A diversity of computer approaches in the homogenization of random composites

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Abstract

A review of the various numerical techniques relating to the homogenization of composites exhibiting random properties is the main aim of this paper. The simulation, spectral and perturbation-based computational techniques are contrasted below to demonstrate their major as well as minor points in determination of probabilistic moments for effective material tensors in various problems. Special attention is given to the existing and future possible application of symbolic computations and those carried out by the finite element method (FEM) commercial programs. As summarized here, the solution for the homogenization problem of random composites consists of a series of finite element analyses for the analogous boundary value problem on the same periodicity cell instead of a single cell problem analyzed in a deterministic situation. A combined application of symbolic and FEM programs is especially efficient in further numerical simulations of random composites and can be used in probabilistic sensitivity analyses for various homogenized composite structures.

Keywords: Composite materials; Homogenization technique; Probabilistic analysis; Finite element method

1. Introduction

Homogenization is an alternative method to traditional analytic and numerical analysis of composite materials and structures. The homogeneous effective material tensors determined algebraically or numerically in the cell problems solutions can be used instead of the original partially constant material characteristics to simplify further modeling. Analogous methodology finds an application in the case of random composites, where material properties and/or geometrical micro- and global parameters are introduced as random variables or fields [1]. Note that the randomness in physical problems is introduced when (a) a response has some random deviation and (b) the response is unknown. According to deterministic problems, computational methods form an inherent part, which influences probabilistic analysis. That is why classical simulation methodology together with spectral perturbation, as well as some symbolic numerical techniques are employed in such an analysis. A collection of most of the numerical methods in this area is the main issue of this paper in the context of parallel finite element method (FEM) and symbolic mathematical computations.

2. Deterministic homogenization problem formulation

Let us consider a periodic displacement function $u(y)$ being a solution of the following boundary value problem:

$$\begin{aligned} &\sigma_{ij,j} = -F_i(y);\ \ \mathbf{y} \in \Omega \\ &\sigma_{ij} = C_{ijkl}(y)\varepsilon_{kl}(\mathbf{u});\quad \mathbf{y} \in \Omega \\ &|\boldsymbol{\sigma}_N| = g(y);\ \ \mathbf{y} \in \Gamma_r\ r = 1,\ \ldots,\ m \end{aligned} \tag{1}$$

where m is the total number of various interface boundaries and Ω denotes the composite region. If the function $g(y)$ represents the additional differences of the elasticity tensor components for various constituents [2], the homogenization function $\chi^{\alpha\beta}$ for $\alpha,\ \beta = 1, 2$ in the plane strain is obtained. The variational form of Eq. (1) may be rewritten as follows for n various components in the composite:

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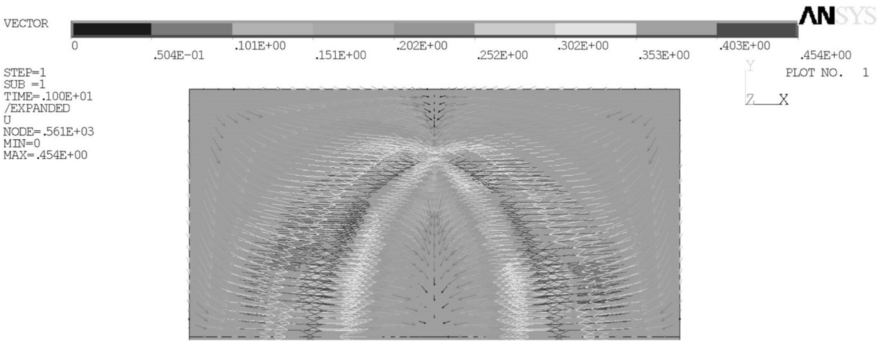

Fig. 1. Homogenization function χ^{11} for the upper half of the RVE.

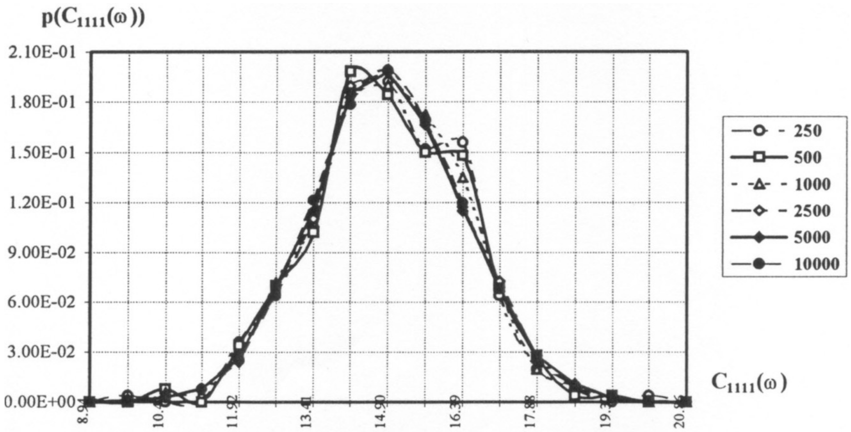

Fig. 2. Probability density function of the effective elasticity tensor.

$$-\sum_{r=1}^{m}\int_{\Gamma_r}\sigma_{ij}n_j u_i \mathrm{d}\Gamma+\sum_{a=1}^{n}\int_{\Omega_a}\sigma_{ij}\,\varepsilon_{ij}(\mathbf{u})\mathrm{d}\Omega=\int_{\Omega}\mathrm{f}_i\mathbf{u}_i\mathrm{d}\Omega \quad (2)$$

for $\mathbf{u}\in U: U=\left\{u_i;\, u_i\in\left[H^1_{per}(\Omega_i)\right]^3;\, [u_i]=0 \text{ on } \Gamma_r;\, r=1,\ \ldots,\ m\right\}$

Numerical solution of three homogenization tests is necessary to calculate effective characteristics in a plane equivalent to the transversal cross section of the fiber-reinforced composite, where the solution vector plot of a for the first problem (χ^{11}) is given in Fig. 1.

3. Monte-Carlo simulation

The Monte-Carlo simulation technique, being the oldest numerical approach in stochastic simulations, consists of an initial generation of all realizations for the random input, sequential solution of the given equilibrium problem, and final statistical estimation of the desired random output quantities. Since the effective elasticity tensor is calculated from two separate components, simulation can be done independently for the spatially averaged elastic properties and homogenizing stresses. One may implement the following combined statistical-analytical formulas for expectations and variances [2]:

$$\mathrm{E}\left[\mathbf{C}^{(\mathrm{eff})}(\omega)\right]=\mathrm{E}\left[\int_{\Omega}\mathbf{C}\mathrm{d}\mathbf{y}\right]+\frac{1}{M}\sum_{i=1}^{M}\int_{\Omega}\boldsymbol{\sigma}^{(i)}(\chi)\,\mathrm{d}\mathbf{y} \quad (3)$$

$$\mathrm{Var}\left(\mathbf{C}^{(\mathrm{eff})}(\omega)\right)=\mathrm{Var}\left(\int_{\Omega}\mathbf{C}\mathrm{d}\mathbf{y}\right)+\frac{1}{\mathrm{M}-1}\sum_{i=1}^{M}\left(\int_{\Omega}\boldsymbol{\sigma}^{(i)}(\chi)\mathrm{d}\mathbf{y}-\mathrm{E}\left[\int_{\Omega}\boldsymbol{\sigma}(\chi)\mathrm{d}\mathbf{y}\right]\right)^2+2\mathrm{Cov}\left(\int_{\Omega}\mathbf{C}\mathrm{d}\mathbf{y},\int_{\Omega}\boldsymbol{\sigma}^{(i)}(\chi)\mathrm{d}\mathbf{y}\right) \quad (4)$$

Furthermore, averaged elastic properties can be defined by the closed form probabilistic moments when material properties of the composite constituents are randomized only and then, simulation is really necessary only for the second component.

As shown in Fig. 2, the power of the Monte-Carlo approach is in providing an opportunity to exact practical computations of any order probabilistic moments and, especially, estimation of the output probability density function. Statistical estimation for this distribution function of the effective elasticity tensor component $C_{1111}^{(\mathrm{eff})}$ for the fiber-reinforced composite with round fiber and material data: $E[e_f] = 84.0\,\mathrm{GPa}$, $\sigma(e_f) = 8.4\,\mathrm{GPa}$ and $E[e_m] = 4.0\,\mathrm{GPa}$, $\sigma(e_m) = 0.4\,\mathrm{GPa}$ is shown for various numbers of random realizations. As can be seen, the simulations number 10^3 is sufficient to obtain satisfactory approximation and to show that the homogenized coefficient is Gaussian (third- and fourth-order probabilistic coefficients take the values 0 and 3).

4. Stochastic perturbation technique in homogenization

Analogously to spectral analysis, discussed further, some expansion is proposed for the random fields present in the problem. The following Taylor formula is applied to express elasticity tensor components:

$$\mathbf{C}(\mathbf{y};\omega) = \mathbf{C}^0(\mathbf{y}) + \sum_{\mathrm{i}=1}^{\mathrm{n}} \frac{\varepsilon^{\mathrm{i}}}{\mathrm{i}!}(\Delta\mathbf{b}(\omega))^{\mathrm{i}}\ \frac{\partial^{\mathrm{i}}\mathbf{C}(\mathbf{y})}{\partial\mathbf{b}^{\mathrm{i}}(\omega)} \tag{5}$$

The nth-order expansion of all parameters in variational formulation reflecting the homogenization cell problem leads to '$n+1$' deterministic equilibrium equations, where up to nth-order displacements, strains and stresses are calculated. They are finally combined into a single formula describing the random effective elasticity tensor as follows:

$$\mathbf{C}^{(\mathrm{eff})}(\omega) = \mathbf{C}^{(\mathrm{eff})0} + \sum_{\mathrm{i}=1}^{\mathrm{n}} \int_\Omega \frac{\varepsilon^{\mathrm{i}}}{\mathrm{i}!}(\Delta\mathbf{b}(\omega))^{\mathrm{i}} \frac{\partial\mathbf{C}^{(\mathrm{i})}(\mathbf{y})}{\partial\mathbf{b}^{\mathrm{i}}(\omega)}\,\mathbf{dy} + \sum_{\mathrm{i}=1}^{\mathrm{n}} \int_\Omega \frac{\varepsilon^{i}}{\mathrm{i}!}(\Delta\mathbf{b}(\omega))^{\mathrm{i}} \frac{\partial^{\mathrm{i}}\boldsymbol{\sigma}(\boldsymbol{\chi})(\mathbf{y})}{\partial\mathbf{b}^{\mathrm{i}}(\omega)}\,\mathbf{dy} \tag{6}$$

As already proven, see [2], the second-order methodology is effective in all those cases, where a dispersion of the input random variables represented by the coefficient of variation is less than or equal to 0.15. Computational implementation may be relatively easily done in any FEM program enhanced with the stochastic perturbation subroutines.

5. Stochastic spectral techniques

The basic idea of this methodology is to make some series representation of the basic random fields using the so-called Karhunen-Loeve method, a homogeneous or polynomial chaos representation [3]. According to this methodology, a random constitutive tensor can be represented by the following expression:

$$\mathbf{C}(\mathbf{y};\omega) = \mathbf{C}^0(\mathbf{y}) + \sum_{\mathrm{i}=1}^{\mathrm{n}} \sqrt{\lambda_{\mathrm{i}}}\xi_{\mathrm{i}}(\omega)\mathbf{C}^{(\mathrm{i})}(\mathbf{y}) \tag{7}$$

where ξ_{i} stands for standardized uncorrelated random variables, λ_{i} and $\mathbf{C}^{(\mathrm{i})}(\mathbf{y})$ are the eigenvalues and eigenvectors describing the elasticity tensor, and $\mathbf{C}^0$ is the additional mean value. An application of analogous expansions for the homogenization functions $\chi_\alpha^{\mathrm{kl}}$ results in the formula for the effective elasticity tensor, which can be proposed as

$$\mathbf{C}^{(\mathrm{eff})}(\omega) = \mathbf{C}^{(\mathrm{eff})0} + \sum_{\mathrm{i}=1}^{\mathrm{n}} \sqrt{\lambda_{\mathrm{i}}}\,\xi_{\mathrm{i}}(\omega) \int_\Omega \mathbf{C}^{(\mathrm{i})}\mathrm{d}(\mathbf{y}) + \sum_{\mathrm{i}=1}^{\mathrm{n}} \int_\Omega \sqrt{\lambda_i}\,\xi_{\mathrm{i}}(\omega)\boldsymbol{\sigma}^{(\mathrm{i})}(\boldsymbol{\chi})\mathbf{dy} \tag{8}$$

Note that $\boldsymbol{\sigma}^{(\mathrm{i})}(\boldsymbol{\chi})$ are obtained from the finite element solution for the eigenproblem on the representative volume element (RVE) with periodic boundary conditions. Also note that if small variations of random input in the perturbation method are not demanded, both spectral and perturbation methods need the first few components of the expansion to ensure satisfactory convergence of the results.

6. Algebraic approximations and bounds for the effective characteristics

In a more general approach when the information about a location and the total number of the fibers in the RVE is incomplete, the algebraic approximations of the homogenized properties are employed [4,5]. The upper bounds for the effective bulk and shear modulus are introduced, for instance, as follows:

$$\begin{cases} \sup\kappa = \left[\sum_{\mathrm{r}=1}^{\mathrm{N}} \mathrm{c}_r(\kappa_{\mathrm{u}} + \kappa_{\mathrm{r}})^{-1}\right]^{-1} - \kappa_{\mathrm{u}} \\ \sup\mu = \left[\sum_{\mathrm{r}=1}^{\mathrm{N}} \mathrm{c}_r(\mu_{\mathrm{u}} + \mu_{\mathrm{r}})^{-1}\right]^{-1} - \mu_{\mathrm{u}} \end{cases}$$

$$\text{where} \quad \begin{cases} \kappa_{\mathrm{u}} = \frac{4}{3}\mu_{\max} \\ \mu_{\mathrm{u}} = \frac{3}{2}\left(\frac{1}{\mu_{\max}} + \frac{10}{9\kappa_{\max}+8\mu_{\max}}\right)^{-1}. \end{cases} \tag{9}$$

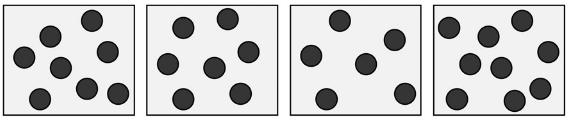

Fig. 3. Random samples of the representative volume element with multiple fibers.

Furthermore, lower bounds for the elasticity tensor are obtained with the same equations where κ_u, μ_u, κ_{max}, μ_{max} are replaced with κ_l, μ_l, κ_{min}, μ_{min}; c_r, $1 \leq r \leq n$ denote volume fractions of the composite components in the RVE. Note that they can be used in conjunction with Monte-Carlo analysis to determine probabilistic characteristics of the bounds in the case of elastic properties defined as random design parameters of the composite. The Monte-Carlo simulation implemented in MAPLE is used to generate a rectangular sample of the composite cross section (see Fig. 3), where the fiber's number is the Poisson random variable. Fibers are embedded in the RVE using the uniform distribution with no contact between each two entities, whilst elastic properties can be given by the Gaussian variables, for instance. Note that, also in the case of upper and lower bound, symbolic simulation, integral formulas for the probabilistic moments and derivation of the characteristic function are numerically available. This case, contrary to the previous methods, obeys the second kind of randomness, where the information about spatial distribution of the fibers or reinforcing particles is not available.

7. Concluding remarks and further perspectives

Therefore, a combined symbolic-FEM computational approach seems to be the most effective in homogenization of random composites with various types of uncertainties appearing in both material properties and its microgeometry. The symbolic computations are employed for either the generation of random spaces (used further for FEM-based random trials) or to derive an algebraic combination of various FEM solutions to get a description of the relevant probabilistic moments. Symbolic programs can be useful in a derivation of up to nth-order derivatives of the state parameters with respect to the input random variables. As shown in Fig. 3, symbolic computational programs can be used to generate random samples of the entire RVE, which can be further processed by the FEM-meshing procedures and structural analyses.

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