Comput. Methods Appl. Mech. Engrg. 254 (2013) 61–82

Contents lists available at SciVerse ScienceDirect

Comput. Methods Appl. Mech. Engrg.

journal homepage: www.elsevier.com/locate/cma

Uncertainty quantification in computational stochastic multiscale analysis of nonlinear elastic materials

A. Clément, C. Soize *, J. Yvonnet

Université Paris-Est, Laboratoire Modélisation et Simulation Multi Echelle, MSME UMR 8208 CNRS, 5 Bd Descartes, 77454 Marne-la-Vallée, France

ARTICLE INFO

Article history:
Received 27 April 2012
Received in revised form 22 October 2012
Accepted 25 October 2012
Available online 3 November 2012

Keywords:
Uncertainty quantification
Multiscale
Nonlinear materials
Computational stochastic mechanics
Nonlinear composites
Hyperelasticity

ABSTRACT

This paper is devoted to a computational stochastic multiscale analysis of nonlinear structures made up of heterogeneous hyperelastic materials. At the microscale level, the nonlinear constitutive equation of the material is characterized by a stochastic potential for which a polynomial chaos representation is used. The geometry of the microstructure is random and characterized by a high number of random parameters. The method is based on a deterministic non-concurrent multiscale approach devoted to micro–macro nonlinear mechanics which leads us to characterize the nonlinear constitutive equation with an explicit continuous form of the strain energy density function with respect to the large scale Cauchy Green strain states. To overcome the curse of dimensionality, due to the high number of involved random variables, the problem is transformed into another one consisting in identifying the potential on a polynomial chaos expansion. Several strategies, based on novel algorithms dedicated to high stochastic dimension, are used and adapted for the class of multi-modal random variables which may characterize the potential. Numerical examples, at both small and large scales, allow analyzing the efficiency of the approach through comparisons with classical methods.

1. Introduction

The problem of the stochastic nonlinear homogenization of heterogeneous random microstructures is a difficult task. Among the many issues related to this objective, the first ones appears at the deterministic level, where, unlike the linear case, the general form of the constitutive equations is unknown. Moreover, the principle of superposition is no longer available and makes unsuitable any analytical homogenization scheme applied to the small elastic strains. Many recent works have been devoted to overcome these difficulties and can be classified in two distinct families. First, approaches based on the extension of classical analytical homogenization methods [8,1] and on second-order homogenization techniques [34,26] both leading to determine the effective constitutive laws of nonlinear composites. Secondly, approaches based on numerical multiscale simulations such as concurrent methods [37,12,46,49,28] and non-concurrent ones [33,44,45,50].

On the other hand, the uncertain nature at the microscopic level of many classes of heterogeneous materials, should be taken into account if one seeks to obtain a reliable model of the effective constitutive law. Thus, many recent works have been devoted to the construction and the identification of stochastic models at the finest scale and to their incorporation in a multiscale analysis through *ad hoc* numerical methods (see [44,18,43] for instance). Naturally, at the present time, the different proposed approaches are only available in the case of linear elasticity and still need further developments to incorporate mechanical nonlinearities at the microscopic level. Moreover, these methods involve very high computational times, especially if one deterministic simulation appears expensive. A great challenge thus comes from the extension of the deterministic methods stated above to the stochastic framework with reasonable computational costs.

Based on a novel efficient non-concurrent multiscale approach developed by Yvonnet and co-workers [50–52], we have extended this method to the stochastic case in Ref. [7]. The so-called Stochastic Numerical EXplicit Potentials method (S-NEXP) aims at numerically determine the apparent strain energy density function according to the large scale strain states and the random variables describing the uncertainties related to the microstructure (geometrical or material parameters). This parametric technique allows one getting efficient solutions but suffers from the "curse of dimensionality" since the interpolation scheme requires a high number of microscopic nonlinear numerical simulations. This problem is similar to the one encountered in the framework of stochastic intrusive techniques, such as Galerkin methods which rely on conventional tensor-product integration rules. However, taking into account a high number of random parameters is of first importance in a stochastic multiscale analysis and we thus propose a different methodology based on polynomial chaos representations. Initiated in Ref. [14], the methodology to construct a

* Corresponding author.
E-mail addresses: christian.soize@univ-paris-est.fr, christian.soize@univ-mlv.fr (C. Soize).

0045-7825/$ - see front matter © 2012 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.cma.2012.10.016

polynomial chaos expansion of random fields has been intensely developed to solve stochastic partial differential equations [3,15,16,13,24,22,29,32,31,35,38,11] but also for the identification of random fields using experimental data and classical inference techniques [17,2] or maximum likelihood estimation [9,10,43,18]. A new methodology has been recently introduced to deal with the identification of polynomial chaos representations in high-dimension [39,41]. We propose to use this novel technique in order to obtain a representation of the stochastic nonlinear constitutive equations which can thus be seen as a stochastic non-intrusive technique as opposed to the Stochastic Numerical EXplicit Potentials method [7] which suffers from the classical tensor-product interpolation rules since it acts as an intrusive technique. Then, we based our approach on the same nonlinear homogenization scheme presented in Ref. [7] but the methodology proposed to characterize the stochastic apparent nonlinear constitutive equations is totally different. Indeed, we use the NEXP approach [52] as a deterministic solver, which is not directly extended to the stochastic framework, and we reformulate the problem into the identification of polynomial chaos expansions in high-dimension.

The paper is organized as follows. Section 2 deals with the homogenization of nonlinear heterogeneous materials at finite strains in a deterministic framework. In the same section, the Numerical EXplicit Potentials method (NEXP) is also briefly presented. Section 3 presents the probabilistic model which allows generating realizations of the microstructure. In Section 4, we then detail the procedure of identification of the reduced-order random variables, resulting from a principal component analysis, on polynomial chaos expansions. Since the problem of identifying multi-modal random variables arises, we define a prior stochastic model based on mixtures of polynomial chaos as introduced in Ref. [30]. Both cases of uni-modal and multi-modal random variables are then addressed. The efficiency of the proposed method is shown in Section 6 with two numerical examples at the microscale and one example at the mesoscale. For each problem, the proposed approach is compared with classical methods showing its efficiency. Some concluding remarks are finally drawn in Section 7.

2. The method of Numerical EXplicit Potentials

In this section, we detail the nonlinear homogenization scheme applied to hyperelastic heterogeneous materials and we present the deterministic method of Numerical EXplicit Potentials [50–52,7] (NEXP) leading to a continuous explicit form of the strain energy density function which characterizes the effective constitutive equations. In the field of homogenization, knowledge on the separation of the scales is vital to perform an appropriate mechanical analysis. We set apart two cases: the case where the two scales are the microscale and the macroscale and the case for which the two scales are the microscale and the mesoscale. More precisely, when the two considered scales are the microscale and the macroscale, the scales are separated. Such a separation is obtained when the spatial correlation lengths of the mechanical fields at the microscale are small enough with respect to the macroscale. The statistical fluctuations at the macroscale are then negligible and the macroscopic mechanical quantities are thus deterministic and are referred as the effective properties. On the other hand, when the two considered scales are the microscale and the mesoscale, the scales are not separated. The statistical fluctuations at the mesoscale are important and the mesoscopic mechanical quantities are stochastic and referred as the apparent properties. The proposed method can be used in both cases, as it will be shown in the numerical examples. Then, in order to simplify the writing of this paper without loss of generality, we use the following terminology. The small scale indicates the microscale and the large scale indicates either the macroscale or the mesoscale. Moreover, both the effective quantities, linked to the macroscale, and the apparent quantities, linked to the mesoscale, are referred as the apparent quantities.

2.1. Nonlinear homogenization scheme

We consider a microstructure, schematically depicted on Fig. 1, which occupies a domain $\Omega \subset \mathbb{R}^d$ where $d \in \{1,2,3\}$ denotes the spatial dimension and where $\partial\Omega$ denotes the boundary of the domain Ω. We identify the position of the material points by the vector $\boldsymbol{X}$ in the reference configuration and by $\boldsymbol{x}$ in the deformed configuration. Those two vectors are related through:

$$\boldsymbol{x} = \boldsymbol{X} + \boldsymbol{u}, \tag{1}$$

where $\boldsymbol{u}$ is the displacement vector of a material point. We introduce the deformation gradient tensor $\boldsymbol{F}$ at point $\boldsymbol{X}$ defined by

$$\boldsymbol{F} = \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}} = \mathbf{1} + \nabla_{\boldsymbol{X}}(\boldsymbol{u}), \tag{2}$$

where $\mathbf{1}$ is the second-order identity tensor and $\nabla_{\boldsymbol{X}}(\cdot)$ is the gradient operator according to the reference configuration. Domain Ω, characterizing the microstructure, is composed of N_p hyperelastic phases defining the N_p domains $\Omega^{(r)}$ with $r \in \{1,\dots,N_p\}$ and such that $\Omega = \bigcup_{r=1}^{N_p} \Omega^{(r)}$. The constitutive equations of each phase can then be characterized by strain energy density functions $\psi^{(r)}$ according to the right-hand Cauchy–Green strain tensor $\boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{F}$ such that the local strain energy density function ψ of Ω can be written as

$$\psi(\boldsymbol{X},\boldsymbol{C}) = \sum_{r=1}^{N_p} \mathbb{I}^{(r)}(\boldsymbol{X})\psi^{(r)}(\boldsymbol{C}), \tag{3}$$

where $\mathbb{I}^{(r)}$ is the characteristic function of domain $\Omega^{(r)}$ which is equal to 1 if $\boldsymbol{X} \in \Omega^{(r)}$ and 0 otherwise. Let us denote by $\boldsymbol{P}$ and $\mathbf{S}$ the first and second Piola–Kirchhoff stress tensors respectively, related by $\boldsymbol{P} = \boldsymbol{F}\mathbf{S}$. In the Lagrangian description, the local constitutive equation is given by (see e.g. [20])

$$\mathbf{S} = 2\frac{\partial \psi}{\partial \boldsymbol{C}}(\boldsymbol{X},\boldsymbol{C}). \tag{4}$$

In the present work, we consider a compressible Neo-Hookean model (see [20] for instance) described by the following potential

$$\psi(\boldsymbol{C}) = \frac{1}{2}\lambda\{\log(J)\}^2 - \mu\log(J) + \frac{1}{2}\mu(tr(\boldsymbol{C}) - 3), \tag{5}$$

where $\log(\cdot)$ indicates the natural logarithm, $J = \det(\boldsymbol{F})$ is the volumetric change, $\lambda = \frac{Ev}{(1+v)(1-2v)}$ and $\mu = \frac{E}{2(1+v)}$ in which E and v are

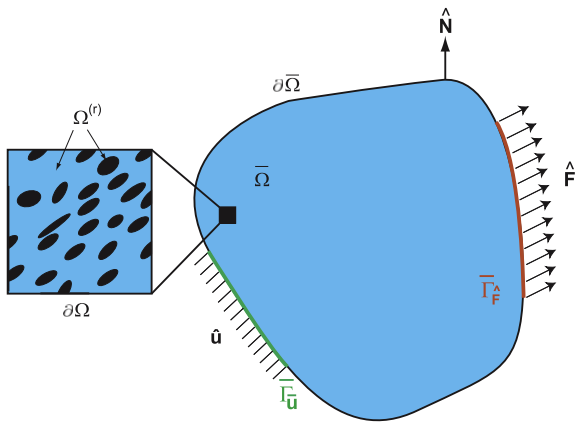

Fig. 1. Model problem: small scale and large scale structures.