A non-concurrent multiscale method for computing the response of hyperelastic heterogeneous structures

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ABSTRACT. *We propose a new numerical method for computing the response of structures made of heterogeneous nonlinear elastic materials. The first step is to define a representative volume element (r.v.e.) associated to the microstructure. Then, the effective potential, or the overall strain density function, is computed numerically for a finite set of points in the macroscopic strains space. In the computation of structure, stress and tangent stiffness tensors can be obtained through interpolation and derivation in the discrete set of potential values. Material properties contrast, anisotropy and morphology of microstructure are arbitrary.*

RÉSUMÉ. *Nous présentons une nouvelle méthode numérique simple pour calculer la réponse de structures constituées de matériaux hétérogènes élastiques non linéaires. Après avoir défini un volume élémentaire représentatif, le potentiel effectif (fonction densité d'énergie des déformations macroscopiques) pour le VER est calculé numériquement pour un ensemble fini de points dans l'espace des déformations macroscopiques. Lors du calcul de structure, les tenseurs des contraintes et tangents peuvent être obtenus par interpolation et dérivation dans le nuage des valeurs discrètes. Les contrastes de propriétés, l'anisotropie et la morphologie de la microstructure sont arbitraires.*

KEYWORDS: *nonlinear homogenization, composites, multiscale methods, method of numerically explicit potentials.*

MOTS-CLÉS : *homogénéisation non linéaire, composites, méthodes multi-échelles, méthode de potentiels numériques explicites.*

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1. Introduction

Computing the response of nonlinear structures is a fundamental problem in engineering. When the material constituting a structure is highly heterogeneous at the microscopic level, a computationally efficient strategy consists in homogenizing the material so as to obtain its macroscopic constitutive law. Though considerable progress has been made in analytical or semi-analytical methods (see e.g. Suquet (1998), Willis (2000)), the restrictive assumptions inherent to analytical methods limit their use for the computation of structures consisting of nonlinear heterogeneous materials of complex microstructure and subjected to arbitrary macroscopic loadings.

On the other hand, the recent drastic increase in the performance of computers has made possible to develop computational multiscale methods for computing structures formed of nonlinear heterogeneous materials. These methods treat separately two or more scales of interest. In non-concurrent multiscale methods (usually restricted to linear problems), a representative volume is defined, and the effective coefficients are computed by solving a limited number of problems associated with different boundary conditions (see e.g. Kanit *et al.* (2003)). In the non-linear case, the number of possible loading cases is in principle infinite, it is thus necessary to couple both scales and to run computations concurrently at both scales (see Figure 1). This family of methods, found in the literature under names such as "Concurrent Multiscale Methods", "Multilevel Finite Element" or "Computational Homogenization" (see, e.g., Smit *et al.* (1998), Feyel (1999), Kouznetsova *et al.* (2004)) are based on a simple idea : each macroscopic integration point is first associated with a representative volume element (r.v.e) of the material. Macroscopic strain relative to the integration point is then prescribed as boundary conditions for the r.v.e. The relevant homogenization problem is finally solved numerically for every increment of the macroscopic loading imposed on the structure. These methods show many attractive features in comparison with the aforementioned analytical approaches : it becomes possible to handle general local constitutive laws as well as complex and evolving microstructures. However, their main shortcoming is the computational cost which is still high even though use is made of techniques like model reduction (Yvonnet *et al.* (2007)) or parallel computing (Feyel (1999)) dedicated to reducing it.

In this work we propose a new numerical method for computing the response of structures made of nonlinear heterogeneous materials. The first step is to define a representative volume element (r.v.e.) associated to the microstructure. Then, the effective potential, or overall strain density function, is computed numerically for a finite set of points in the macroscopic strain space. In the structures computation, stress and tangent tensors can be obtained through interpolation and derivation in the discrete set of potential values. Material properties contrast, anisotropy and morphology of microstructure are arbitrary. The technique, proposed in the small strains elastostatics context in Yvonnet *et al.* (2009), is extended in this paper to finite strains.

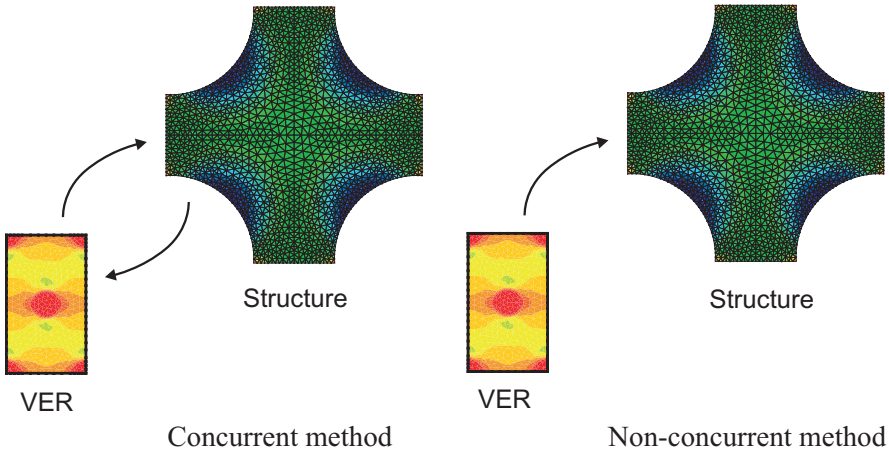

Figure 1. *Schematic view of concurrent and non-concurrent multiscale methods : in concurrent multiscale methods, information is exchanged between scales during the computations ; in non-concurrent multiscale methods, pre-computed data on the microscopic scale are utilized by the macroscopic model*

2. Review of nonlinear homogenization for hyperelastic materials

We consider a representative volume element (r.v.e) Ω with external boundary $\partial\Omega$ in the reference configuration of a composite consisting of N homogeneous hyperelastic phases. The subdomain of Ω occupied by phase $r \in \{1, 2, ..., N\}$ is denoted by Ω_r and described by the characteristic function $\chi^{(r)}$ such that $\chi^{(r)}(\mathbf{X}) = 1$ for $\mathbf{X} \in \Omega_r$ and $\chi^{(r)}(\mathbf{X}) = 0$ for $\mathbf{X} \notin \Omega_r$. We shall symbolize the volume average over Ω_r by $\langle . \rangle_r$ and the one over Ω by $\langle . \rangle$. In particular, $c^{(r)} = \langle \chi^{(r)} \rangle$ is the volume fraction of phase r. The interfaces between the phases of the composite are taken to be perfect.

Let be given the local strain-energy density function Ψ of the composite under investigation by

$$\Psi(\mathbf{X}, \mathbf{C}) = \sum_{r=1}^{N} \chi^{(r)}(\mathbf{X}) \Psi^{(r)}(\mathbf{C}), \qquad [1]$$

where $\Psi^{(r)}$ is the strain-energy density function of phase r, assumed to be convex. A material points is identified by its position vector $\mathbf{X}$ in the reference configuration, while the current position of the same point is denoted by $\mathbf{x}$ in the deformed configuration $\Omega(t)$. The deformation gradient $\mathbf{F}$ at $\mathbf{X}$ is defined as $\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}$. The constitutive behavior of the phases is assumed to be purely elastic and characterized by $\Psi^{(r)}$ which

are functions of the right-Cauchy-Green strain tensor $\mathbf{C} = \mathbf{F}^T\mathbf{F}$. In the Lagrangian description, the local constitutive law is then given by :

$$\mathbf{S}(\mathbf{X}) = 2\frac{\partial \Psi}{\partial \mathbf{C}}(\mathbf{X}, \mathbf{C}). \quad [2]$$

where $\mathbf{S}$ is the second Piola-Kirchhoff stress tensor which must satisfy the equilibrium equation

$$\mathbf{div}(\mathbf{FS}) = \mathbf{0} \text{ in } \Omega \quad [3]$$

in the absence of body forces. Under the length-scale separation hypothesis, the effective stored-energy function $\bar{\Psi}$ of the composite is defined by (Hill (1972))

$$\bar{\Psi}(\bar{\mathbf{C}}) = \underset{\mathbf{C}\in\mathcal{K}(\bar{\mathbf{C}})}{inf} \langle \Psi(\mathbf{X},\mathbf{C}) \rangle = \underset{\mathbf{C}\in\mathcal{K}(\bar{\mathbf{C}})}{inf} \sum_{r=1}^{N} \chi^{(r)} \left\langle \Psi^{(r)}(\mathbf{C}) \right\rangle^{(r)} \quad [4]$$

where $\mathcal{K}$ denotes the set of kinematically admissible strain tensors. From the definition (4), it can be shown that $\bar{\Psi}$ is objective, so that $\bar{\Psi}(\bar{\mathbf{C}}) = \bar{\Psi}(\bar{\mathbf{U}})$, where $\bar{\mathbf{U}}$ is the macroscopic right stretch tensor in the polar decomposition of the macroscopic deformation gradient $\bar{\mathbf{F}} = \bar{\mathbf{R}}\bar{\mathbf{U}}$, with $\bar{\mathbf{R}}$ denoting the macroscopic rotation tensor. Note that $\bar{\mathbf{U}} \neq \langle \mathbf{U} \rangle$ and $\bar{\mathbf{R}} \neq \langle \mathbf{R} \rangle$. It follows from the above definition that the global or macroscopic constitutive relation for the composite is then given by :

$$\bar{\mathbf{S}} = 2\frac{\partial \bar{\Psi}}{\partial \bar{\mathbf{C}}}(\bar{\mathbf{C}}), \quad [5]$$

where $\bar{\mathbf{S}} = \langle \mathbf{F} \rangle^{-1} \langle \mathbf{P} \rangle$ is the macroscopic second Piola-Kirchhoff stress tensor expressed in terms of the average first Piola-Kirchhoff stress tensor $\langle \mathbf{P} \rangle$. Different types of boundary conditions can be considered, such as uniform traction, uniform strain, or periodical boundary conditions. In this work we use the periodical ones, namely

$$\mathbf{u}(\mathbf{X}) = (\bar{\mathbf{F}} - \mathbf{1})\mathbf{X} + \tilde{\mathbf{u}}(\mathbf{X}) \text{ on } \partial\Omega, \quad [6]$$

with $\tilde{\mathbf{u}}(\mathbf{X})$ being periodical on $\partial\Omega$. In this work, we solve the local problem to compute the effective potential $\bar{\Psi}$. As $\bar{\Psi}$ is invariant with respect to a rotation $\bar{\mathbf{R}}$, we can express the boundary conditions with respect to $\bar{\mathbf{C}}$. Using polar decomposition and choosing arbitrarily $\bar{\mathbf{R}} = \mathbf{1}$ we obtain $\bar{\mathbf{F}} = \bar{\mathbf{U}} = \mathbf{C}^{1/2}$ and then :

$$\mathbf{u}(\mathbf{X}) = (\bar{\mathbf{C}}^{1/2} - \mathbf{1})\mathbf{X} + \tilde{\mathbf{u}}(\mathbf{X}) \text{ on } \partial\Omega. \quad [7]$$

In this work, the main purpose of the proposed numerical method is to provide a twice continuously differentiable numerical estimation for the effective strain-energy density function $\bar{\Psi}$.

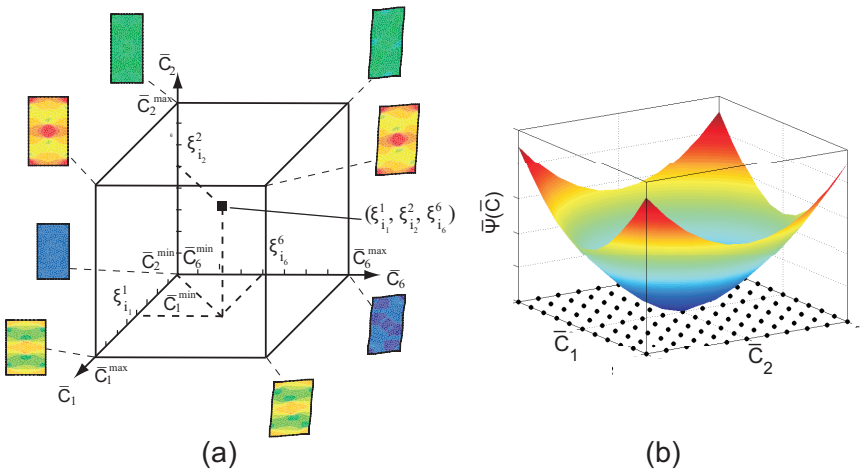

Figure 2. *(a) Macroscopic strain domain for a 2D-compressible problem. Deformed r.v.e. associated with selected macroscopic strains states are depicted ; (b) continuous interpolation of the numerical potential in the $\bar{C}_{11} - \bar{C}_{22}$ plane*

3. The method of numerically explicit potentials

The method of Numerically Explicit Potentials (NEXP for short) was originally proposed in Yvonnet *et al.* (2009) in the case of small elastic strains and is extended in this paper to hyperelasticity. The main idea is to replace the potential $\bar{w}(\bar{\boldsymbol{\varepsilon}})$ by $\bar{\Psi}(\bar{\mathbf{C}})$, though some difficulties related to the definition of the macroscopic strain domain exist. An appropriate methodology is currently developed and will be presented in details in a future work.

When a hyperelastic composite is under investigation, the form of $\bar{\Psi}$ as a function defined over the macroscopic strain space $\mathcal{E}$ is in general unknown and cannot be exactly specified in terms of a finite number of parameters. In other words, $\bar{\Psi}$ has not an exact finite representation. However, once $\bar{\Psi}$ has been accurately evaluated for a sufficient number of points of $\mathcal{E}$, we expect that, under certain regularity conditions for $\bar{\Psi}$, there is a good continuous but finite approximation $\bar{\Psi}^*$ for $\bar{\Psi}$ such that $\bar{\Psi}^*(\bar{\mathbf{C}})$ is close enough to $\bar{\Psi}(\bar{\mathbf{C}})$ for any point $\bar{\mathbf{C}}$ of $\mathcal{E}$.

In this work, we first consider an r.v.e. Ω of the hyperelastic composite and accurately estimate $\bar{\Psi}$ for a sufficient number of points of $\mathcal{E}$ by the finite element method, as illustrated in Figure 2. Then, a continuous approximation $\bar{\Psi}^*$ of $\bar{\Psi}$, is constructed by interpolating the computed discrete values of $\bar{\Psi}$. The interpolation functions used are required to be twice continuously differentiable (or $\mathcal{C}^2$), so that we can finally obtain the approximated effective stress-strain relation and tangent stiffness tensor by calculating the first and second derivatives of $\bar{\Psi}^*$.

3.1. *Discrete representation of the potential*

The space $\mathcal{E}$ consisting of all macroscopic strain tensors $\bar{\mathbf{C}}$ will be referred to as the loading space, since, in the following, the macroscopic variable prescribed on the boundary $\partial\Omega$ of Ω is an element $\bar{\mathbf{C}}$ of $\mathcal{E}$. Let $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ be a three-dimensional (3D) orthonormal basis. Here, we decompose $\bar{C}$ as follows :

$$\bar{\mathbf{C}} = \bar{C}_1\mathbf{e}_1 \otimes \mathbf{e}_1 + \bar{C}_2\mathbf{e}_2 \otimes \mathbf{e}_2 + \bar{C}_3\mathbf{e}_3 \otimes \mathbf{e}_3 + \frac{\bar{C}_4}{\sqrt{2}}(\mathbf{e}_2 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_2)$$

$$+\frac{\bar{C}_5}{\sqrt{2}}(\mathbf{e}_1 \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_1) + \frac{\bar{C}_6}{\sqrt{2}}(\mathbf{e}_1 \otimes \mathbf{e}_2 + \mathbf{e}_2 \otimes \mathbf{e}_1)\ . \qquad [8]$$

The following relations arise :

$$\bar{C}_1 = \bar{C}_{11},\ \bar{C}_2 = \bar{C}_{22},\ \bar{C}_3 = \bar{C}_{33},$$

$$\bar{C}_4 = \sqrt{2}\bar{C}_{23},\ \bar{C}_5 = \sqrt{2}\bar{C}_{31},\ \bar{C}_6 = \sqrt{2}\bar{C}_{12}. \qquad [9]$$

It is well-known that this notation is mathematically more consistent than the traditional Voigt one. In a similar way, we can introduce the components $\bar{S}_\alpha$ $(\alpha = 1, 2, ..., 6)$ and $\bar{S}_{ij}(i, j = 1, 2, 3)$ of the macroscopic stress tensor $\bar{\mathbf{S}}$, which are related by the relations similar to (9).

In the general situation, the potential $\bar{\Psi}$ is defined over $\mathcal{E}$ which can be viewed as a six-dimension vector space, i.e.

$$\bar{\Psi} = \bar{\Psi}(\bar{C}_1, \bar{C}_2, ..., \bar{C}_6), \qquad [10]$$

and the effective stress-strain relation and the effective tangent elastic tensor $\bar{\mathbb{L}} = \partial^2\bar{\Psi}/\partial\bar{C}\partial\bar{C}$ are given by

$$\bar{S}_\alpha = 2\frac{\partial\bar{\Psi}}{\partial\bar{C}_\alpha}, \quad \bar{L}_{\alpha\beta} = \gamma\hat{L}_{\alpha\beta}\ , \hat{L}_{\alpha\beta} = 4\frac{\partial^2\bar{\Psi}}{\partial\bar{C}_\alpha\partial\bar{C}_\beta}. \qquad [11]$$

where the values of γ for the different combinations of α and β are provided in Yvonnet *et al.* (2009). However, we are sometimes interested only in a particular problem, for example a plane-strain problem relative to the plane $x_1 - x_2$. In such a case, $\bar{\Psi}$ depends only on $\bar{C}_1$, $\bar{C}_2$ and $\bar{C}_6$, and the value range of the suffixes α and β in (11) are $\{1, 2, 6\}$. In this section, we focus our attention only on the general situation. When a specific problem is in question, it is relatively easy to adapt the general method presented in this section.

3.2. *Interpolation methods*

Several techniques can be used to interpolate the effective potential data in the macroscopic strain space. In Yvonnet *et al.* (2009), we have proposed two techniques, though many others could be investigated. When the data is structured in the form of a high-dimensional grid, a simple technique is the multidimensional cubic spline interpolation of Habermann *et al.* (2007). However, for high-dimensional stain space, the computational times and memory requirement needed to carry out the interpolation process narrows down its uses. We have proposed an efficient interpolation technique based on separated variables representation of the potential (see e.g. Carol *et al.* (1970), Kiers (2000)). The aim is to find a separated variables representation of the potential in the form :

$$\bar{\Psi}(\bar{C}_1,\bar{C}_2,...,\bar{C}_6) \approx \bar{\Psi}^*(\bar{C}_1,\bar{C}_2,...,\bar{C}_6) = \sum_{r=1}^{R} \tilde{\phi}_1^r(\bar{C}_1)\tilde{\phi}_2^r(\bar{C}_2)...\tilde{\phi}_6^r(\bar{C}_6) \ , \tag{12}$$

where $\tilde{\phi}_j^r(\bar{C}_j)$ are the interpolated values of $\boldsymbol{\phi}_j^r$:

$$\tilde{\phi}_j^r(\bar{C}_j) = \sum_{k=1}^{n} N_k(\bar{C}n_j) \left\{\phi_j^r\right\}_k \ . \tag{13}$$

In Eq. (13), N_k are one-dimensional $\mathcal{C}^2$ interpolation function associated with node k, and n denotes the number of nodes supporting the shape functions $N_k(\bar{C}_j)$ whose value at $\bar{C}_j$ is different from zero. The procedure to construct the vectors $\boldsymbol{\phi}_j^r$ is described in Yvonnet *et al.* (2009). The stress can be expressed by

$$\bar{S}_i^*(\bar{C}_1,\bar{C}_2,...,\bar{C}_6) = 2\sum_{r=1}^{R}\left(\left\{\prod_{k\neq i}\tilde{\phi}_k^r(\bar{C}_k)\right\}\frac{\partial\tilde{\phi}_i^r(\bar{C}_i)}{\partial\bar{C}_i}\right) \ , \tag{14}$$

where

$$\frac{\partial\tilde{\phi}_i^r(\bar{C}_i)}{\partial\bar{C}_i} = \sum_{k=1}^{n}\frac{\partial N_k(\bar{C}_i)}{\partial\bar{C}_i}\left\{\phi_i^r\right\}_k \ . \tag{15}$$

The approximated value $\hat{\mathbb{L}}^*$ of $\hat{\mathbb{L}}$ is evaluated in a similar manner, by using (11). In this work, the functions N_i are chosen to be one-dimensional $\mathcal{C}^2$ cubic spline functions, even though other $\mathcal{C}^2$ interpolation schemes can be considered. For a strain domain of high dimension, this approach only requires finding the coefficients of one-dimensional spline functions, and thus only a small system of equations has to be solved, which saves computational time and memory. Furthermore, the separated representation technique needs only storing one-dimensional discrete functions and thus $p \times d \times R$ values.

4. Numerical example

4.1. *Validation tests*

Firstly, we test the accuracy of the proposed method by comparing it with full FEM calculations. We consider a r.v.e. as depicted in Figure 6c. Each phase is assumed isotropic and governed by a constitutive law deriving from the following strain density function :

$$\Psi(\mathbf{C}) = \frac{1}{2}\lambda\left(log(J)\right)^2 - \mu log(J) + \frac{1}{2}\mu\left(Tr(\mathbf{C}) - 3\right). \quad [16]$$

The corresponding stress (second Piola-Kirchhoff stress) is expressed by

$$\mathbf{S}(\mathbf{C}) = \lambda log(J)\mathbf{C}^{-1} + \mu\left(\mathbf{I} - \mathbf{C}^{-1}\right). \quad [17]$$

The following parameters are used within each phase : E_i = 10000 MPa, ν_i = 0.3, E_m = 100 MPa, ν_m = 0.4, where $\mu = E/(2(1+\nu))$ and $\lambda = E\nu/((1+\nu)(1-2\nu))$, and the indices i and m refer to the inclusion and matrix, respectively. We first compute the NEXP in a strain domain chosen as : $\bar{C}_{11} \in \{0.5; 1.1\}$, $\bar{C}_{22} \in \{0.9; 3.5\}$ and $\bar{C}_{12} \in \{-1.6; 0.1\}$. In this 2D example involving a compressible material, the macroscopic strain domain is three-dimensional. We chose 11 points were defined regularly within each axis. Some points in this strain space led to a divergence of the computations due to very large distortion and entanglement of the materials between the inclusions. For those points, a special extrapolation procedure, defined more in details in a forthcoming paper, has been utilized to carry out the interpolation procedure. We then define some paths along the strain space, not matching the computed data. For each path, we compute the NEXP solution via the above framework, by simply interpolating the data. Both energy and stress solutions are compared with a full FEM computation. We can notice from Figures 3 and 4 that in both cases, very good agreement between the proposed approximation and a full computation is noticed. Deformed configurations corresponding to the strains states A,B and C in Figures 3 and 4 are depicted in Figure 7.

4.2. *A two scales example*

Many numerical examples in the small strains contexts have been presented in Yvonnet *et al.* (2009) to study the accuracy and efficiency of the method in that case. Here we present preliminary results of the computation of structures made of heterogeneous materials at finite strains. The r.v.e. associated with the microstructure is depicted in Figure 6 (c). The same constitutive laws and parameters as in previous example are used within each phase. The microstructure then exhibits a high properties contrast (see phase response in Figure 8). The numerical potential is the one computed in the previous example. The structure, depicted in Figure 6 (a-b), is stretched along the $\mathbf{e}_2$-axis. The response of the composite structure is provided in Figure 8. This example shows that a simple mixture rule (corresponding to the Voigt upper

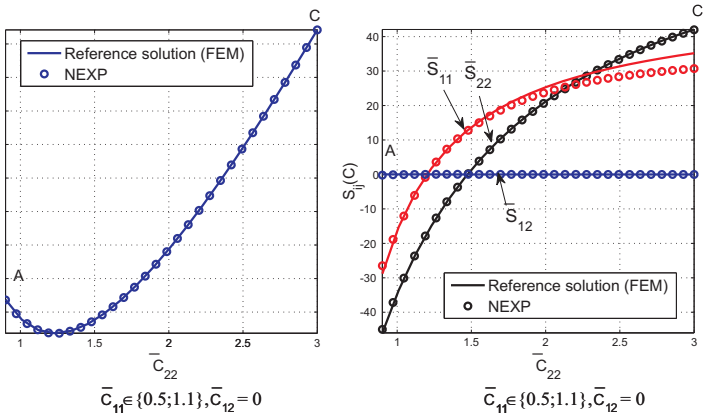

Figure 3. *Computed value of the effective potential (a) and the effective stresses (b) along a strain path. Comparison between NEXP and a full FEM computation. The loading path involves biaxial traction*

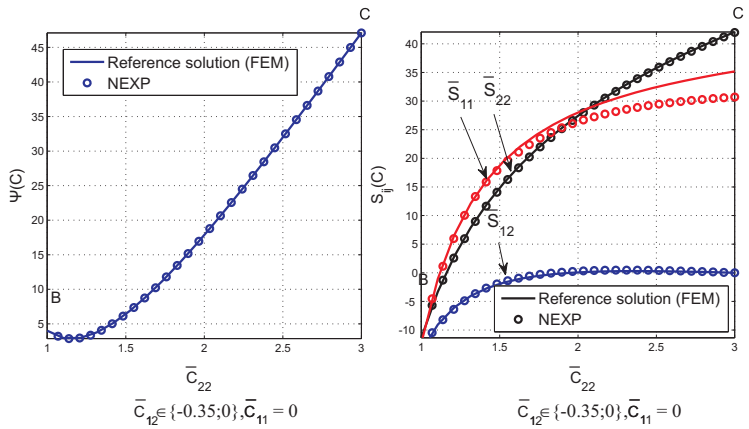

Figure 4. *Computed value of the effective potential (a) and the effective stresses (b) along a strain path. Comparison between NEXP and a full FEM computation. The loading path involves uniaxial stretching combined with shear*

bound) dramatically overestimates the rigidity of the material and highlights the usefulness of the method elaborated. The von Mises stress field of the sample composed of the matrix material, composite and inclusion material, respectively are shown in Figure 7, as well as the deformed configuration of the sample for each case.

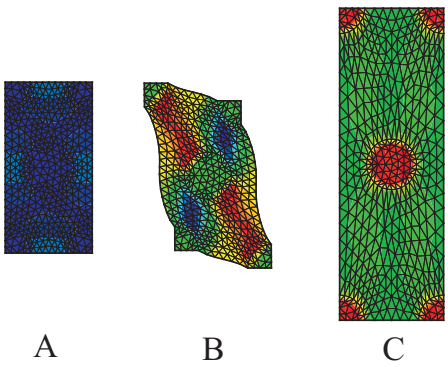

Figure 5. *Deformed configurations of the r.v.e. for loading states A, B and C (see Figures 3 and 4)*

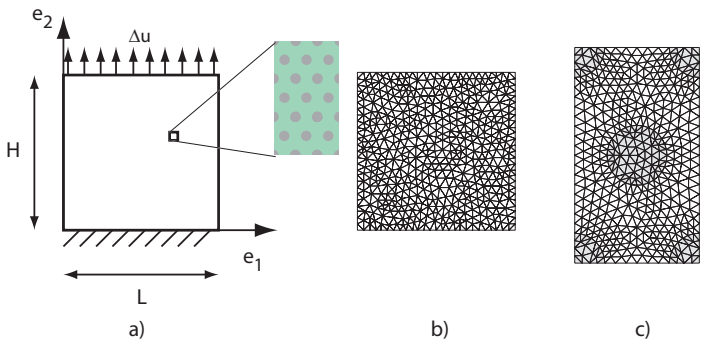

Figure 6. *a) Geometry of the composite tensile sample problem ; b) mesh of a quarter of the structure ; c) mesh of the r.v.e*

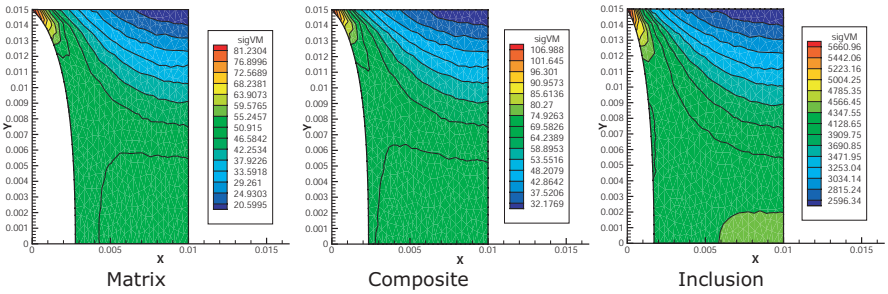

Figure 7. *Deformation of the sample ; comparison between composite response and matrix and inclusion materials*

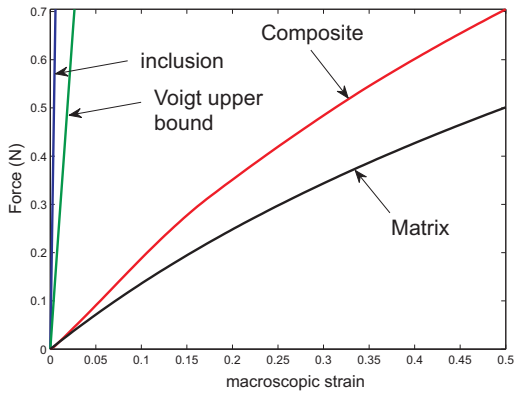

Figure 8. *Response of the tensile sample up to 50 % strain*

5. Conclusion

A non-concurrent multiscale method has been proposed to compute the response of structures made of nonlinearly elastic heterogeneous materials at small and large strains. The key idea is to first compute numerically the effective strain-energy potential for a number of points discretizing the macroscopic strain space. The resulting data are stored in the form of a hypermatrix or a set of vectors. The estimation of the effective strain-energy potential valid for the whole of the macroscopic strain space is then constructed by appropriately interpolating the preliminary discrete results. The effective stress-strain relation and tangent tensor are finally derived in a numerically direct and explicit way via efficient multi-dimensional interpolation techniques. The method possesses the following features :

(a) Once the Numerically Explicit Potential is constructed after the preliminary stage, the stress and elastic tangent tensors can be readily evaluated without any new local FE computations. The numerical treatment necessary to determining the effective stress and elastic tangent tensors is far less than performing a local nonlinear FE computation as in concurrent methods. Nevertheless, the present method is in this work restricted to non-dissipative materials, while concurrent methods have not this limitation.

(b) In concurrent methods, the only way to compute the tangent tensor is to achieve numerical evaluation by a perturbation method (Feyel, 1999), implying additional costly finite element computations. In the present method the tangent elastic tensor can be derived explicitly from the NEXP.

(c) The method is not limited on the use of FEM at the local level, any alternative solver can be used.

(d) The preliminary computations can be costly for 3D problems or very complex microstructures. However, as the local problems for nodal effective responses are independent, parallel computations can be straightforwardly implemented.

However, the present work is limited to nonlinearly elastic heterogeneous materials without internal variables. Extension of the basic idea of the proposed approach to the homogenization of other nonlinear heterogeneous materials is being envisaged and will be presented in forthcoming works. Another future direction of this work is the introduction of uncertainties at the microscopic level to study their influence on the macroscopic response of the material.

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