Topology optimization of continuum structures
made of non-homogeneous materials of isotropic or cubic symmetry

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1. Abstract
The paper concerns optimum design of elastic moduli corresponding to: i) non-homogeneous isotropy, or to ii) cubic symmetry, aimed at minimization of the total compliance. Similarly to the Free Material Design the cost of design is assumed as the integral of the trace of the elastic moduli tensor over the feasible domain. A proof is given that both the optimum design formulations discussed reduce to auxiliary problems being tensorial counterparts of the Monge-Kantorovich scalar problem. The paper comprises numerical analysis of the mentioned auxiliary problems and puts forward case studies concerning isotropy design. A characteristic feature of optimal isotropic designs is emergence of auxetic properties, where Poisson ratio attains negative values.

2. Keywords: Free material design, compliance minimization, anisotropy, cubic symmetry.

3. Introduction
The Free Material Design (FMD) of structures subjected to a single load case leads to optimal material designs being singular, viz. the optimal Hooke tensor occurs to have only one non-zero eigenvalue \( \lambda_1 \). Thus in 3D case the eigenvalues (or Kelvin moduli) of the optimal Hooke tensor are \( (\lambda_1, 0, 0, 0, 0, 0) \), while in 2D the optimal Kelvin moduli are \( (\lambda_1, 0, 0) \), cf. [1, 4, 5, 8]. One of the methods to make the optimal Hooke tensor non-singular is to optimize the structure with respect to multiple loads, cf. [4, 5]. To arrive at positive values of all Kelvin moduli in the 3D case one should optimize the structure with respect to at least six independent load variants. For the 2D case three load cases suffice, see [4, 5].

A non-singular result can also be achieved by imposing isotropy, as shown recently by Czarnecki [6]. In this version of FMD -called IMD or the isotropic material design- the main unknowns are two scalar fields \( k \) and \( \mu \) subjected to the isoperimetric condition expressed by the integral of the trace of Hooke tensor equal to \( 3k + 10\mu \). A less restrictive assumption, like cubic symmetry, leads to optimal values of the moduli among which one becomes zero, see [7]. This version of FMD will be called CSMD (cubic symmetry material design). The aim of the present paper is to publish these theoretical results and augment it with a numerical analysis. It occurs that the problems IMD and CSMD reduce to auxiliary problems similar to those known from the theory of materials with locking and having much in common with Monge-Kantorovich equation. The auxiliary minimization problems (in which test stress fields run through the set of statically admissible stresses corresponding to the given load) are solved, upon discretization, by representing the solutions via singular value decompositions (SVD) and then by performing test stress fields run through the set of statically admissible stresses corresponding to the given load) are solved, upon discretization, by representing the solutions via singular value decompositions (SVD) and then by performing numerical analysis of the mentioned auxiliary problems and puts forward case studies concerning isotropy design. A characteristic feature of optimal isotropic designs is emergence of auxetic properties, where Poisson ratio attains negative values.

The paper puts emphasis on the links between FMD, IMD, CSMD and the minimum compliance problem as set by Bouchité and Buttazzo [3].

4. The FMD problem revisited
Let us recall the stress-based setting of FMD, see [5]. Let the linear form \( f(\mathbf{v}) \) represent the work of given loads on the virtual displacement field \( \mathbf{v} = (v_1, v_2, v_3) \) of the body occupying the domain \( \Omega \). Let \( \Sigma_f \) represent the set of statically admissible stress fields \( \tau = (\tau_j) \) such that

\[
\int_\Omega \tau_j \varepsilon_{ij}(\mathbf{v}) \, dx = f(\mathbf{v}) \quad \forall \mathbf{v} \in V
\]

(1)

where \( V \) is the space of kinematically admissible displacements while \( \varepsilon_{ij}(\mathbf{v}) = \frac{1}{2} (v_{1,j} + v_{j,1}) \) where \( v_{i,j} = \partial v_i / \partial x_j \). Let \( \| \tau \| \) be the Euclidean norm or \( \| \tau \| = (\tau_j \tau_j)^{1/2} \). The Hooke’s law has the form \( \tau_j = C_{ijkl} \varepsilon_{kl}(\mathbf{u}) \) with \( \mathbf{u} \) being the unknown displacement field. This field depends on the tensor field \( \mathbf{C} \) which will be indicated by \( \mathbf{u} = \mathbf{u}(\mathbf{C}) \).
Let $H^1_+(\Omega)$ be the set of positive semidefinite fields $C$ -which locally are elements of the set $\mathbb{R}^4_+$ of fourth rank tensors of appropriate symmetries - satisfying the isoperimetric condition which fixes the value $\Lambda$ of the integral of $\text{tr} C = C_{ijij}$ over the given design domain $\Omega$. In its original setting [1] the FMD problem is formulated as

$$J = \min_{C \in H^1_+(\Omega)} f(u(C))$$

(2)

By expressing $C$ by its spectral decomposition and performing minimization over the projectors, keeping the Kelvin moduli $\lambda_i$ as fixed, one rearranges the problem (2) to the form

$$J = \min_{\tau \in \Sigma_f} \min_{\lambda_i \geq 0} \int_{\Omega} \frac{1}{\lambda_i} \|\tau\|^2 \, dx$$

(3)

Now the minimization over the Kelvin modulus $\lambda_1$ can be performed analytically, which leads to the formula

$$J = Z^2/\Lambda \quad , \quad Z = \min_{\tau \in \Sigma_f} \int_{\Omega} \|\tau\| \, dx$$

(4)

Thus the problem (2) is reduced to the above minimization problem with the integrand of linear growth. The result (4) has been found in an elementary way, hence needs mathematical justification. The main problem lies in the property of the integrand in problem in (4); its linear growth implies that the solutions cannot be, in general, sought in the class of functions; the solutions are measures.

The result (4) can be justified by the methods developed in [3], see Theorem 2.3, p.144 therein. It is worth showing here a complete proof of the estimate: $J \geq Z^2/\Lambda$. The Schwarz inequality is crucial, as seen below. Due to $\tau \in \Sigma_f$ we have

$$f(\nu) = \int_{\Omega} \left( \frac{1}{\sqrt{\lambda_1}} \tau \right) \cdot \left( \frac{1}{\sqrt{\lambda_1}} \epsilon(\nu) \right) \, dx$$

(5)

hence

$$f(\nu) \leq \left( \int_{\Omega} \frac{1}{\lambda_1} \|\tau\|^2 \, dx \right)^{1/2} \left( \int_{\Omega} \frac{1}{\lambda_1} \|\epsilon(\nu)\|^2 \, dx \right)^{1/2}$$

(6)

Let $\|\epsilon(\nu)\| \leq 1$ a.e. on $\Omega$. Then

$$f(\nu) \leq \left( \int_{\Omega} \frac{1}{\lambda_1} \|\tau\|^2 \, dx \right)^{1/2} \left( \int_{\Omega} \lambda_1 \, dx \right)^{1/2} \left( \int_{\Omega} \frac{1}{\lambda_1} \|\tau\|^2 \, dx \right)^{1/2}$$

(7)

since now $\text{tr} C = \lambda_1$. Thus we estimate

$$\int_{\Omega} \frac{1}{\lambda_1} \|\tau\|^2 \, dx \geq \frac{1}{\Lambda} (f(\nu))^2$$

(8)

for $\nu$ such that $\|\epsilon(\nu)\| \leq 1$. Thus (8) implies

$$\inf_{\tau \in \Sigma_f} \inf_{\lambda_i \geq 0} \int_{\Omega} \frac{1}{\lambda_i} \|\tau\|^2 \, dx \geq \frac{1}{\Lambda} \left( \sup_{\|\epsilon(\nu)\| \leq 1} \frac{f(\nu)}{\text{a.e. on } \Omega} \right)^2$$

(9)

where the left hand side is equal to $J$, see (3); this ends the proof of the estimate discussed. In papers [4, 5] the following identity has been put forward

$$\sup\{f(\nu) \mid \|\epsilon(\nu)\| \leq 1 \text{ a.e. on } \Omega\} = \inf\left\{ \int_{\Omega} \|\tau\| \, dx \mid \tau \in \Sigma_f \right\}$$

(10)
by invoking the arguments of Strang and Kohn [9] concerning the Michell truss problem. Just recently the present authors have noted that the identity (10) has been proved by Bouchitté and Valadier [2]. Denoting the value of (10) by $Z$ one can rearrange (9) to the form

$$
\inf_{\tau \in \Sigma_f} \inf_{\lambda_i \geq 0} \left( \frac{1}{\lambda_i} \| \tau \|^2 \right) dx \geq \frac{1}{\Lambda} \left( \inf_{\tau \in \Sigma_f} \int \| \tau \| dx \right)^2
$$

(11)

which proves $J \geq Z^2 / \Lambda$.

Derivation (5) - (11) is inspired by some arguments used to prove Proposition 2.1 in [3]. This derivation is of vital importance, since it shows the passage from the functional (3) having the integrand of the quadratic growth to the functional with the integrand of linear growth at the right hand side of (11).

Much more subtle arguments are necessary to prove that $J \leq Z^2 / \Lambda$ which would complete the proof of (4). In paper [3] and the papers cited therein one can find the equality (10) rearranged to the accurate form. The field $\mathbf{v}$ should be a Lipschitz function from $\text{Lip}_{1,\rho}(\Omega)$ being the closure in the space of continuous functions on $\bar{\Omega}$ of the set of $C^\infty$ functions with compact support vanishing on a given subset of $\Omega$ such that $\rho(\nabla \mathbf{v}) \leq 1$ with $\rho(\nabla \mathbf{v}) = ||| \mathbf{e}(\mathbf{v}) |||$.

Having solved problem (10) one can express the optimal $\lambda_1$ in terms of $\tau^*$ being the minimizer of (4) or (10). The optimal body occupies the subdomain of $\Omega$ being the support of this measure, [4, 5].

5. The cubic symmetry material design (CSMD)

The set of admissible Hooke tensors will be restricted to the set of Hooke tensors of cubic symmetry at each point $x \in \Omega$. Thus we assign to each point $x$ a triplet of unit vectors $(m(x), n(x), p(x))$ and define the tensor

$$
S = n \otimes n \otimes n + m \otimes m \otimes m + p \otimes p \otimes p
$$

(12)

for each point of $\Omega$. Let us recall the expression for components of the unit tensor in $\mathbb{R}^d$

$$
I_{ijkl} = \frac{1}{2} (\delta_{ik} \delta_{lj} + \delta_{ij} \delta_{kl})
$$

(13)

and let $J = \frac{1}{2} (\delta_{ij} \delta_{kl})$. Define $L = I - S$, $M = S - J$. All tensors $C$ of cubic symmetry are represented by Walpole’s formula [10]

$$
C = aL + bM + cM
$$

(14)

with $a, b, c$ being nonnegative moduli. The inverse of $C$ equals

$$
C^{-1} = \frac{1}{a} J + \frac{1}{b} L + \frac{1}{c} M
$$

(15)

provided that all the moduli are positive. The trace of $C$ equals $\text{tr} C = a + 3b + 2c$. The cost of the design is defined as the integral of $\text{tr} C$ over $\Omega$ and is assumed as equal $\Lambda$. The set of tensors $C$ in $\Omega$ represented by (14) and satisfying the mentioned cost constraint will be denoted by $H^1_\Lambda(\Omega)$.

The CSMD problem assumes the form (2) with $H^1_\Lambda$ replaced by $H^2_\Lambda$. One can prove, see [7], that the compliance $J$ is still given by (4) with $Z = Z_2$

$$
Z_2 = \min_{\tau \in \Sigma_f} \int \| \tau \| dx
$$

(16)

and

$$
\| \tau \| = \frac{1}{\sqrt{3}} |\text{tr} \tau| + \sqrt{2} \| \text{dev} \tau |
$$

(17)

where $\text{tr} \tau = \tau_{ii}$ and

$$
\text{dev} \tau = \tau - \frac{1}{3} (\text{tr} \tau) I, \quad I = (\delta_{ij})
$$

(18)

One can prove that $\| \cdot \|_2$ is a norm in $\mathbb{R}^2$. Let

$$
\| |\mathbf{e}| |_2^2 = \sup_{\tau \neq 0} \| \tau \mathbf{e} \|_2
$$

(19)
be the norm dual to (17). The counterpart of the equality (10) reads

$$\sup \{ f(\mathbf{v}) \ | \ ||\mathbf{e}(\mathbf{v})||_2^\ast \leq 1 \} = \inf \left\{ \int_\Omega ||\mathbf{\tau}||_2 \ dx \ | \ \mathbf{\tau} \in \Sigma_f \right\}$$  

(20)

The trial fields \(\mathbf{v}\) are of Lipschitz class previously mentioned, where now \(\rho(\mathbf{V}) = ||\mathbf{e}(\mathbf{v})||_2^\ast\)

The norm \(||.||_2^\ast\) defined by (19) can be expressed explicitly. Appropriate computation gives

$$||\mathbf{e}||_2^\ast = \max \left\{ \frac{\sqrt{\lambda}}{3} ||\mathbf{r}\mathbf{e}||, \frac{\sqrt{\mu}}{2} ||\mathbf{dev}\mathbf{e}|| \right\}$$  

(21)

Thus in the space of principal strains the ball \(||\mathbf{e}||_2^\ast \leq 1\) assumes the shape of a cylindrical domain of length 2 and radius \(2\sqrt{3}/3\).

The problem at the left hand side of (20) is mathematically simpler than the right hand side, but its solution is of lesser importance. The maximizer \(\mathbf{v}^\ast\) does not determine the optimal moduli \(C^\ast_{ijkl}\) directly. To find them one cannot omit solving the problem (16).

Let \(\mathbf{e}^\ast\) be the minimizer of (16). Then the optimal triplet \((m^\ast, n^\ast, p^\ast)\) coincides with the triplet of eigenvectors of \(\mathbf{e}^\ast\). Moreover, the optimal moduli are expressed by

\[
a^\ast(x) = \frac{\Lambda}{\sqrt{2}Z}\|\mathbf{tr}\mathbf{e}^\ast(x)\| \\
b^\ast(x) = 0 \\
c^\ast(x) = \frac{\Lambda}{\sqrt{2}Z}\|\mathbf{dev}\mathbf{e}^\ast(x)\|
\]

(22)

Note that \(\mathbf{tr}\mathbf{C}^\ast(x) = a^\ast(x) + 3b^\ast(x) + 2c^\ast(x) = \frac{\Lambda}{Z}||\mathbf{e}^\ast(x)||_2\) which shows that \(a^\ast, b^\ast, c^\ast\) satisfy the isoperimetric condition.

6. The isotropic material design (IMD)

The set \(H^\ast_{ijk}\) corresponding to isotropy will replace the set \(H^1_{ijk}\) in (2). The tensors \(\mathbf{C}\) are now represented by

\[
\mathbf{C} = 3k\mathbf{J} + 2\mu\mathbf{K}
\]

(23)

with \(\mathbf{K} = \mathbf{I} - \mathbf{J}\) and \(\mathbf{tr}\mathbf{C} = 3k + 10\mu\). As proved by Czarnecki [6], the formula (4) holds good with \(Z\) given by (16) and with the integrand defined as below

$$||\mathbf{\tau}||_3 = \sqrt{10||\mathbf{tr}\mathbf{\tau}|| + 5\sqrt{6}||\mathbf{dev}\mathbf{\tau}||}$$  

(24)

Contrary to obvious discrepancies between isotropic materials and cubic crystals the problem (16) differs only in coefficients in (17) and (24). Assume \(\mathbf{\tau} = \mathbf{\tau}^\ast\) is the minimizer of (4) with \(||.|| = ||.||_1\).

The optimal moduli are expressed by

\[
k^\ast(x) = \frac{\sqrt{10}}{3} \frac{\Lambda}{Z}||\mathbf{tr}\mathbf{e}^\ast(x)|| \ , \ \mu^\ast(x) = \frac{\sqrt{3}}{2} \frac{\Lambda}{Z}||\mathbf{dev}\mathbf{e}^\ast(x)||
\]

(25)

Note that the integral of \(\mathbf{tr}\mathbf{C}^\ast\) is now equal to \(\Lambda\). The support of \(\mathbf{\tau}^\ast\) determines the optimal body. Having the bulk and shear moduli one can compute the optimal Poisson ratio \(\nu^\ast\). The interesting feature of many solutions is that in some large subdomains the optimal Poisson ratio approaches -1 and in other parts of the domain it approaches 1/2. Thus the optimal structures turn out to be of auxetic properties.

7. Construction of optimal solutions and exemplary results

The numerical method for constructing the optimal isotropic material and cubic material designs is based on solving problem (4) with integrands defined by appropriate norms for the trial stress fields. The numerical method has been developed in [4, 5, 6]; it is based on discretization of the set of statically admissible stresses. This linear affine set is represented by the solution of the discretized equilibrium equations with using the singular value decomposition technique (SVD). The free parameters of the representation are determined by performing minimization in the discretized counterpart of (4); for the details the reader is referred to [5]. The aim of the present section is to show only exemplary results: the optimal layouts of isotropic moduli found by the IMD technique outlined in Sec.6.
Consider the girder of dimensions $3.60 \times 0.60$ [m] lying on two non-sliding point supports, see Fig. 1.

A uniformly distributed vertical load of intensity $q = 1.0$ [N/m] is applied along the upper edge. The design cost $\Lambda$, see (3), is assumed as equal to $E_0|\Omega|$, where $\Omega$ represents the area of the design domain. The modulus $E_0$ is assumed as equal 1.0 [N/m], the optimal values of the designed elastic moduli being proportional to $E_0$, see (25). Two optimal designs are constructed: a) for the rectangular design domain without openings, and: b) for the design domain with six hexagonal openings, as shown in Fig. 1. The scatter plots of the Young modulus $E^*$ and Poisson ratio $\nu^*$ of the optimal non-homogeneous isotropic material within the girder domain for both cases a) and b) are shown in Fig. 2. The results have been found with using the bilinear, isoparametric C2D4 finite elements, applied for the approximation of the stress fields. In case (a) the mesh of 5400 elements has been used, in case (b) the number of elements being equal 4555.

For the rectangular design domain the optimal material forms a characteristic arch. The presence of openings

Figure 1: Dimensions of the girder considered

Figure 2: The layouts of Young modulus $E^*$ and Poisson ratio $\nu^*$ in optimal isotropic girders: without openings (case a) and with openings (case b).
brings about creation of stiffenings tangent to the openings, a characteristic feature of available optimal solutions to the scalar Monge-Kantorovich problem, see [3].

A characteristic property of the solution presented is emergence of the domains where the optimal Poisson ratio attains its lower and upper bounds. In the 2D setting these bounds are: -1 and 1, while in the 3D case they are tighter: -1, 1/2. In the 2D case considered we expect the former bounds. Note that in domains shown in the purple color the optimal layout of Poisson ratio reaches its lower bound equal to -1. In contrast, the red color indicates the domain where the Poisson ratio reaches its upper bound being equal to 1. Let us note lastly that in case of 3D optimal solutions constructed by the IMD method both the bounds : -1 and 1/2 are reached in typical optimal 3D designs [6]; selected 3D optimal solutions will be presented during the Conference.

8. Concluding remarks
The three versions of the material design considered come down to the problem (4) with different norms ||.||. To make this problem well posed one should sought the minimizer in the space of measures, as stressed in the paper [3] on shape optimization. The support of the minimizer determines the shape of the optimal body. Thus the material and shape optimizations are indissolubly bonded.

Optimum anisotropy becomes singular unless the strongest assumption of isotropy is imposed. The optimal isotropic bodies exhibit auxetic properties for majority of possible loads.

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10. References


