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Computational nonlinear stochastic homogenization using a non-concurrent multiscale approach for hyperelastic heterogeneous microstructures analysis

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SUMMARY

This paper is devoted to the computational nonlinear stochastic homogenization of a hyperelastic heterogeneous microstructure using a non-concurrent multiscale approach. The geometry of the microstructure is random. The non-concurrent multiscale approach for micro-macro nonlinear mechanics is extended to the stochastic case. Since the non-concurrent multiscale approach is based on the use of a tensorial decomposition, which is then submitted to the curse of dimensionality, we perform an analysis with respect to the stochastic dimension. The technique uses a database describing the strain energy density function (potential) in both the macroscopic Cauchy Green strain space and the geometrical random parameters domain. Each value of the potential is numerically computed by means of the finite element method on an elementary cell whose geometry is given by the random parameters and the corresponding macroscopic strains being prescribed as boundary conditions. An interpolation scheme is finally introduced to obtain a continuous explicit form of the potential, which, by derivation, allows to evaluate the macroscopic stress and elastic tangent tensors during the macroscopic structural computations. Two numerical examples are presented.

KEY WORDS: computational mechanics; stochastic homogenization; nonlinear heterogeneous materials; random microstructures

1. INTRODUCTION

When a structure is made of a highly heterogeneous material at the microscopic level, classical numerical methods used for structural analysis lead to prohibitive memory and computational costs and can hardly be used for standard engineering studies. Homogenization methods represent an effective alternative for determining the macroscopic behavior of such materials. However, the case of nonlinear heterogeneous materials leads us to a set of additional difficulties regarding the linear case: for instance, the general form of the constitutive law is not known and the principle of superposition does not hold which prevents using any analytical homogenization scheme introduced for the case of small elastic strains. To overcome these difficulties two classes of methods have been developed and used during the last two decades. The first one consists in extending classical analytical homogenization approaches by derivation of estimate and exact solutions of some classes of hyperelastic composites [1, 2, 3] or by introducing a second-order homogenization method to determine the effective constitutive laws of nonlinear composites (see [4, 5], for instance). The
second family of methods consists in using numerical multiscale simulations which can be an effective alternative approach when one seeks, for instance, to deal with complex microstructure. Then, concurrent multiscale methods were developed and aim at solving simultaneously the nonlinear problems at both scales (see for instance [6, 7, 8, 9, 10, 11, 12, 13]). The macroscopic problem provides the strain states in all integration points and gives the boundary conditions used to solve each microscopic problem. This kind of techniques allows taking into account different types of nonlinearities but may lead to significant computational costs. Alternatively, the non-concurrent multiscale methods aim at decoupling the numerical simulations at both scales. They consist in identifying parameters characterizing the macroscopic constitutive law from experimental or numerical test [14] or using a database formed of microscopic calculations to build a numerical constitutive law without any assumption on the constitutive equations [15, 16, 17, 18, 19]. In this work, we focus on the methodology proposed in [17, 18, 19].

On the other hand, it may also be necessary to take into account the different sources of uncertainty at the microscopic level if one seeks to obtain a reliable model of the macroscopic behavior of the material. Thus, the general area of stochastic multiscale modeling of complex random heterogeneous microstructures has recently attracted a continuously growing attention in the scientific community. A simple way to solve this kind of problem consists in coupling numerical simulations of random microstructures (based on experimental identification or some geometrical characteristics such that the volume fraction or others parameters such that the spatial and size distributions [20, 21]) with classical finite element computations. Then, one can perform a statistical study of average quantities of interest characterizing the macroscopic behavior of the material (e.g. stress random fields). Recently, more sophisticated methods based on the Maximum Entropy principle have been developed in the case of linear elasticity. The so-called nonparametric approach for uncertainties aims at building prior probability distributions of effective stress tensors with no explicit representation of the random parameters characterizing the microstructure [22, 23, 24, 25]. Parametric approaches have also been used to characterize the macroscopic behavior. In [26, 27, 28], the authors have used spectral stochastic methods (e.g. polynomial chaos approximation) to solve the stochastic boundary value problem involved by the random microstructure. Monte-Carlo simulations may naturally be employed to perform a statistical study on the effective properties of the material (see for instance [29] and [30] where the Monte-Carlo approach is coupled with a X-FEM methodology avoiding the remeshing difficulties). The fundamental objective of the paper is to test a novel non-concurrent approach for solving a nonlinear stochastic homogenization problem. In this context, to the knowledge of the authors, the present paper is the first one devoted to this challenging issue. A choice concerning the mechanical nonlinearities of the microstructure must be made. There are two main types of mechanical nonlinearities: large deformations and displacements with linear constitutive equations (type I) and, small or large deformations with nonlinear constitutive equations (type II). As it is the first research in this field from the authors, we decide to adopt nonlinearities of type I which facilitate the definitio of the potential which is a crucial point of the proposed approach. Further works will be devoted to the extension of the method for different kinds of nonlinearities such as plasticity. On the other hand, the proposed method should, in the future, be applied to a practical example in the field of biomechanics such as the study of living tissues which follow a hyperelastic constitutive behavior. We here focus on fibre reinforced polymer composites, involving a condition of impenetrability between the inclusions, and on the geometrical uncertainties on the microstructure. The first step of the method lies on the construction of a probabilistic model of the random microstructure. This issue has already been assessed by different authors in various ways. In [31, 32], the formalism of random sets is used to generate random heterogeneous microstructures while in [20, 33, 34] the same objective is done based on a Poisson random field model. We also propose to build a random generator of the microstructure which depends on a high number of random variables. We then use a classical statistical reduction through a Karhunen-Loeve expansion [35] which allows controlling the probabilistic model with a few number of reduced random variables. Numerous algorithms given in the literature may replace the one develop in this work. However, the algorithm proposed in Section 3 allows introducing and controlling the correlation structure given to the
geometrical parameters which makes effective the statistical reduction. Then, based on a particular nonlinear homogenization scheme, we propose to extend the method of the Numerical Explicit Potentials (NEXP method) [17, 18, 19] to the stochastic framework. In the deterministic case, this approach is based on the numerical determination of the macroscopic strain energy density function (potential) according to the macroscopic strain state. Through a separated variables representation and an appropriate interpolation scheme, this approach allows obtaining an explicit form of the potential, which, by derivation, yields the stress and elastic tangent tensors which fully characterize the macroscopic constitutive law. In the stochastic framework, the aim is the same but the potential is not only related to the macroscopic strain state but also to the reduced random variables describing the random geometry of the microstructure. Then, the strain energy density function is depending on a set of parameters. This so-called parameters space is discretized into a sufficient number of points corresponding both to a particular macroscopic strain state and a particular geometry of the microstructure which involve a nonlinear boundary value problem numerically solved by a classical finite element method. In order to obtain an explicit form of the potential available for any points belonging to the parameters space, a separated variables representation associated to an appropriate interpolation scheme is adapted from [18, 19]. Thus, the macroscopic structural computations can be easily and efficiently performed using the explicit form of the potential to determine the random macroscopic constitutive law.

Moreover, the probabilistic characterization of such a complex microstructure may require a high number of random variables. Thus, the question of the high dimensionality is also pointed out. We will then focus on the extension of this kind of numerical deterministic solvers to the stochastic framework when one seeks to use a high number of random variables to characterize the probabilistic model.

The paper is organized as follows. Section 2 deals with the homogenization of nonlinear heterogeneous materials at finite strains in a deterministic framework where both, microscale and macroscale problems are detailed. Section 3 presents the probabilistic model leading to a stochastic representation of the microstructure based on a parametric framework. We then detail, in Section 4, the proposed approach, called the method of Stochastic Numerical Explicit Potentials, which allows determining the constitutive law at the upper scale according to the random parameters characterizing the geometry of the microstructure. Numerical examples are finally provided in Section 5 in order to point the advantages and drawbacks of the proposed method. Some concluding remarks are finally drawn in the last section.

2. DETERMINISTIC HOMOGENIZATION OF NONLINEAR HETEROGENEOUS MATERIALS

2.1. Nonlinear homogenization scheme

We consider a microstructure, schematically represented on fig 1, which occupies a domain \( \Omega \subset \mathbb{R}^d \) where \( d \) denotes the spatial dimension (\( d \in \{1, 2, 3\} \)). The boundary of the domain \( \Omega \) is denoted by \( \partial \Omega \) and the position of the material points are identified by the vector \( X \) in the reference configuration and by vector \( x \) in the deformed configuration. These vectors are related through:

\[
x = X + u,
\]

where \( u \) is the displacement vector of a material point. We introduce the deformation gradient tensor \( F \) at point \( X \) defined by

\[
F = \frac{\partial x}{\partial X} = 1 + \nabla_X(u),
\]

where 1 is the second-order identity tensor and \( \nabla_X(\cdot) \) is the gradient operator according to the reference configuration. The microstructure is associated with a multiphased heterogeneous material composed of \( N_p \) hyperelastic phases defined in the \( N_p \) domains \( \Omega^{(r)} \) with \( r \in \{1, \ldots, N_p\} \) and such that \( \Omega = \bigcup_{r=1}^{N_p} \Omega^{(r)} \). The constitutive equation of each phase can then be characterized by strain energy density functions (i.e. elastic potentials) \( \psi^{(r)} \) according to the right-hand Cauchy-Green
strain tensor $C = F^T F$ such that the local strain energy density function $\psi$ of $\Omega$ may be written as

$$
\psi(X, C) = \sum_{r=1}^{N_n} \mathbb{I}^{(r)}(X) \psi^{(r)}(C),
$$

(3)

where $\mathbb{I}^{(r)}$ is the characteristic function of domain $\Omega^{(r)}$ which is equal to 1 if $X \in \Omega^{(r)}$ and 0 otherwise. The local constitutive law is given, in the Lagrangian description, by

$$
S = 2 \frac{\partial \psi}{\partial C}(X, C),
$$

(4)

where $S$ denotes the second Piola-Kirchhoff stress tensor. Several models are available for the hyperelastic constitutive law: we only here consider a compressible Neo-Hookean model described by the following potential

$$
\psi(C) = \frac{1}{2} \lambda \{\log(J)\}^2 - \mu \log(J) + \frac{1}{2} \mu (tr(C) - 3),
$$

(5)

where $J = \det(F)$ is the volumetric change and where $\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}$ and $\mu = \frac{E}{2(1+\nu)}$ with $E$ and $\nu$ respectively the Young modulus and the Poisson ratio. We also introduce the fourth-order tangent elastic tensor $L$ defined by

$$
L = 4 \frac{\partial^2 \psi(X, C)}{\partial C^2}.
$$

(6)

We assume that the elementary cell is associated with a structure at a larger scale which can be a mesoscopic or a macroscopic scale depending on the separation between the considered scales. This issue will be discussed in Section 3. Thus, we define the kinematic quantities as follows:

$$
\overline{F} = \langle F \rangle,
$$

(7)

$$
\overline{C} = F^T F \neq \langle C \rangle,
$$

(8)

where symbol $\langle \cdot \rangle$ denotes the spatial averaging over $\Omega$. The upper scale stress tensors are defined according to

$$
\overline{P} = \langle P \rangle,
$$

(9)

$$
\overline{S} = \overline{F}^{-1} \overline{P} \neq \langle S \rangle,
$$

(10)

where $\overline{P}$ denotes the first Piola-Kirchhoff macroscopic stress tensor. Using equations (7) to (10), it can be shown that

$$
\overline{S} = 2 \frac{\partial \psi(\overline{C})}{\partial \overline{C}},
$$

(11)
where the effective strain energy density function $\overline{\psi}$ is defined by

$$\overline{\psi}(\overline{C}) = \inf_{C \in \mathcal{K}(\overline{C})} \langle \psi(X, C) \rangle. \quad (12)$$

In equation (12), the set $\mathcal{K}(\overline{C})$ gathers all kinematically admissible strain tensors according to $\overline{C}$. Thus, for a given strain state $\overline{C}$, the corresponding value of $\overline{\psi}(\overline{C})$ is determined by taking the spatial average of local strain energy density functions $\psi(X, C)$, where $C(X)$ is the strain field at equilibrium. In a same manner, we can show that the tangent elastic tensor $\mathcal{L}$ can be expressed according to $\overline{\psi}$ such that

$$\mathcal{L} = 4 \frac{\partial^2 \overline{\psi}(\overline{C})}{\partial \overline{C}^2}. \quad (13)$$

Proofs yielding equations (11) and (13) which fully allow characterizing the upper scale constitutive law can be found in [19].

2.2. Involved mechanical problems at different scales

At the microscopic scale the stress must verify the local equilibrium condition:

$$\nabla_X \cdot (FS) = 0 \quad \text{on} \quad \Omega, \quad (14)$$

where $\nabla_X \cdot (\cdot)$ is the gradient operator according to the reference configuration. Boundary conditions must be associated with equation (14) to obtain a unique solution. Several choices are possible: kinematically uniform, statically uniform or periodic boundary conditions. However, since the microstructure is characterized by random geometrical parameters, the implementation of periodic boundary conditions involves numerical difficulties since the finite element mesh is not regular on the boundary. This issue can be encountered using an X-FEM solver with adapted enrichment strategies such as the one proposed in [36] allowing multiple level-sets (i.e., interfaces) cutting the same finite element. We therefore use linear boundary conditions expressed in case of finite strains:

$$u(X) = (\overline{F} - 1)X \quad \text{on} \quad \partial \Omega. \quad (15)$$

At the upper scale, the equilibrium equation must be verified

$$\nabla_X \cdot (\overline{F}S) = 0 \quad \text{on} \quad \overline{\Omega}, \quad (16)$$

with the following boundary conditions

$$\mathbf{r}(\overline{X}) = \hat{u}(\overline{X}) \quad \text{on} \quad \partial \overline{\Omega}_u, \quad \overline{P} \overline{N} = \hat{F} \quad \text{on} \quad \partial \overline{\Omega}_F, \quad (17)$$

where $\overline{\Omega}, \mathbf{r}, \overline{X}, \partial \overline{\Omega}_u, \partial \overline{\Omega}_F, \hat{u}(\overline{X}), \hat{F}$ and $\hat{N}$ are, respectively, the macroscopic domain, the macroscopic displacements, the macroscopic coordinates in the reference configuration, the boundary of macroscopic Dirichlet conditions, the boundary of macroscopic Neumann boundary conditions, the applied displacements, external force and the outward unit normal vector to the boundary $\partial \overline{\Omega}$ of $\overline{\Omega}$. Both nonlinear problems defined by equations (14) and (16) are classically linearized and solved with the Finite Element Method.

3. PROBABILISTIC MODELING

This section deals with the construction of the probabilistic model of the microstructure characterizing a fibre reinforced polymer composite. We first introduce the chosen parametrization of the geometry. We then detail the probabilistic model consisting in a random generator combined with a classical statistical reduction through a principal component analysis.
3.1. Geometrical description of the microstructure

This work is focussed on heterogeneous materials for which the geometrical parameters characterizing the microstructure are random. In particular, we are interested in composites made of polymer matrix and reinforced by non-penetrating long fibers. Manufacturing process of these kind of material involves uncertainties, related to the position of the fibers mainly due to the “fountain effect” of the injector. Moreover, since the 2D-cross section views, used for the microstructure mechanical modeling and for the mechanical numerical analysis, are coming from experimental data, they may involve error on the orientation of the fibers. It thus leads us to another source of uncertainties. Figure 2 illustrates typical section views of this kind of material and clearly shows a correlation between the position and shape of the different fiber which characterize the probabilistic model. The geometrical modeling of the fiber is depicted on figure 3. The microstructural problem illustrated on this figure is different from the one presented on figure 2 since the mean-line of each fiber is parallel to $e_3$. Moreover, in the following, we only use a 2-D model under plane strain assumption, this is why the problem treated in this paper corresponds to a microstructure composing of fiber depicted on figure 3. Therefore, one fiber is represented by an ellipse parametrized by 5 constants: the horizontal and vertical positions $X$ and $Y$ of its center, an aspect ratio $\alpha$, the length of its semi-major axis $a$ and its orientation angle $\gamma$ according to vector $e_3$. Introducing the semi-minor axis $b$, the aspect ratio $\alpha$ is defined by $\alpha = b/a$ with $\alpha \in [0, 1]$. Using this geometrical parametrization, the probabilistic model is detailed in the following section.

3.2. Stochastic modeling of the microstructure

We first introduce the numbers of fiber composing the microstructure denoted by $N_f$ which yields a number $N = 5N_f$ of geometrical parameters. However, if we generate exactly $N$ parameters representing $N_f$ fibers, there is a high probability that several fiber intersect each other and thus do not verify the condition of impenetrability of the fibers detailed in Section 3.2.3 and which is equivalent to a rejection process. We then need to generate a greater number $n \gg N_f$ of “possible” geometrical parameters used in the rejection process. We here adopt a parametric approach to deal with the uncertainties. Let be $m = 5n$. The geometry is modeled by a $\mathbb{R}^m$-valued random variable, defined on a probability space $(\Xi, \mathcal{B}_\Xi, P_\xi)$, whose support of the probability law $P_\xi$ is $\Xi$ which is a subset of $\mathbb{R}^m$. Considering the geometrical parametrization introduced in Section 3.1, the random
“possible” geometrical parameters is represented by the second-order random vector \( \xi \) define by

\[
\xi = (X, Y, \alpha, a, \gamma) = (X_1, ..., X_n, Y_1, ..., Y_n, \alpha_1, ..., \alpha_n, a_1, ..., a_n, \gamma_1, ..., \gamma_n).
\] (18)

The direct construction of \( P_\xi \) is not a trivial task. We thus propose to construct a random generator associated with a statistical reduction method. Consequently, we construct \( P_\xi \) using an indirect approach. The main steps of the development of this stochastic model via the construction of the random generator is given below.

1. Constructing a stochastic model of random vector \( \xi \) and generate a set of independent realizations \( \{ \xi(k) \}_{k=1}^{\nu} \) of \( \xi \), according to the parameters detailed in Section 3.2.1.

2. Performing a statistical reduction of random vector \( \xi \) using a principal component analysis yielding a new random vector \( \zeta = (\zeta_1, ..., \zeta_M) \) with \( M \ll m \) and constructing the \( \nu \) independent realizations (see Section 3.2.2).

3. Selecting the \( \mu \) independent realizations \( \{ \zeta(k) \}_{k=1}^{\mu} \), with \( \mu \leq \nu \), which verify the condition of impenetrability. These realizations completely characterize the stochastic model of the microstructure (see Section 3.2.3).

#### 3.2.1. Stochastic model of \( \xi \) and random generator

The aim is to generate the independent realizations \( \{ \xi^{(k)} \}_{k=1}^{\nu} \) using the order statistics to impose the desired properties for the stochastic model. The random vectors \( X, Y, \alpha, a \) and \( \gamma \), yielding \( \xi \), are characterized by the independent realizations \( \{ X^{(k)} \}_{k=1}^{\nu}, \{ Y^{(k)} \}_{k=1}^{\nu}, \{ \alpha^{(k)} \}_{k=1}^{\nu}, \{ a^{(k)} \}_{k=1}^{\nu} \) and \( \{ \gamma^{(k)} \}_{k=1}^{\nu} \). Since the realizations of each random vector \( X, Y, \alpha, a \) and \( \gamma \), will be generated through the same procedure, we present the methodology for random vector \( X \). To generate the realizations \( \{ X^{(k)} \}_{k=1}^{\nu} \) with the desired properties, we introduce the order statistics. We then denote by \( X^{\text{ord}} = (X^{\text{ord}}_1, ..., X^{\text{ord}}_n) \) the random vector such that \( X^{\text{ord},(k)}_1 < X^{\text{ord},(k)}_2 < \cdots < X^{\text{ord},(k)}_n \) for each realization \( k \) in \( \{1, ..., \nu\} \). Let \( E\{\cdot\} \) be the mathematical expectation. In the construction proposed, the second-order quantities of the second-order random vector \( X^{\text{ord}} \) are controlled by the input parameters of the model, define as follows.

1. The mean vector \( \mu_{X^{\text{ord}}} = E\{X^{\text{ord}}\} \) whose components \( \mu_{X^{\text{ord}}_i}, ..., \mu_{X^{\text{ord}}_n} \) are assumed to be equal to \( \mu_{X^{\text{ord}}} = \mu_{X^{\text{ord}}_1} = \cdots = \mu_{X^{\text{ord}}_n} \).

2. The vector \( \delta_{X^{\text{ord}}} = (\delta_{X^{\text{ord}}_1}, ..., \delta_{X^{\text{ord}}_n}) \) where \( \delta_{X^{\text{ord}}_i} \) is the coefficient of variation of random variable \( X^{\text{ord}}_i \), is assumed to be such that \( \delta_{X^{\text{ord}}} = \delta_{X^{\text{ord}}_1} = \cdots = \delta_{X^{\text{ord}}_n} \).

3. The spatial correlation is controlled by the positive real number \( \rho \).
Let $[C_{\mathbf{X}^{\text{ord}}}]$ be the covariance matrix of random vector $\mathbf{X}^{\text{ord}}$ defined by

$$
[C_{\mathbf{X}^{\text{ord}}}] = \mathbb{E}\{(\mathbf{X}^{\text{ord}} - \mu_{\mathbf{X}^{\text{ord}}})(\mathbf{X}^{\text{ord}} - \mu_{\mathbf{X}^{\text{ord}}})^T\}.
$$

By construction of the stochastic model, the coefficient $[C_{\mathbf{X}^{\text{ord}}}]_{i\ell} = \mathbb{E}\{(X_i^{\text{ord}} - \mu^{\text{ord}})(X_\ell^{\text{ord}} - \mu^{\text{ord}})\}$ are written as

$$
[C_{\mathbf{X}^{\text{ord}}}]_{i\ell} = 1
$$

and

$$
[C_{\mathbf{X}^{\text{ord}}}]_{i\ell} = (\delta^{\text{ord}})^2(\mu^{\text{ord}})^2 \exp\left(\frac{|i - \ell|}{\rho n}\right) \quad \text{if} \quad i \neq \ell.
$$

We now introduce a random vector $\mathbf{U} = (U_1, \ldots, U_n)$ in which $U_1, \ldots, U_n$ are independent uniform random variables on $[0,1]$. Let $\{\mathbf{U}^{(k)}\}_{k=1}^\nu$ be $\nu$ independent realizations of $\mathbf{U}$.

For each realization $k$ in $\{1, \ldots, \nu\}$, we proceed as follows.

1. The components $U_1^{(k)}, \ldots, U_n^{(k)}$ of vector $\mathbf{U}^{(k)}$ are ordered according to the Euclidean distance $|U_1^{(k)} - U_i^{(k)}|$ for $i$ in $\{2, \ldots, n\}$. The resulting non-Gaussian random vector is denoted by $\mathbf{V}^{(k)}$.

2. We compute the vector $\mathbf{X}^{(k)} = \mu_{\mathbf{X}^{\text{ord}}} + [L]_T \mathbf{V}^{(k)}$ in which the matrix $[L]$ is the upper triangular matrix coming from the Cholesky factorization $[C_{\mathbf{X}^{\text{ord}}}] = [L]^T[L]$.

3. The targeted vector $\mathbf{X}^{(k)}$ is then obtained by ordering the vector $\mathbf{X}^{(k)}$. One should notice that, since $\mathbf{V}^{(k)}$ is a non-Gaussian random vector, the Cholesky factorization implies that $\mathbf{X}^{(k)}$ is a non-Gaussian random vector.

By applying the above procedure to the $\nu$ realizations, we finally obtain $\{\mathbf{X}^{\text{ord},(k)}\}_{k=1}^\nu$. The same methodology, with different or identical input parameters, is used to generate the independent realizations of the others random vectors $\mathbf{Y}$, $\mathbf{a}$, and $\gamma$, and finally, to obtain the random vector $\mathbf{ξ}$.

In practice, since dimension $m$ of random vector $\mathbf{ξ}$ is high, it is not possible to directly use $\mathbf{ξ}$ in a parametric probabilistic approach. This difficulty is circumvented in introducing a statistical reduction using a principal component analysis [35] of random vector $\mathbf{ξ}$.

3.2.2. Statistical reduction Let $\mu_{\mathbf{ξ}}$ be the mean value of $\mathbf{ξ}$, estimated by $\mu_{\mathbf{ξ}} \simeq \frac{1}{\nu} \sum_{k=1}^{\nu} \mathbf{ξ}^{(k)}$. Let us denote by $\mathbf{ξ}^{(k)} = \mathbf{ξ}^{(k)} - \mu_{\mathbf{ξ}}$ the centered realizations. The covariance matrix of random vector $\mathbf{ξ}$ is then estimated by

$$
[C_{\mathbf{ξ}}] \simeq \frac{1}{(\nu - 1)} \sum_{k=1}^{\nu} \mathbf{ξ}^{(k)}\mathbf{ξ}^{(k)T}.
$$

Let be $M \leq m$. Let $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_M$ and $\varphi_1, \varphi_2, \ldots, \varphi_M$ be the $M$ largest eigenvalues and the associated eigenvectors, of symmetric positive matrix $[C_{\mathbf{ξ}}]$, such that $[C_{\mathbf{ξ}}] \varphi_j = \lambda_j \varphi_j$. Vectors $\varphi_1, \ldots, \varphi_M$ are orthonormal. Using the principal component analysis, the mean-square approximation of $\mathbf{ξ}$ can be written as $\mathbf{ξ} \simeq \mu_{\mathbf{ξ}} + \sum_{j=1}^{M} \sqrt{\lambda_j} \varphi_j \zeta_j$ for which the second-order random variables $\zeta_1, \ldots, \zeta_M$ are centered and orthonormal, that is to say, $\mathbb{E}\{\zeta_j\} = 0$ and $\mathbb{E}\{\zeta_j\zeta_{j'}\} = \delta_{jj'}$. The integer $M$ is assumed to be sufficient large to reach the mean-square convergence which is controlled by

$$
\sqrt{1 - \frac{\sum_{j=1}^{M} \lambda_j}{\text{tr}[C_{\mathbf{ξ}}]}} = \epsilon_{KL}^M < \epsilon_{KL},
$$

in which $\epsilon_{KL}$ is the tolerance parameter. The random variable $\zeta_j$ is given by $\zeta_j = \frac{1}{\sqrt{\lambda_j}} \varphi_j^T(\mathbf{ξ} - \mu_{\mathbf{ξ}})$ and we introduce the random vector $\mathbf{ζ} = (\zeta_1, \ldots, \zeta_M)$. From these equations, it can be deduced the
representation of the realizations \( \mathbf{\xi}^{(k)} \) of \( \mathbf{\xi} \) which are such that, for all \( k = 1, \ldots, \nu \),

\[
\mathbf{\xi}^{(k)} \simeq \mu_{\mathbf{\xi}} + \sum_{j=1}^{M} \sqrt{\lambda_j} \varphi_j \mathbf{\zeta}^{(k)}_j,
\]

(23)

and the realization \( \mathbf{\zeta}^{(k)}_j \) of \( \mathbf{\zeta}_j \) is given by

\[
\mathbf{\zeta}^{(k)}_j = \frac{1}{\sqrt{\lambda_j}} \varphi_j^T (\mathbf{\xi}^{(k)} - \mu_{\mathbf{\xi}}).
\]

(24)

Introducing the vector \( \mathbf{\zeta}^{(k)} = (\mathbf{\zeta}^{(k)}_1, \ldots, \mathbf{\zeta}^{(k)}_M) \), we deduce that \( \{ \mathbf{\zeta}^{(k)}_j \}_{k=1}^{\nu} \) are the independent realizations of random vector \( \mathbf{\zeta} \) which represents the geometrical parameters of the fiber composing the microstructure.

3.2.3. Condition of impenetrability The final step for obtaining the geometry of the microstructure consists in a selection of the realizations verifying the condition of impenetrability of the fiber which are characterized by domains \( \Omega^{(r)} \) with \( r = 1, \ldots, N_f \). The condition of impenetrability is written as

\[
\bigcap_{r=1}^{N_f} \Omega^{(r)} = \emptyset.
\]

(25)

We will say that the condition of impenetrability is satisfied for a particular realization \( \mathbf{\zeta}^{(k)} \), if there exists a set of domains \( \{ \Omega^{(r)} \}_{r=1}^{N_f} \) that verify equation (25). Each realization of the set \( \{ \mathbf{\zeta}^{(k)}_j \}_{k=1}^{\nu} \) of realizations is tested. If the condition of impenetrability is satisfied the realization is kept, otherwise it is rejected. With this procedure of rejection, we obtain the new set \( \{ \mathbf{\zeta}^{(k)}_j \}_{k=1}^{\nu} \) with \( \mu \leq \nu \). In practice, the condition of impenetrability is verified through a numerical procedure based on a discretization of the elementary cell defined on domain \( \Omega \) into a regular grid of points \( \{ \mathbf{x}_i \}_{i=1}^{N_{\Omega}} \) where \( N_{\Omega} \) is taken sufficiently high to ensure that, at least, one point \( \mathbf{x}_i \) is contained in each domain \( \Omega^{(r)} \). The algorithm used to create the geometry of the microstructure acts as a rejection/acceptation algorithm: the possible fibers are tested one after another (a fiber is rejected or accepted if it does not intersect any existing fiber and stops when the desired number of fiber \( N_f \) is reached.

3.2.4. Study of the probabilistic model Among the various input parameters of the stochastic model, detailed in section 3.2.1, the correlation parameter \( \rho \) plays a major role in the efficiency of the reduction defined by equation (23). Figure 4 illustrates the convergence of error \( \epsilon_{KL}^M \) with respect to the number \( M \) of eigenvalues for several values of \( \rho \) equal to 0.1, 0.3, 0.5, 0.7 and 0.9 while others input parameters are fixed to \( m = 2500, \nu = 5000, \mu_{ord} = 0.5 \) and \( \delta_{ord} = 0.5 \). We can observe a fast decrease of error \( \epsilon_{KL}^M \) according to \( M \) for any value of \( \rho \). As expected, the fastest convergence is reached for the highest value of \( \rho \) but the reduction is also effective for the lower values of \( \rho \). However, even for the case \( \rho = 0.9 \), we can notice that, at least, 9 eigenvalues are required to reach an error inferior to 0.1. Figure 5 displays the graph of the probability density functions for several random variables \( \mathbf{\zeta}_j \) according to different values of the spatial correlation parameter \( \rho \). We can observe that, even though the supports of the probability density functions of random variables \( \mathbf{\zeta}_j \) are essentially the same, the shape of the probability density function is different from a variable to another. The same remark can be pointed out when the spatial correlation parameter varies. It can even be seen, for particular values of \( \rho \), a multimodal probability density function for particular random variable \( \mathbf{\zeta}_j \) (see for instance \( \mathbf{\zeta}_4 \) with \( \rho = 0.5 \)).

As a final illustration of the stochastic model, figure 6 displays some realizations of the random geometry of the microstructure for different values of input parameters.

3.2.5. Remark on the resulting random field In the final part of this section, we study the properties of the random field generated by the proposed stochastic model. In the field of homogenization,
a crucial information comes from the separation of the scales. If the spatial correlation lengths of the mechanical field in the microstructure are small enough with respect of the dimension of the structure, then the scales can be separated and then a stochastic homogenization can be performed. In such a case, the statistical fluctuation at the macroscale are negligible and the effective mechanical properties are deterministic. In the other case, the scales are not separable and the effective properties are random. It is then important to calculate the spatial correlation lengths of the random field $L(X)$ at the microscale. Thus, we propose to focus on the random field $L(X)$ indexed by $\mathbb{R}^d$ through two quantities. The first one is the spatial mean $\mu_{\|L(X)\|_F}$ of $L(X)$ define
Figure 6. Various geometries of the random microstructure corresponding to different values of input parameters.

\[ \mu_{\|L(X)\|_F} = \mathbb{E}\{\|L(X)\|_F\} \]

where \(\|\cdot\|_F\) denotes the Frobenius norm. The second one is the...
correlation function \( r_L(X + \eta, X) \) of \( L(X) \) define by
\[
r_L(X + \eta, X) = \frac{\text{tr}\{E\{(L(X + \eta) - E\{L(X + \eta)\}) (L(X) - E\{L(X)\})^T\}\}}{\sqrt{E\{\|L(X + \eta) - E\{L(X + \eta)\}\|^2_F\} E\{\|L(X) - E\{L(X)\}\|^2_F\}}}
\]
(26)

Figures 7(a) and 7(b) display the graphs of function \( X \mapsto \mu_{\|L(X)\|_F} \) and \( \eta \mapsto r_L(X + \eta, X) \). If the two scales are separated then \( L(X) \) is a mean-square homogeneous second-order random field which involves that \( \mu_{\|L(X)\|_F} \) and \( r_L(X + \eta, X) \) are independent of \( X \). However, figure 7(a) and 7(b) clearly show that \( L(X) \) cannot be considered as a homogeneous random field on the elementary cell. Using equation (26) and using an exponential function to fit the correlation length \( \xi \) we have estimated that \( L_{REV} = 7 \). That is to say that the REV associated to this specific problem should be approximately 7 times longer than the length of the elementary unit cell used in the manuscript where the geometrical characteristics of the fiber remain the same. Only the number \( N_f \) should be increased to \( N_f = 7^2 \times 80 = 3920 \). Thus, we will see in the numerical example 5.1 that the macroscopic mechanical field have significant stochastic fluctuations.

4. METHOD OF STOCHASTIC NUMERICAL EXPLICIT POTENTIALS (S-NEXP)

4.1. Summary of the method
The aim of the S-NEXP method is to numerically determine the strain density energy function \( \psi(C) \) for a finite set of macroscopic boundary conditions depending on tensor \( C \) (see equation (15)) and the different realizations of the random geometries of the microstructure define by the realizations \( \{\zeta^{(h)}\}_{k=1}^{\mu} \). The resulting values are then interpolated according to \( C \) in order to obtain the components of tensors \( \tilde{S} \) and \( \tilde{T} \) required to solve the macroscopic problem (16). The main steps of the approach are define as follows.

1. Define the parameters domain \( \Delta = \Delta_{C} \times \Delta_{\zeta} \), where the domain \( \Delta_{C} \) is related to the components of the right Cauchy-Green strain tensor \( C \) and where the domain \( \Delta_{\zeta} \) is related to the random geometrical parameters generated from the vector \( \zeta \).
2. Discretizing each domain \( \Delta_{C} \) and \( \Delta_{\zeta} \) into a finite number of nodes. For each node, the corresponding values of \( C_{k} \) are used to prescribe boundary conditions on the elementary cell and the corresponding values of \( \zeta_{k} \) are used to define the geometry of the microstructure. For each node the strain energy density function \( \psi(C, \zeta) \) is determined numerically by solving problem (14). The results are stored in a database.
3. Giving the resulting database, a continuous interpolation of the discrete values is realized by an appropriate interpolation scheme associated with a tensorial representation of
\( \bar{\psi}(C, \zeta) \). Then during the macroscopic finite element computations, the effective stress-strain relationship as well as the tangent matrix can be computed by deriving the continuous interpolation.

4.2. Preliminaries

In this work, for the sake of simplicity in the equations, we adopt the following notations, similar to the Voigt ones, to express the components of tensor \( \overline{C} \). Let \( \{e_1, e_2, e_3\} \) be an orthonormal basis, then

\[
\overline{C} = \overline{C}_1 e_1 \otimes e_1 + \overline{C}_2 e_2 \otimes e_2 + \overline{C}_3 e_3 \otimes e_3 + \frac{\overline{C}_4}{\sqrt{2}} (e_2 \otimes e_3 + e_3 \otimes e_2) \\
+ \frac{\overline{C}_5}{\sqrt{2}} (e_1 \otimes e_3 + e_3 \otimes e_1) + \frac{\overline{C}_6}{\sqrt{2}} (e_1 \otimes e_2 + e_2 \otimes e_1),
\]

yielding the following notations

\[
\overline{C}_1 = \overline{C}_{11}, \quad \overline{C}_2 = \overline{C}_{22}, \quad \overline{C}_3 = \overline{C}_{33}, \quad \overline{C}_4 = \sqrt{2} \overline{C}_{23}, \quad \overline{C}_5 = \sqrt{2} \overline{C}_{13}, \quad \overline{C}_6 = \sqrt{2} \overline{C}_{12}.
\]

In a similar manner, the components \( \overline{S}_\alpha \), with \( \alpha = 1, 2, ..., 6 \), of tensor \( \overline{S} \) and \( L_{\alpha\beta} \), with \( \beta = 1, 2, ..., 6 \), of tensor \( \overline{L} \) are such that

\[
\overline{S}_\alpha = 2 \frac{\partial \overline{\psi}}{\partial C_\alpha}, \quad \overline{L}_{\alpha\beta} = 4 \gamma_{\alpha\beta} \frac{\partial^2 \overline{\psi}}{\partial C_\alpha \partial C_\beta},
\]

where \( \gamma_{\alpha\beta} \) takes the values 1, 1/\( \sqrt{2} \) or 1/2 (see [17] for the details).

4.3. Computational details

In this section, we described the main numerical aspects and references, required to implement the different steps of the method listed in Section 4.1.

4.3.1. Definition of domain \( \Delta \)

The global parameters domain \( \Delta \) is split into two domains such that

\[
\Delta = \Delta_{C} \times \Delta_{\zeta} \quad \text{where} \quad \left\{ \begin{array}{l}
\Delta_{C} = \Delta_{C_1} \times \Delta_{C_2} \times \cdots \times \Delta_{C_6} \\
\Delta_{\zeta} = \Delta_{\zeta_1} \times \Delta_{\zeta_2} \times \cdots \times \Delta_{\zeta_M}
\end{array} \right.
\]

The first issue is related to the definition of domain \( \Delta_{C} \) and \( \Delta_{\zeta} \). Extreme values \( \Delta_{C_i}^{\text{min}} \) and \( \Delta_{C_i}^{\text{max}} \) of a domain \( \Delta_{C_i} \) can be arbitrarily chosen. However, this case may involve difficulties during the macroscopic computations since some strain states may correspond to values of \( \overline{C}_i \) which are outside the domain \( \Delta_{C_i} \). To avoid this difficult, preliminary macroscopic simulations can be done with homogeneous behaviors corresponding to each phase of the microstructure. However, there is still a risk that a strain state falls outside the domain \( \Delta_{C_i} \). In that case, one may use the extrapolation technique given in [19] to avoid this problem. Thus, we can determine a priori the range of strains levels in the structure and the values of the extrema \( \Delta_{C_i}^{\text{min}} \) and \( \Delta_{C_i}^{\text{max}} \). Extreme values \( \Delta_{C_i}^{\text{min}} \) and \( \Delta_{C_i}^{\text{max}} \) of a domain \( \Delta_{\zeta_i} \) are naturally chosen using the set \( \{\zeta_i^{(k)}\}_{k=1}^M \). A first way consists in taking the extreme values of the variable \( \zeta_i \) but this strategy may lead to a large range of variation for \( \zeta_i \) and may require a fine discretization of the domain \( \Delta_{\zeta_i} \) only needed for an accurate approximation of values of \( \zeta_i \) corresponding to a low probability. Thus, we propose to define the extreme values \( \Delta_{\zeta_i}^{\text{min}} \) and \( \Delta_{\zeta_i}^{\text{max}} \) on the quantile values (quantiles at 5% and 95% for instance) which allow reducing the support of the variable \( \zeta_i \).

The second issue arises from the discretization of domains \( \Delta_{C} \) and \( \Delta_{\zeta} \). Several ways are possible as non-uniform or uniform discretizations. In this work, we use the same discretization as proposed in [17, 19] yielding a uniform discretization. We choose a rectangular grid leading us to discretize each domain \( \Delta_{C_i} \) into a number \( p \) of nodes homogeneously distributed. Then, the domain \( \Delta_{C_i} \) is
discretized with $p^D$ nodes. Concerning the domains $\Delta_{\zeta}$ related to $\Delta_{\xi}$, the same type of procedure is used. Each domain is discretized into a fixed number $q$ of nodes homogeneously distributed. It then yields a number $q^M$ of nodes for domain $\Delta_{\zeta}$. One can notice that a choice of discretization based on the quantile values is possible and appears to be a more sophisticated way in order to be consistent with the probabilistic content of the problem. This kind of non-homogeneous discretization has been investigated by the authors but has led us to poorer results than the homogeneous one mainly due to the high fluctuation of the solution. Thus the overall parameters domain $\Delta$ is discretized into a number $p^D \times q^M$ of nodes for which nonlinear FEM computations are required to compute the values of the strain energy density function $\psi(\overline{C}, \zeta)$. The FEM computations are not performed independently: for one geometrical realization $\zeta^{(k)}$, we take as an initial guess for the Newton-Raphson algorithm, the solution, among the ones previously calculated, which is the “closest” to the one to be computed. Finally, the different values of $\psi(\overline{C}, \zeta)$ are stored in a hypermatrix $\overline{W}$ which represents the database.

4.3.2. Separated variables interpolation approach Since the hypermatrix $\overline{W}$ is computed, we seek to obtain a continuous explicit form of the potential $\overline{\psi}$ according to tensor $\overline{C}$ and vector $\zeta$. We use the methodology proposed in [19] and we extend it to the stochastic framework. The two distinct steps are the following.

1. Computation of a separated variables representation $\overline{U}$ of $\overline{W}$ through a Parallel Factor Decomposition [37].
2. Computation of a continuous interpolation of $\overline{U}$ using twice continuously differentiable ($C^2$) functions so that we can evaluate the components of tensors $\overline{S}$ and $\overline{C}$.

The separated variables representation consists in decomposing $\overline{W}$ into a tensorial representation $\overline{U}$ such that

$$\overline{W} \approx \overline{U} = \sum_{r=1}^{R} D \sum_{k_1=1}^{D} M \sum_{k_2=1}^{M} \phi_k^r \phi_k^r,$$ (32)

where $\{\phi_k^r, k_1 = 1, \ldots, D\}$ are real-valued vectors related to the macroscopic strain tensor component $\overline{C}_i$, and where $\{\phi_k^r, k_2 = 1, \ldots, M\}$ are real-valued vectors related to the geometrical parameters of the geometry and $R$ is an integer. For a given $R$, the vectors $\phi_k^r$ and $\phi_k^r$ can be constructed by solving the following least square problem,

$$\inf_{\phi_k^1, \phi_k^2} \left\| \overline{W} - \sum_{r=1}^{R} D \sum_{k_1=1}^{D} M \sum_{k_2=1}^{M} \phi_k^r \phi_k^r \right\|^2_F.$$ (33)

Introducing a tolerance parameter $\delta_{sep}$ in order to reach the desired accuracy, integer $R$ is increased until

$$\left\| \overline{W} - \sum_{r=1}^{R} D \sum_{k_1=1}^{D} M \sum_{k_2=1}^{M} \phi_k^r \phi_k^r \right\|_F < \delta_{sep}.$$ (34)

It should be noted that problem defined by equation (33) is nonlinear according to the unknown vectors $\phi_k^r$ and $\phi_k^r$. Thus, we use an iterative procedure to solve the problem with the alternated least square algorithm [38, 39]. In practice, we use the Matlab Tensor Toolbox [40] (parafac.m function) to numerically solve the problem. From equation (32), the continuous interpolation $\overline{\psi}$ of $\overline{\psi}$ can be obtained as

$$\overline{\psi} \approx \overline{\psi} = \sum_{r=1}^{R} D \sum_{k_1=1}^{D} M \sum_{k_2=1}^{M} \phi_k^r (C_{k_1}) \phi_k^r (\zeta_{k_2}).$$ (35)
where \( \tilde{\phi}_j^r(\omega_j) \) are the interpolated values of \( \phi_j^r \) define by

\[
\tilde{\phi}_j^r(\omega_j) = \sum_{k=1}^{n} N_k(\omega_j) \{ \phi_j^r \}_k .
\]  

(36)

In equation (36), \( N_k \) is one-dimensional \( C^2 \) interpolation function associated with node \( k \), \( n \) denotes the number of nodes supporting the shape functions \( N_k(\omega_j) \) and \( \{ \phi_j^r \}_k \) are the discrete values of \( \phi_j^r \). Thus, the second Piola-Kirchhoff stress can be approximated by

\[
\mathbf{S}_i^r(\mathbf{C}_1, \ldots, \mathbf{C}_D, \zeta_1, \ldots, \zeta_M) = 2 \sum_{r=1}^{R} \left( \left\{ \prod_{k_1 \neq i} \tilde{\phi}_k^r(\mathbf{C}_{k_1}) \prod_{k_2} \tilde{\phi}_{k_2}^r(\zeta_{k_2}) \right\} \frac{\partial \tilde{\phi}_j^r(\mathbf{C}_i)}{\partial \mathbf{C}_i} \right),
\]

(37)
in which \( k_1 = 1, \ldots, D \) and \( k_2 = 1, \ldots, M \). In the same manner, the approximated value \( \mathbf{T}^r \) of tangent elastic tensor \( \mathbf{T} \) is given by

\[
\mathbf{T}_{ij} = 4 \gamma_{ij} \sum_{r=1}^{R} \left( \left\{ \prod_{k_1 \neq i,j} \tilde{\phi}_k^r(\mathbf{C}_{k_1}) \prod_{k_2} \tilde{\phi}_{k_2}^r(\zeta_{k_2}) \right\} \frac{\partial \tilde{\phi}_j^r(\mathbf{C}_i)}{\partial \mathbf{C}_i} \frac{\partial \tilde{\phi}_j^r(\mathbf{C}_j)}{\partial \mathbf{C}_j} \right) \mathrm{if} \ i \neq j ,
\]

(38)

\[
\mathbf{L}_{ii} = 4 \gamma_{ii} \sum_{r=1}^{R} \left( \left\{ \prod_{k_1 \neq i} \tilde{\phi}_k^r(\mathbf{C}_{k_1}) \prod_{k_2} \tilde{\phi}_{k_2}^r(\zeta_{k_2}) \right\} \frac{\partial^2 \tilde{\phi}_j^r(\mathbf{C}_i)}{\partial \mathbf{C}_i^2} \right),
\]

(39)

with \( k_1 = 1, \ldots, D \) and \( k_2 = 1, \ldots, M \) and with

\[
\frac{\partial \tilde{\phi}_j^r(\mathbf{C}_j)}{\partial \mathbf{C}_i} = \sum_{k=1}^{n} \frac{\partial N_k(\mathbf{C}_i)}{\partial \mathbf{C}_i} \{ \phi_j^r \}_k \quad \mathrm{and} \quad \frac{\partial^2 \tilde{\phi}_j^r(\mathbf{C}_i)}{\partial \mathbf{C}_i^2} = \sum_{k=1}^{n} \frac{\partial^2 N_k(\mathbf{C}_i)}{\partial \mathbf{C}_i^2} \{ \phi_j^r \}_k .
\]

(40)

Many choices are possible for the interpolation functions \( N_k \). In this work, we use one-dimensional \( C^2 \) cubic spline functions as in [17, 19] for which results of convergence with respect to the number of discretization points have been studied (see for instance [41]). For a parameters domain of high dimension, this approach has the advantage to only determine the coefficient of one-dimensional spline functions and then leads us to solve a small system of equations, which saves both computational time and memory.

5. NUMERICAL EXAMPLES

Two numerical examples are developed in this section. The first one aims at demonstrating the efficiency of the proposed method for the approximation of the macroscopic constitutive behavior through tensors \( \mathbf{S}(\mathbf{C}, \zeta) \) and \( \mathbf{T}(\mathbf{C}, \zeta) \). The numerical potential \( \tilde{\psi}(\mathbf{C}, \zeta) \) obtained in the first example is then used in the second example which deals with a macroscopic problem. For both problems, solutions are compared with reference solutions computed with classical methods.

5.1. Numerical example 1: study of the microscopic problem

5.1.1. Problem definition The aim of this first example is to demonstrate the efficiency of the S-NEXP method and the accuracy of the resulting solution through comparisons with standard approaches (nonlinear FEM computations and Monte-Carlo simulations). For this purpose, we focus on the quantities \( \tilde{\psi}(\mathbf{C}_1, \ldots, \mathbf{C}_D; \zeta_1, \ldots, \zeta_M) \) and \( \mathbf{S}_i(\mathbf{C}_1, \ldots, \mathbf{C}_D; \zeta_1, \ldots, \zeta_M) \) according to macroscopic strains \( \mathbf{C} \) and reduced random variables \( \zeta \) characterizing the random geometry of the microstructure. The parameters of the model are the following ones:

1. Random generator parameters: number of random variables \( m = 6000 \), spatial correlation parameter \( \rho = 0.5 \), number of realizations \( \nu = 1000 \), coefficient of variation \( \delta^{\mathrm{ord}} = 0.5 \) and number of fiber \( N_f = 80 \).
2. Statistical reduction (23): we have chosen $M = 2$ eigenvalues in order to facilitate the understanding for the response surfaces corresponding to $\epsilon_{KL}^1 = 0.8$ and $\epsilon_{KL}^2 = 0.7$. The following values of the tolerance parameter are $\epsilon_{KL}^1 = 0.55, \epsilon_{KL}^2 = 0.38$ and $\epsilon_{KL}^3 = 0.15$.

3. Discretization of domain $\Delta_\psi$, the macroscopic strain domain is chosen such as $\Delta_\psi = \Delta_\psi \times \Delta_\psi \times \Delta_\psi = [1, 1.5] \times [1, 1.5] \times [0, 0.5]$. We use $p = 5$ points for each domain $\Delta_\psi$. A convergence analysis of the deterministic problem only related to the macroscopic strains can be found in [19].

4. Material parameters: we use a compressible Neo-Hookean model given by the potential

$$W = \frac{1}{2} (\lambda_1 + \lambda_2 + \mu_1 + \mu_2 - 3).$$

In this example, we first focus on the efficiency of the method according to the number $q$ of points used for the discretization of parameters domain $\Delta_\psi$. Here, the domain $\Delta_\psi = \Delta_{\psi_1} \times \Delta_{\psi_2} = [q_1, q_{15}] \times [q_2, q_{25}] = [-1.61, 1.63] \times [-1.7, 1.55]$ where $q_1^k$ and $q_2$ are respectively the quantile values at 5% and 95% for the $i$-th random variable. We choose to discretize each domain $\Delta_{\psi_i}$ with different numbers $q = 5, 11$ and 21 of points homogeneously distributed.

5.1.2. Influence of random variable $\zeta_1$ In this section, we study the influence of random variable $\zeta_1$ on the S-NEXP solution and the resulting macroscopic constitutive behavior through the second Piola-Kirchhoff stress tensor $\mathbf{S}$. Figure 8 illustrates the response surfaces of $\psi(\mathbf{C}, \zeta)$, according to $\zeta_1$ and for $\zeta_2$ fixed to zero and to macroscopic strains such that $(\mathbf{C}_{11}, \mathbf{C}_{22}, \mathbf{C}_{12})$ belongs to $[1, 1.5] \times [1, 1.5] \times [0, 0.5]$, for the three choices of discretization of $\Delta_\psi$. Figure 8 also displays a reference solution consisting in a set of direct nonlinear FEM computations for a given grid of $20 \times 20$ points. One can observe a good convergence of the solution towards the reference solution with respect of number of discretization points $q$. The solution corresponding to $q = 21$ is obviously the one which matches the best the reference solution. Figure 9 presents the response surfaces related to component $\mathbf{S}_{11}(\mathbf{C}, \zeta)$ of tensor $\mathbf{S}$ according to the same parameters as in figure 8. We also notice a good convergence of the S-NEXP solution according to the number of discretization points $q$. It is clearly shown that the numerical derivation of the potential $\psi(\mathbf{C}, \zeta)$ allows a good approximation of the macroscopic constitutive behavior. Moreover, one should notice that the post-processing of the S-NEXP solution is very fast thanks to the explicit continuous form of the S-NEXP solution.

In figure 8 and 9, we can observe high variations of the quantities of interest according to parameter $\zeta_1$ which can be naturally related to the stochastic fluctuations. However, with a quite high number of discretization points ($q = 11$ and 21), the S-NEXP method allows us to accurately capture irregularities in the solution. For instance, in figure 9, we can notice an abrupt variation of the solution around the value $\zeta_1 \approx 0$. This is due to a significant change in the geometry as shown on figure 10 where two realizations of the geometry are displayed. The same variations appear in the components of the elastic tangent tensor $\mathbf{T}(\mathbf{C}, \zeta)$ as it is shown in figure 11 where the response surfaces of the component $\mathbf{T}_{1111}$ are displayed for the different S-NEXP solutions and the reference solution.

We then focus on the probability density functions of the previous quantities of interest for a particular macroscopic strain state corresponding to $(\mathbf{C}_{11} = 1.5; \mathbf{C}_{22} = 1.5; \mathbf{C}_{12} = 0.5)$. We use the $\mu$ realizations $\zeta^{(k)}$ which verify the condition of impenetrability given in Section 3.2.3. As a reference solution, we use realizations of the geometry of the microstructure generated with the reduced-order model corresponding to $M = 1$ for which we perform nonlinear FEM computations in order to obtain the reference values of $\psi$ and $\mathbf{S}_{11}$. Figure 12 illustrates these probability density functions for the different chosen discretizations of parameters domain $\Delta_\psi$ and for the reference solution. As for the response surfaces, we can observe a good convergence of the solution according to the number of discretization points $q$.

5.1.3. Influence of random variables $\zeta_1$ and $\zeta_2$ In the previous section, we have noticed that the solution showed a significant variability according to $\zeta_1$. We now focus on the influence of both random variables $\zeta_1$ and $\zeta_2$ on the solution. Figures 13 and 14 illustrate respectively the response surfaces of $\psi$ and $\mathbf{S}_{11}$ according to $\zeta_1$ and $\zeta_2$ for the S-NEXP solution (with $q = 21$) and the
Figure 8. Response surfaces of \( \psi \) according to \( \zeta_1 \) and macroscopic strains such that \((C_{11}, C_{22}, C_{12})\) belongs to \([1, 1.5] \times [1, 1.5] \times [0, 0.5]\) for \( q = 5 \), \( q = 11 \) and \( q = 21 \) and for the reference solution.

reference solution (nonlinear FEM computations). On those two cases the macroscopic strain state corresponds to \( C_{11} = 1.5, C_{22} = 1.5 \) and \( C_{12} = 0.5 \). As expected, we can notice significant global and local variations which disturb the S-NEXP solution. However, the method leads us to acceptable results with respect to the reference solution. As explained in Section 5.1.2, the global variations are due to significant changes in the geometry while the local variations are mainly due to the numerical difficulties involved by problem defined by equation (14) associated with boundary conditions defined by equation (15).

Figure 15 illustrates the probability density functions of \( \psi \) and component \( S_{22} \) for the S-NEXP solution (with \( q = 11 \)) and the reference solution (based on the reduced-order model corresponding to \( M = 2 \)) corresponding to the macroscopic strain state \( C_{11} = 1.5, C_{22} = 1.5 \) and \( C_{12} = 0.5 \). We can observe slight differences between the two solutions. Nevertheless, the S-NEXP solution appears satisfying according to the reference solution.

5.1.4. Accuracy and computational costs of the S-NEXP approximation

In this section we present a convergence analysis in order to estimate the accuracy of the S-NEXP approximation. As we have no \textit{a priori} information on the probabilistic content of the macroscopic strains, we suppose that all components of stress tensors \( \mathbf{S} \) are independent uniform random variables such as \( C_{11} \sim \mathcal{U}(1, 1.5), C_{22} \sim \mathcal{U}(1, 1.5) \) and \( C_{12} \sim \mathcal{U}(0, 0.5) \), in which \( \mathcal{U}(a, b) \) denotes a uniform random variable on \([a, b] \).

We can thus introduce an error indicator \( \epsilon_q \) defined as follows

\[
\epsilon_q = \frac{\| J_q - J_{\text{ref}} \|_{L^2(\Xi, d\mathbb{P})}}{\| J_{\text{ref}} \|_{L^2(\Xi, d\mathbb{P})}},
\]

(41)
Figure 9. Response surfaces of $S_{11}$ according to $\zeta$ and macroscopic strains such that $(C_{11}, C_{22}, C_{12})$ belongs to $[1, 1.5] \times [1, 1.5] \times [0, 0.5]$ for $q = 5$, $q = 11$ and $q = 21$ and for the reference solution.

(a) Mesh of the microstructure corresponding to $\zeta^{(1)} = -0.32$. (b) Mesh of the microstructure corresponding to $\zeta^{(2)} = 0.33$.

Figure 10. Geometries and meshes of the microstructure for two realizations of $\zeta$.

with

$$\|J_{ref}\|_{L^2(\Xi,dP)} \simeq \frac{1}{\mu} \sum_{k=1}^{\mu} |J_{ref}^{(k)}|^2,$$  

(42)
Figure 11. Response surfaces of $L_{1111}$ according to $\zeta_1$ and macroscopic strains such that $(C_{11}, C_{22}, C_{12})$ belong to $[1, 1.5] \times [1, 1.5] \times [0, 0.5]$ for $q = 5$, $q = 11$ and $q = 21$ and for the reference solution.

Figure 12. Probability density functions (Pdf) of $\psi$ and $S_{11}$ corresponding to $C_{11} = 1.5$, $C_{22} = 1.5$ and $C_{12} = 0.5$, for $q = 5$, $q = 11$ and $q = 21$.

where $J_q$ is a quantity of interest corresponding to the post-processing of the S-NEXP solution related to a particular number $q$ and $J_{\text{ref}}$ is the reference quantity of interest. To achieve this computation, we use the set $\{\zeta^{(k)}_i\}_{k=1}^\mu$ and for each $\zeta^{(k)}_i$ we associate a realization of the macroscopic strain state following the uniform distribution. Figure 16 illustrates the convergence of the error indicator $\epsilon_q$ for different quantities of interest (e.g. $\psi$, $S_{11}$, $S_{22}$ and $S_{12}$) according to $q$. Since the number of discretization points $p$ (related to the macroscopic strains domain $\Delta\overline{C}$) is here fixed, it is not possible to reach a level of error close to zero, which would theoretically be
reached with the increase of $p$. However, we can observe a good and fast convergence of $\epsilon_q$. Thus, even for $q = 5$, we notice a low level of error slightly superior to $10^{-3}$ for $\overline{\psi}$, $\overline{S_{11}}$ and $\overline{S_{22}}$, and close to $7 \times 10^{-2}$ for $\overline{S_{12}}$. Figure 17 displays the probability density functions, in semi-log scale, of the sets of realizations used in the computation of the error indicator $\epsilon_q$ for $\overline{\psi}$ and $\overline{S_{11}}$. We can notice a very good match of the results for any number of discretization points $q$ except for the probability
tails for which only the S-NEXP solution corresponding to $q = 21$ matches precisely the reference solution.

We finally focus on the computational costs of the S-NEXP approach. Figure 18 displays the number $Q = p^D \times q^M$ of nonlinear FEM computations needed in the S-NEXP method with respect to number $M$ of random variables $\zeta_j$. On this figure $p = 5$, $D = 3$ and the three lines correspond to $q = 5$, $q = 11$ and $q = 21$. This figure gives an information about the range of applicability of the method proposed. We indeed can observe that the number $Q$ of nonlinear FEM computation becomes very high when $M$ increases. In the case of high dimension (i.e. high values of $M$), the involved computational time would become too important to use this kind of method even with a very efficient solver for the nonlinear boundary value problems. However, the proposed approach remains suitable for low or middle dimension. All the computations have been made on a 40-cores computer and the CPU times for the results given in this example are the following ones:

- $M = 1$: 15 minutes for $q = 5$, 30 minutes for $q = 11$ and 70 minutes for $q = 21$.  


Figure 18. Number $Q$ of nonlinear FEM computations needed in the S-NEXP method as a function of number $M$ of random variables for different number of discretization points $q = (1, 11, 21)$.

- $M = 2$: 7 hours for $q = 11$ and 1 day for $q = 21$.

5.2. Numerical example 2: a two scales structural problem

5.2.1. Problem definitio

In this example, we propose to study the efficiency of the S-NEXP method with a two scales structural problem depicted in Figure 19(a). We consider a structure made of a heterogeneous hyperelastic material where the geometry of the microstructure is random. The microscopic problem corresponds to the one studied in Section 5.1 with the parameters of the probabilistic content given in Section 5.1.1. To characterize the strain energy density function representing the macroscopic constitutive behavior of the material, we use the S-NEXP solutions with the different discretizations (e.g. $q = 5, q = 11$ and $q = 21$). At the macroscopic level, the dimensions of the structure are $L = 1$ m, $H = 1$ m and $e = 0.2$ m and displacements $\Delta u = 5\%$ are imposed on a part $\Gamma$ of the structural domain. For the macroscopic space approximation, we use a mesh composed of 372 3-nodes triangular finite elements depicted on Figure 19(b). To test the efficiency of the method, we build reference solutions with a multilevel Finite Element Method, denoted $\text{FE}^2$ in the following (see [7, 9]), with the same macroscopic mesh used for the S-NEXP calculations.

5.2.2. Accuracy of the S-NEXP solution

We propose to show the efficiency of the S-NEXP method with post-processing of the macroscopic solution. During the macroscopic computation, each integration point in the macroscale discretization must be associated with a microstructure. Two cases are considered.

1. Case (i): the same geometry of the microstructure corresponding to the statistical mean of the stochastic model of the geometry of the microstructure, is used for each integration point.
2. Case (ii): the random geometry of the microstructure constructed with the realizations $\{\zeta^{(k)}\}_{k=1}^\mu$ is used for each integration point.

Case (ii) takes into account the stochastic fluctuation which are significant as shown in Section 5.1. It is worth noticing that the post-processing of the S-NEXP solution is very fast thanks to the explicit continuous form of the potential (less than one minute with a laptop computer for this example) while a complete $\text{FE}^2$ computation takes more than one hour with a computer cluster with 40 cores. Figure 20 displays the von Mises stresses for the macroscopic computations corresponding to the three S-NEXP solution (numerical potential computed with $q = 5, q = 11$ and $q = 21$) and the $\text{FE}^2$ reference solution for case (i). We can observe a good agreement of the results even for a small...
number \( q \) of discretization points. In the same manner, figure 21 displays the von Mises stresses for case (ii). We can also notice a good convergence of the S-NEXP solution towards the reference solution even if the macroscopic solution is not smooth according to the von Mises stress field. However, we can observe that the convergence is slower than the one corresponding to case (i); this is due to the important variations of the potential which are bad approximated with a low number \( q \) of discretization points has shown on figure 9. Thus, a good macroscopic solution required to use a number \( q \) of discretization points which is high enough to capture these irregularities. Finally, figure 22 shows the typical convergence of the macroscopic Newton-Raphson algorithm for both cases. We can observe that behavior of the macroscopic computations are the same for the two cases and thus that the second-order convergence is still reached even for case (ii).

6. CONCLUSIONS

To the knowledge of the authors, the present paper is the first one devoted to the challenging issues concerning the computational nonlinear stochastic homogenization using a non-concurrent multiscale approach for hyperelastic heterogeneous microstructures analysis. The non-concurrent multiscale approach for micro-macro nonlinear mechanics has been validated for the deterministic case in the literature. In this work, we have extended and validated this approach to the stochastic case for hyperelastic heterogeneous microstructures. Since the non-concurrent multiscale approach is based on the use of a tensorial decomposition, which is then submitted to the curse of dimensionality, we have performed an analysis with respect to the stochastic dimension. In order to show the capability of this multiscale approach in the stochastic framework, a prior stochastic model of the microstructure has been introduced, which allows the efficiency to be analyzed with respect to the stochastic dimension. Clearly, such a prior stochastic model could be replaced by any other model which would have the same capabilities. In this work, we have considered a fiber reinforced polymer composites for which the geometry of the microstructure is random. The first point of the proposed method has consisted in building a stochastic model of the random geometry for the microstructure. A major difficulty is related to the impenetrability condition between the fiber and the stochastic dimension induced by the number of fibers. The second point is devoted to the extension of the method of numerical explicit potentials to the stochastic framework. The macroscopic constitutive behavior of the material is defined by a continuous explicit form of the macroscopic strain energy density function (potential) according to the macroscopic strain state and the random geometrical parameters. A separated variables representation associated with an interpolation scheme has allowed obtaining the continuous explicit form of the effective
potential which, by derivation, has allowed determining the components of the stress and the tangent elastic tensors required for the macroscopic computations. Two numerical examples have been presented to validate the proposed approach. However, in the development of the proposed approach, several difficulties have arisen and must be pointed out. First, as the strain energy density function holds irregularities with respect of the geometrical parameters, an important number of discretization points must be employed to capture these local gradients. Thus, the use of a uniform discretization for the parameters domain does not appear as the best choice since unnecessary points are introduced. A non-uniform discretization strategy based, for instance, on the volume fraction will be investigated in a forthcoming paper. Moreover, as the main computational cost comes from the construction of the database, an optimal discretization strategy would allow reducing these costs. Finally, we pointed out that those high computational times prevent from using the approach with an important number of reduced random variables characterizing the geometry of the microstructure. This limitation is classical in the context of parametric stochastic methods when one increases the stochastic dimension. Further works dedicated to circumvent this drawback will be investigated in forthcoming papers.

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Figure 21. Comparison of the von Mises stress field for case (ii): particular realization of the geometry of the microstructure applied to each integration point.

Figure 22. Convergence of the macroscopic Newton-Raphson algorithm for case (i) and case (ii).

REFERENCES


