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Sensitivity and randomness in homogenization of periodic fiber-reinforced composites via the response function method

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ABSTRACT

The main issue this paper addresses is the derivation and implementation of a general homogenization method, including the simultaneous determination of sensitivity gradients and probabilistic moments of the effective elasticity tensor. This is possible with an application of the perturbation method based on Taylor expansion and with the effective modules method. The computational procedure is implemented using plane strain analysis carried out with the finite element method (program MCCEFF) and the symbolic computations system MAPLE. The sensitivity gradients and probabilistic moments are commonly determined on the basis of partial derivatives for the homogenized elasticity tensor, calculated using the response function method with respect to some composite parameters. They are subjected separately to a normalization procedure (in deterministic analysis) and the relevant algebraic combinations (for the stochastic case). This enriched homogenization procedure is tested on a periodic fiber-reinforced two component composite, where the material parameters are taken as design variables and then, the input random quantities. The results of computational analysis are compared against the results of the central finite difference approach in the case of sensitivity gradients determination as well as the direct Monte-Carlo simulation approach. This numerical methodology may be further applied not only in the context of the homogenization method, but also to extend various discrete computational techniques, such as Boundary/Finite element and finite difference together with various meshless methods.

1. Introduction

The variability (or random fluctuations) of elastic characteristics and geometrical dimensions of homogeneous as well as composite elements is a frequent problem in the design of new structures or materials and the inspection of existing ones. This variability in the design process is included during the optimization phase, where, with non-gradient or gradient techniques, the most optimal distribution (in FGM applications (Bhangale and Ganesan, 2006), for instance) or the best choice and contrast (for composites with two or more constituents) is sought. Such fluctuation in design parameters is taken into account a priori and almost always has a clearly deterministic character. On the other hand, experimental testing and a posteriori inspection of engineering structures return statistical or sometimes even stochastic information about the random spatial or spatial–temporal distribution in the material and/or geometrical (both micro- and macro-) parameters. Therefore, sensitivity analysis and probabilistic modeling are very similar from a quantitative point of view. This similarity is even more striking in numerical analysis when the perturbation method is applied to determine sensitivity coefficients or gradients

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with respect to some design parameters, as well as some basic probabilistic moments of structural response; those design parameters are treated as random input variables, fields or processes. The relation between sensitivity and probabilistic analysis appears even closer when we realize that, using higher than the second-order perturbation methodology, it is possible to calculate both higher-order sensitivities and higher-order probabilistic moments after minor changes in the algebraic formulas of the relevant definitions.

The problems raised above are of special importance in the area of composite materials, where not only single particular parameters but multiple characteristics of the same type and, furthermore, their composition may be a subject of such analysis. Even if such phenomena, such as delamination or soft matrix penetration by the rigid fibers typical for specific composites only, are neglected, the sensitivity or probabilistic analysis still has numerous parameters. The homogenization method has been discovered and extended to reduce the number of composite design parameters significantly by the introduction of effective characteristics using potential or complementary energy principles (Markovic and Ibrahimbegovic, 2006). Although this technique, in its modern version, is almost 40 years old (Bensoussan et al., 1978; Luciano and Willis, 2006), there are still some new ideas and applications, such as applications in food industry (Kanit, 2006), some composites made of wood (Lux, 2006), superconductors (Kamiński, 2005; Lefik and Schrefler, 1994), fully and partially saturated heterogeneous solids (Rohan et al., 2006). After fundamental discoveries concerning elastic, thermal and electric effective properties (Christensen, 1979; Milton, 2002), thermo-dynamic wave propagation (Zhang, 2007), various multiscale problems (Fish and Ghouali, 2001; Kamiński, 2005; Zhang, 2005), even for time-dependent cases by "equation free" approach (Samaey et al., 2006); a variety of materially nonlinear multi-component composites can be homogenized also (Castaneda and Suquet, 1998; Friebel et al., 2006; Idiart, 2006; Ma and Hu, 2006). Following numerous engineering applications, the strength of composites can be estimated by the homogenization method (Florence and Sab, 2006; Steeves and Fleck, 2006). Atomistic and nano levels appear to be the smallest resolutions (Clayton and Chung, 2006; Song and Youn, 2006), and some old methods have been revisited recently (Wang, 2006). A lot of attention is obviously paid to random composites (Jeulin and Ostoja-Starzewski, 2001; Kamiński, 2005; Luciano and Willis, 2006; Xu and Graham-Brady, 2005) because of an uncertainty in reinforcement location/shape and/or pore spatial distribution in matrices, and randomness in the components, physical and mechanical characteristics.

The homogenization method is sometimes connected with sensitivity analysis (Kamiński, 2005; Noor and Shah, 1993; Sigmund, 1994) and optimization (see the problem of a homogeneous plate with holes (Chellappa et al., 2004)). Independently, one may consider its usage in conjunction with probabilistic analysis using Monte-Carlo simulation (Cruz and Patera, 1995; Kamiński, 2005) or some spectral methods (Ghanem and Spanos, 1997; Xu and Graham-Brady, 2005) to homogenize random composites. Let us note that even if the mathematical apparatus has a strictly deterministic character, some issues, like the basic correlation dimension or the representativeness of the basic cell subjected to the homogenization process, are nevertheless discussed (Gitman et al., 2006; Kanit, 2006). Considering above it seems to be very difficult to formulate a single universal and general approach to the calculation of effective characteristics, where sensitivity gradients and probabilistic moments can be extracted from the same equations using similar algebra. The duality of sensitivity versus randomness is the main aim of the considerations included in this paper. The perturbation technique based on the nth-order Taylor expansion (Kamiński, 2005) is applied here in conjunction with the effective modules method (Bensoussan et al., 1978; Kamiński, 2005; Sanchez-Palencia, 1980) to determine practically any order of partial derivatives of the homogenized constitutive tensor. The composite subjected to this procedure is linearly elastic and transversely isotropic, where the elastic characteristics of the components are design parameters in the first problem and truncated Gaussian random variables in the second one. They are defined by mean values (in the case of sensitivity coefficients determination) or by the first two probabilistic moments (for the random spaces). The composite remains periodic in both cases in the sense that a long round fiber with constant radius has a periodic distribution in the plane transverse to the fiber directions; all the fibers are perfectly parallel. Material characteristics are the same in each cell for the sensitivity computations, and they have the same first two moments in each cell for random analysis to ensure the perfect periodicity of the composite. The key feature here is the response function reconstruction, where using multiple solutions of the deterministic homogenization problem, each effective tensor component is represented as a polynomial function of the design parameters or input random variables. This is in significant contradiction with previous applications of the perturbation technique, where zeroth- and higher-order equilibrium equations were derived and solved numerically (Kamiński, 2006; Kleiber, 1997). It should be underlined that the idea behind the response function approach is similar to the response surface method (RSM), known from reliability analysis (Xiu-Li and Melchers, 2002), where this function was assumed to be a quadratic polynomial, with or without the mixed terms expressing cross-correlations between various random inputs. Here, an nth-order polynomial function is proposed and implemented without any mixed terms, which reflects the case of a single random input variable. The symbolic computations package MAPLE (Abell and Braselton, 1994) is used here to effectively solve for the coefficients of this polynomial expression as well as to process the normalization of the sensitivity gradients and/or probabilistic moments of the homogenized tensor. With the application of symbolic computations, it is possible to insert the perturbation parameter ε into the polynomial expansion of the random structural response (which is represented by a homogenized tensor) and, furthermore, to calculate higher-order partial derivatives analytically. As it can be seen that this approach enables us to eliminate the limitations of the second-order perturbation technique, to join sensitivity analysis and probabilistic modeling, to shorten the entire computational process (related to Monte-Carlo simulation procedure) as well as to provide the computational process with a given a priori accuracy. Since the finite element method-based plane strain numerical analysis is the core of the solution of the homogenization problem, all error analysis procedures, including adaptivity, may be also included in this implementation (Matache et al., 2000). It is obvious that such a formulation for the implementation of the perturbation method can find a significant number of applications along with any discrete numerical techniques, including boundary elements, finite differences as well as meshless techniques.

2. Homogenization approach

The periodic fiber-reinforced composite structure in plane strain with linearly elastic and transversely isotropic components and random elastic characteristics is the scope of the considerations below. Let us denote the representative volume element (RVE) of Y as Ω; $Y \subset \Re^2$ denotes the section of this composite in the $x_3 = 0$ plane and is constant along the x_3 axis, which is parallel to the fiber direction (see Figs. 1 and 2).

Let us assume that the region Ω contains two perfectly bonded, coherent and disjoint subsets Ω_1 (fiber) and Ω_2 (matrix), and let the scale between corresponding geometrical diameters of Ω and Y be described by the small parameter $\varepsilon > 0$. The parameter ε indexes all the tensors written for the geometrical scale of Ω, and let $\partial\Omega$ denote the external boundary of the Ω, while $\partial\Omega_{12}$ is the interface boundary between the Ω_1 and Ω_2 regions.

Further, it is assumed that the composite is periodic in a random sense if, for an additional ω belonging to a suitable probability space, there exists such a homothety that transforms Ω onto the entire composite Y. Next, let us introduce two different coordinate systems: $\mathbf{y} = (y_1, y_2)$ at the micro scale of the composite and $\mathbf{x} = (x_1, x_2)$ at the macroscale. Let us consider any periodic state function F defined on the region Y; this function can be expressed as

$$F^{\varepsilon}(\mathbf{x}) = F\left(\frac{\mathbf{x}}{\varepsilon}\right) = F(\mathbf{y}). \tag{1}$$

This expression makes it possible to describe the macro functions (connected with the macroscale of a composite) in terms of micro ones and vice versa. The elasticity coefficients can be defined, for instance, as

$$C^{\varepsilon}_{ijkl}(\mathbf{x}) = C_{ijkl}(\mathbf{y}), \tag{2}$$

fulfilling the symmetry, boundedness and ellipticity conditions. Moreover, for any of the composite constituents, this tensor is defined as

$$C_{ijkl}(x) = e(x)\left\{\delta_{ij}\delta_{kl}\frac{v(x)}{(1+v(x))(1-2v(x))} + (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\frac{1}{2(1+v(x))}\right\}. \tag{3}$$

If we introduce

$$A_{ijkl}(\mathbf{x}) = \delta_{ij}\delta_{kl}\frac{v(\mathbf{x})}{(1+v(\mathbf{x}))(1-2v(\mathbf{x}))} + (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\frac{1}{2(1+v(\mathbf{x}))}, \tag{4}$$

then the partial derivatives of the elasticity tensor with respect to Young's modulus in the homogeneous material is equal to

$$\frac{\partial C_{ijkl}}{\partial e} = \delta_{ij}\delta_{kl}\frac{v}{(1+v)(1-2v)} + (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\frac{1}{2(1+v)} = A_{ijkl} \tag{5}$$

and any higher-order partial derivatives equal 0.

The effective tensor $C^{(eff)}_{ijkl}$ is introduced as a tensor that replaces C^{ε}_{ijkl} with $C^{(eff)}_{ijkl}$ in the following equilibrium equations:

$$C^{\varepsilon}_{ijkl}\varepsilon_{kl}(\mathbf{u}^{\varepsilon}) + f_i = 0, \quad \mathbf{x} \in \Omega. \tag{6}$$

$$\varepsilon_{ij}(\mathbf{u}^{\varepsilon}) = \frac{1}{2}(u^{\varepsilon}_{i,j} + u^{\varepsilon}_{j,i}), \quad \mathbf{x} \in \Omega, \tag{7}$$

$$C^{\varepsilon}_{ijkl}(\mathbf{x}) = \chi_1(\mathbf{x})C^{(1)}_{ijkl} + (1-\chi_1(\mathbf{x}))C^{(2)}_{ijkl}, \tag{8}$$

where $\mathbf{u}^0$ is obtained as a solution for a weak limit of $\mathbf{u}^{\varepsilon}$ with $\varepsilon \to 0$ and where the characteristic function is defined as

$$\chi_1(\mathbf{x}) = \begin{cases} 1, & \mathbf{x} \in \Omega_1, \\ 0, & \mathbf{x} \in \Omega_2, \end{cases} \tag{9}$$

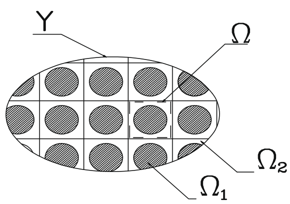

Fig. 1. Periodic fiber reinforced composite, perpendicular cross-section.

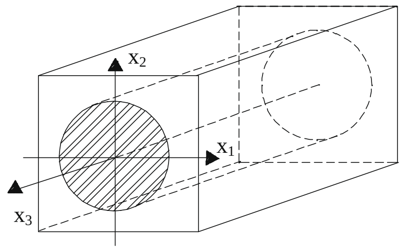

Fig. 2. Periodic fiber reinforced composite, aerial view of the cell.

with the boundary conditions

$$\mathbf{u}^{\varepsilon} = 0, \quad \mathbf{x} \in \partial\Omega. \tag{10}$$

The homogenization problem is to find the limit of the solution $\mathbf{u}^{\varepsilon}$ with ε tending to 0. For this purpose, let us consider a bilinear form $a^{\varepsilon}(\mathbf{u},\mathbf{v})$, defined as follows:

$$a^{\varepsilon}(\mathbf{u},\mathbf{v}) = \int_{\Omega} C_{ijkl}\left(\frac{\mathbf{x}}{\varepsilon}\right)\varepsilon_{ij}(\mathbf{u})\varepsilon_{kl}(\mathbf{v})d\Omega \tag{11}$$

and a following linear form

$$L(\mathbf{v}) = \int_{\Omega} f_i v_i \, d\Omega + \int_{\partial\Omega_{\sigma}} p_i v_i \, d(\partial\Omega). \tag{12}$$

A variational statement equivalent to the equilibrium problem (6)–(10) is to find an $\mathbf{u}^{\varepsilon}$ fulfilling the following equation:

$$a^{\varepsilon}(\mathbf{u}^{\varepsilon},\mathbf{v}) = L(\mathbf{v}) \tag{13}$$

for any kinematic admissible displacement $\mathbf{v}$. Let us denote for any $\mathbf{u}$,$\mathbf{v}$ periodic on Ω:

$$a_y(\mathbf{u},\mathbf{v}) = \int_{\Omega} C_{ijkl}(\mathbf{y})\varepsilon_{kl}(\mathbf{u})\varepsilon_{ij}(\mathbf{v})d\Omega, \tag{14}$$

and let us introduce a homogenization function $\chi_{(ij)k} \in P(\Omega)$ as a solution for the local problem on a periodicity cell:

$$a_y((\chi_{(ij)k} + y_j\delta_{ki})\mathbf{n}_k, \mathbf{w}) = 0 \tag{15}$$

for any periodic $\mathbf{w}$; $\mathbf{n}_k$ is the unit coordinate vector. Now, we are looking for the solution $\mathbf{u}^{\varepsilon}$ that converges weakly

$$\mathbf{u}^{\varepsilon} \to \mathbf{u} \tag{16}$$

if the tensor $C^{\varepsilon}_{ijkl}(\mathbf{y})$ is Ω-periodic. Solution $\mathbf{u}$ is the unique one for the boundary value problem

$$\mathbf{u} \in V : \; D(\mathbf{u},\mathbf{v}) = L(\mathbf{v}) \tag{17}$$

for any admissible displacement $\mathbf{v}$ and

$$D(\mathbf{u},\mathbf{v}) = \int_{Y} D_{ijkl}\varepsilon_{kl}(\mathbf{u})\varepsilon_{ij}(\mathbf{v})dY, \tag{18}$$

where

$$D_{ijkl} = \frac{1}{|\Omega|} a_y((\chi_{(ij)p} + y_i\delta_{pj})\mathbf{n}_p, (\chi_{(kl)q} + y_l\delta_{qk})\mathbf{n}_q). \tag{19}$$

Hence, an equivalent homogeneous orthotropic elastic material is obtained, characterized by the tensor

$$C^{(eff)}_{ijkl} = \frac{1}{|\Omega|}\int_{\Omega}(C_{ijkl}(\mathbf{y}) + C_{ijmn}(\mathbf{y})\varepsilon_{mn}(\chi_{(kl)}(\mathbf{y})))d\Omega. \tag{20}$$

Finally, let us define two fundamental problems P_1 and P_2, the solution of which will be found next:

P_1: Find $\partial^{\alpha}C^{(eff)}_{ijkl}/\partial\mathbf{h}^{\alpha}$ for $\alpha \in N$, where $\mathbf{h} = \mathbf{h}(\mathbf{x}) = \{e_1, e_2\}$ or $\mathbf{h} = \mathbf{h}(\mathbf{x}) = \{v_1, v_2\}$, where

$$\mathbf{h}(\mathbf{x}) = \chi_1(\mathbf{x}) \; h_1 + (1 - \chi_1(\mathbf{x}))h_2. \tag{21}$$

P_2: Find $\mu_{\alpha}(C^{(eff)}_{ijkl})$ where $\alpha \in N$, $\mathbf{b}(\mathbf{x};\omega) = \{e_1(\omega), e_2(\omega)\}$ or $\mathbf{b}(\mathbf{x};\omega) = \{v_1(\omega), v_2(\omega)\}$, where

$$\mu_{\alpha}(\mathbf{b}(\mathbf{x};\omega)) = \chi_1(\mathbf{x})\mu_{\alpha}(b_1(\omega)) + (1 - \chi_1(\mathbf{x}))\mu_{\alpha}(b_2(\omega)), \tag{22}$$

with $\mu_{\alpha}(\mathbf{b}(\mathbf{x};\omega))$ being αth-order central probabilistic moment of $\mathbf{b}(\mathbf{x};\omega)$.

3. Sensitivity analysis in the homogenization of the periodic fiber-reinforced composites

The main aim of the structural design sensitivity analysis of composites is to analyze the interrelations between their state functions and the input design parameters according to variations in these parameters (Ghanem and Spanos, 1997; Kamiński, 2006; Kamiński, 2005; Kleiber, 1997). It is necessary to represent the general composite structure response in terms of displacements, stresses, temperatures, heat and electromagnetic fluxes, and vibrations in terms of volume fractions, spatial distribution and the shape of the reinforcement, layer thicknesses, and material characteristics of the constituents and their contrasts. In contrast to homogeneous structures and materials, even linear elastic problems become complex in terms of such an analysis. As it is known, the sensitivity gradients or coefficients are not the final subject of any computational analysis; generally, they are determined for further usage in an optimization process (Haftka and Gürdal, 1992) for the engineering composite. The sensitivity analysis can be also used in conjunction with the homogenization method frequently used in the analysis of composite materials. It can be done analytically for algebraic approximation of upper and lower bounds on the homogenized tensor components and numerically, when the cell boundary value problem is solved using some plane strain programs (some mixed analytical-numerical approaches are also available (Kamiński, 2006)).

The following functional may be introduced to represent the static structural response of the homogenized system with N degrees of freedom:

$$\Im(\mathbf{C}^{(eff)}(h^d);h^d) = G\lfloor q_\alpha(\mathbf{C}^{(eff)}(h^d)), \mathbf{h}^{(eff)}(h^d), h^d\rfloor, \quad d=1,2,\ldots,D, \;\; \alpha=1,2,\ldots,N, \tag{23}$$

G stands for a given function of its arguments, h^d is a design variables D-dimensional vector and q_α is the vector of the nodal structural response. There holds of course that

$$K_{\alpha\beta}(\mathbf{C}^{(eff)}(h^d);h^d)q_\beta(\mathbf{C}^{(eff)}(h^d);h^d) = Q_\alpha(\mathbf{C}^{(eff)}(h^d);h^d). \tag{24}$$

The stiffness matrix $K_{\alpha\beta}$ and the load vector Q_α are functions of the design variables, so that the solution vector $\mathbf{q}$ is an implicit function of these variables as well. Usually, the main purpose of the SDS numerical analysis is to determine the sensitivity gradient $\partial\Im/\partial h^d$ from

$$\Im^{,d} = G^{,d} + G_{,\alpha}q_\alpha^{,d}, \tag{25}$$

where $(.)^{,d}$ and $(.)_{,\alpha}$ are the first partial derivatives with respect to the dth design variable and the αth nodal displacement, respectively. The differentiation process is decisively more complicated here than for homogeneous structures, because the effective material parameters are used, which are the functions of the initial material parameters of the composite constituents. When the location of some support in a composite structure is a design parameter – it does not influences effective parameter; however, it strongly affects the state functions and the additional functionals. There is no doubt, that the crucial difference between this approach and classical SDS analysis is the determination of the sensitivity gradients for the effective elasticity tensor with respect to material or the other parameters of the composite constituents, which follows the relation

$$K_{\alpha\beta}\frac{\partial q_\beta}{\partial \mathbf{C}^{(eff)}}\frac{\partial \mathbf{C}^{(eff)}}{\partial h^d} = \frac{\partial Q_\alpha}{\partial \mathbf{C}^{(eff)}}\frac{\partial \mathbf{C}^{(eff)}}{\partial h^d} - \frac{\partial K_{\alpha\beta}}{\partial \mathbf{C}^{(eff)}}\frac{\partial \mathbf{C}^{(eff)}}{\partial h^d}q_\beta, \tag{26}$$

where $C^{(eff)}$ substitutes $\mathbf{h}^{(eff)}$. Thus, the sensitivity coefficients of the homogenized elasticity tensor components with respect to the vector $\mathbf{h}$ can be calculated as

$$\frac{dC^{(eff)}_{ijpq}}{d\mathbf{h}} = \frac{1}{|\Omega|}\int_\Omega \frac{\partial C_{ijpq}}{\partial \mathbf{h}}d\Omega + \frac{1}{|\Omega|}\int_\Omega \frac{\partial C_{ijkl}}{\partial \mathbf{h}}\varepsilon_{kl}(\boldsymbol{\chi}_{(\mathrm{pq})})d\Omega + \frac{1}{|\Omega|}\int_\Omega C_{ijkl}\frac{\partial \varepsilon_{kl}(\boldsymbol{\chi}_{(\mathrm{pq})})}{\partial \mathbf{h}}d\Omega. \tag{27}$$

Let us note here that if the design variables vector $\mathbf{h}$ corresponds to the elasticity constants of a given constituent, a result presented in Ponte Castañeda and Suquet (1998)) avoids the complication of having to differentiate the local field.

Contrary to all methods available from the literature of the problem, now the differentiation process is carried out in a fully analytical manner – the components of the spatially averaged elasticity tensor are differentiated according to the formulas displayed below. The analytical function of the second component in Eq. (27) with respect to a single design parameter is approximated first with the response function method. The interval around the mean value of a given design parameter is divided into a finite number of smaller intervals of equal length. Next, the multiple solutions for these inputs allow for a polynomial approximation of the response function, i.e. elasticity tensor components; further derivations are rather easy and straightforward.

Henceforth, let us focus on the partial derivatives of the spatially averaged elasticity tensor for the fiber-reinforced composite. Let us examine first the case where $b \equiv R$. It is apparent that

$$\frac{\partial\langle C_{ijkl}\rangle_\Omega}{\partial R} = \frac{2\pi R}{L^2}\delta_{ij}\delta_{kl}\left\{\frac{\nu_1 e_1}{(1+\nu_1)(1-2\nu_1)} - \frac{\nu_2 e_2}{(1+\nu_2)(1-2\nu_2)}\right\} + \frac{2\pi R}{L^2}(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})\left\{\frac{e_1}{2(1+\nu_1)} - \frac{e_2}{2(1+\nu_2)}\right\} \tag{28}$$

and also

$$\frac{\partial^2\langle C_{ijkl}\rangle_\Omega}{\partial R^2}=\frac{2\pi}{L^2}\delta_{ij}\delta_{kl}\left\{\frac{\nu_1 e_1}{(1+\nu_1)(1-2\nu_1)}-\frac{\nu_2 e_2}{(1+\nu_2)(1-2\nu_2)}\right\}+\frac{2\pi}{L^2}(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})\left\{\frac{e_1}{2(1+\nu_1)}-\frac{e_2}{2(1+\nu_2)}\right\} \tag{29}$$

Let us note that when we replace πR^2 with the term πcd, the periodicity cell of the composite reinforced with the fibers with elliptical cross-section can be analyzed (the variables 'c' and 'd' denote the major semi-axes of this section). Furthermore, the linear dependence of $\langle C_{ijkl}\rangle_\Omega$ and c, d shows that any higher than the first-order partial derivatives equal 0. Thus, $b \equiv R$ is a more interesting case in view of the probabilistic analysis. Let us randomize next the Young modulus of the fiber; then, for $b \equiv e_1$:

$$\frac{\partial\langle C_{ijkl}\rangle_\Omega}{\partial e_1}=\frac{\pi R^2}{L^2}\delta_{ij}\delta_{kl}\frac{\nu_1}{(1+\nu_1)(1-2\nu_1)}+\frac{\pi R^2}{L^2}(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})\frac{1}{2(1+\nu_1)} \tag{30}$$

with any higher-order partial derivatives equal to 0. The case of $b \equiv e_2$ can be derived easily by changing the lower indices in the above two relations as well as in the volumetric phase factor in the first one only. The differentiation with respect to the Poisson ratio leads to the following conclusions:

$$\frac{\partial\langle C_{ijkl}\rangle_\Omega}{\partial \nu_1}=\frac{\pi R^2 e_1}{L^2}\left\{\frac{\delta_{ij}\delta_{kl}}{(1+\nu_1)(1-2\nu_1)}\left(1-\frac{\nu_1}{(1+\nu_1)}+\frac{2\nu_1}{(1-2\nu_1)}\right)-(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})\frac{1}{2(1+\nu_1)^2}\right\} \tag{31}$$

and

$$\begin{aligned}\frac{\partial^2\langle C_{ijkl}\rangle_\Omega}{\partial \nu_1^2}=\frac{\pi R^2 e_1}{L^2}&\left\{\frac{\delta_{ij}\delta_{kl}}{(1+\nu_1)(1-2\nu_1)}\left(-\frac{2}{(1+\nu_1)}+\frac{4}{(1-2\nu_1)}+\frac{2\nu_1}{(1+\nu_1)^2}-\frac{4\nu_1}{(1+\nu_1)(1-2\nu_1)}+\frac{8\nu_1}{(1-2\nu_1)^2}\right)\right.\\ &\left.+(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})\frac{8}{(1+\nu_1)(1-2\nu_1)}\right\}\end{aligned} \tag{32}$$

Of course, as in the case of the Young moduli, first two partial derivatives of the spatially averaged elasticity tensor with respect to the matrix Poisson ratio can be obtained by a change of the volume phase factor to the one relevant for the matrix region and by the additional replacement of all lower indices equal to '1'. Let us also note that

$$\frac{\partial^2\langle C_{ijkl}\rangle_\Omega}{\partial \nu_1 \partial \nu_2}=0, \tag{33}$$

and, therefore, no correlation would result from this term in perturbation-based analysis. Finally, let us note that this analytical (or semi-analytical in conjunction with the FEM) technique may be used for a modeling of the composites with the anisotropic components, however in such a general case (1) quite different definition of the elasticity tensor is necessary and (2) the number of the design (input random parameters) increase significantly. The homogenization procedure itself becomes more complicated because of the essential change in the stress boundary conditions contained in Table 1 at least.

Furthermore, let us note that the sensitivity of $C^{(eff)}_{ijpq}$ components with respect to the fiber shape can be derived analogously to the traditional analysis in that area. However, the final equations for homogenized constitutive parameters for various composites have decisively more complicated forms and can be shown only if the homogenization function can be derived analytically (Sigmund, 1994). Since the sensitivity coefficients should be comparable with each other to distinguish the crucial design parameter, the analyzed function is normalized with respect to the derivation parameter. In case of the homogenized elasticity tensor derivatives, the following normalization rule is applied:

$$\left(\frac{dC^{(eff)}_{ijpq}}{d\mathbf{h}}\right)_{\text{scaled}}=\frac{\partial C^{(eff)}_{ijpq}}{\partial \mathbf{h}}\cdot\frac{h}{C^{(eff)}_{ijpq}(h)}\ \text{(no summation over } j,i,p,q), \tag{34}$$

which makes it possible to establish qualitatively and quantitatively the most influential parameters.

4. Perturbation analysis based on Taylor expansion

Let us introduce the random variable $b(\omega)$ and its probability density function, $p(b)$. The expected value and mth-order central probabilistic moment are defined as (Feller, 1965)

$$E[b] \equiv b^0=\int_{-\infty}^{+\infty} bp(b)db \tag{35}$$

and

$$\mu_m(f(b))=\int_{-\infty}^{+\infty}(f(b)-E[f(b))^m p(b)db. \tag{36}$$

The basic idea of the stochastic perturbation approach is to expand all the input variables and all the state functions of the given problem via Taylor series about their spatial expectations using some small parameter $\varepsilon > 0$. In the case of random function $f(b)$, the following expression is employed:

$$e = e^0 + \sum_{n=1}^{\infty} \frac{1}{n!} \varepsilon^n \frac{\partial^n e}{\partial b^n} (\Delta b)^n, \tag{37}$$

where

$$\Delta b = b - b^0 \tag{38}$$

is the first variation of b about its expected value. The symbol $(.)^0$ represents the function value (.) taken at the expectation b^0, while $(.)^{,b}$ denotes the first partial derivative with respect to b evaluated at b^0. Let us derive the expected values of any random state function $f(b)$ by its expansion via Taylor series with a given small parameter ε as follows (Kamiński, 2005; Vanmarcke, 1983):

$$E[f(b)] = \int_{-\infty}^{+\infty} f(b)p(b)db = \int_{-\infty}^{+\infty} \left(f^0 + \sum_{n=1}^{\infty} \frac{1}{n!} \varepsilon^n \frac{\partial^n f}{\partial b^n} \Delta b^n \right) p(b)db = f^0 + \sum_{n=1}^{\infty} \frac{\varepsilon^n}{n!} \int_{-\infty}^{+\infty} \frac{\partial^n f}{\partial b^n} \Delta b^n p(b)db. \tag{39}$$

This power expansion is valid only if the state function $f(b)$ is analytic with respect to ε, and the Taylor series converge; any criteria of convergence should include the magnitude of the perturbation parameter (which is taken as equal to 1 in numerous practical computations). That is why, contrary to the previous analyses in this area (Kamiński, 2005), the quantity ε is treated as the expansion parameter, and it is included explicitly in all further derivations demanding analytical expressions. Numerical studies performed in the next section demonstrate the influence of this parameter on basic probabilistic moments and characteristics in various orders of the perturbation methodology – all the moments are obtained in the form of polynomials of the additional order with respect to ε.

Obviously, from the numerical point of view, the expansion provided above is carried out for the summation over a finite number of components, and the natural number N bounding this expansion must guarantee a satisfactory precision of the relevant probabilistic moments approximation. It can be done for the expected values and the variances by introducing the following statistical error measures:

- For the expectations

$$\forall_{\delta_1 \in \mathfrak{R}^+} \exists_{N_1 \in N} |E[f_{N_1}(b)] - E[\tilde{f}(b)]| \leqslant \delta_1. \tag{40}$$

- For the variances

$$\forall_{\delta_2 \in \mathfrak{R}^+} \exists_{N_2 \in N} |Var(f_{N_2}(b)) - Var(\tilde{f}(b))| \leqslant \delta_2. \tag{41}$$

The real positive numbers δ_1 and δ_2 denote the admissible errors during the determination of the expectations and variances. Natural quantities N_1 and N_2 correspond to the orders of perturbation resulting in the desired accuracy; the maximum of these two numbers fulfils satisfactory accuracy conditions if only these first two moments are to be computed, where (Bendat and Piersol, 1971)

$$E[\tilde{f}(b)] = \lim_{L\to\infty} \frac{1}{L} \sum_{i=1}^{\infty} \tilde{f}_i(b) \tag{42}$$

and

$$Var(\tilde{f}(b)) = \lim_{L\to\infty} \frac{1}{L-1} \sum_{i=1}^{\infty} (\tilde{f}_i(b) - E[\tilde{f}(b)])^2. \tag{43}$$

L is the total number of random trials in the statistical verification of the estimators for the random function $f(b)$. As it is shown, sufficiently accurate modelling of the moments by the perturbation technique needs initial the Monte-Carlo simulation computations to determine the optimal order of the perturbation for a given boundary value or transient problem.

When higher-order terms are necessary (because of a great random deviation of the input random variable about its expected value), Eq. (39) can be transformed for symmetric probability density functions into the series

$$E[f(b)] = f^0(b) + \frac{1}{2}\varepsilon^2 f^{,bb}(b)\mu_2(b) + \frac{1}{4!}\varepsilon^4 f^{,bbbb}(b)\mu_4(b) + \frac{1}{6!}\varepsilon^6 f^{,bbbbbb}(b)\mu_6(b) + \cdots + \frac{1}{2m!}\varepsilon^{2m} \frac{\partial^{2m} f(b)}{\partial b^{2m}} \mu_{2m}(b)+, \tag{44}$$

where all terms with odd orders are equal to 0. With such an extension of the random output, any desired efficiency of the expected values as well as higher probabilistic moments can be achieved by an appropriate choice of the parameters m and ε, corresponding to the input probability density function (PDF) type, relations between the probabilistic moments, acceptable error of the computations, etc. Analogously to Eq. (39), it is possible to derive the formulas describing higher-order moments, especially in all those cases where m is given. The recursive formula for the central mth-order probabilistic moment in the 10^{th}-order approximation can be determined as

$$\mu_m(f(b)) = \int_{-\infty}^{+\infty} \left(f^0(b) + \sum_{i=1}^{n} \frac{\varepsilon^i}{i!} \Delta b^i \frac{\partial^i f}{\partial b^i} - E[f(b)] \right)^m p(b)db. \tag{45}$$

Let us note that the essential part of the computational implementation of the stochastic perturbation technique is the numerical determination of the partial derivatives of the response function $f(b)$ w.r.t. the random parameter b. Although this differentiation has a purely deterministic character, an extraction of those derivatives from equilibrium equations of increasing order may be very complex. The number of derivatives of various orders systematically increases together with the order of an equation, so the idea of the response function is explored here. Analogously to the sensitivity gradients investigations, the multiple solutions to the homogenization problem around the expected value of random parameter enable us to build analytical polynomial approximations of the effective parameters w.r.t. the input random variable. The coefficients in this polynomial approximation are constant real numbers, so further determination of $\mu_m(C_{ijkl}^{(eff)})$ is rather trivial. Application of such a function, as well as generalization of the upper bound on the perturbation order to any natural number, are the crucial differences between this approach and its previous applications, cf. (Kamiński, 2005).

5. Computational implementation

5.1. Finite element method in homogenization of the fiber-reinforced composite

Let us introduce the following approximation of the homogenization functions $\chi_{(rs)i}^m$ at any point of the considered continuum Ω, for any solution necessary in the response function approximation ($m = 1,\ldots,M$), in terms of a finite number of generalized coordinates $q_{(rs)\alpha}^m$ and shape functions $\varphi_{i\alpha}$ (Bathe, 1996; Kamiński, 2005; Zienkiewicz and Taylor, 2005)

$$\chi_{(rs)i}^m = \varphi_{i\alpha} q_{(rs)\alpha}^m, \quad i,r,s = 1,2, \quad \alpha = 1,\ldots,N, \tag{46}$$

the shape functions remain the same for any approximation test indexed by m. The strain tensor $\varepsilon_{ij}(\chi_{(rs)}^m)$ as well as stress tensor $\sigma_{ij}(\chi_{(rs)}^m)$ are now discretized as

$$\varepsilon_{ij}(\chi_{(rs)}^m) = B_{ij\alpha} q_{(rs)\alpha}^m, \tag{47}$$

$$\sigma_{ij}(\chi_{(rs)}^m) = C_{ijkl}^m \varepsilon_{kl}(\chi_{(rs)}^m) = C_{ijkl}^m B_{kl\alpha} q_{(rs)\alpha}^m, \tag{48}$$

where $B_{kl\alpha}$ represents the shape functions derivatives matrix (no summation on m appears at the right hand side). There holds

$$\int_\Omega \delta\chi_{(rs)i,j}^m C_{ijkl}^m \chi_{(rs)k,l}^m \, d\Omega = \int_{\Gamma_{12}} \delta\chi_{(rs)i}^m [F_{(rs)i}^m]|_{\Gamma_{12}} d\Gamma \quad (\text{no sum on } r,s,m). \tag{49}$$

Next, let us define the global stiffness matrix as

$$K_{\alpha\beta}^m = \sum_{e=1}^{E} K_{\alpha\beta}^{(e)m} = \sum_{e=1}^{E} \int_{\Omega_e} C_{ijkl}^m B_{ij\alpha} B_{kl\beta} \, d\Omega. \tag{50}$$

Introducing this matrix into the virtual work equation (56) and minimizing it with respect to the generalized coordinates, we arrive at

$$K_{\alpha\beta}^m q_{(rs)\beta}^m = Q_{(rs)\alpha}^m, \tag{51}$$

where $Q_{(rs)\alpha}^m$ is the external load vector, which includes the stress boundary conditions applied along the interface (if only fiber and matrix are perfectly bonded) in the following form:

$$\sigma_{ij}(\chi_{(pq)}^m) n_j = \lfloor C_{ijpq}^m \rfloor n_j = F_{(pq)i}^m, \quad \mathbf{x} \in \Gamma_{12}, \tag{52}$$

where n_j is the component of the unit vector normal to the fiber–matrix boundary and directed to the fiber interior, while $[f]$ denotes the difference of the function f values

$$[f] = f^{(2)} - f^{(1)}. \tag{53}$$

The stress boundary conditions corresponding to different homogenization functions are specified in Table 1, so that to compute the function χ_{11}^m we apply the boundary forces with the horizontal components $F_{(pq)1}^m$ and vertical components $F_{(pq)2}^m$ given in the first column.

Having computed in the similar manner all the homogenization function components, i.e. χ_{11}^m, χ_{12}^m and χ_{22}^m the final determination of the homogenized elasticity tensor proceeds M times according to the formula (54).

$$C_{ijkl}^{(eff)m} = \frac{1}{|\Omega|} \int_\Omega (C_{ijkl}^m(\mathbf{y}) + C_{ijpq}^m(\mathbf{y}) \varepsilon_{pq}^m(\chi_{(kl)}(\mathbf{y}))) d\Omega. \tag{54}$$

It should be underlined that taking into account the interface phenomena in engineering composites, the fiber and matrix boundaries may have somewhat different contours (due to the lack of contact between the components), which may be the result of composite processing thermal stresses. Finally, let us note that to ensure the symmetry conditions on the periodicity cell quarter, the orthogonal displacements and rotations for every nodal point belonging to the external boundaries of Ω are fixed.

Table 1
The components of forces $F^m_{(pq)i}$

	χ^m_{11}	χ^m_{12}	χ^m_{22}
$F^m_{(pq)1}$	$C^{(2)m}_{1111} - C^{(1)m}_{1111}$	$C^{(2)m}_{1212} - C^{(1)m}_{1212}$	$C^{(2)m}_{1122} - C^{(1)m}_{1122}$
$F^m_{(pq)2}$	$C^{(2)m}_{2211} - C^{(1)m}_{2211}$	$C^{(2)m}_{1212} - C^{(1)m}_{1212}$	$C^{(2)m}_{2222} - C^{(1)m}_{2222}$

5.2. Response function for the effective elasticity tensor approximation

As shown during derivation of equations for the generalized perturbation based approach, one of the most complicated issues is numerical determination of up to nth-order partial derivatives of the structural response function with respect to the randomized parameter. It is possible to determine this function first by multiple solutions of the boundary value problem around the expectation of the random parameter to complete this task. The response function for each component of the homogenized tensor is built up from uniform symmetric discretization in the neighborhood of this expectation, with equidistant intervals. A set of classical deterministic re-computations of the homogenized tensor components leads to the final formation of the responses function for all $C^{(eff)}_{\alpha\beta\gamma\delta}$. That is why we consider further a problem of the unknown response function approximation by the following polynomial of $n-1$ order:

$$C^{(eff)}_{\alpha\beta\gamma\delta} = A_1^{\alpha\beta\gamma\delta} b^{n-1} + A_2^{\alpha\beta\gamma\delta} b^{n-2} + \cdots + A_n^{\alpha\beta\gamma\delta} b^0, \tag{55}$$

having the values of this function determined computationally for n different arguments. With this representation, the algebraic system of equations is formed

$$\begin{cases} A_1^{\alpha\beta\gamma\delta} b_1^{n-1} + A_2^{\alpha\beta\gamma\delta} b_1^{n-2} + \cdots + A_n^{\alpha\beta\gamma\delta} b_1^0 = C^{(eff)}_{\alpha\beta\gamma\delta(1)}, \\ A_1^{\alpha\beta\gamma\delta} b_2^{n-1} + A_2^{\alpha\beta\gamma\delta} b_2^{n-2} + \cdots + A_n^{\alpha\beta\gamma\delta} b_2^0 = C^{(eff)}_{\alpha\beta\gamma\delta(2)}, \\ \vdots \\ A_1^{\alpha\beta\gamma\delta} b_n^{n-1} + A_2^{\alpha\beta\gamma\delta} b_n^{n-2} + \cdots + A_n^{\alpha\beta\gamma\delta} b_n^0 = C^{(eff)}_{\alpha\beta\gamma\delta(n)}, \end{cases} \tag{56}$$

where the coefficients $C^{(eff)}_{\alpha\beta\gamma\delta(i)}$ for $i = 1,\ldots,n$ denote the approximated function values in ascending order of the arguments b_i. Therefore, the following algebraic system of equations is formed to determine the polynomial coefficients $A_i^{\alpha\beta\gamma\delta}$:

$$\begin{bmatrix} b_1^{n-1} & b_1^{n-2} & \ldots & b_1^0 \\ b_2^{n-1} & b_2^{n-2} & & b_2^0 \\ \vdots & \vdots & & \vdots \\ b_n^{n-1} & b_n^{n-2} & \ldots & b_n^0 \end{bmatrix} \begin{Bmatrix} A_1^{\alpha\beta\gamma\delta} \\ A_2^{\alpha\beta\gamma\delta} \\ \vdots \\ A_n^{\alpha\beta\gamma\delta} \end{Bmatrix} = \begin{Bmatrix} C^{(eff)1}_{\alpha\beta\gamma\delta} \\ C^{(eff)2}_{\alpha\beta\gamma\delta} \\ \vdots \\ C^{(eff)n}_{\alpha\beta\gamma\delta} \end{Bmatrix}. \tag{57}$$

The crucial point of this method is a proper determination of the set of input parameters $\{b_1^0, \ldots, b_n^0\}$ inserted into this equation. This determination is started with a choice of the computational domain $[b\text{-}\Delta b, b + \Delta b]$, where $2\Delta b = 0.05b$. Then, this domain is subdivided into the set of equidistant $n-1$ intervals with the length $\Delta b = \frac{2\Delta b}{n-1}$ for any $m = 1,\ldots,n-1$. So that assuming that $b_0 = b - \Delta b$ it is obtained that $b_m = b - \Delta b + m\frac{2\Delta b}{n-1}$. Let us note that since this linear system of equations is non-symmetric, its solution cannot be done by the integration with the FEM solver, and some separate numerical procedure based on the Gauss–Jordan elimination scheme must be employed. The unique solution for this system makes it possible to calculate up to the nth-order ordinary derivatives of the homogenized elasticity tensor with respect to the parameter b at the given b_0 as

- 1st-order derivative

$$\frac{\partial C^{(eff)}_{\alpha\beta\gamma\delta}}{\partial b} = (n-1) A_1^{\alpha\beta\gamma\delta} b^{n-2} + (n-2) A_2^{\alpha\beta\gamma\delta} b^{n-3} + \cdots + A_{n-1}^{\alpha\beta\gamma\delta}, \tag{58}$$

- 2nd-order derivative

$$\frac{\partial^2 C^{(eff)}_{\alpha\beta\gamma\delta}}{\partial b^2} = (n-1)(n-2) A_1^{\alpha\beta\gamma\delta} b^{n-3} + (n-2)(n-3) A_2^{\alpha\beta\gamma\delta} b^{n-4} + \cdots + A_{n-2}^{\alpha\beta\gamma\delta}, \tag{59}$$

- kth-order derivative

$$\frac{\partial^k C^{(eff)}_{\alpha\beta\gamma\delta}}{\partial b^k} = \prod_{i=1}^{k} (n-i) A_1^{\alpha\beta\gamma\delta} b^{n-k} + \prod_{i=2}^{k} (n-i) A_2^{\alpha\beta\gamma\delta} b^{n-(k+1)} + \cdots + A_{n-k}^{\alpha\beta\gamma\delta}. \tag{60}$$

Providing that the response function of the effective elasticity tensor has a single independent argument, that is, the input random variable of the problem, it is possible to employ the stochastic perturbation technique based on the Taylor representation to compute up to the mth-order probabilistic moments $\mu_m(C^{(eff)}_{\alpha\beta\gamma\delta})$. It is clear from the derivation above that to complete the mth-order approximation we need to solve the initial deterministic problem m times, with its number of degrees of freedom and a single system of algebraic equations $m \times m$, to find a single response function. Including the formulas above for the derivatives of the response function in a definition of the probabilistic moments for f, one can determine the expectations, variances as well as any order random characteristics of the structural response.

6. Numerical experiments

6.1. Numerical determination of the sensitivity coefficients

The main purpose of this analysis is to determine via combined analytical–numerical and numerical methods the sensitivity coefficients for the in-plane EET components. This is performed using the response function method (RFM) explained above and, for a comparison, the central difference method previously implemented for this problem. The combined approach is based on the MAPLE computations of the sensitivity gradients of the spatially averaged elasticity tensor components with respect to various design parameters. The spatially averaged stress tensor components calculated from the homogenization function are approximated using the response function approach, and differentiation is performed symbolically in MAPLE as well. A full straightforward numerical technique is implemented in this system using the RFM technique, applied to both spatially averaged elasticity and homogenizing stress tensor components. A separate solver for the RFM computations based on the least squares method is implemented in the MAPLE symbolic environment, together with the normalization procedures for all sensitivity coefficients computed. It is necessary to note that the core of the homogenization process is realized in the finite element-based program MCCEFF, where the plane strain problem is solved.

Let us consider a composite with a quarter of the periodicity cell – the fiber has round cross-section and the entire cell is square. The composite analyzed is perfectly periodic: fibers are distributed uniformly transverse to the cross-sectional plane presented, while the reinforcement ratio is equal to 50% of the total area of the RVE. The material characteristics for the computational analysis are the following: e_1 = 84.0 GPa, v_1 = 0.22 as well as e_2 = 4.0 GPa, v_2 = 0.34; the FEM discretization using sixty-two 4-noded elements with 76 nodal points for the plane strain analysis implemented in the system MCCEFF is presented below. Let us note that it is possible to automatically generate the quarters, the halves of the RVE as well as the cells with a single and multiple fibers in it.

Numerical analysis in this section is focused on the computation of the sensitivity gradients for the effective and spatially averaged in-plane elasticity tensor components. They are computed using the response function method, where the approximating polynomial was of the 9th order and further compared against the results obtained with the central finite difference application. The normalized sensitivity coefficients for the effective elasticity tensor (EET) are collected in Table 2, and the elasticity tensor components spatially averaged over the RVE (AET) are in Table 3; the design variables were taken separately, including the Young moduli of the fiber and the matrix, together with the additional Poisson ratios. Table 2 is arranged so that the first value in all the main rows corresponds to the RFM developed in the paper, and the second corresponds to the central finite difference (CFD) method. The CFD results for the RVE containing the full fiber with the surrounding matrix, which are taken from (Kamiński, 2008) are included in the brackets below (CFD*). The next table collects the sensitivity gradients for the AET components (1) computed analytically, (2) by the RFM implementation and, finally, with the use of the CFD technique. Let us note that all the results computed using the central finite difference scheme were obtained for an increment of the perturbed parameter equal to 1%, which follows the conclusions from previous numerical modeling (Kamiński, 2008).

Table 2
Sensitivity coefficients for the effective elasticity tensor

h		$\partial C^{(eff)}_{1111}/\partial h$	$\partial C^{(eff)}_{1122}/\partial h$	$\partial C^{(eff)}_{1212}/\partial h$
e_1	RFM	0.110	0.026	0.955
	CFD	0.110	0.029	0.955
v_1	RFM	0.011	0.142	−0.178
	CFD	0.012	0.138	−0.178
e_2	RFM	0.881	0.932	0.039
	CFD	0.882	0.940	0.040
	CFD*	(0.867)	(0.926)	(0.044)
v_2	RFM	1.081	2.505	−0.009
	CFD	1.101	2.557	−0.010
	CFD*	(1.205)	(2.814)	(−0.011)

Table 3
Sensitivity coefficients for the averaged elasticity tensor

h		$\partial C^{(eff)}_{1111}/\partial h$	$\partial C^{(eff)}_{1122}/\partial h$	$\partial C^{(eff)}_{1212}/\partial h$
e_1	Analytical	0.940	0.896	0.959
	RSM	0.941	0.894	0.958
	CFD	0.941	0.894	0.958
v_1	Analytical	0.060	0.104	0.041
	RSM	0.060	0.105	0.041
	CFD	0.060	0.105	0.042
e_2	Analytical	0.304	1.438	−0.173
	RSM	0.304	1.437	−0.173
	CFD	0.304	1.435	−0.173
v_2	Analytical	0.081	0.298	−0.010
	RSM	0.080	0.296	−0.010
	CFD	0.082	0.302	−0.010

The first and the most important conclusion that can be made from those results is the almost perfect agreement between the various numerical approaches – the homogenized characteristics response function approach and the finite difference technique in the first case, as well as both of them with pure analytical differentiation implemented in MAPLE. This indicates that for the needs of the homogenization method and the computational implementation of sensitivity analysis, all of those methods are accurate and can be used equivalently, depending on engineering software employed for a simulation. It should be clear that the use of the response function method is independent of any further numerical parameters, such as the parameter increments in the CFD computations; no closed formulas are necessary as in the analytical approach, and it does not really need any technical interventions into the source codes for FEM homogenization-oriented codes. Therefore, the apparent efficiency of this technique compared to the remaining methodologies yields a new modeling tool for sensitivity analysis as well as for random modeling, as seen in the next section.

Let us also note here that the mesh in the RVE is completed using a rather small number of finite elements; therefore, it is not necessary to create a very detailed mesh to obtain reliable results from the sensitivity analysis. In further numerical simulations, it would be interesting to check the influence of the number of fibers of the RVE discretized on the values of those gradients, and in the case of random distribution of those fibers into the computational domain. According to previous studies in this area, it can be confirmed on the RVE quarter that the most important role in such a composite is played by the elastic characteristics of the matrix. The Young moduli of the fibers have a smaller influence, whereas their Poisson ratio can be practically neglected (during the optimization process). Some of those parameters, namely the Poisson ratio, can result in negative sensitivity coefficients, so that by increasing those design parameter values, one can decrease some homogenized elasticity tensor components.

6.2. Computations of probabilistic moments of the EET

The probabilistic RFM-related technique is implemented here in two different ways. The first approach can be classified as a combined analytical–numerical methodology, where the 0th order spatially averaged elasticity tensor, together with its higher order derivatives with respect to the input random variable, are determined using MAPLE only. The second part, consisting of the homogenizing stresses spatially averaged over the RVE, is partially computed in the MCCEFF finite element-based system and then included in MAPLE to approximate the response functions of the spatially averaged homogenizing stress tensor components w.r.t. random input quantities. The procedure has been programmed with the use of the homogenization-oriented computer program MCCEFF (Kamiński, 2005), used previously for computations of the probabilistic moments of the effective elasticity tensor components with use of the Monte-Carlo simulation technique. Both methods return almost the same results, so the results of the second methodology are analyzed here.

Let us consider a composite with a quarter of the periodicity cell – the fiber has round cross-section and the entire cell is square. The composite analyzed is perfectly periodic, fibers are distributed uniformly and transverse to the cross-sectional plane presented, and the reinforcement ratio is equal to 50% of the total area of the RVE. The elastic properties of the glass fiber and resin matrix are assumed as follows: the Young moduli expected values are $E[e_1]$ = 84 GPa, $E[e_2]$ = 4.0 GPa, while the Poisson ratios are taken as equal to $E[v_1]$ = 0.22 for the fibers and $E[v_2]$ = 0.34 for the matrix (each parameter is randomized separately, and then the expectations of the remaining properties become simply their deterministic values); all the parameters are assumed to be truncated Gaussian random variables (Fig. 3).

The preliminary results of the computational analysis are presented in Fig. 4 as the response functions of all the homogenized elastic tensor components, where the Poisson ratio of the matrix is taken as the input random variable. This choice was justified by the fact that all previous computational studies (Kamiński, 2005) show that this particular composite is most sensitive to variations in this ratio. As is it is clear from all the graphs included together as Fig. 4, a very smooth function is obtained for the expectation of this parameter, but at both edges of the computational domain the polynomial representa-

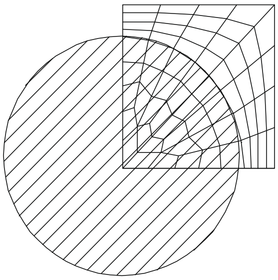

Fig. 3. FEM discretization of the RVE quarter.

tion of the 10th order returns some fluctuations in the response function. It may lead, in future implementations of this method, to (a) higher-order response function polynomia, and (b) non-uniform discretization of the response function domain (such as the exponential one, for instance).

Figs. 5–8 show the expected values of the first component for the effective elasticity tensor, $E[C^{(eff)}_{1111}]$, as functions of the perturbation order of the method – from the 2nd to 10th – as well as of the input coefficient of the variation of the random

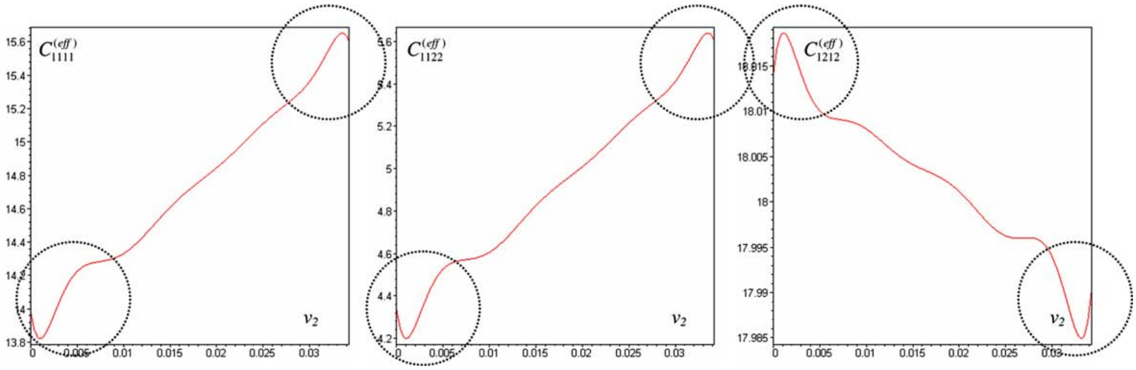

Fig. 4. The probabilistic response functions around the expectations for the homogenized tensor components.

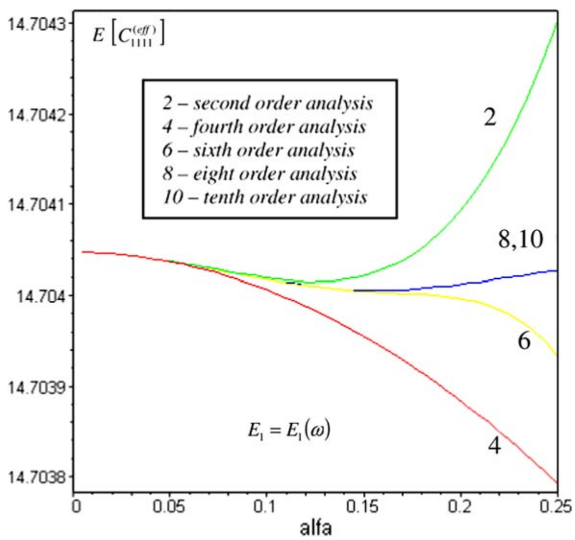

Fig. 5. The expected values of $C^{(eff)}_{1111}$ for the randomized Young modulus of the fiber.

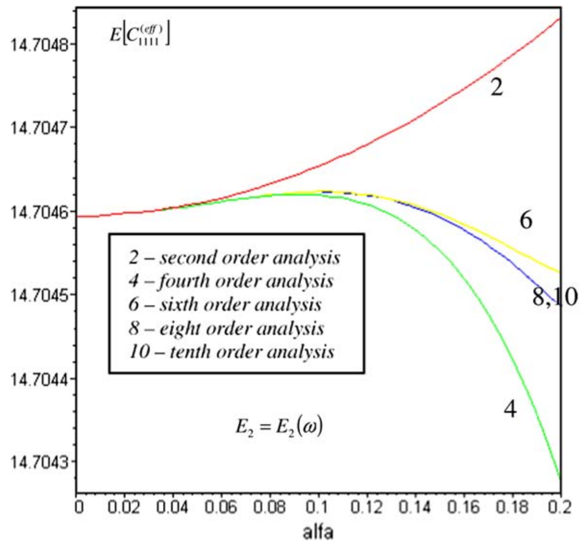

Fig. 6. The expected values of $C_{1111}^{(eff)}$ for the randomized Young modulus of the matrix.

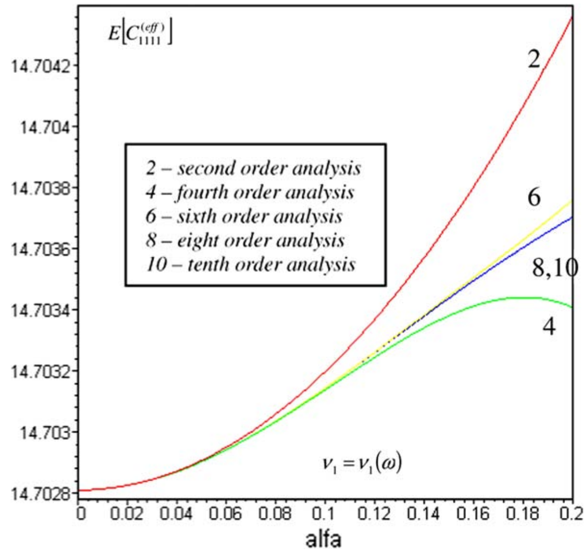

Fig. 7. The expected values of $C_{1111}^{(eff)}$ for the randomized Poisson ratio of the fiber.

input parameter (each test contains only a single random input): first the Young modulus of the fiber, then the Young modulus of the matrix, then the Poisson ratio of the fiber, and finally the Poisson ratio for the matrix. First, the most general observation is that even for the largest value of the input coefficient of the variation, the method implemented is convergent, so that there is practically no difference between the expectations computed according to the 8th- and the 10th-order perturbation formulations. Since the largest coefficients of the variation of the random input variables are very rare in solid mechanics applications, this coefficient has been restricted to a value of 0.2. By the way, one can notice the differences between the 2nd order method, known from the literature, and higher-order results, even if this coefficient does not exceed the recommended value of 0.1. It is very characteristic that the probabilistic convergence of all those expected values has a different type depending strongly on the random input type, but generally has a definitely nonlinear character (with respect to the coefficient of variance). Some expectations monotonously increase, some of them decrease and the remaining demonstrate more complicated behavior. Those promising results will lead to the further analogous computations of higher moments and coefficients using the response function method, where perhaps higher-order perturbations will be necessary. As it was demonstrated however, such an implementation is neither very complicated nor very demanding, regardless of both computational power and time.

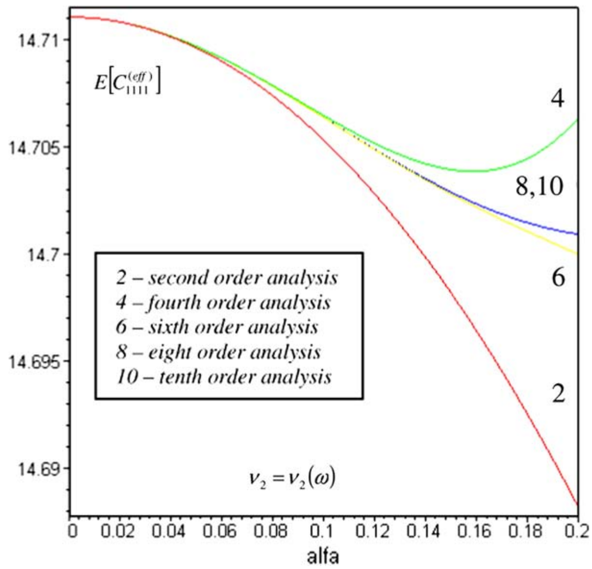

Fig. 8. The expected values of $C_{1111}^{(eff)}$ for the randomized Young modulus of the matrix.

7. Conclusions

1. The results obtained in this paper show how powerful the Taylor expansion-based perturbation technique can be in sensitivity and stochastic analyses of the homogenization problem. As it was shown by the computational analysis presented here, the sensitivity gradients obtained with the RFM are almost equal to those obtained before using the CFD. However, the first method implemented and tested here is significantly more efficient than the central finite difference approach in the sensitivity analysis, because it is free from a dependence on the increment of the input design parameter chosen for the partial differentiation.
2. As it was suggested in the Introduction, the RFM technique is also suitable for the homogenization of the random composites, where straightforward stochastic perturbation analysis as well as the Monte-Carlo simulation techniques were employed before. Contrary to the simulation-based approaches, the method proposed here does not need such a large time effort – instead of at least 10,000 random samples (Kamiński, 2005) only 10 iterative solutions of the same deterministic character is used here to approximate the expected values. Further computational studies will show, whether the same set of solutions is necessary to get a satisfactory comparison in terms of higher-order moments of the homogenized tensor components. Let us note that the stochastic second order perturbation technique applied before (Kamiński, 2005) does now allowed for (1) higher than the second moments computations, (2) is not appropriate for the input coefficients of variation larger than 0.1, so that there is no doubt that the RFM is computationally much more efficient. As it is demonstrated (3) here with additional numerical studies, the expected values of various homogenized tensor components appear to be stochastically convergent, where the 10th-order perturbation-based approach appears to be a quite satisfactory approximation of those expectations. Therefore, any higher-order moments and coefficients of the homogenized elasticity tensor may be computed using this approach without application of the time-consuming Monte-Carlo simulation technique, although it may need larger than 9th-order response function approximation. A randomization of the geometrical parameters requires more computational effort, however, it is also possible using the response function method. Therefore, this sensitivity and probabilistic technique may be used for design optimization as well as reliability analysis of some composites-based engineering structures, such as the superconducting strands (Kamiński, 2006; Lefik and Schrefler, 1994).

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