Multi-parameter underlying micro-structures in the FE inverse homogenization process towards extreme isotropic composites

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Abstract

The objective of this work is to determine the microstructure of the periodic composites with assumed effective isotropic properties constructed by using 2nd rank orthogonal laminates. The microstructure is recovered by the inverse homogenization process on a basic cell of periodicity Y uniformly divided into finite elements. At each element, the underlying material is characterized by three independent scalar parameters unlike in the 1-parameter SIMP-like models. These parameters constitute the set of decision variables for the optimization problem. The effective properties of the underlying material are calculated by the exact Lurie-Cherkaev-Fiodorov formula. The optimization problem thus formulated is nonconvex and nonlinear and is solved by Sequential Linear Programming (SLP) method with a multipoint start. The effective moduli as well as the gradient of the objective function are computed according to the homogenization algorithm for periodic media [5]. In comparison to the widely utilised method based on the SIMP-like interpolation of the underlying material, the use of such a simple tri-parameter model of orthogonal laminates gives much better results, significantly reduces the number of the decision variables involved in the process and the time of computation.

Keywords: inverse homogenization, isotropic composites, orthogonal laminates, microstructures

1. Introduction

The isotropic elastic mixtures composed of two isotropic materials of the bulk moduli ($\kappa_2>\kappa_1$) and shear moduli ($\mu_2>\mu_1$) are characterized by the effective bulk and shear moduli (κ^*, μ^*). In the planar problems the theoretically admissible pairs (κ^*, μ^*), for given volume fraction ρ^0 of material (κ_2, μ_2), lie within a rectangular domain determined by the Hashin-Shtrikman (HS). The tightest bounds in 2D known up till now are due to Cherkaev and Gibiansky (CG) [2]. Theoretically admissible (κ^*, μ^*) for (E_1, ν_1) = (1/20, 0.3), (E_2, ν_2) = (1, 0.3) and ρ^0 = 0.5 are shown in Fig. (1) and Fig. (2). CG bounds are expressed by κ and μ moduli instead of Young modulus E and Poisson ratio ν. The constitutive matrix $\mathbf{E}$ of the 2D problem shows relationships between these two sets of moduli.

$$\mathbf{E}^{2D}=\frac{\mathrm{E}}{1-\nu^2}\begin{Bmatrix}1 & \nu & 0\\ \nu & 1 & 0\\ 0 & 0 & (1-\nu)/2\end{Bmatrix}=\begin{Bmatrix}\kappa+\mu & \kappa-\mu & 0\\ \kappa-\mu & \kappa+\mu & 0\\ 0 & 0 & \mu\end{Bmatrix} \tag{1}$$

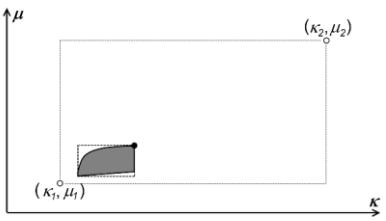

Figure 1: CG area (greyed) an HS rectangle (dotted).

The microstructures corresponding to the interior of the CG area can be of arbitrary rank, in the meaning of the hierarchical homogenization.

The challenge is to design a microstructure whose effective properties correspond to the extreme points of the CG bounds. Some "close to" extreme composite structures are shown in [7], yet there are some points on the boundaries of the CG area for which the structure is not known until today (e.g. point D). Many optimization techniques have been used to attain the CG bounds, including the Method of Moving Asymptotes (MMA) [10], SLP [8] and other. Nevertheless, due to numerical properties of the FE method used for homogenisation, the problem is still tough to solve and only approximate solutions can be obtained.

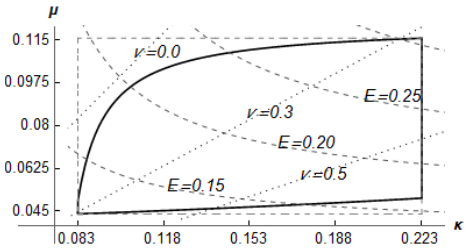

Figure 2: Contour lines of E and ν in the CG area (thick, black) and HS bounds (thin, grey) in (κ, μ) coordinates.

2. Inverse homogenization

The inverse homogenization problems state the questions on the optimal layout of several materials usually with given proportions within Y. Here, optimal means such a layout that gives assumed homogenized properties $\mathbf{E}^*$ of the periodic composite. As such, the problem can be treated as a topology optimization problem: to minimize the gap between the given $\mathbf{E}^*$ and the calculated $\mathbf{E}^{\mathrm{H}}$. Here, the minimized objective function $P(\bullet)$ has a form:

$$P(\bullet)=\left[\left(\kappa^*-\kappa(\bullet)\right)/\kappa^*\right]^2+\left[\left(\mu^*-\mu(\bullet)\right)/\mu^*\right]^2 \tag{2}$$

The conventional process of the optimization is carried out on the Y uniformly divided into n finite-elements Ω_k. Let $\mathbf{E}_i=\mathbf{E}(\kappa_i, \mu_i)$. For each element a variable ρ_k is assigned such that: $\rho_k=0 \Rightarrow \Omega_k.\in \mathbf{E}_1$, $\rho_k=1 \Rightarrow \Omega_k.\in \mathbf{E}_2$. By creating a few configurations of $\boldsymbol{\rho}=\{\rho_k\}$, i.e., layouts of materials, one can try

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to get the expected result described by the assumed $\mathbf{E}^*$. Solution of such a pure 0-1 element-wise optimization problem by some 'hard-kill' method or others does not guarantee achieving the global or even local optimum. The relaxation of the problem allows for variation of $\rho_k \in \langle 0, 1\rangle$ i.e. the material characteristics in each element are dependent on "pseudo-density" variables ρ_k. This requires, for intermediate values of ρ_k, a proper calculating of $\mathbf{E}(\rho_k)$ by adopting some material interpolation scheme, e.g., SIMP [1], RAMP [9], GRAMP [3] or HSρ [6]. This point is crucial for relaxed topology optimization problems because the final solution must be characterized only by $\rho_k = \{0, 1\}$.

2.1. Orthogonal laminate of 2nd rank as a underlying micro-structures

Instead of artificial isotropic one-parameter models, the multi-parameter (•) microstructures (MpM) can be adopted as underlying structures. For laminates, used as MpM, calculating $\mathbf{E}_k(\bullet)$ can be done exactly. For the 1st rank in-plane laminate, composed of periodically repeating layers of materials of any constitutive properties, the effective constitutive matrix $\mathbf{E}^I$ is given by Lurie-Cherkaev-Fiodorov formula (2).

$$\mathbf{H}^I = \langle \mathbf{H} \rangle - (1-\rho)\,\rho\,\Delta\mathbf{H}\,\mathbf{Q}\left[\mathbf{Q}^T\,\mathbf{H}^{*a}\,\mathbf{Q}\right]^{-1}\mathbf{Q}^T\,\Delta\mathbf{H}, \tag{3}$$

where (for selected basis):

$$\mathbf{Q} = \frac{\sqrt{2}}{2}\begin{bmatrix} \sqrt{2}\cos^2(\alpha) & -\sin(2\alpha) \\ \sqrt{2}\sin^2(\alpha) & \sin(2\alpha) \\ \sin(2\alpha) & \sqrt{2}\cos(2\alpha) \end{bmatrix}, \quad \mathbf{H} = \begin{bmatrix} E_{11} & E_{12} & \sqrt{2}E_{13} \\ & E_{22} & \sqrt{2}E_{23} \\ \text{sym.} & & 2H_{33} \end{bmatrix}$$

In above, $\mathbf{H}$ is the matrix representation of Hooke's tensor and α is the angle of the direction of lamination, for details see [4]. The 1st rank laminate $\mathbf{E}^I$ thus obtained can be used for the construction of the 2nd rank laminate $\mathbf{E}^{II}$, calculated again by formula (3). Assumed MpM model of the laminate of two isotropic materials with orthogonal layers i.e. $\alpha = \{90°, 0°\}$ can be described by three parameters ρ, η, φ as shown in Fig. 3.

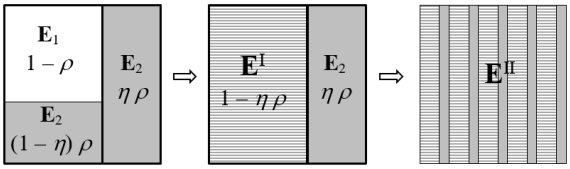

Figure 3: Construction of the 2nd rank orthogonal laminate.

The first lamination, ($\alpha = 90°$, $\rho^I = 1 - \eta\rho$) consist of $(1-\rho)/\rho^I$ and $(1-\eta)\rho/\rho^I$ fractions of materials $\mathbf{E}_1$ and $\mathbf{E}_2$ respectively, determines the properties of $\mathbf{E}^I$. The next one, for $\alpha = 0°$ contains $1-\eta\rho$ fraction of $\mathbf{E}^I$ and $\eta\rho$ fraction of $\mathbf{E}_2$ gives $\mathbf{E}^{II}$ next rotated by the angle φ which defines the orientation of the laminate in the coordination system of the cell Y. Such model allows for the exact description of:

- isotropic material, $\rho = 0 \Rightarrow \mathbf{E}^{II} \equiv \mathbf{E}_1$, $\rho = 1 \Rightarrow \mathbf{E}^{II} \equiv \mathbf{E}_2$,
- 1st rank orthotropic laminate for $\eta = 1$ or $\eta = 0$ and $\rho > 0$,
- 2nd rank orthotropic laminate.

3. Results

To achieve the boundary of the CG domain, variety of isotropic composites are constructed based on $\mathbf{E}^{II}$ underlying laminates. At the starting point, the triplets (ρ_k, η_k, φ_k) are selected randomly yet satisfying the isoperimetric condition $\rho^0 = 0.5$. The obtained results (black dots) for 128 x 3 decision variables are presented in Fig. 4. Grey lines show the convex hull of results obtained for 3200 decision variables each (single-parameter elements) by using the HSρ interpolation scheme.

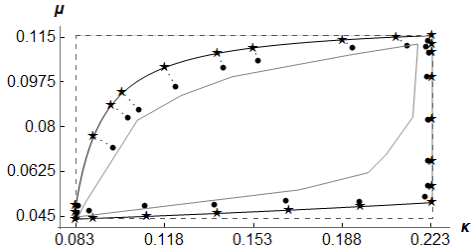

Figure 4: Effective ● (κ^H, μ^H) obtained for assumed ★ (κ^*, μ^*) (connected by dotted lines respectively).

4. Final remarks

A new inverse homogenization technique is developed to construct extremal microstructures of effective isotropic moduli. The constructed layouts correspond to the points lying very closely to the contour of the CG domain. The number of the decision variables for the proposed MpM model is nearly 10 times smaller than for first rank microstructures, which significantly reduces the time of computation. The local basic cell problems are set on a hexagonal cell Y possessing rotational symmetry of angle 120°. Such a non-conventional choice of a basic cell generates automatically the family of isotropic mixtures. It should however be noted that the MpM approach causes great limitations – the resulting solution by definition is limited to a narrow class of the assumed microstructures – here to orthogonal laminates of at most 2nd rank.

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