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ON SENSITIVITY ANALYSIS IN HOMOGENIZATION OF SOME COMPOSITE MATERIALS

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Abstract

Main purpose of the paper is to present theoretical aspects and Finite Element Method implementation of the sensitivity analysis in homogenization of multicomponent materials in the linear range; the problem is solved by using of the effective modules homogenization approach. The deterministic sensitivity analysis is worked out in general form and is illustrated on the example of some material parameters such as the heat conductivity coefficients and Young moduli of the component materials, for instance, as well as for particular 1d periodic two-component composite. The results of sensitivity analysis presented in the paper may be successfully applied to computational optimization of engineering composites, to the shape sensitivity studies and, after some extensions, to random composites analysis.

1. Introduction

As it is known, the sensitivity analysis in engineering sciences is provided to verify how some input structural parameters of specific engineering problem influence the state functions analyzed (displacements, stresses, temperatures or another potential state functions) [1,7-10,12,17-18]. This sensitivity is computed by the use of the partial derivatives of the state function considered with respect to the chosen input parameter of the structure. These derivatives can be computed starting from fundamental algebraic equations system obtained for the problem being solved. It is important to underline that this methodology is common for different discrete numerical techniques: Boundary Element Method (BEM), Finite Difference Method (FDM), Finite Element Method (FEM) or, alternatively, some hybrid and meshless strategies [16]. From the computational point of view there are the Direct Differentiation Method (DDM) used in the paper, the Adjoint Variable Method (AVM) or computational finite difference scheme in the domain of structural design sensitivity analysis.

The paper is devoted generally to some sensitivity studies in the homogenization of some two-component fiber-reinforced composite materials. The composite model assumes that the structure constituents are linear elastic and transversely isotropic in the context of effective elasticity tensor components derivation and linear isotropic in heat conduction (generally linear potential field) problem. The main purpose of this study is to obtain numerical algorithm for verification of the most crucial material parameters of the composite. It is done to effectively optimize these materials in the context of designing their constituents as well as their volume fraction. The homogenization method improved here is the intermediate numerical tool to exclude the necessity of composite micro-scale discretization and, at the same time, to reduce the total number of the structure degrees of freedom; analogous studies have been done previously in [20] but in the numerical phenomenological approach only. The main value of the sensitivity approach proposed is that the effective tensors sensitivities computed do not vary on the arguments increments - differentiation with respect to the input parameters (Young moduli and heat conductivities, for instance) is provided by the mathematical closed equations only.

2. Periodic composite model

Let us consider a periodic fiber-reinforced two component composite in plane strain in the unstressed and undeformed state. We assume that the composite is built up with the fibers parallel to the x_3 direction; the cross-section of the structure $Y \subset \Re^2$ with $x_3 = 0$ the plane, orthogonal to the longitudinal direction, is shown in Fig. 1. Let us consider the periodicity cell Ω (Representative Volume Element - RVE) of Y with the rectangular shape parallel to x_1 and x_2 axes, respectively, and defined by the external lengths l_1 and l_2. Let further all geometric dimensions of Ω be related to the corresponding dimensions of Y by a small parameter $\delta > 0$.

Let us note that interface boundary (or simply interface) is the continuous contour dividing two different materials in the periodicity cell; in this context it is assumed that fiber and matrix are perfectly bonded. Considering further mathematical formulations the interface is assumed to be the regular and sufficiently smooth contour, however it should be outlined that some nonsmoothnesses can be observed within the interfaces and, moreover, interface defects between fiber and matrix may occur [4,15].

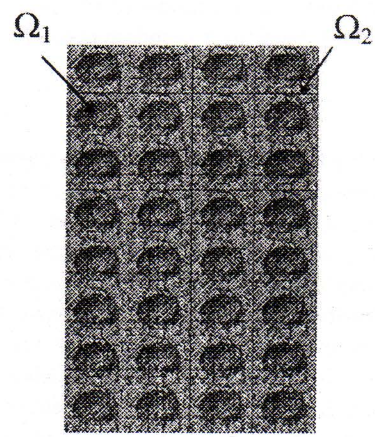

Fig. 1. The RVE of fiber-reinforced composite

Both components of composite are assumed to be linear elastic and transversely isotropic in the case of elastostatic problem while linear and isotropic in the case of linear potential field problem homogenization [14]. Thus, material parameters of the components are piecewise constant functions of the position only

$$\mathbf{p}(\mathbf{x}) = \begin{cases} \mathbf{p}_1; \mathbf{x} \in \Omega_1 \\ \mathbf{p}_2; \mathbf{x} \in \Omega_2 \end{cases} \tag{1}$$

It should be mentioned that the homogenization method presented for the fiber-reinforced composite may be applied for instance to homogenize n-component materials continuous and containing some microvoids [6] as well as granular media built up with the grains of different shape and different physical and mechanical properties.

3. Homogenization method

3.1. Linear elastostatics problem

To derive the expressions for the effective elasticity tensor components let us rewrite the principle of virtual work for the homogenization boundary problem defined on the periodicity cell Ω as follows [3,14,21]:

$$\int_{\Omega} C_{ijkl}\varepsilon_{kl}\left(\chi_{(pq)}\right)\varepsilon_{ij}(\mathbf{v})\,d\Omega = \int_{\Omega} f_i v_i d\Omega \tag{2}$$

where $\mathbf{v}$ is any kinematically admissible periodic displacement function while $\chi_{(pq)}$ represent periodic displacement fields to be determined and called homogenization function. To obtain the solution, the L.H.S. of Eq. (2) is divided into the components corresponding to regions Ω_1, Ω_2. Neglecting body forces of the composite there holds

$$\begin{aligned}&\int_{\Omega_1} C_{ijkl}\varepsilon_{kl}\left(\chi_{(pq)}\right)\varepsilon_{ij}(\mathbf{v})\,d\Omega + \int_{\Omega_2} C_{ijkl}\varepsilon_{kl}\left(\chi_{(pq)}\right)\varepsilon_{ij}(\mathbf{v})\,d\Omega = \\ &= \int_{\partial\Omega_{12}}\left(\sigma_{ij}^{(1)} - \sigma_{ij}^{(2)}\right)n_j v_i\, d(\partial\Omega)\end{aligned} \tag{3}$$

where $\sigma_{ij}^{(1)}$, $\sigma_{ij}^{(2)}$ are the interface stresses at the $\partial\Omega_{12}$. To calculate the homogenization functions $\chi_{(pq)}$ the following stress boundary conditions are applied:

$$\sigma_{ij}\left(\chi_{(pq)}\right)n_j = \left[C_{ijpq}\right]_{\partial\Omega_{12}} n_j = F_{(pq)i}\Big|_{\partial\Omega_{12}}; \ \mathbf{x} \in \partial\Omega_{12} \tag{4}$$

while periodicity of $\chi_{(pq)}$ leads us to the following displacement type boundary conditions:

$$\left[\chi_{(pq)}\right] = 0; \ \mathbf{x} \in \partial\Omega \tag{5}$$

$$\frac{\partial\chi_{(pq)}}{\partial x_i} = 0; \ x_i = 0, l_i \tag{6}$$

The component of unit vector normal to the interface $\partial\Omega_{12}$ and directed to the fiber interior is denoted by n_j, while $\left[C_{ijpq}\right]_{\partial\Omega_{12}}$ is the difference of the elasticity tensor components for fiber and matrix. Thus, Eq. (3) can be rewritten as

$$\begin{aligned}&\int_{\Omega_1} C_{ijkl}\varepsilon_{kl}\left(\chi_{(pq)}\right)\varepsilon_{ij}(\mathbf{v})\,d\Omega + \int_{\Omega_2} C_{ijkl}\varepsilon_{kl}\left(\chi_{(pq)}\right)\varepsilon_{ij}(\mathbf{v})\,d\Omega = \\ &= \int_{\partial\Omega_{12}} \left[C_{ijpq}\right]_{\partial\Omega_{12}} n_j v_i\, d(\partial\Omega)\end{aligned} \tag{7}$$

what allows to compute the functions $\chi_{(11)}$, $\chi_{(12)}$ and $\chi_{(22)}$. Next, the effective elasticity tensor components are calculated. To this purpose it is shown that

$$\int_{\partial\Omega_{12}} \left[C_{ijpq}\right]_{\partial\Omega_{12}} n_j v_i \, d(\partial\Omega) = \int_{\Omega} C_{ijpq} \, \varepsilon_{ij}(v) \, d\Omega \tag{8}$$

Since that we arrive at

$$\int_{\Omega} C_{ijkl} \varepsilon_{kl}\left(\chi_{(pq)}\right) \varepsilon_{ij}(v) \, d\Omega = -\int_{\Omega} C_{ijpq} \, \varepsilon_{ij}(v) \, d\Omega, \tag{12}$$

or, alternatively

$$\int_{\Omega} \left(C_{ijpq} + C_{ijkl} \varepsilon_{kl}\left(\chi_{(pq)}\right)\right) \varepsilon_{ij}(v) \, d\Omega = 0. \tag{13}$$

Since the fact that the effective elasticity tensor components are to be constant within the composite there holds

$$C_{ijpq}^{(eff)} = \frac{1}{|\Omega|} \int_{\Omega} \left(C_{ijpq} + C_{ijkl} \varepsilon_{kl}\left(\chi_{(pq)}\right)\right) d\Omega. \tag{14}$$

3.2. Heat conduction as the illustration for the linear potential field problems

By the analogy to previous considerations, single temperature homogenization function Φ is derived and, on its basis, the effective conductivity coefficient $k^{(eff)}$ constant for the whole composite is determined. To calculate Φ and $k^{(eff)}$ it is assumed that the periodicity of the essential and natural boundary conditions for $\mathbf{x} \in \partial\Omega$

$$\Phi\Big|_{x \in \partial\Omega_\Phi} = \text{const.}, \; q\Big|_{x \in \partial\Omega_q} = 0. \tag{15}$$

Variational statement of the heat conduction homogenization problem can be written as [14]

$$\sum_{i=1,2} \left(\int_{\Omega_1} \left[\delta\Phi\left(k_i^{(1)} \Phi_{,i}\right)\right]_{,i} d\Omega + \int_{\Omega_2} \left[\delta\Phi\left(k_i^{(2)} \Phi_{,i}\right)\right]_{,i} d\Omega \right) = \int_{\partial\Omega_{12}} \delta\Phi\left(\left[k_n^{(1)} - k_n^{(2)}\right]\Phi_{,n}\right) d(\partial\Omega). \tag{16}$$

Due to the divergence theorem [3,21], Eq. (17) takes the form

$$\sum_{i=1,2} \left(\int_{\Omega_1} \left[\delta\Phi\left(k_i^{(1)} \Phi_{,i}\right)\right]_{,i} d\Omega + \int_{\Omega_2} \left[\delta\Phi\left(k_i^{(2)} \Phi_{,i}\right)\right]_{,i} d\Omega \right) = \sum_{i=1,2} \left(\int_{\partial\Omega_{12}} \delta\Phi\left(\left[k_i\right]\Phi_{,i}\right) n_i d(\partial\Omega) \right), \tag{17}$$

where $[\mathbf{k}]$ denotes the difference of composite constituents heat conductivities at the interface $\partial\Omega_{12}$. Next, we have

$$\begin{aligned} \int_{\Omega} \left(\delta\Phi \, k_i\right)_{,i} d\Omega &= \int_{\Omega} \delta\Phi_i \; k_i \; d\Omega + \int_{\Omega} \delta\Phi \; k_{i,i} d\Omega = \\ &= \int_{\partial\Omega} k_i n_i \delta\Phi \; d(\partial\Omega) - \int_{\partial\Omega_{12}} \left[k_i\right] n_i \delta\Phi \; d(\partial\Omega) + \int_{\Omega} \delta\Phi \; k_{i,i} d\Omega \end{aligned} \tag{18}$$

and we arrive at

$$\int_{\Omega} (\delta\Phi\, k_i)_{,i} d\Omega = -\int_{\partial\Omega_{12}} [k_i]\, n_i \delta\Phi\, d(\partial\Omega) \tag{19}$$

what, included into Eq. (17), gives

$$\sum_{i=1,2}\left(\int_{\Omega} \left[\delta\Phi(k_i \Phi_{,i})\right]_{,i} d\Omega\right) = -\int_{\Omega} [\delta\Phi\, k_i]_{,i}\, d\Omega. \tag{20}$$

Thus, since the isotropic character of composite components in the plane considered, the effective conductivity can be calculated as follows:

$$k^{(eff)} = \frac{1}{|\Omega|}\int_{\Omega} k\, d\Omega + \frac{1}{|\Omega|}\int_{\Omega} k\, 1_i \Phi_{,i}\, d\Omega, \tag{21}$$

where 1_i denotes the unity operator. The effective heat conductivity coefficient calculated using the procedure presented above may be compared against the corresponding upper and lower bounds for effective conductivity coefficient, cf. [5,11,19].

4. Sensitivity problem formulation

4.1. Effective elastic behavior sensitivity analysis

Starting from Eq. (14), the sensitivity of effective elasticity tensor components with respect to sensitivity parameters vector **h** can be calculated as

$$\frac{\partial C^{(eff)}_{ijpq}}{\partial \mathbf{h}} = \frac{\partial}{\partial \mathbf{h}}\left\{\frac{1}{|\Omega|}\int_{\Omega} C_{ijpq} d\Omega\right\} + \frac{\partial}{\partial \mathbf{h}}\left\{\frac{1}{|\Omega|}\int_{\Omega} C_{ijkl}\varepsilon_{kl}\left(\chi_{(pq)}\right) d\Omega\right\}. \tag{22}$$

We can rewrite this equation in the following form:

$$\frac{\partial C^{(eff)}_{ijpq}}{\partial \mathbf{h}} = \frac{1}{|\Omega|}\int_{\Omega}\frac{\partial C_{ijpq}}{\partial \mathbf{h}} d\Omega + \frac{1}{|\Omega|}\int_{\Omega}\frac{\partial C_{ijkl}}{\partial \mathbf{h}}\varepsilon_{kl}\left(\chi_{(pq)}\right) d\Omega + \frac{1}{|\Omega|}\int_{\Omega} C_{ijkl}\frac{\partial \varepsilon_{kl}\left(\chi_{(pq)}\right)}{\partial \mathbf{h}} d\Omega, \tag{23}$$

and we observe that if the input sensitivity parameters are not the arguments of the elasticity tensor C_{ijkl}, there holds

$$\frac{\partial C^{(eff)}_{ijpq}}{\partial \mathbf{h}} = \frac{1}{|\Omega|}\int_{\Omega} C_{ijkl}\frac{\partial \varepsilon_{kl}\left(\chi_{(pq)}\right)}{\partial \mathbf{h}} d\Omega. \tag{24}$$

while the derivatives of homogenization functions $\chi_{(pq)}$ with respect to the vector **h** components can be obtained computationally only. By the analogous way the sensitivity of $C^{(eff)}_{ijpq}$ components with respect to fiber shape [7] can be derived, however final equations have decisively more complicated form and can be shown if only homogenization function can be derived analytically.

4.2. Sensitivity in homogenization of the heat conduction

The sensitivity of effective conductivity tensor $k_{ij}^{(eff)}$ with respect to design parameters vector **h** components can be calculated as

$$\frac{\partial k_{ij}^{(eff)}}{\partial \mathbf{h}} = \frac{\partial}{\partial \mathbf{h}}\left\{\frac{1}{|\Omega|}\int_{\Omega} k_{ij}\, d\Omega\right\} + \frac{\partial}{\partial \mathbf{h}}\left\{\frac{1}{|\Omega|}\int_{\Omega} k_{ij} 1_m \Phi_{,m}\, d\Omega\right\}. \tag{25}$$

The differentiation over the region Ω may be carried out by the following way:

$$\frac{\partial k_{ij}^{(eff)}}{\partial \mathbf{h}} = \frac{1}{|\Omega|}\int_{\Omega} \frac{\partial k_{ij}}{\partial \mathbf{h}}\, d\Omega + \frac{1}{|\Omega|}\int_{\Omega} \frac{\partial k_{ij}}{\partial \mathbf{h}} 1_m \Phi_{,m}\, d\Omega + \frac{1}{|\Omega|}\int_{\Omega} k_{ij} 1_m \frac{\partial \Phi_{,m}}{\partial \mathbf{h}}\, d\Omega. \tag{26}$$

Let us note that while the partial derivatives of heat conductivity with respect to the sensitivity parameters vector may be derived explicitly, the partial derivatives of the homogenization functions derivatives $\Phi_{,m}$ have to be obtained numerically only. In the case where the vector of design sensitivity variables is not included in the heat conductivity coefficients there holds

$$\frac{\partial k_{ij}^{(eff)}}{\partial \mathbf{h}} = \frac{1}{|\Omega|}\int_{\Omega} k_{ij} 1_m \frac{\partial \Phi_{,m}}{\partial \mathbf{h}}\, d\Omega. \tag{27}$$

It should be mentioned that, as it is shown in the numerical illustration presented further, detailed results on sensitivity analysis can be obtained from Eqs. (24,27) if only effective characteristics have closed analytical form.

5. Finite Element discretization of the homogenization problem

5.1. Homogenization of linear elastostatics

Let us introduce the following approximation of homogenization functions $\chi_{(rs)i}$ for i,r,s=1,2 at any point of Ω in terms of a finite number of generalized coordinates $q_{(rs)\alpha}$ and shape functions $\varphi_{i\alpha}$ [2]

$$\chi_{(rs)i} = \varphi_{i\alpha} q_{(rs)\alpha},\ i,r,s = 1,2,\ \alpha = 1,\ldots,N \tag{28}$$

where N is the total number of degrees of freedom of the structure. By the same way the strain $\varepsilon_{ij}(\chi_{(rs)})$ and stress $\sigma_{ij}(\chi_{(rs)})$ tensors components are expressed

$$\varepsilon_{ij}(\chi_{(rs)}) = B_{ij\alpha} q_{(rs)\alpha} \tag{29}$$

$$\sigma_{ij(rs)} = \sigma_{ij}(\chi_{(rs)}) = C_{ijkl}\varepsilon_{kl}(\chi_{(rs)}) = C_{ijkl}B_{kl\alpha}q_{(rs)\alpha}, \tag{30}$$

where $B_{kl\alpha}$ represents the shape functions derivatives. Introducing Eqs. (28-30) into the homogenization virtual work principle it is obtained that

$$\int_{\Omega} \delta\chi_{(rs)i,j} C_{ijkl} \chi_{(rs)k,l}\, d\Omega = \int_{\partial\Omega_{12}} \delta\chi_{(rs)i} F_{(rs)i}\, d(\partial\Omega). \quad \text{(no sum on r,s)} \tag{31}$$

where, cf. Eq. (4)

$$F_{(rs)i} = \left[C_{rsij}\right]_{\partial\Omega_{12}} n_j . \tag{32}$$

Furthermore, let us define the composite global stiffness matrix as

$$K_{\alpha\beta} = \sum_{e=1}^{E} K_{\alpha\beta}^{(e)} = \sum_{e=1}^{E} \int_{\Omega_e} C_{ijkl} B_{ij\alpha} B_{kl\beta} d\Omega \tag{33}$$

for $\alpha, \beta = 1, \ldots, N$. Using the matrix into Eq. (33) and minimizing the variational principle with respect to the generalized coordinates, we arrive at

$$K_{\alpha\beta} q_{(rs)\alpha} = Q_{(rs)\alpha}, \tag{34}$$

where $Q_{(rs)\alpha}$ is the external load vector containing the boundary forces defined by Eq. (34), homogenization functions $\chi_{(rs)i}$ are obtained in three numerical tests for r,s=1,2. To assure the symmetry conditions on a periodicity cell, the orthogonal displacements and rotations for any nodal point belonging to $\partial\Omega$ are fixed. Starting from the functions $\chi_{(rs)i}$ so obtained the stresses $\sigma_{ij}(\chi_{(rs)})$ are calculated and averaged over the RVE due to the formula (14).

5.2. Homogenization of heat conduction problem

Let us assume that region Ω is discretized by a set of finite elements and the scalar temperature field Φ is described by the nodal temperatures vector Ψ_α corresponding to homogenization function as [2]

$$\Phi(x_i) = H_\alpha(x_i)\,\Psi_\alpha ;\ i=1,2. \tag{35}$$

It follows that

$$\Phi_{,i} = H_{\alpha,i}\,\Psi_\alpha \tag{36}$$

Then heat conductivity matrix $K_{\alpha\beta}$ and the vector P_α may be expressed as

$$K_{\alpha\beta} = \int_\Omega k_{ij} H_{\alpha,i} H_{\beta,j} d\Omega \tag{37}$$

and

$$P_\alpha = \int_\Omega g\, H_\alpha d\Omega + \int_{\partial\Omega} \hat{q}\, H_\alpha d(\partial\Omega). \tag{38}$$

This leads to the following equations system:

$$K_{\alpha\beta}\Psi_\beta = P_\alpha \tag{39}$$

To complete considerations on the homogenization problem implementation, it should be noticed that three elastostatic tests are needed to compute effective elastic characteristics of the composite, while the only one is to be solved to obtain the effective coefficient for linear potential field problem. Then, in the case of coupled thermoelastic problems all these functions can be found by the use of parallel computational procedures.

6. Discrete approach to the sensitivity analysis in homogenization

6.1. Finite element discretization of the effective tensor sensitivities

The classical deterministic discretized elastostatics problem given by Eq. (36) is rewritten as follows:

$$\frac{\partial \mathbf{K}_{\alpha\beta}}{\partial \mathbf{h}} q_{(rs)\alpha} + \mathbf{K}_{\alpha\beta} \frac{\partial q_{(rs)\alpha}}{\partial \mathbf{h}} = \frac{\partial \mathbf{Q}_{(rs)\alpha}}{\partial \mathbf{h}}, \tag{40}$$

to calculate sensitivities of homogenization function components as

$$\frac{\partial q_{(rs)\alpha}}{\partial \mathbf{h}} = \mathbf{K}_{\alpha\beta}^{-1} \left(\frac{\partial \mathbf{Q}_{(rs)\alpha}}{\partial \mathbf{h}} - \frac{\partial \mathbf{K}_{\alpha\beta}}{\partial \mathbf{h}} q_{(rs)\alpha} \right). \tag{41}$$

If design variables are not the arguments of the R.H.S. vector, it is obtained that

$$\frac{\partial q_{(rs)\alpha}}{\partial \mathbf{h}} = -\mathbf{K}_{\alpha\beta}^{-1} \frac{\partial \mathbf{K}_{\alpha\beta}}{\partial \mathbf{h}} q_{(rs)\alpha}. \tag{42}$$

where the derivatives $\frac{\partial \mathbf{K}_{\alpha\beta}}{\partial \mathbf{h}}$ may be computed explicitly or thanks to the finite difference scheme [17]. Next, the sensitivity of the effective elasticity tensor components is calculated starting from Eqs. (14,24) as follows:

$$\begin{aligned}
\frac{\partial C_{ijkl}^{(eff)}}{\partial \mathbf{h}} &= \frac{1}{|\Omega|}\int_\Omega \frac{\partial C_{ijkl}}{\partial \mathbf{h}} d\Omega + \frac{1}{|\Omega|}\int_\Omega \frac{\partial C_{ijpq}}{\partial \mathbf{h}} B_{kl\gamma} q_{(pq)\gamma} d\Omega + \\
&+ \frac{1}{|\Omega|}\int_\Omega C_{ijkl} B_{kl\gamma} \frac{\partial q_{(pq)\gamma}}{\partial \mathbf{h}} d\Omega = \\
&= \frac{1}{|\Omega|}\int_\Omega \frac{\partial C_{ijkl}}{\partial \mathbf{h}} d\Omega + \frac{1}{|\Omega|}\int_\Omega \frac{\partial C_{ijpq}}{\partial \mathbf{h}} B_{kl\gamma} K_{\beta\gamma}^{-1} Q_{(pq)\beta} d\Omega + \\
&+ \frac{1}{|\Omega|}\int_\Omega C_{ijkl} B_{kl\gamma} \frac{\partial K_{\beta\gamma}^{-1}}{\partial \mathbf{h}} Q_{(pq)\beta} d\Omega + \frac{1}{|\Omega|}\int_\Omega C_{ijkl} B_{kl\gamma} K_{\beta\gamma}^{-1} \frac{\partial Q_{(pq)\beta}}{\partial \mathbf{h}} d\Omega
\end{aligned} \tag{43}$$

for $\alpha, \beta, \gamma = 1, \ldots, N$. If for example the sensitivity parameter is introduced in the form of the Young modulus $\mathbf{h} \equiv e$, then we introduce the elasticity tensor as

$$C_{ijkl}(e(\mathbf{x}); \nu(\mathbf{x})) = e(\mathbf{x})\, A_{ijkl}(\nu(\mathbf{x})) \tag{44}$$

and

$$\frac{\partial C_{ijkl}(e(\mathbf{x}); \nu(\mathbf{x}))}{\partial e} = A_{ijkl}(\nu(\mathbf{x})), \tag{45}$$

while finite element stiffness matrix component corresponding to a-th material parameters can be expressed as

$$K^{(a)}_{\alpha\beta} = \int_{\Omega_a} C^{(a)}_{ijkl} B_{ij\alpha} B_{kl\beta} d\Omega = \int_{\Omega_a} e^{(a)} A^{(a)}_{ijkl} B_{ij\alpha} B_{kl\beta} d\Omega . \tag{46}$$

As a result, the sensitivity of i-th finite element stiffness matrix component with respect to a-th material Young modulus is calculated as

$$\frac{\partial K^{(i)}_{\alpha\beta}}{\partial e^{(a)}} = \begin{cases} \int_{\Omega_a} A^{(a)}_{ijkl} B_{ij\alpha} B_{kl\beta} d\Omega; \; x \in \Omega_a \\ 0; \text{ elsewhere} \end{cases} \tag{47}$$

Further, the sensitivities of the R.H.S. vector are obtained in general form

$$\frac{\partial Q_{(pq)\alpha}}{\partial \mathbf{h}} = \frac{\partial \left(\left[C_{pq\alpha j} \right] \right) n_j}{\partial e} = \left[A_{pq\alpha j} \right] n_j . \tag{48}$$

while the sensitivity of the effective elasticity tensor to Young modulus is equal to

$$\begin{aligned} \frac{\partial C^{(eff)}_{ijkl}}{\partial e} = & \frac{1}{|\Omega|} \int_{\Omega} A_{ijkl} d\Omega + \frac{1}{|\Omega|} \int_{\Omega} A_{ijkl} B_{ij\gamma} K^{-1}_{\gamma\beta} Q_{(pq)\beta} d\Omega + \\ & + \frac{1}{|\Omega|} \int_{\Omega} C_{ijkl} B_{ij\gamma} \left[\sum_{a=1}^{E} \int_{\Omega_a} A^{(a)}_{ijkl} B_{ij\gamma} B_{kl\beta} d\Omega \right] Q_{(pq)\beta} d\Omega + \\ & + \frac{1}{|\Omega|} \int_{\Omega} C_{ijkl} B_{ij\gamma} K^{-1}_{\beta\gamma} \left[A^{(a)}_{pq\beta j} \right] n_j d\Omega \end{aligned} \tag{49}$$

By the analogous way the effective elasticity tensor components with respect to the Poisson's ratios of composite components can be calculated. Since the complicated form of elasticity tensor description as a function of the ratios, the derivation is omitted here.

6.2. Sensitivity analysis for heat conduction homogenization problem

Taking into account the finite element implementation for the classical deterministic cell problem, cf. Eq. (41), the sensitivity of the temperature homogenization function can be obtained as

$$\frac{\partial K_{\alpha\beta}}{\partial \mathbf{h}} \Psi_\beta + K_{\alpha\beta} \frac{\partial \Psi_\beta}{\partial \mathbf{h}} = \frac{\partial P_\alpha}{\partial \mathbf{h}} , \tag{50}$$

what gives as a result

$$\frac{\partial \Psi_\beta}{\partial \mathbf{h}} = K^{-1}_{\alpha\beta} \left(\frac{\partial P_\alpha}{\partial \mathbf{h}} - \frac{\partial K_{\alpha\beta}}{\partial \mathbf{h}} \Psi_\beta \right) . \tag{51}$$

If only the R.H.S. vector is not a function of the design parameters vector **h**, Eq. (51) is simplified to the following one:

$$\frac{\partial \Psi_\beta}{\partial \mathbf{h}} = -K^{-1}_{\alpha\beta} \frac{\partial K_{\alpha\beta}}{\partial \mathbf{h}} \Psi_\beta , \tag{52}$$

where the partial derivatives $\frac{\partial K_{\alpha\beta}}{\partial \mathbf{h}}$ may be computed explicitly or, alternatively, obtained by using the finite difference scheme as

$$\frac{\partial K^{(e)}_{\alpha\beta}}{\partial h^{d}} \approx \frac{1}{\varepsilon}\left[K^{(e)}_{\alpha\beta}\left(h + \mathbf{1}_{(d)}\varepsilon\right) - K^{(e)}_{\alpha\beta}(h)\right], \tag{53}$$

where $K^{(e)}_{\alpha\beta}(\mathbf{h})$ is the e-th element stiffness matrix, h^{d} is the d-th component of the D-dimensional design variable vector $\mathbf{h}$, ε represents a small perturbation and the D-dimensional vector $\mathbf{1}_{(d)}$ has the values equal to 1 for the d-th component and zeroes elsewhere (analogously to the classical FEM shape functions). As it is known from sensitivity numerical analysis the final result of stiffness matrix derivative value shows some variability with respect to value of the parameter ε.

Moreover, taking into account considerations improved in Sec. 4, the discretization of effective conductivity tensor components sensitivity with respect to the vector $\mathbf{h}$ can be formulated as

$$\begin{aligned}\frac{\partial k^{(eff)}_{ij}}{\partial \mathbf{h}} &= \frac{1}{|\Omega|}\int_{\Omega}\frac{\partial k_{ij}}{\partial \mathbf{h}}\,d\Omega + \frac{1}{|\Omega|}\int_{\Omega}\frac{\partial k_{ij}}{\partial \mathbf{h}} 1_m H_{\alpha,m}\Psi_{\alpha}\,d\Omega + \frac{1}{|\Omega|}\int_{\Omega} k_{ij} 1_m \frac{\partial\left(H_{\alpha,m}\Psi_{\alpha}\right)}{\partial \mathbf{h}}\,d\Omega = \\ &= \frac{1}{|\Omega|}\int_{\Omega}\frac{\partial k_{ij}}{\partial \mathbf{h}}\,d\Omega + \frac{1}{|\Omega|}\int_{\Omega}\frac{\partial k_{ij}}{\partial \mathbf{h}} 1_m H_{\alpha,m}\Psi_{\alpha}\,d\Omega + \frac{1}{|\Omega|}\int_{\Omega} k_{ij} 1_m H_{\alpha,m}\frac{\partial\left(\Psi_{\alpha}\right)}{\partial \mathbf{h}}\,d\Omega\end{aligned} \tag{54}$$

Taking into account the result of Eq. (52) it is obtained that

$$\begin{aligned}\frac{\partial k^{(eff)}_{ij}}{\partial \mathbf{h}} &= \frac{1}{|\Omega|}\int_{\Omega}\frac{\partial k_{ij}}{\partial \mathbf{h}}\,d\Omega + \frac{1}{|\Omega|}\int_{\Omega}\frac{\partial k_{ij}}{\partial \mathbf{h}} 1_m H_{\alpha,m}K^{-1}_{\beta\alpha}P_{\beta}\,d\Omega + \\ &+ \frac{1}{|\Omega|}\int_{\Omega} k_{ij} 1_m H_{\alpha,m}K^{-1}_{\beta\alpha}\left(\frac{\partial P_{\beta}}{\partial \mathbf{h}} - \frac{\partial K_{\beta\gamma}}{\partial \mathbf{h}}\Psi_{\gamma}\right)d\Omega\end{aligned} \tag{55}$$

If heat conductivity tensor is taken as design parameter then

$$\frac{\partial K_{\beta\gamma}}{\partial \mathbf{h}} = \int_{\Omega}\delta_{ij}H_{\beta,i}H_{\gamma,j}\,d\Omega \tag{56}$$

and

$$\begin{aligned}\frac{\partial k^{(eff)}_{ij}}{\partial \mathbf{h}} &= \frac{1}{|\Omega|}\int_{\Omega}\delta_{ij}\,d\Omega + \frac{1}{|\Omega|}\int_{\Omega}\delta_{ij} 1_m H_{\alpha,m}K^{-1}_{\beta\alpha}P_{\beta}\,d\Omega + \\ &+ \frac{1}{|\Omega|}\int_{\Omega} k_{ij} 1_m H_{\alpha,m}K^{-1}_{\beta\alpha}\left(\delta_{ij}H_{\beta,i}H_{\gamma,j}\Psi_{\gamma}\right)d\Omega\end{aligned} \tag{57}$$

Further, for the case of $\mathbf{h} \equiv k^{(a)}_{ij}$ there holds

$$\frac{\partial k_{ij}^{(eff)}}{\partial k_{ij}^{(a)}} = \frac{1}{|\Omega|}\int_{\Omega} \chi_a \delta_{ij} \, d\Omega + \frac{1}{|\Omega|}\int_{\Omega} \chi_a \delta_{ij} 1_m H_{\alpha,m} K_{\beta\alpha}^{-1} P_\alpha \, d\Omega + \frac{1}{|\Omega|}\int_{\Omega} k_{ij} 1_m H_{\alpha,m} K_{\beta\alpha}^{-1} \left(\delta_{ij} H_{\beta,i} H_{\gamma,j} \Psi_\gamma\right) d\Omega \tag{58}$$

From the engineering point of view the sensitivity analysis of the effective conductivity tensor components to the coefficients of particular composite constituents has more applications. In particular, the most decisive component can be found during composite design studies what makes it possible to optimize effective heat conductivity coefficient with respect to this component neglecting variability of the other material parameters.

7. Some results for 1d structure homogenization

Let us consider for illustration of the procedure presented above the layered structure with piecewise constant material and geometrical properties. In that case it can be shown that effective Young moduli or effective heat conductivity coefficient can be described as

$$k^{(eff)} = \frac{1}{\int_{\Omega} \frac{1}{k(y)} dy}; \tag{59}$$

there is no need to introduce any homogenization function in this case. Let us consider the RVE built up with n components defined on Ω by the use of (k_i, A_i, l_i) where k_i=const. for $y \in l_i$ and such that $k_i \neq k_j$ for i,j=1,...,n. Hence, the integration in formula (59) can be rewritten as

$$k^{(eff)} = \frac{1}{\sum_{i=1}^{n} \frac{A_i l_i}{k_i}}, \tag{60}$$

where variables A_i, l_i denote the cross-sectional area and the length of i-th element. After some algebraic transformations we arrive at

$$k^{(eff)} = \frac{\prod_{i=1}^{n} k_i}{\sum_{i=1}^{n} A_i l_i k_1 k_2 \ldots k_{i-1} k_{i+1} \ldots k_n}. \tag{61}$$

According to previous considerations, the sensitivity of effective parameter $k^{(eff)}$ with respect to the coefficient k_j, j=1,...,N can be calculated generally as

$$\frac{\partial k^{(eff)}}{\partial k_j} = \frac{\prod_{i=1}^{j-1} k_i \prod_{j+1}^{n} k_i \left(\sum_{i=1}^{n} A_i l_i k_1 k_2 \ldots k_{i-1} k_{i+1} \ldots k_n\right)}{\left(\sum_{i=1}^{n} A_i l_i k_1 k_2 \ldots k_{i-1} k_{i+1} \ldots k_n\right)^2} + \\ - \frac{\prod_{i=1}^{n} k_i \frac{1}{k_j}\left(\sum_{i=1}^{j-1} A_i l_i k_1 k_2 \ldots k_{i-1} k_{i+1} \ldots k_n + \sum_{j+1}^{n} A_i l_i k_1 k_2 \ldots k_{i-1} k_{i+1} \ldots k_n\right)}{\left(\sum_{i=1}^{n} A_i l_i k_1 k_2 \ldots k_{i-1} k_{i+1} \ldots k_n\right)^2} \tag{62}$$

while geometrical sensitivity with respect to the cross-sectional area A_j as

$$\frac{\partial k^{(eff)}}{\partial A_j} = -\frac{\prod_{i=1}^{n} k_i \left(l_j k_1 k_2 \ldots k_{j-1} k_{j+1} \ldots k_n\right)}{\left(\sum_{i=1}^{n} A_i l_i k_1 k_2 \ldots k_{i-1} k_{i+1} \ldots k_n\right)^2}. \quad (63)$$

Analogously, geometrical sensitivity with respect to l_j is obtained as

$$\frac{\partial k^{(eff)}}{\partial l_j} = -\frac{\prod_{i=1}^{n} k_i \left(A_j k_1 k_2 \ldots k_{j-1} k_{j+1} \ldots k_n\right)}{\left(\sum_{i=1}^{n} A_i l_i k_1 k_2 \ldots k_{i-1} k_{i+1} \ldots k_n\right)^2}. \quad (64)$$

It should be underlined that the equations obtained above can be incorporated in 1d FEM formulation for elastostatics as well as heat conduction problems both in deterministic and stochastic computational analyses. These equations are rewritten for illustration in the case of the two-component composite with the RVE presented in Fig. 2.

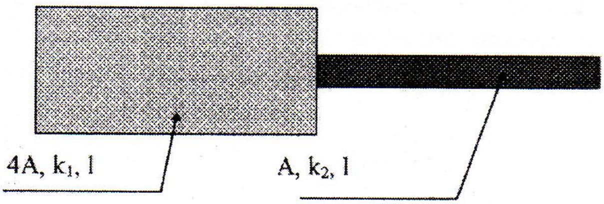

Fig. 2. Two-component composite bar

The homogenization procedure give the effective conductivity as

$$k^{(eff)} = \frac{k_1 k_2}{4Alk_2 + Alk_1}, \quad (65)$$

while corresponding sensitivities are obtained as

$$\frac{\partial k^{(eff)}}{\partial k_1} = \frac{4k_2^2}{Al\left(4k_2 + k_1\right)^2}, \quad \frac{\partial k^{(eff)}}{\partial k_2} = \frac{k_1^2}{Al\left(4k_2 + k_1\right)^2} \quad (66)$$

as well as geometrical sensitivities in the following form:

$$\frac{\partial k^{(eff)}}{\partial A} = -\frac{k_1 k_2}{A^2 l\left(4k_2 + k_1\right)}, \quad \frac{\partial k^{(eff)}}{\partial l} = -\frac{k_1 k_2}{Al^2\left(4k_2 + k_1\right)}. \quad (67)$$

The general result of that analysis is intuitionally clear - increasing of structural geometrical parameters results in decreasing of the effective parameter value (negative derivative sign) and vice versa. Analogously it is observed that increasing any heat conductivity coefficient of composite components, the increase of effective homogenized parameter is obtained. Quantitative verification of the most decisive parameter depends on interrelations between particular material and geometrical characteristics and may be studied further in details.

8. Concluding remarks

The sensitivity analysis of the heat conduction homogenization problem introduced in the paper may be applied for any linear potential field problem - irrotational and incompressible fluid flow, film lubrication, acoustic vibration as well as for electric conduction, electrostatic field, electromagnetic waves. To use the results presented in the paper to homogenization of another engineering field problems, the well-known field analogies may be used introduced to transform the heat conductivity coefficients computed to another physical field parameters, cf. seepage permeability, shear modulus, electrostatic permittivity or electric conductivity.

Using all equations posed above we can introduce the incremental description of the structural sensitivity analysis for elastostatics and linear potential field problems as well as elastodynamics and thermodynamics which may find an application in some further composite materials analyses - deterministic as well as stochastic [13,15].

Considering the assumption that the scale factor between the periodicity cell and the whole composite structure tends to 0 and, on the other hand, that this quantity in real composites is small but different from 0, the sensitivity of effective characteristics to this parameter are to be calculated next starting from the so-called micro-macro approach [22]. To carry out such analysis, the scale parameter has to be introduced in the equations describing effective quantities and next, the influence of δ relating composite micro- and macrostructure may be shown. On the other hand, the sensitivity of the effective characteristics of the composite to the external shape of the RVE as well as the shapes of its components can be studied.

The stochastic sensitivity of the effective elasticity and conductivity tensors can be computed starting from equations posed above using generally two different approaches: Monte-Carlo simulation technique which can be formulated on the basis of the sensitivity approach presented here and the Stochastic Finite Element Method (SFEM) [17].

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Notation

$\mathbf{C}^{(\mathrm{eff})}$	effective elasticity tensor
$\mathbf{h}$	design variable vector
$\mathbf{k}^{(\mathrm{eff})}$	effective heat conductivity tensor
$K_{\alpha\beta}$	stiffness (conductivity) matrix
δ_{ij}	Kronecker delta
$\varphi_{i\alpha}$, H_α	shape functions
ε_{ij}	strain tensor components
σ_{ij}	stress tensor components
χ_{pq}	homogenization function for elastostatics
Φ	homogenization function for heat conduction
Ω	the Representative Volume Element