computation technique in ABAQUS Implicit, where a python script and user subroutines UMAT have been developed for this goal. Finally numerical results are presented for a 3D composite structure.

**Mots Clés :** calcul multi-échelle ( $FE^2$ ), homogénéisation périodique, matériaux composite, comportement elastoviscoplastique, endommagement.

**Keywords:** multiscale Finite Element computation ( $FE^2$ ), periodic homogenization, Composite materials, elastoviscoplastic behavior, damage.

## 1. Introduction

Nowadays, composite materials are considered to be a good technological solution for automobile and aeronautic industries, because of their lightness and their structural durability. For this reason, the identification of the mechanical properties of these materials triggered intense researches during the past decades. In order to investigate and describe the behavior of the composite materials and structures, advanced modeling and simulation methods are necessary. Several numerical approaches have been proposed for modeling the nonlinear behavior of composite structures including the LATIN method [1-2], the sequential multi-scale method [3] and the multi scale finite element method (FE<sup>2</sup> method) introduced by Feyel [5-6-7].

In this work, a two-level finite element method (FE<sup>2</sup>), based on the concept of periodic homogenization is proposed. The method predicts the 3D nonlinear macroscopic behavior for a composite with periodic microstructure by considering that each macroscopic integration point has its own unit cell, which includes the material and geometrical characteristics of the constituents in the microstructure. To this end, a FE<sup>2</sup> analysis process has been developed using an implicit resolution scheme, with the use of a Newton Raphson algorithm to solve the nonlinear system of equations at the macroscopic and the microscopic scales.

The main advantage of this methodology is that it can account for any type of nonlinear behavior, as well as any form of periodic microstructure. This idea was originally introduced by Renard and Marmonier in 1987 [4], and various authors have implemented the original approach or proposed extensions [8-5-6-7-9-10-11]. The computational scheme of the method is in brief the following: at each macroscopic strain increment, the macroscopic tangent modulus and the macroscopic stress are computed at each macroscopic integration point by solving iteratively a FE problem at the microscopic level. In this paper, the method is implemented in a 3D structure, with a 3D unit cell and accounts for viscoplastic and damage mechanisms.

The layout of this paper is as follows: in section 2, the theoretical formulation of the microscopic and the macroscopic problems is described as well as the principle of scale transition between the local and the global fields. In section 3, details of the numerical implementation of FE<sup>2</sup> method is given for a 3D nonlinear problem. In section 4, the approach is validated on a real 3D composite structure exhibiting heterogeneous strain fields, in which the microstructure consists of an elastoviscoplastic polymer matrix with ductile damage, reinforced by short glass fibers.

## 2. Theoretical formulation of micro-macro level

The objective of the periodic homogenization theory is to define a fictitious homogeneous medium having similar behavior with the average response of the periodic unit cell that represents the microstructure. The framework presented in this section follows the works of [12-13] where more details can be found.

A periodic medium is defined by a repeated unit cell that is translated along three vectors. It is important to point out that the concept of periodic homogenization works fine as long as a separation of scales is possible. This means that the dimensions of the unit cell, defining the microscopic level, must be much smaller than the macroscopic dimensions of the medium.

According to the average stress and strain theorems, it can be shown that the stress and the strain averages within a unit cell are equal to the stress and the strain applied at its boundaries, which are considered as the macroscopic stress and strain respectively. The relationship between the two scales is given by the following equations:

$$\bar{\sigma} = \langle \sigma \rangle = \frac{1}{V} \int_V \sigma dV = \frac{1}{V} \int_V \sigma \cdot n \otimes x dS, \quad (\text{Eq. 2.1})$$

$$\bar{\varepsilon} = \langle \varepsilon \rangle = \frac{1}{V} \int_V \varepsilon dV = \frac{1}{2V} \int_V (u \otimes n + n \otimes u) dS, \quad (\text{Eq. 2.2})$$

where  $\sigma$ ,  $\varepsilon$ ,  $\bar{\sigma}$  and  $\bar{\varepsilon}$  denote the microscopic and the macroscopic stress and strain tensors respectively,  $V$  is the volume of the unit cell.  $x$  and  $u$  are the position and the displacement vectors respectively,  $n$  is the outgoing normal of the unit cell boundary  $\partial V$ .  $\langle \bullet \rangle$  is the mean operator and  $\otimes$  the dyadic product.

## 2.1 Microscopic problem

The assumption of periodicity implies that the displacement vector  $u$  of any material point located in  $x$  can be written under the form of an affine part and periodic fluctuation part  $u'$ :

$$u(x) = \bar{\varepsilon} \cdot x + u'(x) \quad (\text{Eq. 2.3})$$

The fluctuation part of the displacement  $u'$  is periodic and it takes the same value on opposite sides of the unit cell. The strain average produced by  $u'$  is null and the average strain in the unit cell is given by:

$$\langle \varepsilon(u) \rangle = \bar{\varepsilon} + \langle \varepsilon(u') \rangle = \bar{\varepsilon} \quad (\text{Eq. 2.4})$$

The stress field is also periodic and satisfies the conditions of equilibrium within the unit cell. The local problem is formulated as follow:

$$\begin{cases} \sigma(x) = F(x, \bar{\varepsilon} + \varepsilon(u'(x))), & \forall x \in V, \\ \text{div}(\sigma(x)) = 0, & \forall x \in V, \\ u'(x_+) = u'(x_-), \quad \sigma(x_+) \cdot n = -\sigma(x_-) \cdot n, & \forall x \in \partial V \end{cases} \quad (\text{Eq. 2.5})$$

where  $x_+$  and  $x_-$  are the coordinates of each pair of opposite points of the unit cell boundary,  $\text{div}(\bullet)$  denotes the divergence operator and  $F(\bullet)$  is an operator that defines the relationship between local stress and strain (possibly nonlinear). In linear elasticity the microscopic stress/strain relationship is given by:

$$\sigma(x) = C(x) : (\bar{\varepsilon} + \varepsilon(u'(x))), \forall x \in V, \quad (\text{Eq. 2.6})$$

where  $C$  is the fourth order stiffness tensor and  $:$  denotes the twice contracted product.

## 2.2 Macroscopic problem

It is assumed that the material is heterogeneous and characterized by a periodic microstructure. The macroscopic stress can be calculated by averaging the local stress using the (Eq. 2.1). The equilibrium at the macroscopic level in the absence of body forces is written as follows:

$$\text{div}(\bar{\sigma}(\bar{x})) = 0 \quad (\text{Eq. 2.7})$$

where  $\bar{\sigma}(\bar{x})$  is the Cauchy stress tensor associated with the point  $\bar{x}$  of the macrostructure. The macroscopic stress/strain linear relationship is given in Voigt notation by:

$$\begin{Bmatrix} \bar{\sigma}_1 \\ \bar{\sigma}_2 \\ \bar{\sigma}_3 \\ \bar{\sigma}_4 \\ \bar{\sigma}_5 \\ \bar{\sigma}_6 \end{Bmatrix} = \begin{pmatrix} \bar{C}_{11} & \bar{C}_{12} & \bar{C}_{13} & \bar{C}_{14} & \bar{C}_{15} & \bar{C}_{16} \\ & \bar{C}_{22} & \bar{C}_{23} & \bar{C}_{24} & \bar{C}_{25} & \bar{C}_{26} \\ & & \bar{C}_{33} & \bar{C}_{34} & \bar{C}_{35} & \bar{C}_{36} \\ & & & \bar{C}_{44} & \bar{C}_{45} & \bar{C}_{46} \\ & & & & \bar{C}_{55} & \bar{C}_{56} \\ & & & & & \bar{C}_{66} \end{pmatrix} \times \begin{Bmatrix} \bar{\varepsilon}_1 \\ \bar{\varepsilon}_2 \\ \bar{\varepsilon}_3 \\ \bar{\varepsilon}_4 \\ \bar{\varepsilon}_5 \\ \bar{\varepsilon}_6 \end{Bmatrix} \quad (\text{Eq. 2.8})$$

where  $\bar{\mathbb{C}}$  is the macroscopic stiffness tensor that can be recovered by calculating the macroscopic stress resulting from the six elementary strain states given in (Eq. 2.9) also in Voigt notation

$$\begin{cases} \bar{\varepsilon}_1 = (k \ 0 \ 0 \ 0 \ 0 \ 0)^T \\ \bar{\varepsilon}_2 = (0 \ k \ 0 \ 0 \ 0 \ 0)^T \\ \bar{\varepsilon}_3 = (0 \ 0 \ k \ 0 \ 0 \ 0)^T \\ \bar{\varepsilon}_4 = (0 \ 0 \ 0 \ k \ 0 \ 0)^T \\ \bar{\varepsilon}_5 = (0 \ 0 \ 0 \ 0 \ k \ 0)^T \\ \bar{\varepsilon}_6 = (0 \ 0 \ 0 \ 0 \ 0 \ k)^T \end{cases} \quad (\text{Eq. 2.9})$$

with  $k = 1$ . Then, the  $ij$  component of the stiffness tensor is given by the  $i^{th}$  component of the stress vector calculated with the  $j^{th}$  elementary strain state, divided by the  $j^{th}$  component of the strain vector of the  $j^{th}$  elementary strain state that is equal to  $k$ :

$$\bar{C}_{ij} = \frac{\bar{\sigma}_{i(j)}}{k}, \quad i, j = 1, 2, 3, 4, 5, 6 \quad (\text{Eq. 2.10})$$

For non-linear materials, the macroscopic stress/strain relationship cannot be explicitly provided by a stiffness tensor. Nevertheless, for a given macroscopic strain, the macroscopic stress response can be computed using an implicit resolution scheme, where the local behavior is linearized and corrected at each strain increment. Then using the same principle the macroscopic behavior can also be linearized in order to predict the next increment. This linearization requires to write the microscopic and macroscopic constitutive law in the rate form as follows:

$$\dot{\sigma}(x) = C_t(x) : \left( \dot{\bar{\varepsilon}} + \dot{\varepsilon}(\dot{u}'(x)) \right), \quad \forall x \in V \quad (\text{Eq. 2.11})$$

$$\dot{\bar{\sigma}} = \langle \dot{\sigma}(x) \rangle = \langle C_t(x) : \left( \dot{\bar{\varepsilon}} + \dot{\varepsilon}(\dot{u}'(x)) \right) \rangle, \quad \forall x \in V \quad (\text{Eq. 2.12})$$

where  $C_t$  is the local tangent stiffness tensor defined as the differentiation of the stress with respect to the total strain. In order to connect the microscopic problem with any macroscopic problem, the global tangent stiffness tensor  $\bar{C}_t$  is computed by applying the six elementary strain states in the same way as previously described for linear elasticity.

### 3. Numerical implementation in ABAQUS

The developed approach lies within the general category of multiscale models. It consists of three main goals according to F. Feyel [5]:

- (1) A geometrical description and a FE model for the unit cell
- (2) The local constitutive laws expressing the response of each component of the composite within the unit cell.

(3) Scale transition relationships that define the connection between the local and the global fields (stress and strain).

The scale transition is obtained by considering periodic homogenization, which is expressed using specific boundary conditions on the unit cell. The macroscopic fields (stress and strain) are introduced with the help of additional degrees of freedom (DOFs) that are connected to the unit cell using kinematic equations. Thus, the behavior of a 3D macroscopic structure is predicted by considering that the material response of each integration point is determined from the homogenization of a unit cell, which includes the local constitutive laws and the geometrical characteristics of the microstructure (Fig. 1).

The proposed FE<sup>2</sup> process has been developed using an implicit resolution scheme, with the use of a Newton-Raphson algorithm that solves the nonlinear system of equations at the macroscopic and the microscopic scales. At each macroscopic strain increment, the macroscopic tangent modulus and the macroscopic stress are computed at each macroscopic integration point by solving iteratively a FE problem at the microscopic level. The steps of the multi-scale computational strategy are described below:

The microscopic problem is rewritten in the nonlinear form given by the following equations:

$$\begin{cases} \Delta\sigma(x) = C_t(x) : (\Delta\bar{\varepsilon} + \Delta\varepsilon(\Delta u')) & \forall x \in V \\ \operatorname{div}(\Delta\sigma(x)) = 0, & \forall x \in V \\ \Delta u_i - \Delta u_j = \Delta\bar{\varepsilon}_{ij} \cdot (x_i - x_j) & \forall x \in \partial V \end{cases} \quad (\text{Eq. 3.1})$$

To start the process, the local problem is solved by applying the PBCs. The initial tangent modulus  $\bar{C}_t$  is computed by using the six elementary strain states written in section 2.2 (the initial tangent modulus is the elastic stiffness tensor). Once  $\bar{C}_t$  is computed, the analysis at the macro-level is then performed and the first macroscopic strain increment  $\Delta\bar{\varepsilon}$  is given by the Meta-UMAT user subroutine. This increment is used in the subsequent step through the periodic boundary condition (PBCs) for the calculation of the microscopic response in the unit cell by using the developed user subroutine UMAT. By averaging the microscopic stresses, the macroscopic stress is computed. The updating of the macroscopic stress is performed for each integration point.

At each time increment the macroscopic strain is obtained by a prediction provided by the macroscopic FE model. This macroscopic strain is then applied to the local problem (unit cell) that, once solved, gives the macroscopic stress. Next, the local tangent moduli are mapped on the unit cell and, by applying the six elementary strain states, the global tangent modulus is computed. To proceed to the second step, the solution dependent variable (SDVs) and the local stress are saved as initial conditions using (\*Initial Conditions, type=) available in ABAQUS, in order to be used in the next iteration step.

The global convergence of the FE<sup>2</sup> technique is checked at the macroscopic stress. The two quantities previously computed ( $\bar{\sigma}$ ,  $\bar{C}_t$ ) are transferred to the macroscopic FE solver by using the Meta UMAT user subroutine. The convergence of  $\bar{\sigma}$  is examined before proceeding to the next time increment.

The two scale algorithm for the nonlinear computational homogenization in ABAQUS is presented in tab. 1.

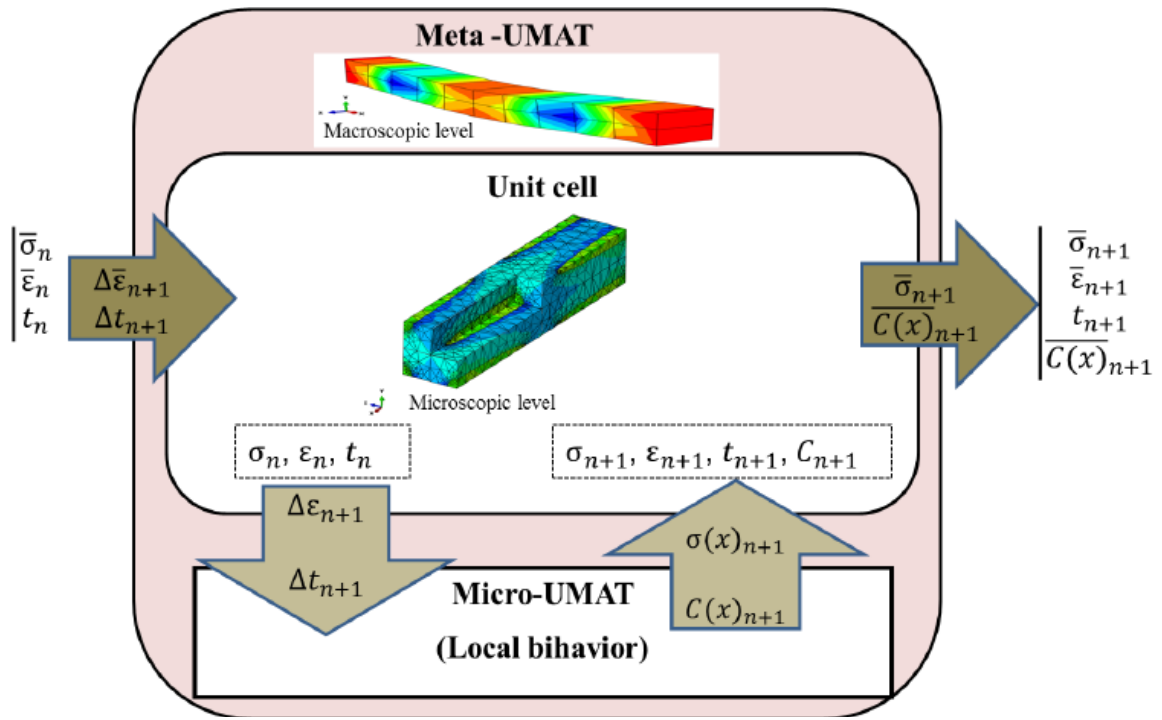


Fig. 1. The overall behavior of the composite is implemented in the form of a "Meta-UMAT" which uses the microscopic problem (unit cell) at each strain / time increment. The microscopic problem is fed by the laws of behavior of the constituents, implemented in the form of a "Micro-UMAT".

Micro	Macro
<p><b>1- Initialization</b></p> <ul style="list-style-type: none"> <li>➤ Apply periodic boundary condition on the unit cell.</li> <li>➤ Solve the problem microscopic with the local nonlinear behavior</li> <li>➤ Compute the initial macroscopic stress by averaging <math>\bar{\sigma} = \langle \sigma \rangle</math>.</li> <li>➤ Compute the initial macroscopic tangent modulus <math>\bar{C}_t</math></li> </ul> <p><b>2- Updating</b></p> <ul style="list-style-type: none"> <li>➤ Restart the analysis in the microscopic level from the previous step.</li> <li>➤ Compute the macroscopic stress <math>\bar{\sigma}</math>.</li> <li>➤ Compute the macroscopic tangent modulus <math>\bar{C}_t</math>.</li> </ul>	<p>❖ <u>Input filed for the Meta-UMAT</u></p> <ul style="list-style-type: none"> <li>➤ Define <math>\bar{\sigma}</math> in the Meta-UMAT</li> <li>➤ Define <math>\bar{C}_t</math> in the Meta-UMAT</li> </ul> <p>➤ Resolve the macroscopic problem</p> <p>➤ Get the macroscopic strain increment <math>\Delta \bar{\epsilon}_{n+1}</math></p> <p><b>3- Convergence testing :</b></p> <ul style="list-style-type: none"> <li>➤ Introduce the <math>\bar{\sigma}</math> in the Meta-UMAT</li> <li>➤ Convergence analysis. <ul style="list-style-type: none"> <li>○ if OK : we proceed to the next increment : step 4</li> <li>○ Else, iteration Intel convergence: step 2, 3 and 4.</li> </ul> </li> </ul> <p><b>4- Next increment:</b></p> <ul style="list-style-type: none"> <li>➤ Call the python script for restart the microscopic analysis with the new strain increment <math>\Delta \bar{\epsilon}_{n+1}</math></li> <li>➤ Solve the problem microscopic in the unit cell step 2, 3 and 4.</li> </ul>

Tab. 1. The two-scale FE<sup>2</sup> algorithm in ABAQUS Implicit in the nonlinear case

## 4. Numerical example

### 4.1 Validation with a semi analytical solution

The developed multiscale ABAQUS approach has been validated by comparing the numerical results with a semi analytical solution for a multilayer composite structure with elastoplastic phases [15]. The unit cell consists of two phases, one elastic and the other plastic (Fig. 2).

The two approaches yield the same response, demonstrating hence the accuracy of the FE<sup>2</sup> strategy.

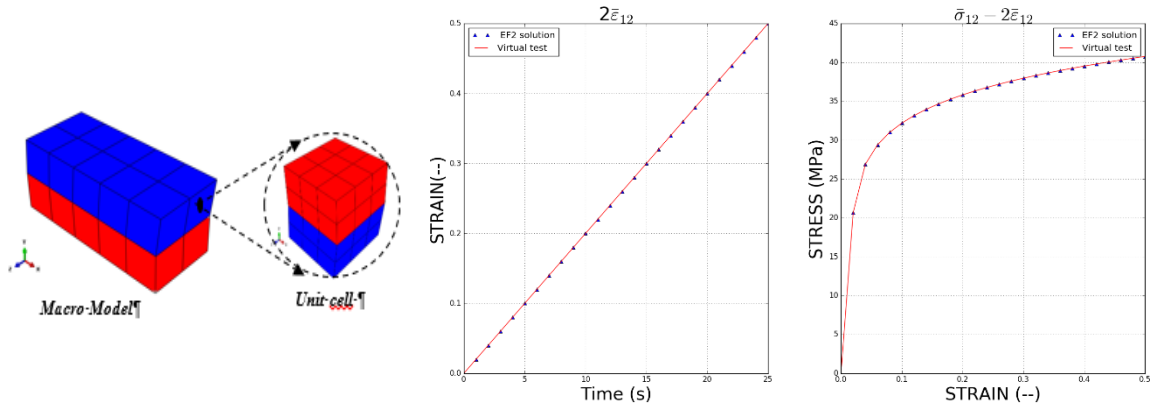


Fig. 2. : Comparison of the solution FE<sup>2</sup> with semi-analytical solution on a multilayer with elastoplastic behavior.

### 4.2 Validation with a virtual test on the unit cell

To further validate the proposed model under complex temporal loadings, a second validation example is examined. In this second example, a composite, consisting of a viscoplastic-damageable matrix reinforced with elastic short fibers with ellipsoidal shape, is subjected to the macroscopic strain loading path of (Fig 3a) The solution obtained by the FE<sup>2</sup> method on a single macroscopic finite element has been compared to a virtual test (the same macroscopic loading path has been applied on a single unit). The comparison of the results with the two methods (Fig. 3.b-c-d) illustrate the accuracy of the developed framework.

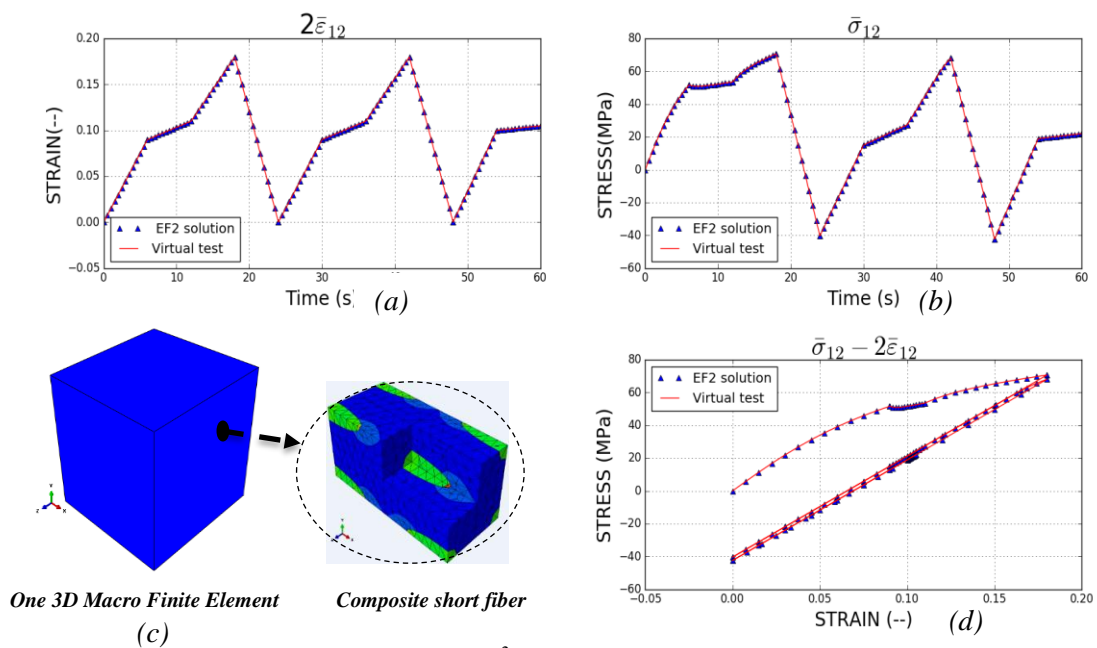


Fig 3. Comparison of FE<sup>2</sup> strategy with the virtual testing



### 4.3 Two-scale analysis on 3D composite structure

In order to demonstrate the capability of the developed approach, the complex 3D composite structure of (Fig. 4a), subjected to the loading path of (Fig. 4b), is simulated. The structure is made of a thermoplastic aligned short fiber reinforced composite in which the matrix phase exhibits a coupled damageable elastoviscoplastic response. The multiscale nonlinear behavior and the effects of such periodic microstructure on the macroscopic response of the structure are shown in Fig. 5. The results illustrate that the response of the composite is highly influenced by the presence of the matrix, exhibiting both viscoplastic response (through creep and relaxation phenomena), as well as stiffness reduction during unloading due to the ductile damage.

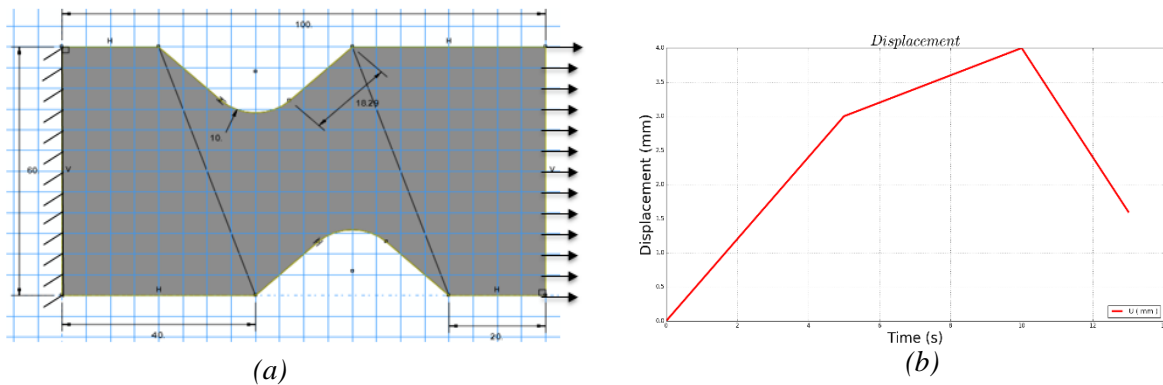


Fig. 4. Tensile and compression test on the Meuwissen test tube [14] with temporal loading

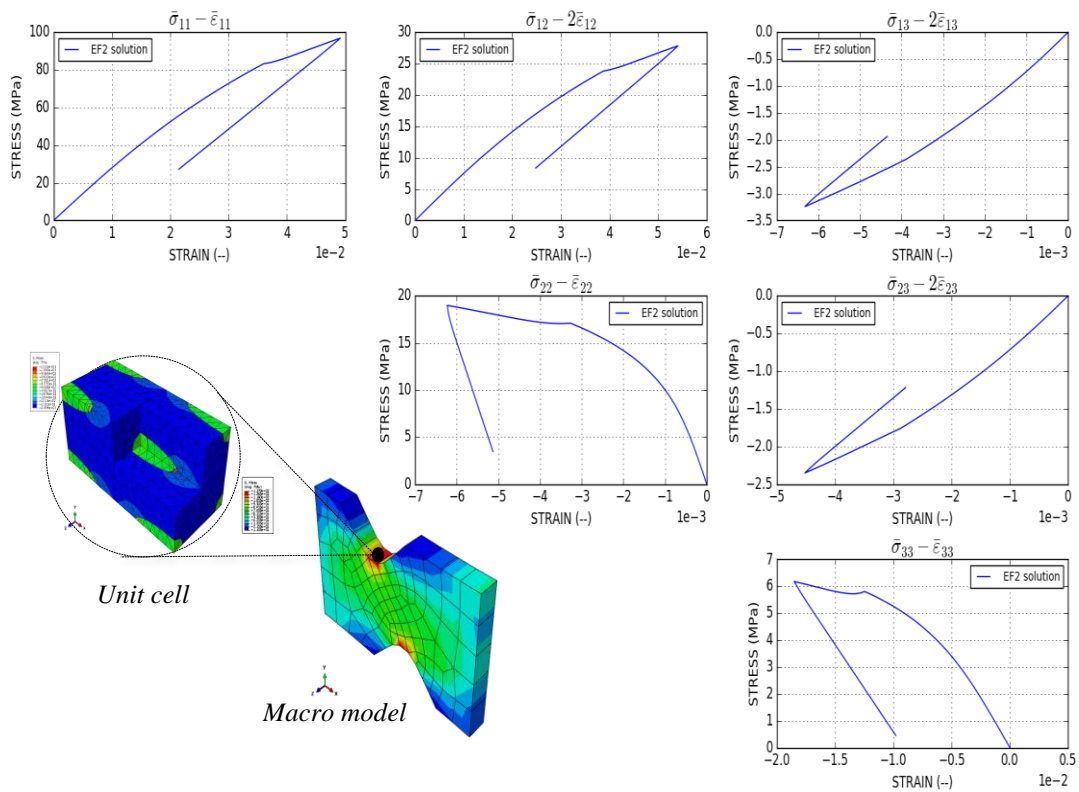


Fig. 5. Temporal loading test on 3D composite structure with microstructure is a matrix phase exhibits a coupled damageable elastoviscoplastic response.

## 5. Summary and Conclusion

This work presents a nonlinear 3D two-scale finite-element (FE<sup>2</sup>) framework. The framework allows to simulate 3D heterogeneous composite structures with any kind of nonlinear behavior at the microscopic level and various types of periodic microstructures.

The developed multiscale strategy in the Finite Element Analysis (FEA) package ABAQUS Implicit has been validated with two independent examples: In the first example, a multilayer composite structure with elastoplastic phases is simulated and the results are compared with a semi analytical solution. In the second example, a short fiber composite with elastoviscoplastic-damageable matrix under uniform macroscopic conditions is studied through the FE<sup>2</sup> framework and a virtual testing machine that solves a single unit cell.

A periodic 3D composite structure exhibiting heterogeneous strain fields is simulated, in which the microstructure consists of an elastoviscoplastic polymer matrix with ductile damage, which is reinforced by aligned short glass fibers. The response of the structure clearly highlights creep and relaxation phenomena, which are characteristic for rate dependent responses. This viscous behavior and the stiffness reduction observed during unloading have been induced by the viscoplastic nature of the polymer matrix.

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