Homogenization of fibre reinforced composite with gradient enhanced damage model

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Abstract

Classical finite element simulations face the problems of losing uniqueness and strain localization when the strain softening of materials is involved. Thus, when using continuum damage model or plasticity softening model, numerical convergence will not be obtained with the refinement of the finite element discretization when strain localization occurs.

Gradient-enhanced softening and non-local continua models have been proposed by several researchers in order to solve this problem. In such approaches, high-order spatial gradients of state variables are incorporated in the macroscopic constitutive equations. However, when dealing with complex heterogeneous materials, a direct simulation of the macroscopic structures is unreachable, motivating the development of non-local homogenization schemes.

In this work, a non-local homogenization procedure is proposed for fiber reinforced materials. In this approach, the fiber is assumed to remain linear elastic while the matrix material is modeled as elasto-plastic coupled with a damage law described by a non-local constitutive model. Toward this end, the mean-field homogenization is based on the knowledge of the macroscopic deformation tensors, internal variables and their gradients, which are applied to a micro-structural representative volume element (RVE). Macro-stress is then obtained from a homogenization process.

1 Introduction

As direct numerical simulations of composites taking directly into account the individual phases are often too complex to handle and the computation expenses are unaffordable, homogenized properties are usually sought to perform structures analyzes. Homogenization techniques are known to be efficient tools to derive those homogenized material properties analytically [1, 2, 3], among others, and/or numerically [4, 5], among others, see [6] for an exhaustive overview.

Among those different methods, the mean-field homogenization (MFH) approach [3] provides predictions for the macroscopic behavior of heterogeneous materials at a reasonable computational cost and is thus of particular interest for the modeling of particle or fiber reinforced composites. Efficient MFH methods have been available for a long time for linear elastic problems [7, 1] and are based on the single inclusion Eshelby solution [8]. When extending MFH methods to the non-linear regime, the so-called incremental formulation rewrites the constitutive equations in a pseudo-linear form relating the stress and strain rates [9, 10].

To be more realistic to real composite behaviors, such an incremental homogenization scheme could be extended to capture the degradation process that may happen during irreversible deformations, by

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considering damage variables. However, when formulating such a multiscale method able to capture degradation at the micro or macro scale, the governing partial differential equations may lose ellipticity at the strain-softening onset and the problem becomes ill-posed.

One way to avoid the loss of uniqueness happening at strain softening onset, is to supply the formulation with higher-order derivatives, which introduces an internal length scale, and leads to a non-local approach. One efficient non-local formulation developed for continuum mechanics, which avoids the necessity of evaluating explicitly internal variable derivatives, was proposed in [11]. In this approach, the non-local kernel has been reformulated in such a way that a new non-local variable, representative of an internal variable and its derivatives, results from the resolution of a new boundary value problem.

In this paper, the incremental MFH approach is extended to account for the damage behavior happening in the matrix-material at the micro-scale, with the aim of extracting the effective properties of particle or fiber reinforced composites. In order to avoid the strain/damage localization caused by matrix material softening, the gradient-enhanced formulation [12] is adopted during the homogenization process. As a result this new formulation allows simulating the ply-level response under quasi-static loading conditions resulting from the coupled plasticity-damage model considered at the micro matrix scale [13].

2 Non-Local MFH for elasto-plastic materials with damage model

2.1 MFH background

In a multiscale approach, at each macro-point \( X \) of the structure, the macro-strain \( \bar{\varepsilon} \) is known, and the macro-stress \( \bar{\sigma} \) is sought from a micro-scale boundary value problem (BVP). At the micro-level, the macro-point is viewed as the center of a RVE of domain and the Hill-Mandell condition, expressing the equality between energies at both scales, transforms the relation between macro-strains \( \bar{\varepsilon} \) and stresses \( \bar{\sigma} \) into the relation between average strains \( \langle \varepsilon \rangle \) and stresses \( \langle \sigma \rangle \) over the RVE.

For a two-phase isothermal composite with the respective volume fractions \( v_0 + v_1 = 1 \) (subscript 0 refers to the matrix and I to the inclusions), the average quantities are expressed in terms of the phases average as

\[
\bar{\varepsilon} = v_0 \langle \varepsilon \rangle_{\omega_0} + v_1 \langle \varepsilon \rangle_{\omega_1} \quad \text{and} \quad \bar{\sigma} = v_0 \langle \sigma \rangle_{\omega_0} + v_1 \langle \sigma \rangle_{\omega_1} .
\]  

(1)

In linear elasticity, MFH allows writing

\[
\bar{\sigma} = \bar{C} : \bar{\varepsilon} ,
\]  

(2)

where \( \bar{C} \) is the homogenized macro-stiffness which is computed from the constitutive material stiffness tensors \( C_0 \) of the matrix and \( C_1 \) of the inclusions. The relation between \( \bar{C} \) and both \( C_0 \) and \( C_1 \) can be expressed as

\[
\bar{C} = [v_1 C_1 : B^e + v_0 C_0] : [v_1 B^e + v_0 I]^{-1} ,
\]  

(3)

where \( B^e \) is the strain concentration tensor. This last tensor states the relation between the deformation in the two phases as

\[
\langle \varepsilon \rangle_{\omega_1} = B^e : \langle \varepsilon \rangle_{\omega_0} ,
\]  

(4)

and can only be obtained analytically under some assumptions on the micro-mechanics [1, 7]. In this paper, the Mori-Tanaka (M-T) expression of \( B^e \), which assumes that the strain at infinity corresponds to the average strain in the matrix phase, is used.

For two-phase elasto-plastic composites, the MFH methods revolve around an incremental formulation [9] based on a so-called linear comparison composite (LCC). During a finite incremental process,
the constitutive equations are discretized in time intervals \([t_n, t_{n+1}]\), and the expression sought during that interval is of the form

\[
\Delta \sigma = \bar{C} : \Delta \epsilon \, .
\]  

(5)

Toward this end, the macro linearizations of strain and stress tensors (1) are still obtained from the average linearizations of strain and stress in the phases with, respectively,

\[
\delta \epsilon = v_0 \langle \delta \epsilon \rangle_{\omega_0} + v_1 \langle \delta \epsilon \rangle_{\omega_1} \, , \quad \text{and}
\]

\[
\delta \sigma = v_0 \langle \delta \sigma \rangle_{\omega_0} + v_1 \langle \delta \sigma \rangle_{\omega_1} \, .
\]  

(6)

(7)

The same relations hold when considering finite variations \(\Delta\) on the time interval \([t_n, t_{n+1}]\), with

\[
\Delta \epsilon = v_0 \langle \Delta \epsilon \rangle_{\omega_0} + v_1 \langle \Delta \epsilon \rangle_{\omega_1} \, , \quad \text{and}
\]

\[
\Delta \sigma = v_0 \langle \Delta \sigma \rangle_{\omega_0} + v_1 \langle \Delta \sigma \rangle_{\omega_1} \, .
\]  

(8)

(9)

The so-called linear comparison composite states a relation between the average incremental strains in the two phases (4) of the equivalent linear phases such that

\[
\langle \Delta \epsilon \rangle_{\omega_1} = B^* (I, \bar{C}^{\text{alg}}_1, \bar{C}^{\text{alg}}_0) : \langle \Delta \epsilon \rangle_{\omega_0} \, ,
\]  

(10)

where \(\bar{C}^{\text{alg}}_0\) and \(\bar{C}^{\text{alg}}_1\) are the average values of the consistent algorithmic tangent moduli of the two phases. Similarly to the elastic counter part (2), the macroscopic homogenized stress increment \(\Delta \sigma\) can be related to the macroscopic homogenized stress increment \(\Delta \epsilon\) through (5), where

\[
\bar{C} = [v_0 \bar{C}^{\text{alg}}_1 : B^* + v_0 \bar{C}^{\text{alg}}_0] : [v_0 B^* + v_0 I]^{-1}
\]  

(11)

is the macro-moduli of the homogenized elasto-plastic two-phase composite. In this last expression, the Mori-Tanaka strain concentration tensor \(B^*\) is computed from the isotropic parts of \(\bar{C}^{\text{alg}}_0\) to improve prediction results [10].

Finally, when solving the problem at the finite element level using a Newton-Raphson procedure, one needs to linearize the stress tensor at time \(t_{n+1}\), such that

\[
\delta \sigma = \bar{C}^{\text{alg}} : \delta \epsilon \, ,
\]  

(12)

where \(\bar{C}^{\text{alg}}\) is the consistent algorithmic homogenized tangent moduli that is defined from the MFH process.

### 2.2 The non-local implicit model

In order to avoid loss of solution uniqueness and strain localization problem when extending MFH to damage theory, the model should be written in a non-local from involving gradient enrichment. Toward this end, some internal variables \(a\) (which can be strains, accumulated plastic strain, damage...) are replaced by their weighted average \(\tilde{a}\) over a characteristic volume \((\hat{V}_C)\) to reflect the interaction between neighboring material points:

\[
\tilde{a}(X) = \frac{1}{\hat{V}_C} \int_{V_C} a(y) \phi(y; X) \, dV \, ,
\]  

(13)

where \(y\) denotes the position in the infinitesimal volume \(dV_C\) and where \(\phi(y; X)\) are the weight functions.

Practically, in order to avoid the direct computation of (13) in a finite element framework, this expression can be substituted by an explicit approximated that neglects terms of fourth-order and higher:

\[
\tilde{a} = a + I^2 \nabla^2 a \, ,
\]  

(14)
where the Laplacian operator \( \nabla^2 = \sum_i \partial^2 / \partial x_i^2 \), and where the internal length scale of the non-local model is preserved in the gradient coefficient \( \ell \). On top of the difficulty of applying adequate boundary conditions, the numerical evaluation of relation (14) in a traditional finite element framework is not straightforward as elements are usually not satisfying high order continuity, which motivated the development of the so-called implicit method [12].

Considering Green functions \( G(\mathbf{y}; \mathbf{x}) \) as weighting functions \( \phi(\mathbf{y}; \mathbf{X}) \) in (13), an alternative second-order gradient approximation leads to

\[
\tilde{a} - \ell^2 \nabla^2 \tilde{a} = a. \tag{15}
\]

In contrast to the definition (14), the non-local internal variables \( \tilde{a} \) is not given explicitly in terms of \( a \) and its derivatives, but is the solution of a new boundary value problem consisting of the Helmholtz equation (15) completed by appropriate boundary conditions.

In particular, the non-local implicit approach can be applied to damage model in order of avoiding any loss of ellipticity. The damage model can be linear damage, exponential damage, Lemaitre - Chaboche ductile damage and so on. In this paper, we focus on Lemaitre - Chaboche ductile damage model [14] in which the damage evolution is defined as

\[
\dot{D} = \begin{cases} 
0, & \text{if } p \leq p_C; \\
\left( \frac{Y}{S_0} \right)^s \dot{p}, & \text{if } p > p_C.
\end{cases} \tag{16}
\]

In this expression, \( p \) is the accumulated plastic strain, \( p_C \) is a plastic threshold for the evolution of damage, \( S_0 \) and \( s \) are the material parameters, and \( Y = \frac{1}{2} \varepsilon_{el} : C_{el} : \varepsilon_{el} \) is the strain energy release rate computed from the elastic strain tensors.

In order to render this damage model non-local, the non-local accumulated plastic strain \( \tilde{p} \) is applied to calculate the damage evolution, and Eqs. (16) is rewritten

\[
\dot{\tilde{D}} = \begin{cases} 
0, & \text{if } \tilde{p} \leq p_C; \\
\left( \frac{Y}{S_0} \right)^s \dot{\tilde{p}}, & \text{if } \tilde{p} > p_C.
\end{cases} \tag{17}
\]

The non-local accumulated plastic strain \( \tilde{p} \) is computed from the implicit formulation (15), which becomes

\[
\tilde{p} - \ell^2 \nabla^2 \tilde{p} = p. \tag{18}
\]

### 2.3 Non-local MFH with damage

In this work, the LCC MFH for elasto-plastic composite is extended to damage. Fibers are considered elastic, and damage is introduced in the matrix elasto-plastic material only, with the usual assumption that the strain observed in the actual body and in its undamaged representation are equivalent [15, 16]. From the usual definition of the average effective stress in the matrix, one has

\[
\delta \sigma_0 = \sigma_0 / (1 - D), \tag{19}
\]

where \( D \) is the representation of the matrix damage on the RVE. Thus, the linearization of the average stress in the matrix is easily derived, see [13] for details, as

\[
\dot{\sigma}_0 = (1 - D) \dot{C}_0^el : \dot{\varepsilon}_0^el - \dot{D} C_0^el : \varepsilon_0^el, \\
\delta \sigma_0 = (1 - D) \dot{C}_0^{alg} : \delta \varepsilon_0 - \dot{\sigma}_0 \delta D. \tag{20}
\]

Following the incremental formulation of MFH, the stress linearization (7) can be rewritten as:

\[
\delta \sigma = v_0 \dot{C}_0^{alg} : \delta \varepsilon_0 + v_1 \dot{C}_1^{alg} : \delta \varepsilon_1, \tag{21}
\]
where $\bar{C}_0^{\text{alg}}$ and $\bar{C}_1^{\text{alg}}$ are the averaged “consistent” tangent operators for the matrix and the fibers respectively. Combining Eqs. (20) and (21) leads to

$$\delta \bar{\sigma} = v_1 \bar{C}_1^{\text{alg}} : \delta \bar{\varepsilon} + v_0 (1 - D) \bar{C}_0^{\text{alg}} : \delta \bar{\varepsilon} - v_0 \bar{\sigma} \delta D.$$  \hfill (22)

Remembering that for the non-local formulation, the damage depends on both $\varepsilon_0$ and on $\tilde{p}$, the last term of this result can be rewritten as

$$\delta D(\varepsilon_0, \tilde{p}) = \frac{\partial D}{\partial \varepsilon_0} \delta \varepsilon_0 + \frac{\partial D}{\partial \tilde{p}} \delta \tilde{p}.$$  \hfill (23)

Using (23), Eq. (22) can be rewritten in the form

$$\delta \bar{\sigma} = v_1 \bar{C}_1^{\text{alg}} : \delta \bar{\varepsilon} + v_0 \bar{C}_0^{\text{algD}} : \delta \varepsilon_0 - v_0 \bar{\sigma} \left( \frac{\partial D}{\partial \varepsilon_0} \right) : \delta \varepsilon_0 - v_0 \bar{\sigma} \frac{\partial D}{\partial \tilde{p}} \delta \tilde{p},$$  \hfill (24)

where

$$\bar{C}_0^{\text{algD}} = (1 - D) \bar{C}_0^{\text{alg}}.$$  \hfill (25)

The first two terms at the right hand side of Eq. (24) represent the stress variation of a composite with a fictitious matrix material of constant non-local damage, which is a non-local representation of an internal variable of the matrix only. Thus we assume that the incremental Mori-Tanaka process can be applied on the first two terms of Eq. (24), leading to

$$\delta \bar{\sigma} = \left[ \bar{C}_0^{\text{algD}} - v_0 \bar{\sigma} \left( \frac{\partial D}{\partial \varepsilon_0} \right) : \frac{d \varepsilon_0}{d \bar{\varepsilon}} \right] : \delta \bar{\varepsilon} - v_0 \bar{\sigma} \frac{\partial D}{\partial \tilde{p}} \delta \tilde{p},$$  \hfill (26)

where $\bar{C}_0^{\text{algD}}$ is the tangent operator of the composite with damaged matrix. Both $\bar{C}_0^{\text{algD}}$ and $\frac{d \varepsilon_0}{d \bar{\varepsilon}}$ are obtained from the MFH procedure, see [13] for details. For completeness, the last two terms of Eq. (24) are related to the softening of the matrix due to the damage in the matrix, and are not considered in the Mori-Tanaka process. Indeed M-T is only defined when the two tangent moduli are definite positive, which would not be the case in the softening part. So in this paper, we choose to consider the slope $(1 - D) \bar{C}_0^{\text{alg}}$ for the damage tangent matrix. This introduces an error as the softening of the matrix does not lead to a relaxing of the fiber. However, this is an error of the same order of magnitude as for elasto-plasticity behaviors. Indeed MFH using the LCC incremental formulation does not correct the previous stress increments, although a correction should result from a modification of the material stiffness. Thus we expect the MFH to produce stress and damage slightly above the solution obtained with a finite element simulation, e.g.

### 2.4 Governing equations

The problem is limited to small deformations and static analysis. The governing equations of the homogenized material using the implicit gradient enhanced elastic-plasticity read

$$\nabla \cdot \sigma + f = 0 \quad \text{for the material},$$  \hfill (27)

$$\tilde{p} - t^2 \nabla^2 \tilde{p} = p \quad \text{for the matrix material only},$$  \hfill (28)

where $f$ represents the body force vector, and $\tilde{p}$ is a homogenized representation of the non-local accumulated plastic strain of the matrix material.

At the macro-scale, a finite element formulation, based on the weak form of the governing equations is implemented, see [13] for details. This finite element formulation accounts for a new degree of freedom on each node which results from the resolution of the new Helmholtz-type equations governing the implicit formulation of the gradient-enhanced damage model.
3 Numerical simulation

In this section, the gradient enhanced MFH model is used to compute the effective response of unidirectional fiber reinforced elasto-plastic composites. The considered composites consist in a continuous elasto-plastic matrix, experiencing damage, reinforced by unidirectional continuous fibers with linear elastic behavior.

As an example, the matrix considered is made of epoxy and the reinforcements are continuous carbon fibers. The properties of the matrix are: Young’s modulus $E_0 = 2.89$ GPa, Poisson ration $\nu_0 = 0.3$ and yielding stress $\sigma_Y = 35.0$ MPa. The hardening law of the epoxy material follows an exponential law

$$R(p) = h_0[1 - e^{-mp}],$$

where $h_0 = 73.0$ MPa and $m = 60$. The damage law obeys Eq. (17), with the parameters $S_0 = 2.0$ MPa, $s = 0.5$ and $p_C = 0.0$. The characteristic length of the non-local model $l$ is set such that $l^2 = 2.0$ mm$^2$. The carbon fibers are linear elastic, with $E_I = 238$ GPa and $\nu_I = 0.26$. Moreover, the carbon fibers are assumed to be isotropic, which is far from being true, to enhance the difference of material properties in the transverse direction and, thus to illustrate the ability of the method to perform the homogenization.

Reference results are provided by finite element computations performed on unit cells where the microstructure is fully meshed. Two kinds of unit cells are applied for the validation. The first one is the small unit cell with periodical distribution of fibers in the transverse direction, and the second one is the larger cell with random distribution of fibers in the transverse direction. As in the second case, the characteristic length of the unit cell is not much larger than the characteristic length of the microstructure, six different occurrences, with random fibers distribution are simultaneously considered in order to capture the scattering effect due to the violation of the length scale separation. The comparisons between simulations are successively achieved for 15, 30 and 50 % volume fraction of fibers.

![Stress-strain behavior of the epoxy fiber reinforced composite for different fiber volume ratios under transverse loading.](image)

(a) $\nu_I = 0.15$  
(b) $\nu_I = 0.30$  
(c) $\nu_I = 0.50$

Figure 1: Stress-strain behavior of the epoxy fiber reinforced composite for different fiber volume ratios under transverse loading.

A loading-unloading cycle is applied in the direction transverse to the fibers. A maximal deformation of 10 % is reached before the unloading proceeds to zero-transverse deformation. Boundary conditions correspond to uniform displacements, with controlled deformation in the loading direction, plane stress state in the other transverse direction and plane strain in the longitudinal direction. The plane-stress condition in the fibers direction correspond to the state of composite ply, while the combination of
plane-stress, strain-controlled displacements in the transverse direction gives good convergence results in terms of unit-cell size.

The effective behaviors predicted by the MFH models and the FE results for the three fiber volume ratios are presented in Fig. 1. For the three fiber volume ratios, the homogenized property is dominated by the properties of matrix, with an obvious elasto-plastic behavior exhibiting softening. The 6 random cells occurrences converged as they exhibit a solution similar to the periodical unit cell. For the fiber volume fractions of $v_I = 15\%$ and $30\%$, rather good predictions are given by the MFH model, with, as expected, higher macroscopic stress and damage predicted by the MFH due to the incremental LCC formulation. However for $v_I = 50\%$, the MFH model overestimates the macroscopic stress. This error comes from the assumption of Mori - Tanaka based MFH, which can give an accurate prediction when the volume fraction of inclusions is lower than $30\%$. Also for the computations of random cells of $v_I = 50\%$, only one random cell reaches the end of the loading-unloading cycle. This might because of the abrupt increase of damage, which can reach 1.0 in high stress concentration area even before the maximum loading stage.

For illustration purpose, the von Mises stress, the matrix accumulated plastic strain and matrix damage for the $30\%$ inclusion random cell are presented in Fig. 2 for the maximum deformation reached and in Fig. 3 at zero-strain after unloading. As comparison, those values obtained from the MFH are also presented. In the random unit cell, the distribution of the von Mises stress is quite homogeneous (Fig. 2(a)), higher damage is found between the fibers along the loading direction (Fig. 2(c)), and higher accumulated plastic strain appears in a $45^\circ$-band (Fig. 2(b)). Highest values of those in matrix are seen at the fiber/matrix interfaces. On the contrary, uniform values of the von Mises stress, accumulated plastic strain and damage are obtained by the cell with the MFH process (Fig. 2(d)-Fig. 2(f)). This was expected, but as the homogenized material exhibits softening, it is important to make sure any localization problems are avoided under uniform loading, which is the case in this formulation. Interestingly, the damage predicted in the matrix by the MFH ((Fig. 2(f)) is of similar order of magnitude as the damage obtained with the direct numerical simulation (Fig. 2(c)). The same observations hold after unloading, see Fig. 3.
Figure 3: The von Mises stress, accumulated plastic strain and damage at zero-strain after unloading, for a 30% inclusion random unit cell (a)∼(c), and those of a 30% inclusion homogenized cell (d)∼(f) under transverse loading.

4 Conclusions

In this paper, a gradient enhanced mean-field homogenization (MFH) scheme, based on the so-called linear comparison composite (LCC) approach, for damage-enhanced elasto-plastic composites was presented. In order of avoiding issues related to softening behaviors, as mesh-dependency, arbitrary strain localization ... the damage of the matrix was formulated in a non-local way, using the so-called implicit approach.

As an illustration, this approach was applied to unidirectional carbon-fiber, epoxy-matrix composites, and the responses under uniform strain obtained with the new MFH non-local formulation was compared to the responses obtained with the direct numerical simulation of unit cells and RVEs.

For low fiber volume ratios (≤ 30 %) results are in excellent agreement, including during the softening and unloading parts of the loading history. For average fiber volume ratios (up to 50 %), the method is less accurate (error ∼ 15 % during the loading part and up to 50 % in the unloading part), which is mainly explained by the M-T assumption, and the incremental MFH approach adopted in this paper. Indeed MFH using the LCC incremental formulation does not correct the previous stress increments from a modification of the material stiffness, due to the plastic or damage behavior.

References


