Two-phase composites with prescribed Kelvin moduli. The inverse homogenization problem

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Abstract

The paper deals with the plane inverse homogenization problem: to reconstruct the layout of two elastic and isotropic materials within a given periodicity cell, corresponding to the predefined values of the Kelvin moduli of the effective composite. The effective moduli are computed according to the homogenization algorithm, with using appropriate Finite Elements (FE) techniques along with periodicity assumptions. The inverse problem thus formulated is solved numerically by the gradient method.

Keywords: composite, finite element methods, homogenization, inverse problems, optimization.

1. Introduction

The direct homogenization means evaluating effective moduli of a composite knowing all microproperties of its representative volume element (RVE). It occurs that treating RVE as repetitive cell *Y* delivers accurate approximations under some commonly accepted assumptions of randomness, see [10]. Therefore, *Y*-periodicity is not a restrictive assumptions, which justifies using the formal methods of periodic homogenization to describe real composite behaviour [6]. According to the homogenization theory the effective moduli are expressed by the formulae involving solutions to the so-called basic cell problems. The latter problems can be attacked by the FE method, preceded by a careful discretization of the RVE identified here with a periodicity cell *Y* [3], [11], [5].

The inverse homogenization means reconstructing the layout of given materials (usually isotropic) within RVE to achieve prescribed effective properties of the composite [8], [9]. This topic is indissolubly bonded with the topology optimization since the optimal designs turn out to possess composite structure with highly complicated local properties of the underlying microstructure [2].

The present paper refers to the topology optimization formulation in which the Kelvin moduli are predefined at each point of the plane feasible domain [4]. The present paper puts forward a numerical algorithm to reconstruct in RVE the layout of two isotropic materials of a common Poisson ratio ν and of given Young moduli E_0 and $E_{\max}= \alpha E_0$, $\alpha \geq 1$

The layout of the material properties is parameterized by the density function ρ, distributed element-wise constant within *Y*.

Let *Y* be divided into Ω_k elements. At each element we assume

$$E_k = E_0\rho_k\,, \qquad \rho_k = \eta^{\alpha_k}\,, \quad \eta = E_{\max}/E_0 \tag{1}$$

2. Numerical homogenization by FE method

The algorithm used follows from imposing the FE approximation on the solution to the basic cell problems of the homogenization theory. This algorithm can be summarized as follows: the nodal displacement **q** determine the displacement field $\mathbf{u} = \mathbf{Nq}$ and the strain field $\boldsymbol{\varepsilon}= \mathbf{Bq}$ within Ω_k, with **N** being shape functions and **B** being the geometric matrix. For the case of Ω_k being the Q4 quadrilateral finite element we have $\mathbf{B}= \mathbf{B}_k$ and $\boldsymbol{\varepsilon}=\boldsymbol{\varepsilon}_k$ in the k-th element and the stress matrix is given by $\boldsymbol{\sigma}_k=\mathbf{E}\boldsymbol{\varepsilon}_k$. We define

$$\mathbf{H}_k = \int_{\Omega_k} \mathbf{E}_k\mathbf{B}_k\,d\Omega_k\,, \quad \mathbf{K}_k = \int_{\Omega_k} \mathbf{B}_k^T\mathbf{E}_k\mathbf{B}_k\,d\Omega_k \tag{2}$$

for each element k.

Let $\lfloor * \rfloor$ stands for the FE aggregations and $\langle * \rangle$ means averaging over the Y. The effective constitutive matrix reads

$$\mathbf{E} = \langle \lfloor \mathbf{E}_k \rfloor \rangle - \langle \lfloor \mathbf{H}_k \rfloor \rangle \langle \lfloor \mathbf{K}_k \rfloor \rangle^{-1} \langle \lfloor \mathbf{H}_k \rfloor \rangle^T \tag{3}$$

or

$$\mathbf{E} = \mathbf{E}^{Avg} - \left(\mathbf{H}\mathbf{K}^{-1}\mathbf{H}^T\right)|Y|^{-1} \tag{4}$$

3. Kelvin moduli of the composite

Let **C** be a constitutive tensor corresponding to the matrix **E**. Let us recall the spectral decomposition of **C** [7]

$$\mathbf{C} = \lambda_1\mathbf{P}_1 + \lambda_2\mathbf{P}_2 + \lambda_3\mathbf{P}_3\,, \tag{5}$$

where λ_1, λ_2, λ_3 are called Kelvin's moduli ($\lambda_1 \geq \lambda_2 \geq \lambda_3 > 0$) and $\mathbf{P}_1$, $\mathbf{P}_2$, $\mathbf{P}_3$ are projectors satisfying $\mathbf{P}_r\,\mathbf{P}_s= \mathbf{0}$ if $r \neq s$ and $\mathbf{P}_1+\mathbf{P}_2+\mathbf{P}_3 = \mathbf{I}$, **I** being the unit tensor.

4. Optimization problem

Prior to solving the optimization problem we construct the formulae for the gradient of **E** with respect to the variables α_k. They read

$$\partial\mathbf{E}/\partial\alpha_k = \left(\ln(\eta)\eta^{\alpha_k}A_k\mathbf{E}_0 - \left[2\breve{\mathbf{H}}_k - \mathbf{R}^T\breve{\mathbf{K}}_k\right]\mathbf{R}\right)|Y|^{-1} \tag{6}$$

where $A_k = |\Omega_k|$ and

$$\mathbf{R}=\mathbf{K}^{-1}\mathbf{H}^T\,, \quad \breve{\mathbf{H}}_k = \partial\mathbf{H}/\partial\alpha_k\,, \quad \breve{\mathbf{K}}_k = \partial\mathbf{K}/\partial\alpha_k \tag{7}$$

Acknowledgement. The paper was prepared within the Research Grant no N506 071338, financed by the Polish Ministry of Science and Higher Education, entitled: *Topology Optimization of Engineering Structures. Simultaneous shaping and local material properties determination*.

We write also the differentiation rules

$$\partial\lambda_r / \partial\alpha_k = (\partial \mathbf{C} / \partial\alpha_k).\mathbf{P}_r \tag{8}$$

We are looking for the two-material layout within Y corresponding to prescribed Kelvin moduli λ_1^0, λ_2^0, λ_3^0. The objective function for the discussed inverse problem is chosen as below

$$\min_{\alpha_k} \left(\sum_r w_r \left(\lambda_r(\alpha_k) - \lambda_r^0\right)^2 + \right.$$
$$\left. + w_\rho \sum_k \left(\alpha_k(1-\alpha_k)\right)^2 + w_p \sum_k f(p_k, \alpha_k) \right) \tag{10}$$

where w_r are weighting factors given as below (constants or of a α_k dependent variables)

$$\mathrm{w}_r = \left[\left(\lambda_1^0\right)^{-1}, \left(\lambda_1^0\right)^{-1}, \left(\lambda_1^0\right)^{-1} \right] \quad \text{or} \quad \mathrm{w}_r = \left[\lambda_1^{-1}, \lambda_2^{-1}, \lambda_3^{-1}\right], \tag{11}$$

The two last components of (10) are penalty terms to push the solution towards the "white-black" layout in which the intermediate properties do not occur. Both are weighted by its own scalar weighting coefficients, respectively, w_ρ, w_p which should be calculated independently, at each step of optimization process, to speed up the convergence. It is clear that first of them reaches a minimum for α_k= (0,1). The last one, tentatively called *push-out (to 1 or 0) function* acts similarly to the second. The parameters p_k have the same meaning as α_k. In this work it is assumed that at each iteration step s of the optimization process we put

$$p_k^{(s)} = \alpha_k^{(s-1)}. \tag{14}$$

Moreover, the function f has the following properties

$$\begin{aligned} & f(p, a) = 0 \\ & \partial f / \partial\alpha_k(p, a) = 0 \qquad \partial f / \partial\alpha_k(p, p) = 0 \end{aligned} \tag{15}$$

for a = 0 or a = 1. The above requirements concerning the derivative of f can be easily met by adopting proper form of this function, here applying two cubic splines, each of them being defined by four points.

5. Results

The process starts from a cell consisting of few square grains with randomly selected variables α_k ranging between 0 and 1. The mesh is generated over the cell with such density that each grain is divided into at least four finite elements. The current value of the objective function and its gradient are calculated for given α_k and λ_1, λ_2, λ_3. In successive steps the gradient method is applied with one or with both penalty terms. In the next stage the grains are refined and the process repeats until reaches an assumed accuracy. In case of benchmark examples of Fig.1 the routines give good results. The structures tested are recovered independently of the choice of the starting point of the optimization process.

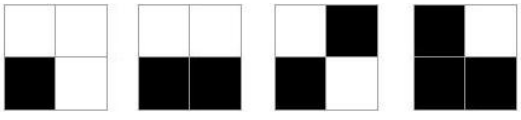

Figure 1: Benchmark structures which are recovered.

The structure of the composite recovered by this process (bilinear Q4 elements and the second penalty term only) is shown in Fig. 2. For specific data $\lambda_1^0 = 4$, $\lambda_2^0 = \lambda_3^0 = 2$ and assumed E_0=1 (white), E_{max}=10 (black), $\nu = 0.3$, we obtain finally the composite structure with λ_1 =3.83, λ_2 = 2.16, λ_3 = 1.97.

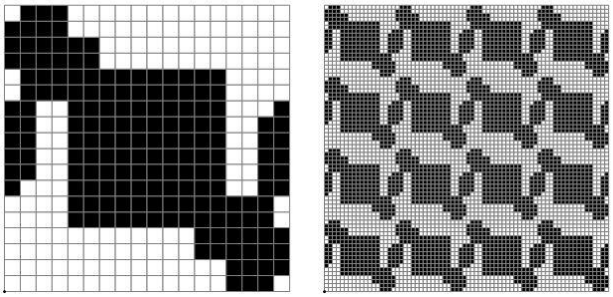

Figure 2: Recovered representative cell and the corresponding composite structure.

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