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Dual probabilistic homogenization of the rubber-based composite with random carbon black particle reinforcement

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ABSTRACT

This study concerns numerical determination of the basic statistics of the effective elasticity tensor for the rubber reinforced with the carbon black particles. This goal is achieved by an application of the iterative and generalized stochastic perturbation technique implemented as the Stochastic Finite Element Method and applied to the homogenization problem of such a composite. A fundamental difference of this approach to the traditional Taylor expansion is in development of the basic equations for higher order probabilistic characteristics, where traditional linearization procedure (expectation is approximated by the zeroth order term) has been replaced by sequential (iterative) symbolic calculation of these characteristics. The radius of the carbon black particle has been chosen as the input Gaussian random parameter and it affects both FEM-based and also analytical method of the effective tensor components determination. Sensitivity analysis in addition to this radius together with the FEM computational error for the homogenization problem are carried out here prior to the principal stochastic analysis. We contrast the iterative SFEM with two other probabilistic numerical methods, namely the classical Monte-Carlo scheme and also semi-analytical probabilistic FEM strategy. Both stochastic perturbation and semi-analytical method are related to the same polynomial response functions of the input random particle radius, but the first employs Taylor series expansion while the second – symbolic integration with Gaussian PDF to calculate the final probabilistic characteristics of the effective tensor. This study shows some remarkable differences in-between numerical and analytical homogenization methods in the context of geometrical uncertainty in the RVE of such a composite.

1. Introduction

Probabilistic analysis of the composite materials at different geometrical scales and for various types of engineering materials still affects modern trends in computational, experimental and theoretical mechanics [6,9]. It is applied either with the use of historically the oldest statistically motivated Monte-Carlo simulation method, Bayesian approach, polynomial chaos [26], semi-analytical strategies [8], kriging approach [12] or, alternatively, with the use of stochastic perturbation technique [17]. It is essential to underline that the research focused on optimization of the existing stochastic numerical techniques is still very extensive towards minimization of the computational effort and maximization of the resulting characteristics reliability and precision. Determination of higher order statistics is connected in the modern engineering literature with an application of the Monte-Carlo simulation, semi-analytical approach and the generalized stochastic perturbation technique, for instance [8,9], while the remaining methods offer only the first two probabilistic moments. Computational analyses generally include composite materials models in their original heterogeneous multiscale configuration or may be related to some applications of the homogenization method, where the effective equivalent medium is determined. The first group of numerical simulations carried out dominantly with the Stochastic Finite Element Method (SFEM) [9,24] focuses on both material [1,14] and geometrical uncertainties [28] with Gaussian [7,8] and non-Gaussian parameters [19] treated as random variables [9] and fields [4,20]. The relevant studies deals with the linear elastic, viscoelastic [29], elastoplastic deformations [28] as well as with failure initiation [10], its propagation [22] and overall strength prediction [27] for various composites. Considering particular components of these composites one may of course notice polymers [5,28,29] also in the form of nanocomposites [30] and widely applied in civil engineering CFRPs [19,20] and various foams including especially metallic materials [1,21]. These are grouped into the following sub-classes: fiber-reinforced [16,23], particle-reinforced materials [7], laminates [19] as well as honeycomb [10] heterogeneous structures.

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An alternative approach is based on the homogenization method, connected with the same probabilistic methods, where equivalent statistically homogeneous medium is to be numerically determined [6]. Various deterministic counterparts are based on asymptotic homogenization method [2,18], characteristic deformations of the RVE under uniform extensions [11] implemented with the use of Finite Element Method [15] or using the direct variational estimates of homogenized material characteristics [3]. This alternative has also some novel ideas as an application of the asymptotic approach to the nanocomposites [30], for instance. Homogenization method has been and still is applied in the context of different composites sensitivities to their geometrical and material parameters taking into account their shape, topology and elastic properties contrast optimization [7,8,25].

The main objective of this work is to apply the novel iterative generalized stochastic perturbation technique [8] implemented together with the Finite Element Method [9,15] to calculate the first four probabilistic characteristics of the effective elastic properties for the rubber-carbon black particle reinforced composites. This very specific example has been chosen to analyze a composite with an incompressible matrix, extreme contrast of the elastic moduli for both components as well as Gaussian uncertainty in the particle radius [7]. This study is focused also on numerical error of the FEM solution itself obtained for different 3D solid finite elements types (tetrahedra and hexahedra) and density of the mesh increasing far beyond most popular numerical experiments as well as deterministic sensitivity of the effective characteristics in addition to the particle radius inside the cubic RVE. Probabilistic realization of this problem is based on the Weighted Least Squares Method (WLSM) approximation with the polynomial basis relating effective tensor components with this radius, where statistical optimization of its order is implemented. The weighting scheme follows Dirac function to associate the largest importance to the mean value of the input parameter being equal to the overall importance of all the remaining trial test points. This optimal approximation is further employed in the iterative perturbation-based SFEM, Monte-Carlo simulation and semi-analytical integration technique to determine expectations, coefficients of variations, skewness and kurtosis of the effective tensor components as the functions of the input coefficient of variation of the particle radius. This analysis is carried out to determine the validity ranges for the iterative perturbation method for homogenization problems with specific geometrical uncertainty inside the RVE.

2. Mathematical model of the composite

Let us consider a statistically heterogeneous and bounded continuum $\Omega \subset \Re^3$ with no initial stresses and strains consisting of spherical carbon particles statistically uniformly distributed into the homogeneous polymeric matrix (Fig. 1). We assume a perfect contact in-between these two constituents throughout all the interfaces and also a complete lack of any contact of any two neighboring particles. The rubber and polymer phases work both in the linear elastic regime and their material characteristics are uniquely defined by their Young moduli and Poisson ratios, which are given in a deterministic manner. We assume that the filler particles have random Gaussian size distribution defined by the expectation and standard deviation of their radii, namely $E[R]$ and $\sigma(R)$. These operators are traditionally defined as [1,13] (see Figs. 1 and 2)

$$E[R] = \int_{-\infty}^{+\infty} R\, p_R(x)\, dx, \tag{1}$$

and

$$\sigma(R) = \sqrt{Var(R)} = \left\{ \int_{-\infty}^{+\infty} (R - E[R])^2\, p_R(x)\, dx \right\}^{\frac{1}{2}}, \tag{2}$$

where $p_R(x)$ is the probability density function assumed to have the form

$$p_R(x) = \frac{1}{\sigma(R)\sqrt{2\pi}} \exp\left(-\frac{(x - E[R])^2}{2\sigma^2(R)} \right). \tag{3}$$

We use further also skewness and kurtosis classically introduced in probability theory in the following form (Monte–Carlo simulation explores a variety of estimators, whose accuracy depends on the few parameters):

$$\beta(R) = \frac{\mu_3(R)}{\sigma^3(R)}, \quad \kappa(R) = \frac{\mu_4(R)}{\sigma^4(R)} - 3, \tag{4}$$

which equal both to 0 for Gaussian variables and where

$$\mu_m(R) = \int_{-\infty}^{+\infty} (R - E[R])^m\, p_R(x)\, dx, \tag{5}$$

denotes the mth central probabilistic moment of the variable R for any natural number m. The main goal of further considerations is to determine the basic probabilistic material characteristics of the equivalent homogenized medium and we introduce for this purpose the Representative Volume Element (Fig. 1) consisting of a single rubber particle within the surrounding polymeric matrix in the form of a cube (due to the same importance of all directions related to Cartesian coordinates, which is affected by statistical isotropy of the matrix and the whole composite themselves). We determine numerically for this purpose the random displacement fields $u_i^{x_1}$, $u_i^{x_2}$, $u_i^{x_{12}}$ and random stress tensors $\sigma_{ij}^{x_1}$, $\sigma_{ij}^{x_2}$, $\sigma_{ij}^{x_{12}}$ satisfying three specific linear elasticity elliptic boundary–value problems – of uniaxial extension of the RVE (x_1), of uniaxial extension (x_2) and also of the biaxial extension of the RVE (x_{12}). We assume for the needs of numerical analysis that there are non-empty subsets of external boundaries of the domain Ω (with the dimensions $2\delta \times 2\delta \times 2\delta$), namely $\partial\Omega_\sigma$ and $\partial\Omega_u$, where the stress and displacement boundary conditions are defined.

According to the main idea of the generalized stochastic perturbation technique [13], we need to solve the entire set of the boundary value problems with the same boundary conditions and with additionally modified input random radius $R \equiv R^{(\zeta)}$, $\zeta = 1, \ldots, N$ to approximate the response function relating the effective tensor components with this parameter using some polynomial deterministic function. We look for the set of solutions to the boundary–differential equation systems describing static equilibrium around the mean value of this parameter, so that

$$\sigma_{ij}^{(\zeta)}(\mathbf{x};\omega) = C_{ijkl}\varepsilon_{kl}^{(\zeta)}(\mathbf{x};\omega), \tag{6}$$

$$\varepsilon_{kl}^{(\zeta)}(\mathbf{x};\omega) = \frac{1}{2}\left(\frac{\partial u_k^{(\zeta)}(\mathbf{x};\omega)}{\partial x_l} + \frac{\partial u_l^{(\zeta)}(\mathbf{x};\omega)}{\partial x_k} \right), \tag{7}$$

$$\sigma_{ij,j}^{(\zeta)}(\mathbf{x};\omega) = 0, \tag{8}$$

$$u_i^{(\zeta)}(\mathbf{x}) = \hat{u}_i(\mathbf{x}); \quad \mathbf{x} \in \partial\Omega_u, \tag{9}$$

$$\sigma_{ij}^{(\zeta)}(\mathbf{x};\omega)n_j = \tilde{t}_i^{(\zeta)}(\mathbf{x};\omega); \quad \mathbf{x} \in \partial\Omega_\sigma. \tag{10}$$

Then we follow the finite set of integral variational equations to get an appropriate numerical solution for the strain energy in the context of the Finite Element Method. It yields

$$\int_\Omega C_{ijkl}\varepsilon_{ij}^{(\zeta)}\,\delta\varepsilon_{kl}^{(\zeta)} d\Omega = \int_{\partial\Omega_\sigma} \tilde{t}_i \delta u_i^{(\zeta)} d(\partial\Omega), \tag{11}$$

where the left hand side of Eq. (11) corresponds to elastic behavior of the structure and the R.H.S. (Right Hand Side) is equivalent to the stress boundary conditions applied. It needs to be mentioned that indexing with respect to the RFM (Response Function Method)