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Multiscale finite element analysis of uncertain-but-bounded heterogeneous materials at finite deformation

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ABSTRACT

A new computationally interval homogenization modelling for heterogeneous materials with uncertain-but-bounded parameters is presented in a deformation controlled setting, and the homogenization analysis in the context of elasticity at finite deformation is then addressed by an integrative approach of finite element method with the optimization algorithms where the interval uncertainty in the microstructure of the material is fully considered. Different deformation-controlled boundary conditions are imposed on the representative volume element, and the interval effective quantities involving the tangent tensor and the first Piola–Kirchhoff stress tensor as well as the strain energy together with the effective moduli are obtained. The influences of different uncertain cases on the interval effective quantities are also analyzed. For the purpose of verification, the results from particle swarm optimization (PSO) algorithm are compared with those obtained from genetic algorithm (GA) and Monte-carlo simulation. The feasibility and validity of the proposed modelling method are evidenced by the well-agreed consequences among the above algorithms.

1. Introduction

Multiscale material modelling is tightly related to theory and simulation of material properties and behavior across length and time scales from the atomistic to the macroscopic [1]. The applications of these techniques are mainly focused on simulations of microstructure and mechanical properties of kinds of materials including polymers, ceramics, semiconductors and metals, etc [2]. In the last decade, many techniques of multiscale material modelling have been developed [3]. Among these modelling techniques, a distinction is made between the hierarchical approach [2], which involves running separate models with some sort of parametric coupling, and the hybrid approach, in which models are run concurrently over different spatial regions of a simulation [4]. Furthermore, JA Elliott [2] classified the hierarchy of multiscale modelling methods into the following three categories, atomistic and molecular modelling, mesoscale and continuum modelling, and engineering and process unit design as well, to effectively represent the characteristics of different methods in depicting temporal and spatial scales. The atomistic and molecular modelling methods cover the Quasicontinuum method [5], molecular dynamics [6], the Handshaking method [7], the Bridging-domain method [3], coupling methods based on lattice dynamics [8] and hybrid quantum mechanic–molecular mechanic methods [9], etc.

Mesoscopic regime lies between discrete atomic particles and FE representations of a continuum. As far as mesoscale and continuum modelling of multiscale material is concerned, modelling techniques involves coarse graining method [2] and dissipative particle dynamics [2] as well as direct micro-macro method [10], etc. Especially, from the viewpoint of micromechanics, a homogenization theory has been constructed for the heterogeneous materials in a series of theoretical papers. In the context of micromechanics, the effective physical behavior of a heterogeneous structure, to be considered here as a matrix material with separated inclusions, strongly depends on the size, shape properties and spatial distribution of the second phase [10]. Because the length scale of a macrostructure made up of a heterogeneous material is typically much larger than the length scale of the heterogeneities, during standard numerical analysis methods required for the solution of problems posed on the macrostructural scale, a direct resolution of the microstructure is not

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feasible. To overcome this problem some homogenization techniques have been created to obtain a suitable constitutive model to be inserted at the macroscopic level [10].

The goal of homogenization is to determine the apparent physical properties of a heterogeneous material based on the knowledge of geometry and material properties of their microstructure [11]. The method relies on a statistically representative sample of material on the mesoscale, referred to as a representative volume element (RVE), and on establishing a suitable scale transition procedure between the microscale features and the macroscale response [12]. Homogenization techniques are both of computational [13,14] and analytical [15–17] nature, particularly, computational homogenization technique based on finite element has been developed as well [11].

In this work, the problem of homogenization is addressed in the context of elasticity in the finite deformation regime. There have been some reports published about the heterogeneous materials in the setting of large deformations. Kouznetsova, Brekelmans and Baaijens [10] presented a direct micro-macro strategy suitable for modelling the mechanical response of heterogeneous materials at large deformations and non-linear history dependent material behavior, in which the behavior was determined through the detailed modelling of the microstructure within the context of finite element implementation. Homogenization in the non-linear elastic regime was pioneered by the works of Hill [12], Hill and Rice [17] as well as Ogden [18]. An analytical approach to the problem was developed by constructing bounds on the effective strain energy [19]. However, non-uniqueness of the solution at finite deformations, the non-convexity of the strain energy function, and the non-invertibility of the stress-strain relationship [20] render these results applicable only in a limited range of deformation and for a limited class of materials [21]. Moreover, in general, there is no apparent constitutive equation that characterizes the macroscopic behavior [22]. In this case, the computational homogenization method is undoubtedly the most appropriate choice.

The uncertainty existing in the input and material parameters [23] recently motivated a continuous attention to random heterogeneous materials [14,24,25], and numbers of study have been proposed in the framework of stochastic homogenization analysis [26–29]. The key to random analysis is to determine the probability density function of each random parameter, in which sufficient statistical information is needed. For the uncertain problems with small samples or poor information, the probability statistics of the random parameters are difficult to obtain. The direct consequence of such complication is that the results of stochastic analysis become less confident, or even inaccurate in some cases [30]. Therefore, there is urgent necessity to further develop other types of uncertainty analysis simply because that stochastic approach does not have sufficient universality to solve all problems in real-life engineering [31]. Interval method is only concerned with the value intervals of the uncertain parameters, and it is not necessary to determine the probability distributions of uncertain parameters. In the interval analysis, interval problems can be transformed into the optimization problems since the upper and lower bounds of results are respectively corresponding to the maximum and minimum values of the system outputs, and the work on the interval analysis of uncertain structures has also been reported [32–34]. Actually, the homogenization for heterogeneous materials with uncertain-but-bounded parameters may also be addressed with the interval analysis method, which, however, has never been considered so far, and there are little reports about homogenization of heterogeneous materials containing interval uncertainty.

The present work focuses on the interval homogenization of a three-dimensional (3D) heterogeneous material in the frame of finite element (FE) implementation, and the aim is to predict the mechanical behavior of heterogeneous materials with uncertain-but-bounded parameters. The problem is addressed in the context of elasticity in the finite deformation regime, and the solution is based on the work of Hill [12], Hill and Rice [17], Nemat-Nasser [35] and Ogden [18]. The uncertain-but-bounded parameters in the microstructure of heterogeneous materials are fully accounted for, and a computationally homogenization technique based on FE method combined with the optimization strategy is first formulated in a deformation controlled setting. A detailed investigation on the influences of the uncertain-but-bounded parameters on the homogenized results is reported, and some important conclusions are obtained as well.

2. Homogenization in non-linear elasticity based on multiscale finite element technique

In this section, the homogenization of a non-linear elasticity problem is summarized, and a heterogeneous material M consisting of homogeneous isotropic matrix M_1 and inclusions M_2 is considered (see Fig. 1).

2.1. Macroscopic constitutive characterization

Consider the two-phase heterogeneous material M, associated with the reference configuration R_0, with constitutive equation $\boldsymbol{S} = \widehat{\boldsymbol{S}}(\boldsymbol{X}, \boldsymbol{E})$, where $\boldsymbol{S}$ and $\boldsymbol{E}$ are respectively the second Piola-Kirchhoff stress tensor and the Green-Lagrange strain tensor. Two homogeneous isotropic materials, the matrix (M_1) and inclusions (M_2) (see Fig. 1), are characterized by their respective constitutive equations $\widehat{\boldsymbol{S}}^I(\boldsymbol{E})$.

A mechanical boundary value problem [11] on this heterogeneous macrostructure M is to determine $\boldsymbol{x}(\boldsymbol{X}, t)$ so that

$$\mathrm{Div}(\boldsymbol{P}) + \rho_0 \boldsymbol{b} = \rho_0 \ddot{\boldsymbol{x}} \text{ in } R_0 \tag{1}$$

with boundary conditions $\boldsymbol{x} = \overline{\boldsymbol{x}}$ on boundary ∂R_0^x, and $\boldsymbol{p} = \boldsymbol{P}\boldsymbol{N} = \overline{\boldsymbol{p}}$ on boundary ∂R_0^p, and constitutive equation is $\boldsymbol{P} = \boldsymbol{P}(\boldsymbol{X}, F)$, where $\boldsymbol{x}$ and $\boldsymbol{X}$ are respectively the positions of a point on the spatial configuration R and reference configuration R_0 of the material according to the continuum mechanics, $\boldsymbol{p}$ is the traction on the surface ∂R_0^p with outward unit normal $\boldsymbol{N}, \boldsymbol{P}$ is the first Piola-Kirchhoff stress, $\boldsymbol{F}$ is the microscopic deformation gradient, ρ_0 is the density, and $\rho_0 \boldsymbol{b}$ and $\rho_0 \ddot{\boldsymbol{x}}$ are respectively the macro-

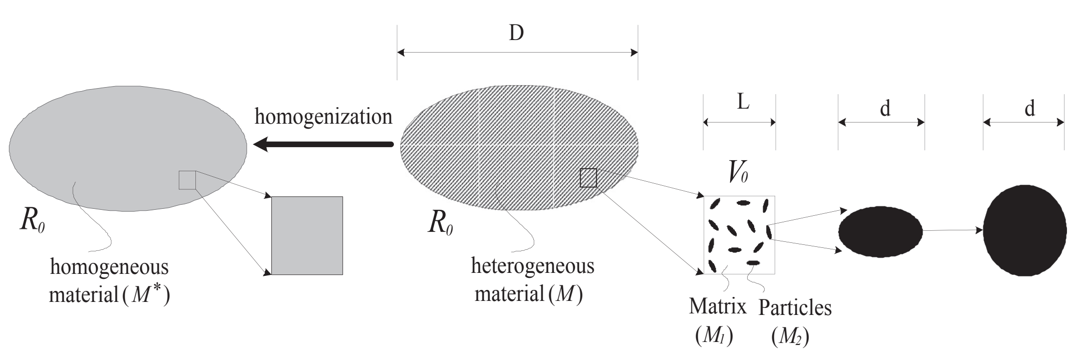

Fig. 1. Homogenization problem of a two-phase heterogeneous material (the original heterogeneous material of the macrostructure is replaced by the effective material) and the micro (d: inclusions) –meso (L: RVE) –macro (D) principle of the homogenization.