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Application of the Isotropic Material Design and Inverse Homogenization in 3D printing

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Homogenization-based approach to structural optimization and Free Material Design (FMD) technique are discussed in case of isotropy. The problem is elaborated from the perspective provided by: (i) the theory of composites and (ii) Isotropic Material Design (IMD) – a variant of FMD. Results provided by IMD are interpreted in light of the Hashin-Shtrikman bounds on the effective isotropic properties of material-void mixtures. This in turn provides practical guidelines for 3D printing.

Key words: Hashin-Shtrikman bounds, Free Material Design, 3D printing.

1. Introduction

In this paper we investigate the links between two techniques for structural compliance minimization: (i) the homogenization-based approach, and (ii) Free Material Design (FMD). Such study is justified by significant differences in the mathematical structure of the above-mentioned optimization procedures.

Loosely speaking, both techniques ask for the optimal constitutive tensor at each point of the design domain. The set of feasible solutions in the FMD approach is rather weakly restricted in the space of all Hooke's tensors E_s^4 hence straightforward analytical solutions are available for a wide class of optimization problems.

Conversely, in the homogenization-based approach optimal tensor belongs to a set $E_s^4 \supset G$ whose elements are unknown in general. Therefore, in most cases, numerical methods are necessary for the solution. The Reader is referred to e.g. [1, 4, 5] for details on homogenization theory and FMD in the context of linearized elasticity.

In the sequel we restrict our attention to isotropy. Such choice allows us to study the relation between: (i) the Hashin-Shtrikman (HS) bounds on the effective properties of a porous (material-void) composite, and (ii) the results of the Isotropic Material Design (IMD) – a variant of FMD – developed in [3]. Recall that the HS bounds are explicitly given in two- and three-dimensional elasticity; it is also proven that they are simultaneously achieved on certain microstructures, see [1] for details.

2. Notation

Let $\overline{\Omega} \subset R^2$ and set $\overline{\Omega} = \Omega \cup \partial\Omega$, where $\partial\Omega$ denotes the boundary of Ω. Next, suppose that $\overline{\Omega}$ represents the middle plane of a thin plate with constant thickness h, and consider the generalized plane stress problem of linearized elasticity posed on $\overline{\Omega} \times [-h/2, h/2]$, see e.g. [6] for details of such setting. Here and subsequently, most of the mathematical technicalities are omitted for the reason of space.

Write V for the linear space of kinematically admissible displacement fields, i.e. functions satisfying certain boundary conditions on $\partial\Omega_u \subset \partial\Omega$. For given $\mathbf{v} \in V$ define the small strain tensor field $\boldsymbol{\varepsilon}(\mathbf{v}) = [\nabla\mathbf{v} + (\nabla\mathbf{v})^{\mathrm{T}}]/2$, $\boldsymbol{\varepsilon} \in L^2(\Omega;\, E_s^2)$, where E_s^2 stands for the space of symmetric second-order tensors.

Assume that the plate is subjected to a one-parameter load $\mathbf{p} \in L^2(\partial\Omega_\tau; R^2)$ at $\partial\Omega_\tau \subset \partial\Omega$. Stress fields $\boldsymbol{\tau}$ are called statically admissible if they belong to the set

$$\Sigma = \left\{ \boldsymbol{\tau} \in L^2(\Omega\,; E_s^2) \;\middle|\; \int_\Omega \boldsymbol{\tau} : \boldsymbol{\varepsilon}(\mathbf{v}) dx = \int_{\partial\Omega_\tau} \mathbf{p} \cdot \mathbf{v} ds \quad \forall \mathbf{v} \in V \right\},$$

where symbols " : ", " · " denote the inner product operations in respective spaces.

Optimization problems discussed in this paper assume the common setting

$$\text{(P)} \qquad \left| \begin{array}{l} Y = \min\left\{ J(\mathbf{C}) \;\middle|\; \mathbf{C} \in X \right\}, \\[2ex] J(\mathbf{C}) = \min\left\{ \displaystyle\int_\Omega \boldsymbol{\tau} : (\mathbf{C}^{-1}\boldsymbol{\tau})\, dx \;\middle|\; \tau \in \Sigma \right\}, \end{array} \right.$$

where $\mathbf{C} \in L^\infty(\Omega\,; E_s^4)$ denotes the constitutive (Hooke's) tensor field and X stands for a set of restrictions imposed on $\mathbf{C}$. Recall that $J(\mathbf{C})$ in (P) defines the compliance of the plate. It turns out that solutions to (P) can be expressed as

$$Y = \frac{Z^2}{\Lambda}, \qquad Z = \min\left\{ \int_\Omega \|\boldsymbol{\tau}\| \, dx \,\middle|\, \boldsymbol{\tau} \in \Sigma \right\}$$

with Λ, $\|\boldsymbol{\tau}\|$ and Z appropriately defined.

In the sequel we frequently refer to the spectral decomposition of the isotropic Hooke's tensors of material stiffness and compliance, respectively given by

$$\mathbf{C} = 2k\,\mathbf{P}_1 + 2\mu\,\mathbf{P}_2, \qquad k = \frac{E}{2(1-\nu)}, \qquad \mu = \frac{E}{2(1+\nu)},$$
$$\mathbf{C}^{-1} = \frac{1}{2}K\,\mathbf{P}_1 + \frac{1}{2}L\,\mathbf{P}_2, \qquad K = \frac{1}{k}, \qquad L = \frac{1}{\mu},$$

where $\mathbf{P}_1$, $\mathbf{P}_2 \in E_s^4$ denote the projectors on spherical and deviatoric subspaces of E_s^4.

3. Optimal effective moduli of the isotropic material-void composite

Classical topology optimization deals with the optimal distribution of a given, isotropic material characterized by the moduli E_0 and ν_0. Total amount of this basic material in a design domain Ω is fixed by $\Lambda_H = |\Omega|\,\theta_0$, $0 < \theta_0 < 1$. The task, initially ill-posed, is regularized (relaxed) in the framework of homogenization theory. With the additional assumption on isotropy it takes the form

$$(\mathrm{P}_H) \qquad \left| \begin{array}{l} Y_H = \min\left\{ J(\mathbf{C}) \;\middle|\; \mathbf{C} \in X_H \right\}, \\ J(\mathbf{C}) = \min\left\{ \displaystyle\int_\Omega \boldsymbol{\tau} : (\mathbf{C}^{-1}\boldsymbol{\tau})\, dx \;\middle|\; \boldsymbol{\tau} \in \Sigma \right\}, \end{array} \right.$$

where the set X_H is defined by

$$X_H = \Bigg\{ \mathbf{C} = 2k_H\,\mathbf{P}_1 + 2\mu_H\,\mathbf{P}_2 \;|(k_H, \mu_H) \quad \text{as in (3.1)},$$
$$\theta \in L^\infty(\Omega\,; [0,\,1]), \; \int_\Omega \theta\, dx = \Lambda_H \Bigg\},$$

$$(3.1) \qquad \frac{1}{k_H} = \frac{1}{\theta}(K_0 + \alpha_K) - \alpha_K, \qquad \frac{1}{\mu_H} = \frac{1}{\theta}(L_0 + \alpha_L) - \alpha_L,$$

with $\alpha_K = L_0$, $\alpha_L = 2K_0 + L_0$. Formulae in (3.1) define the Hashin-Shtrikman bounds on effective properties of two-dimensional, linearly elastic, isotropic material-void composite and θ denotes the material density in the mixture.

Mathematically, (P_H) is a special case of the general topology optimization problem discussed e.g. in [1]. Making use of the same arguments leads to the following bound on Y_H

$$Y_H \leqslant \frac{(Z_H)^2}{\theta_0}, \qquad Z_H = \min\left\{ \int_\Omega \|\boldsymbol{\tau}\|_H \, dx \;\middle|\; \boldsymbol{\tau} \in \Sigma \right\}, \tag{3.2}$$

where

$$\|\boldsymbol{\tau}\|_H = \sqrt{\frac{1}{4}\left[K_0 + \alpha_K(1-\theta_0)\right](tr\,\boldsymbol{\tau})^2 + \frac{1}{2}\left[L_0 + \alpha_L(1-\theta_0)\right]\|dev\,\boldsymbol{\tau}\|^2}.$$

Assume $\boldsymbol{\sigma}$ for a minimizer in (3.2). Effective Young's modulus and Poisson's ratio are thus given by

$$E_H^* = \frac{\theta^*}{3-2\theta^*}E_0, \qquad \nu_H^* = \frac{1-\theta^*(1-\nu_0)}{3-2\theta^*} \qquad \theta^* = \Lambda_H \frac{f(\boldsymbol{\sigma})}{\int_\Omega f(\boldsymbol{\sigma})\, dx}, \tag{3.3}$$

where

$$f(\boldsymbol{\sigma}) = \sqrt{\frac{1}{4}(K_0 + \alpha_K)(tr\,\boldsymbol{\sigma})^2 + \frac{1}{2}(L_0 + \alpha_L)\|dev\,\boldsymbol{\sigma}\|^2}.$$

Note that (3.1) and (3.3) couple (k_H^*, μ_H^*) through θ^*.

Validity of (3.2) and (3.3) is restricted by

$$\theta_0 \leqslant 1 + \min\left\{\frac{1+\nu_0}{3-\nu_0}, \frac{1-\nu_0}{1+\nu_0}\right\}, \qquad \theta_0 \leqslant \min_{x\in\Omega}\left\{\frac{\frac{1}{|\Omega|}\int_\Omega f(\boldsymbol{\sigma})\, dx}{f(\boldsymbol{\sigma})}\right\}. \tag{3.4}$$

Restrictions in (3.4) are not derived here for the reason of space. Note that the first inequality is trivially fulfilled due to $-1 \leqslant \nu_0 \leqslant 1$ in plane stress and assumed $0 < \theta_0 < 1$.

4. Matching the effective composite moduli and IMD results

4.1. Brief exposition of the IMD

Following [3], we set (P) in the form suitable for two-dimensional considerations in the framework of the Isotropic Material Design (IMD)

$$(\mathrm{P}_I) \qquad \left| \begin{array}{l} Y_I = \min\{J(\mathbf{C}) \mid \mathbf{C} \in X_I\},, \\[2ex] J(\mathbf{C}) = \min\left\{ \int_\Omega \tau : (\mathbf{C}^{-1}\boldsymbol{\tau})\, dx \;\middle|\; \boldsymbol{\tau} \in \Sigma \right\}, \end{array} \right.$$

with

$$X_I = \left\{ \mathbf{C} = 2k_I\,\mathbf{P}_1 + 2\mu_I\,\mathbf{P}_2 \;\middle|\; \int_\Omega tr\,\mathbf{C}\,dx = \Lambda \right\}$$

and $\Lambda = |\Omega| C_0$, where C_0 is a reference modulus and $tr\,\mathbf{C} = 2k_I + 4\mu_I$. Solution to (P_I) reads

$$Y_I = \frac{(Z_I)^2}{\Lambda}, \qquad Z_I = \min\left\{ \int_\Omega \|\boldsymbol{\tau}\|_I\,dx \;\middle|\; \boldsymbol{\tau} \in \Sigma \right\}, \tag{4.1}$$

where

$$\|\boldsymbol{\tau}\|_I = \frac{\sqrt{2}}{2}\,|tr\,\boldsymbol{\tau}| + \sqrt{2}\,\|dev\,\boldsymbol{\tau}\|.$$

On assuming $\boldsymbol{\sigma}$ for a minimizer in (4.1) we obtain the formulae for optimal moduli of isotropy

$$k_I^* = \frac{\sqrt{2}}{4}\Lambda\frac{|tr\,\boldsymbol{\sigma}|}{\int_\Omega \|\boldsymbol{\sigma}\|_I\,dx}, \qquad \mu_I^* = \frac{\sqrt{2}}{4}\Lambda\frac{\|dev\,\boldsymbol{\sigma}\|}{\int_\Omega \|\boldsymbol{\sigma}\|_I\,dx}. \tag{4.2}$$

Note that (k_I^*, μ_I^*) in (4.2) are independently controlled by the invariants of optimal stress tensor $\boldsymbol{\sigma}$. Therefore (k_I^*, μ_I^*) are uncoupled, conversely to (k_H^*, μ_H^*), see the remark at the end of Sec. 3. Thus, matching the effective moduli of the composite and the IMD result in the whole design space is impossible in general.

By assuming that the function defining the Poisson ratio $\nu_Y = \nu_Y(x)$ is known in Ω, one may recast the IMD problem to the YMD form recently proposed by S. Czarnecki and T. Lewiński in a yet unpublished report. Fixing $\nu_Y = \nu_H^*$, see (3.3), is the first step towards matching the effective isotropic composite moduli and the YMD results.

Solution of $(\mathrm{P}_Y) \equiv (\mathrm{P}_I)$ is now given by

$$Y_Y = \frac{(Z_Y)^2}{\Lambda}, \qquad Z_Y = \min\left\{ \int_\Omega \|\boldsymbol{\tau}\|_Y\,dx \;\middle|\; \boldsymbol{\tau} \in \Sigma \right\}, \tag{4.3}$$

where

$$\|\boldsymbol{\tau}\|_Y = \sqrt{\frac{3-\nu_Y}{2(1+\nu_Y)}(tr\,\boldsymbol{\tau})^2 + \frac{3-\nu_Y}{1-\nu_Y}\,\|dev\,\boldsymbol{\tau}\|^2}, \qquad \nu_Y = \nu_H^*. \tag{4.4}$$

On assuming $\boldsymbol{\sigma}$ for a minimizer in (4.3) we obtain the optimal Young's modulus

$$E_Y^* = \Lambda \frac{1-(\nu_Y)^2}{3-\nu_Y} \frac{\|\boldsymbol{\sigma}\|_Y}{\int\limits_\Omega \|\boldsymbol{\sigma}\|_Y \, dx}. \tag{4.5}$$

4.2. Applying the YMD results in 3D printing

In addition to illustrating how the IMD (YMD) formulas work in the context of the theory of composites, our considerations provide guidelines for the practical application of optimal designs.

Consider the 3D printing technology. Our task now is to match the YMD results and the parameters of a material-void composite for the identification of:

a) the constitutive parameters E_0 and ν_0 of the basic material ("ink" for the 3D printer) and its density θ^* at each point of Ω;
b) microstructural arrangement of the basic material at each point of Ω (the printing pattern).

The first goal is achieved in the following way:

a) density of a basic material in a composite

$$\theta^* = \frac{3E_Y^*}{E_0 + 2E_Y^*} \tag{4.6}$$

is obtained by substituting (3.3) and (4.5) in $E_H^* = E_Y^*$;

b) lower estimate on E_0

$$\frac{E_0}{C_0} \geqslant \max_{x\in\Omega} \left\{ \frac{1-(\nu_Y)^2}{3-\nu_Y} \frac{\|\boldsymbol{\sigma}\|_Y}{\frac{1}{|\Omega|}\int\limits_\Omega \|\boldsymbol{\sigma}\|_Y \, dx} \right\}, \tag{4.7}$$

where $\boldsymbol{\sigma}$ stands for a minimizer in (4.3), is provided by the restriction $0 \leqslant \theta^* \leqslant 1$;

c) the total amount of basic material needed for the 3D print is estimated by

$$\Lambda_H = \int\limits_\Omega \frac{3E_Y^*}{E_0 + 2E_Y^*} \, dx. \tag{4.8}$$

Note that the above-mentioned calculations require an iterative procedure as E_Y^* depends on ν_H^* and θ^*.

In case of high porosity (low density) of the composite, i.e. in case when the values of $\theta^* = \theta^*(x)$ are small everywhere in the design domain, the 3D printing pattern may be assumed as a single-scale, equilateral triangular lattice, or Kagomé lattice, see [2] for mathematical justification of this observation. In both layouts, the layers of materials intersect at 60° and their thickness are equal to $\theta^*/3$.

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