A class of tensor-valued random fields for random anisotropic elastic microstructure modeling and stochastic homogenization
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ABSTRACT: A generic micro-scale stochastic model is presented for a large class of random anisotropic elastic microstructures allowing a parametric analysis of the Representative Volume Element (RVE) size to be performed. This new approach can be useful for a direct experimental identification of random anisotropic elastic microstructures when the standard method cannot easily be applied. Such a RVE is used to construct the macroscopic properties in the context of stochastic homogenization. The probability analysis is not performed as usual for a given particular random microstructure defined in terms of its constituents, but is performed for a large class of random anisotropic elastic microstructures. For this class, the probability distribution of the random effective stiffness tensor is explicitly constructed and allows a full probability analysis of the RVE size to be carried out with respect to the spatial correlation length of the random microstructure.

Keywords: microstructures, probability and statistics, anisotropic material, elastic material, inhomogeneous material

1 INTRODUCTION

The probabilistic model of a random microstructure (such as a composite constituted of several constituents) can directly be constructed from the geometry and mechanical properties of its constituents. This is the case for the class of random heterogeneous materials whose microstructures can be modeled as a distribution of inclusions or cavities of well-defined geometry in a given matrix, see for instance (Willis, 1982; Torquato and Stell, 1985; Drugan and Willis, 1996; Torquato, 1997; Quintanilla and Torquato, 1997; Nemat-Nasser and Hori, 1999; Quintanilla, 1999; Ostoja-Starzewski, 1998; Kachanov et al., 2001; Milton, 2002; Roberts and Garboczi, 2002; Torquato, 2002; Drugan, 2003; Monetto and Drugan, 2004). Generally, the statistics-based bounding techniques only use the lower-order statistics (first- and second-order moments) and the probability distributions which give the detailed probabilistic information are not taken into account. Recently, a global stochastic model of the local stiffness tensor of the random microstructure has been constructed using chaos decomposition (Jardak and Ghanem, 2004). The random microstructure can be homogenized if there is a representative volume element (RVE) size such that the random fluctuations of the random effective stiffness tensor around the statistical mean value of the random effective stiffness tensor is “negligible”. RVE size has received a particular attention; see for instance (Cailletaud et al., 1994; Drugan and Willis, 1996; Gusev, 1997; Nemat-Nasser and Hori, 1999; Kanit et al., 2003; Monetto and Drugan, 2004; Sab and Nedjar, 2005). The prime objective of this paper is not to analyse a particular random isotropic or anisotropic microstructure described in terms of its constituents, but is to propose (when the standard method cannot easily be applied to anisotropic elastic microstructures) a new way which could be useful for a direct experimental identification of random anisotropic elastic microstructures introducing a micro-scale stochastic model. The main idea of this paper is then to directly introduce a micro-scale stochastic model of the random anisotropic elastic microstructure, which is not deduced from the stochastic models of its constituents. Such a micro-scale stochastic model must verify fundamental mathematical properties to obtain a physical model of any anisotropic elastic microstructure. The random anisotropic elastic microstructure (for instance a mortar constituted of a cement paste with embedded sand particles, some porous media such as plaster boards, some cortical bones, some biological membranes and more generally, some living tissues, etc) is then modeled by an equivalent random continuous anisotropic elastic medium which is completely defined by its local stiffness fourth-order tensor-valued random field $x \mapsto C(x) = \{C_{ijkl}(x)\}_{ijkl}$. The random field $C$ is then constructed of 21 mutually dependent real-valued random fields modeling the anisotropic microstructure.
at the micro-scale level. The theory proposed allows strong anisotropic random fluctuations to be taken into account. Such an equivalent random anisotropic elastic medium can also be viewed (but it is not necessary) as the stochastic homogenization of the random anisotropic microstructure on a micro-scale RVE. The great interest of such a direct construction of a micro-scale stochastic model of the random anisotropic elastic microstructure is the capability to identify the parameters of the random field \( x \mapsto \mathbb{C}(x) \) using strain measurements on the boundary of tested specimens at the RVE- or macro-scale and solving an inverse stochastic problem. It is then necessary to choose a stochastic representation of \( x \mapsto \mathbb{C}(x) \) in a class of random fields for which only a few parameters are required to define its system of marginal probability distributions. Therefore, the inverse problem related to such an experimental identification of \( x \mapsto \mathbb{C}(x) \) is more feasible. In addition, such a class of random fields \( x \mapsto \mathbb{C}(x) \) must be constructed using only the available information and not “hypothetical” information for which no statistics are available or for which the number of experimental specimens is too small to obtain a good convergence of the statistical estimators. For the tensor-valued random field, \( x \mapsto \mathbb{C}(x) \), the largest class can be constructed using as available information: the symmetry properties, the mean value \( x \mapsto \mathbb{C}(x) \) which is assumed to be known and a stochastic nonuniform ellipticity condition for the corresponding linear elasticity stochastic differential operator. Clearly, any random anisotropic elastic microstructure belongs to this class. The results presented in this paper could allow the micro-scale stochastic model to be identified from RVE- or macro-scale measurements solving an inverse stochastic problem.

2 MACROSCOPIC PROPERTIES OF A RANDOM ANISOTROPIC MICROSTRUCTURE

Consider a random microstructure constituted of a random heterogeneous anisotropic elastic linear medium. The random local (or microscopic) constitutive equation is written as \( \sigma(x) = \mathbb{C}(x) : \varepsilon(x) \) which means \( \sigma_{jk}(x) = \mathbb{C}_{jk\ell m}(x) \varepsilon_{\ell m}(x) \), in which \( x \mapsto \sigma_{jk}(x) \) is the random local stress tensor field, \( \varepsilon_{jk}(\mathbb{D}(x)) = \frac{1}{2} (\partial D_{\ell}(x)/\partial x_{\ell} + \partial D_{m}(x)/\partial x_{m}) \) is the random local strain tensor field, \( x \mapsto \mathbb{D}(x) = (D_{1}(x), D_{2}(x), D_{3}(x)) \) is the random local displacement field, \( x \mapsto \mathbb{C}(x) \) is the fourth-order tensor-valued random field allowing the elastic properties of the random microstructure to be characterized and where \( x = (x_{1}, x_{2}, x_{3}) \) is a point of the RVE which is a 3D bounded open domain \( \Omega \) in \( \mathbb{R}^{3} \). The random effective (or macroscopic) stress and strain tensors are usually defined as the average in the RVE of the random local stress and strain tensor fields,

\[
<\sigma> = \frac{1}{|\Omega|} \int_{\Omega} \sigma(x) dx, \quad <\varepsilon> = \frac{1}{|\Omega|} \int_{\Omega} \varepsilon(x) dx. \tag{1}
\]

2.1 Localization and random effective stiffness tensor

The localization is done with a given random effective strain \( \varepsilon \) on the boundary \( \partial \Omega \) of the RVE which is independent of \( x \). Consequently, the random local displacement field \( \mathbb{D} \) in the microstructure \( \Omega \) can be constructed by solving the following stochastic boundary value problem (BVP) in \( \Omega \),

\[
-\text{div} \sigma = 0 \text{ in } \Omega, \quad \mathbb{D}(x) = \varepsilon(x) \text{ on } \partial \Omega. \tag{2}
\]

Since the solution \( \mathbb{D} \) of Eq. (2) depends linearly on \( \varepsilon \), the random local strain tensor can be written as

\[
\varepsilon(\mathbb{D}(x)) = \mathbb{H}(x) : \varepsilon, \tag{3}
\]

in which the symmetric fourth-order tensor-valued random field \( x \mapsto \mathbb{H}(x) \) corresponds to the strain localization associated with the stochastic BVP defined by Eq. (2). In order to construct the random field \( \mathbb{H} \), for all \( \ell \) and \( m \) in \( \{1, 2, 3\} \), the second-order tensors \( g^{\ell m} \) are introduced such that

\[
g_{jk}^{\ell m} = \frac{1}{2} (\delta_{jk} \delta_{lm} + \delta_{jm} \delta_{kl}), \tag{4}
\]

in which \( \delta_{jk} \) is the Kronecker symbol. For all \( \ell \) and \( m \) in \( \{1, 2, 3\} \), let \( \mathbb{D}^{\ell m} \) be the random local displacement field which is the solution of the following stochastic BVP in \( \Omega \),

\[
-\text{div} \sigma^{\ell m} = 0 \text{ in } \Omega, \quad \mathbb{D}^{\ell m}(x) = g^{\ell m} \varepsilon(x) \text{ on } \partial \Omega, \tag{5}
\]

in which \( \sigma^{\ell m}(x) = \mathbb{C}(x) : \varepsilon(\mathbb{D}^{\ell m}(x)) \). We then have

\[
\mathbb{H}_{jk\ell m}(x) = \varepsilon_{\ell m}(\mathbb{D}^{\ell m}(x)), \tag{6}
\]

with the property \( <\mathbb{H}_{jk\ell m}> = g^{\ell m}_{jk} \). The symmetric fourth-order random effective stiffness tensor \( \mathbb{C}^{\text{eff}} \) which is defined by \( <\sigma> = \mathbb{C}^{\text{eff}} : <\varepsilon> \) can then be calculated by

\[
\mathbb{C}^{\text{eff}} = <\mathbb{C} : \mathbb{H}>. \tag{7}
\]

2.2 Micro-scale stochastic model for random anisotropic elastic microstructures

For all \( x \) fixed in \( \Omega \), the random fourth-order tensor \( \mathbb{C}(x) \) has a given mean value, must verify the symmetry property and a stochastic nonuniform ellipticity condition related to positive-definiteness.
properties. The random field \( C \) is constituted of 21 mutually dependent real-valued random fields and the system of marginal probability distributions of \( C \) is required because the unknown random solution \( x \mapsto D^m(x) \) of the stochastic BVP defined by Eq. (5) is a nonlinear mapping of the random field \( C \).

The mean value of the random field \( C \) is a deterministic tensor-valued field \( x \mapsto \{ C_{\ell j k}(x) \}_{\ell j k} \). The microscale stochastic model has to be such that \( E \{ C_{\ell j k}(x) \} = C_{\ell j k}(x) \) for all \( x \), where \( E \) is the mathematical expectation. The known symmetries can be taken into account with the mean model random variable with values in the set \( \{ ( ) \} \) of \( \ell \) and \( k \) around the mean tensor. This paper deals with the case for which the random fluctuation tensor \( \{ C_{\ell j k}(x) - C_{\ell j k}(x) \}_{\ell j k} \) around the mean tensor is purely anisotropic, with any symmetries.

We present an extension of the probability model proposed in (Soize, 2004 and 2006) which only uses the available information. The usual uniform ellipticity condition is not introduced to construct this probability model because such a condition does not correspond to available information (objective data). For the proposed stochastic model, a nonuniform ellipticity condition is introduced for \( x \mapsto C(x) \) which corresponds to the available information and which, for all \( \ell \) and \( m \) fixed in \{1, 2, 3\}, allows the random field \( C(x) \) defined in Section 3.

\#\#3 STOCHASTIC MODEL OF THE RANDOM FIELDS \([G]\) AND \([A]\)

Let \( d \geq 1 \) and \( n \geq 1 \) be two given integers. The random field \( x = (x_1, \ldots, x_d) \mapsto \{ G(x) \} \) is indexed by \( \mathbb{R}^d \) with values in \( M_6^+(\mathbb{R}) \). In Eq. (11), we have \( d = 3 \) and \( n = 6 \). As explained in Section 2.2, the extended probability model presented below is based on the construction and the mathematical analysis of the random field \( [G] \) performed in (Soize, 2006). The results which allow the numerical calculation to be performed are summarized below. The random field \( x \mapsto \{ G(x) \} \) is constructed as a homogeneous and normalized non-Gaussian positive-definite matrix-valued random field, defined on probability space \((\Theta, \tau, P)\), indexed by \( \mathbb{R}^d \), with values in \( M_6^+(\mathbb{R}) \). This random field is constructed as a nonlinear mapping of stochastic germs.

3.1 Random fields \( U_{ij}' \) as the stochastic germs of the random field \([G]\)

The stochastic germs are constituted of \( n(n+1)/2 \) independent second-order centered homogeneous Gaussian random fields \( x \mapsto U_{ij}(x), 1 \leq j \leq j' \leq n \), defined on the probability space \((\Theta, \tau, P)\), indexed by \( \mathbb{R}^d \), with values in \( \mathbb{R} \) and such that \( E \{ U_{ij}(x) \} = 0 \) and \( E \{ U_{ij}(x)^2 \} = 1 \). Consequently, all these random fields are completely and uniquely defined by the \( n(n+1)/2 \) correlation functions \( R_{ij}(\eta) = E \{ U_{ij}(x) U_{ij'}(x + \eta) \} \) defined for all \( \eta = \eta_1, \ldots, \eta_d \) in \( \mathbb{R}^d \) and such that \( R_{ij}(0) = 1 \). In order to obtain a class having a reasonable number of parameters, these autocorrelation functions are written as \( R_{ij}(\eta) = \rho_{ij}^{\eta} \rho_{ij'}^{\eta} \ldots \rho_{ij''}^{\eta} \) in which,
for all \( k = 1, \ldots, d \), one has \( \rho^\gamma_k(0) = 1 \) and for all \( \eta_k \neq 0 \),

\[
\rho^\gamma_k(\eta_k) = \frac{4(L_k^\gamma)^2}{(\pi^2 \eta_k^2) \sin^2(\pi \eta_k / (2L_k^\gamma))},
\]

in which \( L_1^\gamma, \ldots, L_d^\gamma \) are positive real numbers. Each random field \( U_{ji} \) is then mean-square continuous on \( \mathbb{R}^d \) and it power spectral measure has a compact support. Such a model has \( d(n+1)/2 \) real parameters \( L_1^\gamma, \ldots, L_d^\gamma \) for \( 1 \leq j \leq j' \leq n \) which represent the spatial correlation lengths of the stochastic germs \( U_{ji} \).

3.2 Defining an adapted family of functions

The construction of the random field \([G]\) requires the introduction of an adapted family of functions \( \{u \mapsto h(\alpha, u)\}_{\alpha > 0} \). Let \( \alpha \) be a positive real number. The function \( u \mapsto h(\alpha, u) \) from \( \mathbb{R} \) into \([0, +\infty)\) is introduced such that \( \Gamma_{\alpha} = h(\alpha, U) \) is a gamma random variable with parameter \( \alpha \) while \( U \) is a normalized Gaussian random variable \( (E[U] = 0 \text{ and } E[U^2] = 1) \). Consequently, for all \( u \) in \( \mathbb{R} \), we have

\[
h(\alpha, u) = F_{\Gamma_{\alpha}}^{-1}(F_U(u)).
\]

in which \( u \mapsto F_U(u) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{u} e^{-v^2/2} dv \) is the cumulative distribution function of the normalized Gaussian random variable \( U \). The function \( p \mapsto F_{\Gamma_{\alpha}}(p) \) from \([0, 1]\) into \([0, +\infty)\) is the reciprocal function of the cumulative distribution function \( \gamma \mapsto F_{\Gamma_{\alpha}}(\gamma) = \int_{0}^{\gamma} t^{\alpha-1} e^{-t} dt \) of the gamma random variable \( \Gamma_{\alpha} \) with parameter \( \alpha \) in which \( \Gamma(\alpha) = \int_{0}^{\infty} t^{\alpha-1} e^{-t} dt \).

3.3 Defining the random field \([G]\)

The random field \( x \mapsto [G(x)] \), defined on the probability space \((\Theta, \mathcal{T}, P)\), indexed by \( \mathbb{R}^d \), with values in \( \mathbb{M}_n(\mathbb{R}) \) is constructed as follows:

(i) Let \( \{U_{ji}(x), x \in \mathbb{R}^d\}_{1 \leq j \leq j' \leq n} \) be the \( n(n+1)/2 \) independent random fields introduced in Section 3.1. For all \( x \) in \( \mathbb{R}^d \) and for all \( i \) and \( j \) such that \( 1 \leq j \leq j' \leq n \), we have

\[
E\{U_{ji}(x)^2\} = 0, \quad E\{U_{ji}(x)^2\} = 1.
\]

(ii) Let \( \delta \) be the real number, independent of \( x \) and \( n \), such that \( 0 < \delta < \sqrt{(n+1)(n+5)}^{-1} < 1 \). This parameter which is assumed to be known (resulting, for instance, from an experimental identification solving an inverse problem) allows the dispersion of the random field \([G]\) to be controlled.

(iii) For all \( x \) in \( \mathbb{R}^d \), the random matrix \([G(x)]\) is written

\[
[G(x)] = [L(x)]^T [L(x)],
\]

in which \([L(x)]\) is the upper \((n \times n)\) real triangular random matrix defined as follows:

For \( 1 \leq j \leq j' \leq n \), the \( n(n+1)/2 \) random fields \( x \mapsto [L(x)]_{ji} \) are independent.

For \( j < j' \), the real-valued random field \( x \mapsto [L(x)]_{ji} \), indexed by \( \mathbb{R}^d \), is defined by \([L(x)]_{ji} = \sigma U_{ji}(x)\) in which \( \sigma \) is such that \( \sigma = \delta(n+1)^{-1/2} \).

For \( j = j' \), the positive-valued random field \( x \mapsto [L(x)]_{ji} \), indexed by \( \mathbb{R}^d \), is defined by \([L(x)]_{ji} = \sigma \sqrt{2b(\alpha, U_{ji})}X\) in which \( \alpha_j = (n+1)/2(\delta^2) + (1-j)/2 \).

Let \([B]\) be a random matrix, defined on \((\Theta, \mathcal{T}, P)\), with values in the set \( \mathbb{M}_n(\mathbb{R}) \) of all the \((m \times m)\) real matrices. For \( \theta \in \Theta \), let \([B(\theta)] \in \mathbb{M}_n(\mathbb{R})\) be a realization of \([B]\). The norm \( \|B(\theta)\| \) of \([B(\theta)]\) induced by the Euclidean norm \( \|v\| \) of \( v \) in \( \mathbb{R}^m \) is such that

\[
\|B(\theta)\| = \sup_{\|v\| = 1} \|B(\theta)v\|, \quad v \in \mathbb{R}^m.
\]

It can be proven the following fundamental property (non uniform ellipticity condition replacing the usual uniform ellipticity condition which is not introduced): let \( \Omega \) be any bounded open domain of \( \mathbb{R}^d \) and let \( \overline{\Omega} = \Omega \cup \partial \Omega \) be its closure. We then have

\[
E\{\sup_{x \in \Omega} \|G(x)\| \} = c_G^2 < +\infty,
\]

in which sup is the supremum and where \( 0 < c_G < +\infty \) is a finite positive constant. Note that the mathematical proof of Eq. (17) can easily be derived from (Soize, 2006) for the extended class introduced in Section 3.1.

3.4 Basic properties of the random field \([A]\) and its parameters

The random field \( x \mapsto [A(x)] \) is a second-order random field on \( \Omega: E\{\|A(x)\|^2\} \leq E\{\|A(x)\|^2\} < +\infty \) in which \( \|\cdot\|_F \) is the Frobenius norm. The system of the marginal probability distributions of the random field \( x \mapsto [A(x)] \) is completely defined, is not Gaussian and is deduced from the system of the marginal probability distributions of the random field \( x \mapsto [G(x)] \) by using Eq. (11). In general, since \([a(x)]\) depends on \( x \), then the random field \( \{[A(x)], x \in \Omega\} \) is non homogeneous. For all fixed \( x \), the dispersion parameter \( \delta_A(x) \) of the random matrix \([A(x)]\), which is defined by

\[
\delta_A(x)^2 = E\{\|A(x) - [a(x)]\|^2_F\}/\|a(x)\|^2_F,
\]

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is such that

\[
\delta_\ell(x) = \frac{\delta}{\sqrt{n+1}} \left\{ 1 + \frac{(\text{tr}[A(x)])^2}{\text{tr}[g(x)]^2} \right\}^{1/2}.
\] (19)

The random field \( x \mapsto [G(x)] \) almost surely has continuous trajectories. If the function \( x \mapsto [g(x)] \) is continuous on \( \Omega \), then the random field \( x \mapsto [A(x)] \) almost surely has continuous trajectories on \( \Omega \). Nevertheless, if the function \( x \mapsto [g(x)] \) is not continuous on \( \Omega \), then the random field \( x \mapsto [A(x)] \) almost surely does not have continuous trajectories on \( \Omega \).

Then the random field \( x \mapsto [G(x)] \) is completely and uniquely defined by the following parameters: the \( M^\ell_1(\mathbb{R}) \)-valued mean function \( x \mapsto [\bar{g}(x)] \), the positive real parameter \( \delta \) and the 63 positive real parameters \( L_1, L_2, L_3 \) for \( 1 \leq j \leq j' \leq 6 \). The smallest number of parameters corresponds to the following case: \( x \mapsto [\bar{g}(x)] \), \( \delta \) and \( L_1=L_2=L_3=L_4 \) for all \( 1 \leq j \leq j' \leq 6 \).

3.5 Spatial correlation lengths of the random field \([A]\) for the homogeneous case

If \( [g(x)] = [\bar{g}] \) is independent of \( x \), then the random field \( \{[A(x)] = [L] + [G(x)] - [L] \} \) can be viewed as the restriction to \( \Omega \) of a homogeneous random field indexed by \( \mathbb{R}^3 \). Then the dispersion function defined by Eq. (18) is independent of \( x \) and then \( \delta_\ell(x) = \delta_\ell \). Let \( \eta = (\eta_1, \eta_2, \eta_3) \mapsto r^A(\eta) \) be the function defined from \( \mathbb{R}^3 \) into \( \mathbb{R} \) by

\[
r^A(\eta) = \text{tr} E\{([A(x + \eta)] - [\bar{g}])([A(x)] - [\bar{g}])\}.
\] (20)

It can be seen that \( r^A(0) = 1 \) and \( r^A(\eta) = r^A(\eta) \). For \( k = 1, 2, 3 \), the spatial correlation length \( L'_k \) of \( x \mapsto [A(x)] \) and relative to the coordinate \( x_k \) can then be defined by

\[
L'_k = \int_0^{\infty} r^A(\eta^k) \, d\eta_k,
\] (21)

in which \( \eta^k = (\eta_1, 0, 0), \eta^2 = (0, \eta_2, 0) \) and \( \eta^3 = (0, 0, \eta_3) \).

4 DISCRETIZING WITH STOCHASTIC FINITE ELEMENTS AND SOLVING THE RANDOM EQUATION

For all \( \ell \) and \( m \) in \{1, 2, 3\}, we have to (1) solve the stochastic BVP defined by Eq. (5) with \( \sigma^{\ell m}(x) = \varepsilon(D^{m}(x)) \) in order to construct the random local displacement field \( D^{m} \); (2) calculate the fourth-order tensor-valued random field \( H \) defined by Eq. (6) and corresponding to the strain localization; (3) estimate the probabilistic properties of the fourth-order random effective stiffness tensor \( C^{\varepsilon \theta} \) defined by Eq. (7).

In order to solve this problem, the following computational stochastic method is used.

The weak formulation of the stochastic BVP is constructed and the existence of a unique second-order stochastic solution can be proven. Note that the usual proof of the existence of a solution can be directly deduced if a uniform ellipticity condition and a uniform boundness condition for the fourth-order tensor valued random field \( x \mapsto \varepsilon(D) \) is used. This usual proof cannot be used for the present case due to the non introduction of these uniformness conditions which are substituted by the more realistic probabilistic hypothesis which has been introduced and which corresponds to the introduction of the non uniformness condition. The adapted proof can be obtained thanks to Eq. (17).

The stochastic finite element method is used for discretizing the weak formulation and Eq. (5). For such a numerical approximation, the random local stiffness tensor field \( x \mapsto \varepsilon_{\varepsilon \theta}^{(m)}(x) \) and the random local strain tensor field \( x \mapsto \varepsilon_{\varepsilon \theta}^{(d)}(D^{m}(x)) \) are discretized at all the Gauss-Legendre quadrature points of the finite elements.

The probabilistic quantities are then estimated by using the Monte Carlo simulation method which is made up of 3 main steps: (a) developing a generator for constructing \( n \) independent realizations \{\( x \mapsto C(x, \theta_r), r = 1, \ldots, n \)\} of the random field \( x \mapsto C(x) \) using the probability model presented in Section 3; (b) for each realization \( x \mapsto C(x, \theta_r) \), calculating the corresponding realization \( C^{\varepsilon \theta}(D^{m}(x)) \) of the effective tensor (and related quantities such as the random eigenvalues of the random tensor \( C^{\varepsilon \theta} \)) by solving a deterministic matrix equation; (c) with the \( n \) independent realizations, estimating the probabilistic quantities (moments, probability distributions) using the mathematical statistics and studying the convergence with respect to \( n \).

4.1 Finite element discretization

Let \( V = L^2(\Theta, V) \) be the real Hilbert space of all the second-order random variables \( \theta \mapsto \{x \mapsto D(x, \theta)\} \) defined on probability space \( (\Theta, \tau, P) \), with values in the Hilbert space \( V = (H^2(\Omega))^3 \). Let \( e(d) \) be the strain vector defined by \( e(d) = (\varepsilon_{11}(d), \varepsilon_{22}(d), \varepsilon_{33}(d), 2 \varepsilon_{12}(d), 2 \varepsilon_{15}(d), 2 \varepsilon_{23}(d)) \) and let \( (D, \delta D) \) be the random bilinear form on \( V \times V \) defined by

\[
K(D, \delta D) = \int_{\Omega} <[A(x)] e(D(x)), e(\delta D(x))> \, dx.
\] (22)

The stochastic finite element method is used to discretize the weak formulation. A finite element mesh of domain is carried out using 3D solid finite elements.
We then have $\Omega = \bigcup \Omega_e$ in which $\Omega_e$ is the domain of the finite element number $e$. Any displacement field $x \mapsto d(x)$ in $V$ and its associated strain vector field $x \mapsto e(x)$ are then approximated by
\[
d(x) = [B(x)]w, \quad x \in \overline{\Omega}, \quad e(x) = [S(x)]w, \quad x \in \Omega,
\]
in which $w = (w_1, \ldots, w_V)$ is the vector of the $V$ degrees of freedom corresponding to the values of the components of the field $d$ at the nodes of the mesh. The $(3 \times V)$ real matrices $[B(x)]$ and $[S(x)]$ are known matrices usually constructed by using the interpolation functions of the finite elements. For any integrable function $x \mapsto f(x)$ defined on $\Omega$ and continuous on $\Omega$, the following usual numerical approximation can be written as
\[
\int_{\Omega} f(x)dx = \sum_{k=1}^{N_e} \omega_k f(x_k),
\]
in which $\{\omega_1, \ldots, \omega_{N_e}\}$ and $\{x_1, \ldots, x_{N_e}\}$ are the sets of all the $N_e$ weights and the $N_e$ Gauss-Legendre quadrature points for the finite element $\Omega_e$. Consequently, it can be written that
\[
\int_{\Omega} f(x)dx = \sum_{k=1}^{N_e} \omega_k f(x_k),
\]
in which $\{\omega_1, \ldots, \omega_{N_e}\}$ and $\{x_1, \ldots, x_{N_e}\}$ are the sets of all the $N_e$ weights and the $N_e$ Gauss-Legendre quadrature points for $\Omega = \cup e \Omega_e$, with $N = \sum_e N_e$.

For all $x$ in $\overline{\Omega}$, the finite element approximation of all $D$ and $\delta D$ in $V$ is then written as $D(x) = [B(x)]W$ and $\delta D(x) = [B(x)]\delta W$, in which $W$ and $\delta W$ are $\mathbb{R}^V$-valued second-order random vectors. Therefore, the corresponding finite element approximation of the random bilinear form defined by Eq. (22) is such that
\[
\int_{\Omega} f(x)dx = \sum_{k=1}^{N_e} \omega_k f(x_k),
\]
in which $\{\omega_1, \ldots, \omega_{N_e}\}$ and $\{x_1, \ldots, x_{N_e}\}$ are the sets of all the $N_e$ weights and the $N_e$ Gauss-Legendre quadrature points for $\Omega = \cup e \Omega_e$, with $N = \sum_e N_e$.

The random stiffness matrix $[K]$ defined by Eq. (23) can then be approximated by the random matrix $[K]_N$ such that
\[
[K]_N = \sum_{\alpha=1}^{N_e} [S(x_\alpha)]^T [A(x_\alpha)] [S(x_\alpha)] dx,
\]
in which $[S(x_\alpha)]^T [A(x_\alpha)] [S(x_\alpha)] dx$ is the vector of the $v$ degrees of freedom for the nodes inside the domain $\Omega$ and where $w_i(x)$ is the $\mathbb{R}^V$-valued second-order random vector of the $v$ degrees of freedom for the nodes belonging to the boundary $\partial \Omega$. This last vector is such that $d(x) = [B(x)]w_i(x)$ for all $x$ in $\partial \Omega$ and $[K]_N = \sum_{\alpha=1}^{N_e} [S(x_\alpha)]^T [A(x_\alpha)] [S(x_\alpha)] dx$.

The finite element approximation of Eq. (5) is then given by the following random matrix equation allowing the unknown random vector $W_{\text{fem}}$ to be calculated,
\[
[K]_N W_{\text{fem}} = -[\delta K]_N W_{\text{fem}}. \tag{25}
\]

The random values $\mathbb{H}(x_1), \ldots, \mathbb{H}(x_N)$ of $\mathbb{H}$ are calculated by using Eq. (6). Let $\mathbb{C}(x_\alpha), \ldots, \mathbb{C}(x_\alpha)$ be the random values of $\mathbb{C}$. The finite element approximation of the fourth-order random effective stiffness tensor $\mathbb{C}_{\text{eff}}$ defined by Eq. (7) can then be written as
\[
\mathbb{C}_{\text{eff}} \approx \frac{1}{|\Omega|} \sum_{\alpha=1}^{N_e} \omega_\alpha \mathbb{C}(x_\alpha) : [H](x_\alpha). \tag{26}
\]

The $M_{\alpha}(\mathbb{R})$-valued random matrix $[A^\alpha]$ of the fourth order random effective stiffness tensor $\mathbb{C}_{\text{eff}}$ is such that
\[
[A^\alpha]_{\ell, j} \sim \mathbb{C}_{\text{eff}, j, k}. \tag{27}
\]

### 4.2 Defining the probabilistic quantities for the random effective stiffness matrix

It is assumed that the mean model of the microstructure is homogeneous, that is to say $[a(x)] = [\overline{a}]$ is independent of $x$. Consequently, the random field $[A]$ describing the fourth-order tensor-valued random field $\mathbb{C}$ can be viewed as the restriction to $\Omega$ of a homogeneous random field indexed by $\mathbb{R}^3$. Using Eq. (19), the dispersion parameter $\delta_a$ which is then independent of $x$ can easily be deduced from the value of the dispersion parameter $\delta$. The spatial correlation lengths $L_i^\text{eff}$ and $L_j^\text{eff}$ defined by Eq. (21) depend on the values of the parameters $L_i^\text{eff}, L_j^\text{eff}$ for $1 \leq i \leq j \leq 6$. Let $z \mapsto p(z)$ be the probability density function with respect to $dz$ of the random variable $Z$ defined by
4.3 Solving the random equation and computing the statistical estimations

The stochastic problem defined by Eqs. (25) to (28) is solved by using the Monte Carlo numerical simulation method with $n_i$ independent realizations $\theta_i, \ldots, \theta_j$ in $\Theta$. The independent stochastic germs $U_{ij}$ for $1 \leq i \leq j \leq 6$ are simulated in the $N$ Gauss-Legendre quadrature points $x_1, \ldots, x_N$. The mathematical expectation of any random quantity $R$ is estimated by $E[R] = 1/n_i \sum_{i=1}^{n_i} R(\theta_i)$. The cumulative probability distribution $F_Z$ defined by Eq. (28) is estimated with the usual estimator (Serfling, 1980). Let $[A_{\text{eff}}]$ be the random effective stiffness matrix calculated with the finite element model having $v$ degrees of freedom. For a given value of $v$, the convergence of the Monte Carlo numerical simulation with respect to $n_s$ can be controlled by studying the function

$$n_s \mapsto \text{conv}(n_s, v) \frac{1}{\| A_{\text{eff}} \|} \left( \frac{1}{n_s} \sum_{i=1}^{n_s} \| A_{\text{eff}}(\theta_i) \| \right)^{1/2}$$

(30)

in which $\| A_{\text{eff}}(\theta_i) \|$ is the realization $\theta_i$ of the random variable $\| A_{\text{eff}} \|$. If the mean model of the microstructure is homogeneous, then the local stiffness matrix $[a]$ is independent of $x$ and then $[A_{\text{eff}}] = [a]$. The right hand side of Eq. (30) corresponds to the statistical estimation of the norm $\| A_{\text{eff}} \| = E(\| A_{\text{eff}} \|^2)^{1/2}$ of the random matrix $[A_{\text{eff}}]$. For a given value of $n_s$, the convergence with respect to the number $v$ of degrees of freedom of the finite element model is given by the function $v \mapsto \text{conv}(n_s, v)$.

5 APPLICATION TO AN ANISOTROPIC RANDOM MICROSTRUCTURE

5.1 Mean model and finite element discretization of the mean model of the microstructure

The open bounded domain $\Omega$ (the RVE) of $\mathbb{R}^3$ is such that $\Omega = (0, 1)^3$. The mean model of the microstructure corresponds to a homogeneous anisotropic linear elastic medium whose local stiffness matrix $[a]$ belonging to $\mathbb{M}_n^+(\mathbb{R})$ with $n = 6$ is then independent of $x$ and such that $[a] = 10^{10}$

$$\begin{bmatrix} 3.3617 & 1.7027 & 1.3637 & -0.1049 & -0.2278 & 2.1013 \\ 1.7027 & 1.6092 & 0.7262 & 0.0437 & -0.1197 & 0.8612 \\ 1.3637 & 0.7262 & 1.4653 & -0.1174 & -0.1506 & 1.0587 \\ -0.1049 & 0.0437 & -0.1174 & 0.1319 & 0.0093 & -0.1574 \\ -0.2278 & -0.1197 & -0.1506 & 0.0093 & 0.1530 & -0.1303 \\ 2.1013 & 0.8612 & 1.0587 & -0.1574 & -0.1303 & 1.7446 \end{bmatrix}$$

The finite element model is a regular mesh of $12 \times 12 \times 12 = 1728$ nodes and $11 \times 11 \times 11 = 1331$ finite elements which are 8-nodes solid elements with $2 \times 2 \times 2$ Gauss-Legendre quadrature points. Therefore there are 5184 degrees of freedom, $N = 10648$ Gauss-Legendre quadrature points, $v = 3000$ degrees of freedom for the nodes inside domain $\Omega$ and $v_b = 2184$ degrees of freedom for the nodes belonging to boundary $\partial \Omega$. In this case, the weights $\omega_1, \omega_2, \omega_3$ are such that $\omega_1 = |\Omega|/N$ and consequently, Eq. (26) can be rewritten as

$$C_{\text{eff}} \simeq \frac{1}{N} \sum_{\alpha=1}^{N} C(\mathbf{x}^\alpha) : H(\mathbf{x}^\alpha).$$

5.2 Micro-scale stochastic model, computational parameters and stochastic response

(i) Micro-scale stochastic model. The stochastic model of the elasticity tensor of the random anisotropic microstructure is defined in Sections 2.2 and 3. The random field $x \mapsto [A(x)]$, indexed by $\Omega$, with values in $\mathbb{M}_n^+(\mathbb{R})$, with $n = 6$, is such that (see Eq. (11)), $[A(x)] = [L]^{T} [G(x)] [L]$ in which the matrix $[a]$, defined in Section 5.1 is written (see Eq. (10)) as $[a] = [L]^{T} [L]$. The stochastic field $x \mapsto [G(x)]$, indexed by $\mathbb{R}^3$, with values in $\mathbb{M}_3^+(\mathbb{R})$, is defined in Section 3.

(ii) Dispersion parameter. The dispersion parameter $\delta_{\text{eff}}$ defined by Eq. (18) is then independent of $x$ and can be calculated as a function of the parameter $\delta$ by using Eq. (19) and yields $\delta_{\text{eff}} = 0.6192 \times \delta$. For $\delta = 0.1, 0.2, 0.3$ and 0.4, one then has $\delta_{\text{eff}} = 0.0619, 0.1238, 0.1858$ and 0.2477 respectively. Below, all the results are given as function of $\delta$ instead of $\delta_{\text{eff}}$.

(iii) Parameters of the stochastic germs and spatial correlation lengths of the random field $[A]$. In is assumed that the parameters $L_{ij}^{\text{eff}}, L_{ij}^{\text{eff}}, L_{ij}^{\text{eff}}$ for $1 \leq j \leq j' \leq 6$ of the stochastic germs are such that $L_{ij}^{\text{eff}} = L_{ij}^{\text{eff}} = L_{ij}^{\text{eff}} = L_{ij}$ for all $j$ and $j'$ in which $L_{ij}$ is the unique parameter relative to the length-scales of the stochastic germs. For each given
Stochastic convergence analysis for the random effective stiffness matrix.

The mean-square convergence with respect to \( n_z \) has been studied by constructing the function \( n_z \mapsto \).
conv\( (n_\nu, \nu) \) defined by Eq. (30). For \( \delta = 0.4 \) (the largest value considered for the dispersion parameter), for \( L_\delta = 0.1 \) (the smallest value considered for this parameter) and for a finite element model having \( \nu = 5184 \) degrees of freedom and corresponding to \( 11 \times 11 \times 11 \) finite elements, convergence is reached for \( n_\nu \geq 500 \).

The mean-square convergence with respect to the number \( \nu \) of degrees of freedom of the finite element model is studied by constructing the function \( \nu \mapsto \text{conv}(n_\nu, \nu) \) defined by Eq. (30). Figure 2 displays the graph of \( \nu \mapsto \text{conv}(n_\nu, \nu) \) for \( \delta = 0.4, L_\delta = 0.1 \) and \( n_\nu = 900 \). Clearly, convergence is reached for \( 11 \times 11 \times 11 \) finite elements corresponding to \( \nu = 5184 \).

All the results presented below have been computed with \( n_\nu = 900 \) and \( 11 \times 11 \times 11 \) finite elements corresponding to \( \nu = 5184 \). Convergence is reached for the values of \( L_\delta \) and \( \delta \) which are considered below.

5.3 Probabilistic analysis of the RVE size

Let \( \beta \) be a positive real number. Let \( \beta \mapsto \mathbb{P}(\beta) \) be the function defined by

\[
\mathbb{P}(\beta) = P\{1 - \beta < Z \leq 1 + \beta\} = F_Z(1 + \beta) - F_Z(1 - \beta).
\]

For \( \delta = 0.4 \) and for \( L_\delta \) belonging to \([0.1, 0.7]\), Fig. 3 displays the graph of the function \( \mathbb{P} \). For instance, for \( L_\delta = 0.2 \) and for \( \delta = 0.02, 0.04 \) and 0.08, one has \( \mathbb{P} = 0.36, 0.65 \) and 0.95, which means that \( P\{0.98 < Z \leq 1.02\} = 0.36, P\{0.96 < Z \leq 1.04\} = 0.65 \) and \( P\{0.92 < Z \leq 1.08\} = 0.95 \). For instance, for \( \delta = 0.4 \) (i.e., \( \delta_\kappa = 0.2477 \)), if stochastic homogenization is performed with a RVE whose size is five times the spatial correlation length (RVE size = 1 and spatial correlation length \( L_\delta = 0.2226 \)), then the probability for which the random fluctuations of the effective stiffness tensor is less than 2\%, 4\% or 8\%, is 0.36, 0.65 or 0.95 respectively.

6 CONCLUSIONS

We have presented an approach introducing a micro-scale stochastic model which can be used when the standard method cannot be applied to anisotropic elastic microstructures. This new approach is useful for a direct experimental identification of random anisotropic elastic microstructures. A parametric probabilistic study of the RVE size has been performed with respect to the intensity \( \delta_\kappa \) of the stochastic fluctuations of the local stiffness tensor-valued random field describing the micro-scale stochastic model and in function of its correlation lengths \( L_\delta \). Such a study is also useful to get information on the RVE size for which stochastic fluctuations are still significant and consequently, can be measured. Then the results presented in this paper could allow the micro-scale stochastic model to be identified from RVE- or macro-scale measurements solving an inverse stochastic problem. For fixed spatial correlation lengths and dispersion parameter \( \delta_\kappa \), the effective RVE size can effectively be calculated in a probability sense using the cumulative distribution function of the random variable measuring the random fluctuations of the effective stiffness tensor. A large numerical simulation has been carried out and the numerical results obtained allow a probability analysis of the representative volume element size to be performed.

REFERENCES


