On the comparison of material interpolation schemes and optimal composite properties in plane shape optimization

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Abstract This paper deals with the classical problem of material distribution for minimal compliance of two-dimensional structures loaded in-plane. The main objective of the research consists in investigating the properties of the exact solution to the minimal compliance problem and incorporating them into an approximate solid-void interpolation model. Consequently, a proposition of a constitutive relation for a porous material arise. The non-smoothness of stress energy functional known from the approach based on homogenization may be thus avoided which is beneficial for the numerical implementation of the scheme. It is next shown that the simplified variant of the proposed formula justifies and generalizes the RAMP (Rational Approximation of Material Properties) interpolation model of Stolpe and Svanberg (Struct Multidisc Optim 22:116–124). In the second part of the paper, explicit formulae for function $\theta : \Omega \rightarrow [0, 1]$ describing the distribution of basic isotropic material in the design space $\Omega \in \mathbb{R}^2$ are derived for various interpolation schemes by the requirement of optimality imposed at each $x \in \Omega$. Theoretical considerations are illustrated by a code written in MATLAB for typical optimization problems of a cantilever and MBB beam.

Keywords Topology optimization · Minimal compliance · Two-dimensional elasticity · Interpolation scheme · Effective properties

1 Introduction

The classical optimization problem of minimal structural compliance was set in the late 1960s. Roughly speaking, the goal is to search the set of characteristic functions $\chi : \Omega \rightarrow \{0, 1\}$, where Ω denotes the design area, for a minimizer χ_{opt} such that the compliance $J = J(\chi)$ of a structure subjected to a given load achieves its minimal value $\underline{J} = J(\chi_{\text{opt}})$. At the early stage of research the above-mentioned task had proven to be badly posed due to the general non-convergence of sequences $\{\chi_n\}$ in the standard norm of $L^\infty(\Omega, \{0, 1\})$ (see e.g. Kozłowski and Mróz 1969; Rozvany et al. 1982), hence χ_{opt} could not be computed. This phenomenon, often referred to as “non-existence of classical solutions”, revealed a need for regularizing the optimal design problem.

One of the regularization methods assumes replacing the classical design set $L^\infty(\Omega, \{0, 1\})$ with its larger counterpart $L^\infty(\Omega, [0, 1])$, i.e. the set of generalized designs θ whose main property is that these functions can take any value between 0 and 1. From the mechanical point of view, the extension of this type results in allowing the microstructural composites of basic material and void in the analysis of the problem. The mathematical foundation of such method, known as the homogenization theory, is being developed simultaneously with its mechanical applications from 1970s. Detailed exposition of this topic lays outside of scope of the paper, hence we refer the reader to Cherkhaev (2000), Lewiński and Telega (2000), Milton (2002) and Tartar (2000) for further references.

It turns out that the shape optimization problem posed in the linear elasticity setting in two space dimensions has an explicit and accurate solution in terms of principal values $N_I(x)$, $N_{II}(x)$, $x \in \Omega$ of the force resultant tensor N . Namely, one may analytically determine the material

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distribution function $\theta_{\text{opt}} = \theta_{\text{opt}}(x)$ realizing $\underline{J} = J(\theta_{\text{opt}})$ as well as the local microstructural geometrical properties. Consequently, the macroscopic effective constitutive characteristics of a composite made of basic material and void locally mixed in proportions $\theta_{\text{opt}}(x)$ and $1 - \theta_{\text{opt}}(x)$ respectively can also be computed. This feature is thoroughly dealt with in Allaire (2002). Nevertheless, the numerical implementation of a homogenization-based results is hampered by the non-smoothness of stress energy functional $W(N, \theta)$ for $N_I N_{II} = 0$. Namely, if this is the case, then the constitutive formula is not unique, hence it cannot be directly inverted into the stress-displacement form which serves as a natural base for a numerical implementation by FEM. As a possible remedy, one may either make use of the solution to the problem of optimal layout formulated for a two-material structure, see Lewiński (2004), or seek the smooth, thus invertible, approximation of $W(N, \theta)$. In the sequel, the latter option is investigated.

According to the homogenization approach, $\theta_{\text{opt}}(x)$ ranges from 0 to 1 in the design area Ω hence the generalized material distribution function may serve as a reference solution to certain suboptimal, though practical and manufacturable, “0–1” designs stemming from the simplified material-void interpolation models. The most popular SIMP (Solid Isotropic Material with Penalization) scheme emerged from the papers of Bendsøe (1989) or Zhou and Rozvany (1991) and it is now widely used in solving various engineering optimization problems, see (Bendsøe and Sigmund 2003) for their extensive review. The mathematical foundation of SIMP is also subject to continuous research, see e.g. Rietz (2001), Martínez (2005), Almeida et al. (2010), Amstutz (2011) and Azegami et al. (2011). Another power law-like model of the material-void composite constitutive behavior, called RAMP (Rational Approximation of Material Properties), was proposed by Stolpe and Svanberg (2001b) following Rietz (2001). Both SIMP and RAMP interpolation schemes incorporate a certain real parameter which can be adjusted during the optimization procedure to penalize the intermediate densities of the basic material in the effective composite thus the almost “0–1” designs can be created. Deep discussion of problems corresponding to penalization and numerous filtering techniques is a subject of e.g. Sigmund and Petersson (1998), Bourdin (2001), Bruns and Tortorelli (2001), Stolpe and Svanberg (2001a), Rietz (2007) and Sigmund (2007).

The constitutive properties of a composite and, consequently, the value of the energy accumulated in a particle of an effective medium depend on the material interpolation scheme. Hence, the range of the SIMP or RAMP parameters is restricted by the requirement $W_{\text{opt}} \leq W_{\text{app}}$, where W_{opt} denotes the stress energy related to the optimal solution based on the homogenization approach and W_{app} stands for its approximation corresponding to the

chosen interpolation scheme. Even more restrictive is the requirement of the macrostructural isotropy of the solid-void composite. Bounds on the effective isotropic properties of a two-material mixture were introduced by Hashin and Shtrikman (1963) and improved by Cherkaev and Gibiansky (1993). It is worth pointing out, however, that both results coincide for the mixture of material and void hence in the sequel we will write $W_{\text{HS}} \leq W_{\text{app}}$ to denote the requirement of effective isotropy.

The paper is organized as follows: The notation necessary for the presentation of the topic is introduced in Section 2 together with a brief recall of optimal solution to the minimal compliance problem for material and void in a two-dimensional setting. Section 3 contains a derivation of an energy-based solid-void interpolation scheme in its general two-parameter form related to the homogenization approach. It is shown that a certain, simplified variant of the scheme allows for uniform estimation of the optimal stress energy functional and justifies the RAMP interpolation function of Stolpe and Svanberg (2001b). Hence, the proposed solid-void constitutive formula is nicknamed as generalized RAMP (GRAMP). Thus obtained scheme is next confronted with the Hashin-Shtrikman and SIMP estimates. Section 4 is devoted to the derivation of the explicit formulae for material distribution functions corresponding to various interpolation models. Numerical examples obtained with the help of GRAMP are presented in Section 5 and compared with the exact solutions and those based on SIMP and classical RAMP schemes.

2 Background of the research

2.1 Notation

Set $\Omega \in \mathbb{R}^2$ with a Cartesian basis $\{e_1, e_2\}$ for a middle plane of a thin plate. Let $x \in \Omega$ and set $t = 1$ for the uniform thickness of a plate. Next, introduce the basis

$$\begin{aligned} E_1 &= \frac{1}{\sqrt{2}} (e_1 \otimes e_1 + e_2 \otimes e_2), \\ E_2 &= \frac{1}{\sqrt{2}} (e_1 \otimes e_1 - e_2 \otimes e_2), \\ E_3 &= \frac{1}{\sqrt{2}} (e_1 \otimes e_2 + e_2 \otimes e_1), \end{aligned} \quad (1)$$

see e.g. Rychlewski (1995), allowing for representing the symmetric second-order tensors and Hooke's fourth-order tensors as vectors and symmetric matrices in $\mathbb{R}^3$ respectively.

From now on, Greek indices take values 1 or 2 while the Latin ones range from 1 to 3 and usual summation

convention applies. Moreover, in the sequel we write $f_{,\alpha} = \partial f / \partial (x_\alpha)$ for the differential operator; $\mathbf{A}\mathbf{B}$ for the contraction of the Hooke tensor $\mathbf{A}$ (bold upright) and symmetric second-order tensor $\mathbf{B}$ (bold italic) and $\mathbf{A} \cdot \mathbf{B}$ for the scalar product of two symmetric second-order tensors.

Throughout the paper we frequently refer to the in-plane force resultant tensor $\mathbf{N} = N_{\alpha\beta} \mathbf{e}_\alpha \otimes \mathbf{e}_\beta = N_i \mathbf{E}_i$ where

$$[N_i] = \frac{1}{\sqrt{2}} [N_{11} + N_{22}, N_{11} - N_{22}, 2N_{12}]^T, \quad (2)$$

and isotropic compliance tensor $\mathbf{A} = A_{\alpha\beta\lambda\mu} \mathbf{e}_\alpha \otimes \mathbf{e}_\beta \otimes \mathbf{e}_\lambda \otimes \mathbf{e}_\mu = A_{ij} \mathbf{E}_i \otimes \mathbf{E}_j$ where

$$[A_{ij}] = \text{diag} \left[\frac{1}{2}K, \frac{1}{2}L, \frac{1}{2}L \right], \quad (3)$$

with

$$K = \frac{2(1-\nu)}{E}, \quad L = \frac{2(1+\nu)}{E}, \quad (4)$$

expressed by Young's modulus E and Poisson's ratio ν .

Formula $\boldsymbol{\varepsilon} = \mathbf{A}\mathbf{N}$ links the force resultant tensor with the deformation tensor $\boldsymbol{\varepsilon}(\mathbf{u})$ whose components are derived from the kinematically admissible displacement vector $\mathbf{u}$ by $2\varepsilon_{\alpha\beta} = u_{\alpha,\beta} + u_{\beta,\alpha}$.

Assume that the plate is loaded by the in-plane load $\mathbf{p} = p_\alpha \mathbf{e}_\alpha$. Tensor $\mathbf{N}$ is statically admissible and we write $\mathbf{N} \in \mathcal{S}$ iff the equilibrium equation

$$\int_{\Omega} \mathbf{N} \cdot \boldsymbol{\varepsilon}(\mathbf{v}) dx = \int_{\Omega} p_\alpha v_\alpha dx \quad (5)$$

is satisfied for each $\mathbf{v}$ kinematically admissible.

Let $\theta : \Omega \rightarrow [0, 1]$ denote the function describing the layout of a given isotropic material $\mathbf{A}_0$ in Ω . Its total amount is limited by the isoperimetric condition

$$\frac{1}{|\Omega|} \int_{\Omega} \theta(x) dx \leq m, \quad m \in [0, 1]. \quad (6)$$

The compliance of a plate related to given θ is thus expressed by

$$J(\theta) = \int_{\Omega} p_\alpha v_\alpha dx, \quad (7)$$

or equivalently, by the Castigliano Theorem, as

$$J(\theta) = \min_{\mathbf{N} \in \mathcal{S}} \int_{\Omega} 2W(\mathbf{N}, \theta) dx, \quad (8)$$

where W denotes the stress energy value calculated at given $x \in \Omega$, i.e. $2W(\mathbf{N}, \theta) = \mathbf{N} \cdot (\mathbf{A}(\theta)\mathbf{N})$ with $\mathbf{N} = \mathbf{N}(x)$ and $\theta = \theta(x)$ by abuse of notation. By substituting (4) in (3) and with $N_{11} = N_I$, $N_{22} = N_{II}$, $N_{12} = 0$ standing for the principal values of $\mathbf{N}$ in (2) we may write

$$2W(\mathbf{N}, \theta) = \frac{1}{E(\theta)} (N_I^2 + N_{II}^2) - 2 \frac{\nu(\theta)}{E(\theta)} N_I N_{II}. \quad (9)$$

Coefficients $E(\theta)$, $\nu(\theta)$ denote the constitutive properties of an isotropic and non-homogeneous plate locally composed of given material $\mathbf{A}_0$ and void mixed in proportions θ , $1 - \theta$ respectively. In what follows, the equivalent form of (9) is utilized, namely

$$2W(\mathbf{N}, \theta) = \frac{N_{II}^2}{\theta E_0} U(\zeta, \theta), \quad (10)$$

$$U(\zeta, \theta) = a(\theta) (1 + \zeta^2) + 2b(\theta) \zeta,$$

where $\zeta = N_I/N_{II}$, $N_{II} \neq 0$ and

$$E(\theta) = \frac{\theta E_0}{a(\theta)}, \quad \nu(\theta) = -\frac{b(\theta)}{a(\theta)}. \quad (11)$$

It is worth pointing out that all considerations in the sequel remain valid if one swaps N_I with N_{II} in (9) thus redefining ζ and the expressions in (10) accordingly. This operation is possible due to the assumed isotropy of $\mathbf{A}(\theta)$ and allows for the straightforward application of the subsequent results in the limiting cases of $N_I = 0$ and $N_{II} = 0$. We assume that $N_I = N_{II} = 0$ and $W = 0$ if $\theta = 0$.

Optimal material distribution, or shape optimization problem, amounts to finding the minimal compliance of a structure through

$$\underline{J} = \min_{\theta: \Omega \rightarrow [0, 1]} \min_{\mathbf{N} \in \mathcal{S}} \int_{\Omega} (2W(\mathbf{N}, \theta) + \ell \theta) dx, \quad (12)$$

where $\theta \in L^\infty(\Omega, [0, 1])$ and ℓ denotes the Langrange multiplier for isoperimetric condition (6). Once minimizations in (12) are swapped over, it is possible that the “minimum over θ ” operation is exchanged with integration due to the Rockafellar Theorem (Rockafellar 1976) which leads to

$$\underline{J} = \min_{\mathbf{N} \in \mathcal{S}} \int_{\Omega} \min_{\theta(x) \in [0, 1]} [2W(\mathbf{N}(x), \theta(x)) + \ell \theta(x)] dx. \quad (13)$$

As this Theorem is crucial for further considerations, let us discuss its conditions in optimal design setting. First, note that the existence of a minimizer $\theta_{\min} \in L^\infty(\Omega, [0, 1])$ in (12) is provided by the homogenization theory, see Allaire (2002, Th. 4.2.6). Moreover, structural compliance calculated for any material distribution is represented by a finite

number, hence $\underline{J} < +\infty$ for given $\theta_{\min}$. By this, one of the Rockafellar's Theorem assumptions is fulfilled.

In the original formulation of the Theorem it is expected that the minimizing function $\theta_{\min}$ is looked for in the decomposable linear space of measurable functions. Therefore, the set $L^\infty(\Omega, [0, 1])$ should be extended to $L^\infty(\Omega, \mathbb{R})$ thus admitting $\theta_{\min}(x) < 0$ and $\theta_{\min}(x) > 1$ as possible solutions in (13). The extension, however, is formal and pose no additional problems. Indeed, by the inspection of results in the sequel one may check that the values $\theta_{\min}(x)$ and $-\theta_{\min}(x)$ saturate the extremum of the integrand in (13) at $x \in \Omega$, but the minimizer is always given by $\theta_{\min}(x) > 0$. On the other hand, it is always possible to set $\theta_{\min}(x) = 1$ if the upper bound of the $[0, 1]$ interval is violated but such restriction has to be compensated by adjusting the Lagrange multiplier ℓ which is necessary to retain the isoperimetric condition (6).

The last two assumptions sufficient for (13) to hold are that the integrand is lower semicontinuous in θ for any $x \in \Omega$ and that its epigraph is a measurable function. The former condition is fulfilled as $a(\theta)$ and $b(\theta)$ defining $U(\zeta, \theta)$, see (10), are continuous in θ for all cases considered in the remainder of this paper. Consequently, the latter condition is also satisfied.

Having disposed of this step, one may conclude that the optimal material distribution function is locally determined through the condition

$$\frac{d}{d\theta}(2W(N, \theta) + \ell\theta) = 0. \quad (14)$$

Functions satisfying (14) vary for different material-void interpolation schemes. Their explicit forms are derived in subsequent sections.

2.2 Properties of the explicit solution to the problem of material layout for minimal compliance

From the considerations in Cherkaev (2000) and Allaire (2002) it turns out that for given (N, θ) , the value of stress energy in (12) can be calculated in terms of a real parameter $\alpha \in [-K_0, L_0]$ as

$$4W_{\text{opt}}(N, \theta) = \frac{K_0 + \alpha(1 - \theta)}{\theta} \left(\frac{1}{\sqrt{2}} \text{tr} N \right)^2 + \frac{L_0 - \alpha(1 - \theta)}{\theta} \|\text{dev} N\|^2, \quad (15)$$

or explicitly in terms of principal values of tensor N as

$$8W_{\text{opt}}(N, \theta) = \frac{K_0 + \alpha(1 - \theta)}{\theta} (N_I + N_{II})^2 + \frac{L_0 - \alpha(1 - \theta)}{\theta} (N_I - N_{II})^2, \quad (16)$$

where

$$\alpha = \begin{cases} -K_0 & \text{if } N_I N_{II} \leq 0, \\ L_0 & \text{if } N_I N_{II} \geq 0. \end{cases} \quad (17)$$

We refer the reader to the above-mentioned references for complete discussion of this result, here we only recall its certain properties that are necessary in further considerations.

Formula (15) for W_{opt} is isotropic as it is a function of the invariants of N only. By substituting (4) with $E = E_0$ and $\nu = \nu_0$ in (17) and then in (16), W_{opt} takes the equivalent form

$$2W_{\text{opt}}(N, \theta) = \frac{1}{\theta E_0} (|N_I| + |N_{II}|)^2 + -2 \frac{1 + \text{sgn}(N_I N_{II}) \nu_0}{E_0} |N_I| |N_{II}|. \quad (18)$$

Indeed, for $N_I N_{II} \leq 0$, formula (16) is given by

$$2W_{\text{opt}}(N, \theta) = \frac{1}{\theta E_0} (N_I - N_{II})^2 + 2 \frac{1 - \nu_0}{E_0} N_I N_{II}, \quad (19)$$

while for $N_I N_{II} \geq 0$ it reads

$$2W_{\text{opt}}(N, \theta) = \frac{1}{\theta E_0} (N_I + N_{II})^2 - 2 \frac{1 + \nu_0}{E_0} N_I N_{II}. \quad (20)$$

Combining (19) and (20) in one expression leads to (18).

Consequently, the optimal material distribution θ_{opt} obtained through (14) is determined by

$$\theta_{\text{opt}}(N) = \min \left\{ 1, \frac{|N_{II}|}{\sqrt{\ell E_0}} (|\zeta| + 1) \right\}. \quad (21)$$

Re-writing (18) similarly to (10) yields

$$U_{\text{opt}}(\zeta, \theta) = a_{\text{opt}}(\zeta, \theta) (1 + \zeta^2) + 2b_{\text{opt}}(\zeta, \theta) \zeta, \quad (22)$$

where, by making use of $\text{sgn}(N_I N_{II}) = \text{sgn}(\zeta)$,

$$\begin{aligned} a_{\text{opt}}(\zeta, \theta) &= 1, \\ b_{\text{opt}}(\zeta, \theta) &= -\theta \nu_0 + (1 - \theta) \text{sgn}(\zeta). \end{aligned} \quad (23)$$

3 Solid-void interpolation scheme based on the properties of optimal stress energy

3.1 Derivation of the interpolation function

Expressing the stress energy in the form given by (10) allows for analyzing the functional U instead of W in

further considerations. Therefore, we continue in this fashion to obtain the approximation U_{app} of U_{opt} by taking (22) as the reference expression in determining $a_{\text{app}}(\theta)$ and $b_{\text{app}}(\theta)$ which are required to be independent of the sign of ζ and such that

$$U_{\text{app}}(\zeta, \theta) \geq U_{\text{opt}}(\zeta, \theta) \quad (24)$$

is satisfied for any pair (ζ, θ) . It turns out that by simplified variant of this approach one may also justify and generalize the RAMP interpolation scheme of Stolpe and Svanberg (2001b).

For any θ , the sought approximation with the above required properties is realized at U_{app} sharing the common tangent with U_{opt} at two distinct points ζ_1 and ζ_2 . Setting $\zeta_1 = 1/q_1$ and $\zeta_2 = -1/q_2$ followed by

$$\begin{aligned} \frac{\partial U_{\text{app}}}{\partial \zeta} \left(\frac{1}{q_1}, \theta \right) &= \frac{\partial U_{\text{opt}}}{\partial \zeta} \left(\frac{1}{q_1}, \theta \right), \\ \frac{\partial U_{\text{app}}}{\partial \zeta} \left(-\frac{1}{q_2}, \theta \right) &= \frac{\partial U_{\text{opt}}}{\partial \zeta} \left(-\frac{1}{q_2}, \theta \right), \end{aligned} \quad (25)$$

leads to

$$\begin{aligned} a_{\text{app}}(\theta) &= 1 + 2(1 - \theta) \frac{q_1 q_2}{q_1 + q_2}, \\ b_{\text{app}}(\theta) &= (1 - \theta) \frac{q_1 - q_2}{q_1 + q_2} - \theta v_0. \end{aligned} \quad (26)$$

Requirement (24) restricts the range of q_α to

$$q_\alpha \in [1, +\infty). \quad (27)$$

In this way, the two-parameter solid-void interpolation scheme is established with the approximate stress energy function W_{app} defined through (10) and (26). It follows that U_{app} shares the common tangent with U_{opt} and $U_{\text{app}} = U_{\text{opt}}$ at two distinct points iff $q_1 = q_2 = 1$.

The simplified, one-parameter variant of the above is obtained by setting $q_1 = q_2 = q$ in (26). This choice is heuristic, however it seems quite legitimate as it leads to the uniform approximation of the functional U_{opt} as it is shown in the sequel. As a result one may claim the generalized Rational Approximation of Material Properties (GRAMP) in the following form

$$\begin{aligned} a_{\text{GRAMP}}(\theta) &= 1 + q(1 - \theta), \\ b_{\text{GRAMP}}(\theta) &= -\theta v_0 \end{aligned} \quad (28)$$

and

$$\text{(GRAMP)} : \begin{cases} \frac{E(\theta)}{E_0} = f_q(\theta), & \frac{\nu(\theta)}{\nu_0} = f_q(\theta), \\ f_q(\theta) = \frac{\theta}{1 + q(1 - \theta)}, \end{cases} \quad (29)$$

where $f_q(\theta)$ denotes the common interpolation function for $E(\theta)$ and $\nu(\theta)$. Recall that the original RAMP scheme assumes $\nu(\theta) = \text{const.}$ which gives

$$\begin{aligned} a_{\text{RAMP}}(\theta) &= 1 + q(1 - \theta), \\ b_{\text{RAMP}}(\theta) &= -\nu_0 [1 + q(1 - \theta)]. \end{aligned} \quad (30)$$

The set of plots in Fig. 1 shows f_q for different values of parameter q .

Assuming the solid-void interpolation scheme in a GRAMP form has a great impact on the quality of approximation U_{app} . For given $\zeta_0 > 0$, it can be measured as

$$\Delta(U_{\text{app}}) = \frac{\int_{-\zeta_0}^0 |U_{\text{app}}(\zeta, \theta) - U_{\text{opt}}(\zeta, \theta)| d\zeta}{\int_0^{\zeta_0} |U_{\text{app}}(\zeta, \theta) - U_{\text{opt}}(\zeta, \theta)| d\zeta}, \quad (31)$$

thus expressing a simple requirement of approximation uniformity for different signs of ζ . One may calculate that $\Delta(U_{\text{GRAMP}}) = 1$ which is not the case for neither of other approximation schemes discussed in this paper.

Fig. 1 Interpolation function f_q plotted for $q = 1$ (solid line), $q = 3$ (dashed line) and $q = 10$ (dotted line)

3.2 Relation to the Hashin-Shtrikman bounds and SIMP model

At this point of discussion it is worth following through the mutual relations among U_{GRAMP} , U_{opt} , U_{HS} and U_{SIMP} where the latter two stress energy functions are respectively related to the Hashin-Shtrikman and SIMP (Solid Isotropic Material with Penalization) interpolation models. Formula determining U_{HS} can be expressed by (10) with

$$a_{\text{HS}}(\theta) = 3 - 2\theta, \quad b_{\text{HS}}(\theta) = -\theta\nu_0 - (1 - \theta), \quad (32)$$

while U_{SIMP} admits

$$a_{\text{SIMP}}(\theta) = \frac{1}{\theta^{p-1}}, \quad b_{\text{SIMP}}(\theta) = -\frac{\nu_0}{\theta^{p-1}}, \quad (33)$$

where p stands for the penalization factor in SIMP scheme. Equation (11) links the coefficients of stress energy functionals and material properties $E(\theta)$, $\nu(\theta)$.

Let us emphasize that both U_{HS} and U_{opt} establish certain lower limits on the stress energy accumulated in a particle of a structure. The difference in their formulae are, roughly speaking, due to the fact that the calculations of U_{HS} incorporate the control over the isotropy of the effective material which is not the case for U_{opt} .

Indeed, the derivation of Hashin-Shtrikman bounds consists of two independent steps. Application of a hydrostatic field $\mathbf{N} = N_{\text{H}}\mathbf{E}_1$ allows for defining the minimal value of $K(\theta)$, while obtaining the minimal value of $L(\theta)$ requires subjecting a composite to the deviatoric field $\mathbf{N} = N_{\text{D}}(\mathbf{E}_2 + \mathbf{E}_3)$.

Conversely, U_{opt} measures the energy of a composite subjected to an arbitrary field $\mathbf{N}$. However, if we assume that $\mathbf{e}_\alpha$ stand for the eigenbasis of some $\mathbf{N}$ at given $x \in \Omega$, and if we set $N_{\text{I}} = N_{\text{II}} = N$ (i.e. $\zeta = 1$) then we obtain $U_{\text{HS}} = U_{\text{opt}}$, as $\mathbf{N} = (\sqrt{2}N)\mathbf{E}_1$ is a hydrostatic field. On the contrary, setting $N_{\text{I}} = -N_{\text{II}} = N$ (i.e. $\zeta = -1$) does not lead to a similar conclusion on the equality of energies because applying the deviatoric field $\mathbf{N} = (\sqrt{2}N)\mathbf{E}_2$

and controlling the response of a composite medium in the direction $\mathbf{E}_3$ at the same time is impossible.

Table 1 presents the lower bounds imposed on the parameters of GRAMP, RAMP and SIMP approximations. They stem from two requirements which has to be fulfilled by any approximate stress energy functional U_{app} . Inequality $U_{\text{app}} - U_{\text{opt}} \geq 0$, see (24), restricts the values of parameters to those for which the approximate energy takes the form of an isotropic function (10) while $U_{\text{app}} - U_{\text{HS}} \geq 0$ imposes the effective isotropy of a composite material as an additional constraint. Partial results related to the Hashin-Shtrikman restrictions are reported in e.g. Bendsøe and Sigmund (1999) and Stolpe and Svanberg (2001b).

In case of the GRAMP model, the isotropy of an approximate stress function U_{GRAMP} is satisfied for any $q \geq 1$, see (27). By making use of (28) and (32) one may conclude that $U_{\text{GRAMP}} - U_{\text{HS}} \geq 0$ if

$$(1 - \theta)((q - 2)(1 + \zeta^2) + 2\zeta) \geq 0 \quad (34)$$

demanding in this way the macroscopic material isotropy. From (34) it follows that

$$q \geq \frac{2(\zeta^2 - \zeta + 1)}{\zeta^2 + 1} \quad (35)$$

which has to be fulfilled for any ζ . Consequently, one obtains $q \geq 3$ as the function on the r.h.s. of (35) takes its maximum for $\zeta = -1$.

Similar calculations can be performed for SIMP and RAMP schemes. It is worth pointing out that in the GRAMP scheme parameters are independent of the basic material's Poisson ratio value ν_0 and density θ . On the contrary, in the course of calculations related to RAMP and SIMP schemes one has to set $\theta = 1$ in order to assure the validity of expressions in Table 1 for any $\theta \in [0, 1]$. The comparison of U_{opt} , U_{HS} and U_{GRAMP} , U_{RAMP} , U_{SIMP} with parameters of lowest possible values are shown for $\nu_0 = 1/3$ (Fig. 2) and $\nu_0 = -1/3$ (Fig. 3). In the latter case of an auxetic material, values of parameters in the RAMP and SIMP

Table 1 Requirements on the parameters in GRAMP, RAMP and SIMP interpolation schemes imposed by the conditions of optimality ($U_{\text{app}} \geq U_{\text{opt}}$) or material isotropy ($U_{\text{app}} \geq U_{\text{HS}}$)

	$U_{\text{app}} = U_{\text{GRAMP}}^{\text{a}}$	$U_{\text{app}} = U_{\text{RAMP}}^{\text{b}}$	$U_{\text{app}} = U_{\text{SIMP}}^{\text{b}}$
$U_{\text{app}} \geq U_{\text{opt}}$	$q \geq 1$	$q \geq \max \left\{ \frac{1 + \nu_0}{1 - \nu_0}, \frac{1 - \nu_0}{1 + \nu_0} \right\}$	$p \geq \max \left\{ \frac{2}{1 - \nu_0}, \frac{2}{1 + \nu_0} \right\}$
$U_{\text{app}} \geq U_{\text{HS}}$	$q \geq 3$	$q \geq \max \left\{ \frac{1 + \nu_0}{1 - \nu_0}, \frac{3 - \nu_0}{1 + \nu_0} \right\}$	$p \geq \max \left\{ \frac{2}{1 - \nu_0}, \frac{4}{1 + \nu_0} \right\}$

^aparameters are independent of the basic material's Poisson ratio value ν_0 and density θ

^bexpressions are calculated for $\theta = 1$ in order to enforce their validity for the whole range $\theta \in [0, 1]$

Fig. 2 Plots of functions U_{opt} (lower solid line), U_{HS} (upper solid line), U_{GRAMP} with $q = 1$ (lower dotted line), U_{GRAMP} with $q = 3$ (upper dotted line), U_{SIMP} with $q = 3$ (dashdotted line). Plots match up with $v_0 = 1/3$ (in this unique case $U_{\text{HS}} = U_{\text{RAMP}}$ with $q = 2$) and $\theta = 0.7$

schemes are significantly higher than for the solid with positive Poisson's ratio. This in turn, reflects in higher values of the predicted stress energy and may influence the structural compliance and optimal solid-void layout.

Fig. 3 Plots of functions U_{opt} (lower solid line), U_{HS} (upper solid line), U_{GRAMP} with $q = 1$ (lower dotted line), U_{GRAMP} with $q = 3$ (upper dotted line), U_{RAMP} with $q = 5$ (dashed line), U_{SIMP} with $q = 6$ (dashdotted line). Plots match up with $v_0 = -1/3$ and $\theta = 0.7$

Constitutive properties predicted by Hashin-Shtrikman approach are realizable on certain isotropic microstructures like 3rd rank sequential laminates (Francfort and Murat 1986) or coated circles (Hashin 1962; Grabovsky and Kohn 1995a). On the other hand, composites of minimal compliance can be arranged as orthotropic 2nd rank orthogonal sequential laminates or, if $\det N > 0$, in a form of the Vigdergauz microstructures (Vigdergauz 1989; Grabovsky and Kohn 1995b) or 4th rank sequential laminates (Allaire and Aubry 1999).

In light of the studies in this section it seems that one may neglect the requirement of the macrostructural isotropy if the best possible macroscale material distribution is considered as a primal goal of the optimization problem. Nevertheless, thus obtained solution may serve as a good starting point of the continuation method where the change of a parameter in the interpolation scheme (like e.g. q in RAMP or GRAMP) reflects in the tendency to the pure “0-1” distribution of a basic isotropic material in the domain of an analyzed structure. Problems related to the microscopic layout of material and void in optimized structures are detailed at length in e.g. Allaire (2002), Cherkaev (2000) and Bendsøe and Sigmund (2003), see also references therein.

4 Material distribution functions for minimal compliance

Our next objective is to derive the material distribution functions that correspond to various interpolation schemes. Repeated application of (14) where $W(N, \theta)$ is given by (10) and appropriate expressions for $a(\theta)$ and $b(\theta)$ enables us to write the sought formulae in their explicit forms similarly to (21).

Indeed, for (28) we obtain the function

$$\theta_{\text{GRAMP}}(N) = \min \left\{ 1, \frac{|N_{\text{II}}|}{\sqrt{\ell E_0}} \sqrt{(1+q)(\zeta^2 + 1)} \right\} \quad (36)$$

whereas for (30),

$$\theta_{\text{RAMP}}(N) = \min \left\{ 1, \frac{|N_{\text{II}}|}{\sqrt{\ell E_0}} \sqrt{(1+q)(\zeta^2 - 2v_0\zeta + 1)} \right\} \quad (37)$$

in the original RAMP scheme and the Hashin-Shtrikman framework with (32) provides

$$\theta_{\text{HS}}(N) = \min \left\{ 1, \frac{|N_{\text{II}}|}{\sqrt{\ell E_0}} \sqrt{(\zeta + 1)^2 + 2(\zeta - 1)^2} \right\}. \quad (38)$$

Material distribution function predicted by the SIMP model with (33) is given by

$$\theta_{\text{SIMP}}(N) = \min \left\{ 1, \left[p \frac{N_{\text{II}}^2}{\ell E_0} (\zeta^2 - 2\nu_0 \zeta + 1) \right]^{\frac{1}{1+p}} \right\}. \quad (39)$$

It follows that functions $\theta(N)$ in SIMP, RAMP and Hashin-Shtrikman interpolation schemes are sensitive to the sign of ζ and ν_0 which is not the case for the material distribution based on GRAMP or exact homogenization approach.

Figure 4 illustrates the material distribution functions with the parameters set to the values for which the respective functionals U_{GRAMP} , U_{RAMP} and U_{SIMP} do not violate the lower bounds on the stress energy given by U_{opt} and U_{HS} for $\nu_0 = 1/3$. In this sense Fig. 4 corresponds to Fig. 2.

Figure 5 in turn displays the same functions $\theta(N)$ but the values of parameters are such that the energy functionals U_{opt} and U_{HS} are not violated for $\nu_0 = -1/3$. In this sense Fig. 5 corresponds to Fig. 3.

Explicit formulae for material distribution can be directly applied in numerical codes for compliance minimization problem in this way allowing to avoid the heuristic density updating schemes.

Fig. 4 Plots of the material distribution functions $\theta_{\text{opt}}(N)$ (lower solid line), $\theta_{\text{HS}}(N)$ (upper solid line) and their closest approximations corresponding to the following interpolation schemes: GRAMP with $q = 1$ (lower dotted line), GRAMP with $q = 3$ (upper dotted line), SIMP with $p = 3$ (dashdotted line). Plots match up with $\nu_0 = 1/3$ (in this unique case $\theta_{\text{HS}} = \theta_{\text{RAMP}}$ with $q = 2$) and $(N_{\text{II}}^2)/(\ell E_0) = 1/12$

Fig. 5 Plots of the material distribution functions $\theta_{\text{opt}}(N)$ (lower solid line), $\theta_{\text{HS}}(N)$ (upper solid line) and their closest approximations corresponding to the following interpolation schemes: GRAMP with $q = 1$ (lower dotted line), GRAMP with $q = 3$ (upper dotted line), RAMP with $q = 5$ (dashed line), SIMP with $p = 6$ (dashdotted line). Plots match up with $\nu_0 = -1/3$ and $(N_{\text{II}}^2)/(\ell E_0) = 1/12$

5 Examples of material layouts

5.1 General comments on numerical implementation

The GRAMP interpolation scheme is applied to find the suboptimal layout of basic isotropic material in classical problems of a cantilever and half of a MBB beam. Results obtained in this way are compared to the distribution of materials ensuing from the homogenization theory as well as those related to the original RAMP or SIMP approach. Designs associated with both exemplary problems are shown in Figs. 6, 7, 8 and 9. The dimensions of a rectangular design area Ω are given by $l \times h = 2 \times 1$ and the material fraction of Ω is set to $m = 0.5$. Young's modulus of an isotropic solid is denoted by $E_0 = 1$ and two cases of Poisson's ratio are considered in the course of calculations, i.e. $\nu_0 = \pm 1/3$. The structure is due to a concentrated load $P = 1$.

All calculations are coded in MATLAB and performed by FEM using the mesh of 200×100 square, four-node elements with two degrees of freedom per node. The idea of programming is to supplement the applications published at the TopOpt research group website (www.topopt.dtu.dk) hence the codes presented in the Appendices have a structure based on the program written by Andreassen et al. (2011) for topology optimization in 2D.

Fig. 6 Layouts of material with a Poisson ratio $\nu_0 = 1/3$ and corresponding compliances J ; **a** Geometry, load and boundary conditions for a cantilever; **b** Optimal solution by the homogenization method; **c** Solution by GRAMP with $q = 1$; **d** Solution by RAMP with $q = 2$; **e** Solution by GRAMP with $q = 3$; **f** Solution by SIMP with $p = 3$. In cases **d–f** the penalization parameters are set to lowest values satisfying the isotropy of a composite and the density filter is enabled

Fig. 7 Layouts of material with a Poisson ratio $\nu_0 = -1/3$ and corresponding compliances J ; **a** Solution by RAMP with $q = 5$; **b** Solution by GRAMP with $q = 3$; **c** Solution by SIMP with $p = 6$. Penalization parameters are set to lowest values satisfying the isotropy of a composite and the density filter is enabled

Fig. 8 Layouts of material with a Poisson ratio $\nu_0 = 1/3$ and corresponding compliances J ; **a** Geometry, load and boundary conditions for a half of an MBB beam; **b** Optimal solution by the homogenization method; **c** Solution by GRAMP with $q = 1$; **d** Solution by RAMP with $q = 2$; **e** Solution by GRAMP with $q = 3$; **f** Solution by SIMP with $p = 3$. In cases **d–f** the penalization parameters are set to lowest values satisfying the isotropy of a composite and the density filter is enabled

Fig. 9 Layouts of material with a Poisson ratio $\nu_0 = -1/3$ and corresponding compliances J ; **a** Solution by RAMP with $q = 5$; **b** Solution by GRAMP with $q = 3$; **c** Solution by SIMP with $p = 6$. Penalization parameters are set to lowest values satisfying the isotropy of a composite and the density filter is enabled

Typical, k -th step of the optimization loop consists of two substeps. First, the FE analysis is performed for fixed vector $\mathbf{x}^{k-1}$ representing the values of θ obtained in the previous run. Next, vectors of principal values of stress resultant N_I^k and N_{II}^k are determined. Components of each vector are calculated either at the Gauss points or in the middle of each element, see Sections 5.2 and 5.3 for further details.

Set $d = \dim N_I = \dim N_{II}$ and $\Delta N = N^k - N^{k-1}$. If, for given small $\epsilon > 0$,

$$\sqrt{\sum_{i=1}^d \left[(\Delta N_I^i)^2 + (\Delta N_{II}^i)^2 \right]} < \epsilon \quad (40)$$

then the optimization routine is stopped. Otherwise, the material distribution function is updated by applying (21) or one of the formulae (36)–(39) depending on the interpolation scheme. In this way vector $\mathbf{x}^k$ is determined. Finally, the constitutive properties of a composite are modified and the $(k + 1)$ -th step of the routine is executed. The l.h.s. in (40) can be understood as a counterpart of the L^2 norm of function ΔN posed in a discrete setting.

Here we set $\epsilon = 10^{-2}$ but this value can be adjusted to meet the required accuracy. It has to be pointed out that the convergence measured by (40) is fairly slow. Some authors prefer to rewrite this criterion in terms of the material density vector $\mathbf{x}$, see the numerical codes in Bendsøe and Sigmund (2003) and Andreassen et al. (2011).

Minimal compliance problem tackled in this paper falls into the category of constrained optimization. The necessary conditions for optimum are thus obtained by applying the Karush-Kuhn-Tucker (KKT) Theorem, see e.g. Haftka and Kamat (1985) for further details in context of structural optimization. Discussed formulation (12) is a double minimization with respect to N and θ . The KKT conditions of optimality admit the Lagrange multiplier ℓ for the isoperimetric constraint (6). The requirement of static admissibility imposed on N by (5) can be accounted for in a similar way with the Lagrange multiplier assumed in a functional form. Both constraints are to be satisfied at the stationary point of an objective function. In this way, the stopping criterion of the numerical algorithm is provided.

In the corresponding numerical algorithm the unknowns N and θ are respectively referred to as vectors N and $\mathbf{x}$. Iterative numerical implementation of (12) with alternating minimization in both variables guarantees that the objective function converges to a stationary point. Indeed, determining N^k for fixed $\mathbf{x}^{k-1}$ reduces to solving the linear elasticity problem. Consequently, the stress energy is minimized hence the value of the objective function decreases. Upon updating the stress resultant vector, the objective function is

Table 2 Computational details of the solutions to the half-MBB beam problem shown in Fig. 8

Interpolation scheme	Compliance	Number of iterations	Computing time in seconds
Homogenization Fig. 8b	70,94	437	514
GRAMP ($q = 1$) Fig. 8c	71,17	191	254
RAMP ($q = 2$) Fig. 8d	79,72	166	186
GRAMP ($q = 3$) Fig. 8e	80,88	218	197
SIMP ($p = 3$) Fig. 8f	81,56	346	355

minimized explicitly by $\mathbf{x}^k$ obtained through (21) or one of (36)–(39) depending on the solid-void interpolation model. The Lagrange multiplier ℓ is adjusted in order to enforce the corresponding KKT condition. Formula (40) serves as the stopping condition of a numerical algorithm. Its fulfilment shows the convergence of N and the convergence of the objective function follows.

Tables 2 and 3 give some details concerning the optimization procedure implemented in MATLAB for the half-MBB beam problem. The results were obtained using a DELL XPS M1330 laptop with Intel Core2 Duo CPU (model T9300), 4 GB RAM, Windows 7 (64-bit) and MATLAB 7.11.0 (R2010b).

5.2 Comments on the homogenization-based approach

Stress functional U_{opt} obtained by the homogenization approach is continuous but not smooth at $\zeta = 0$, see Figs. 2

Table 3 Computational details of the solutions to the half-MBB beam problem shown in Fig. 9

Interpolation scheme	Compliance	Number of iterations	Computing time in seconds
RAMP ($q = 5$) Fig. 9a	81,75	439	435
GRAMP ($q = 3$) Fig. 9b	80,08	226	205
SIMP ($p = 6$) Fig. 9c	85,39	417	423

and 3. This, in turn, poses a serious drawback of direct application of the stress-based results in numerical computations. However, the results reported in Lewiński (2004) for a two-material problem make it possible to reformulate the topology optimization problem in the displacement setting. Consequently, for $\varepsilon_I, \varepsilon_{II}$ denoting the principal values of a deformation tensor $\boldsymbol{\varepsilon}$ and for $k_0 = 1/K_0, \mu_0 = 1/L_0$ one may set

$$\zeta_\varepsilon = \left| \frac{\varepsilon_I - \varepsilon_{II}}{\varepsilon_I + \varepsilon_{II}} \right|, \quad \zeta_1 = \frac{k_0 + (1 - \theta)\mu_0}{\theta\mu_0}, \quad \zeta_2 = \frac{\theta k_0}{\mu_0 + (1 - \theta)k_0}, \quad (41)$$

followed by

$$k_{\text{opt}} = \begin{cases} \frac{\theta k_0 \mu_0}{\mu_0 + (1 - \theta)k_0} & 0 \leq \zeta_\varepsilon \leq \zeta_2, \\ \frac{\theta k_0 \mu_0 (1 + \zeta_\varepsilon)}{k_0 + \mu_0} & \zeta_2 \leq \zeta_\varepsilon \leq \zeta_1, \\ k_0 & \zeta_1 \leq \zeta_\varepsilon, \end{cases} \quad (42)$$

$$\mu_{\text{opt}} = \begin{cases} \mu_0 & 0 \leq \zeta_\varepsilon \leq \zeta_2, \\ \frac{\theta k_0 \mu_0 (1 + \zeta_\varepsilon^{-1})}{k_0 + \mu_0} & \zeta_2 \leq \zeta_\varepsilon \leq \zeta_1, \\ \frac{\theta k_0 \mu_0}{k_0 + (1 - \theta)\mu_0} & \zeta_1 \leq \zeta_\varepsilon, \end{cases} \quad (43)$$

thus defining the optimal stiffness tensor $\mathbf{C}_{\text{opt}}$ represented by $[C_{ij}^{\text{opt}}] = \text{diag}[2k_{\text{opt}}, 2\mu_{\text{opt}}, 2\mu_{\text{opt}}]$ in basis (1).

In order to reduce the checkerboard-like instability of solutions, all element-wise calculations in the homogenization-based approach are performed at four integration points. The stiffness matrix of e -th element is thus determined according to

$$\mathbf{K}_e = \frac{1}{4} \sum_{i=1}^4 \mathbf{B}_i^T \mathbf{C}_i^{\text{opt}} \mathbf{B}_i = \frac{1}{4} \left(\sum_{i=1}^4 2k_i^{\text{opt}} \mathbf{b}_{1i}^T \otimes \mathbf{b}_{1i} + \sum_{i=1}^4 2\mu_i^{\text{opt}} (\mathbf{b}_{2i}^T \otimes \mathbf{b}_{2i} + \mathbf{b}_{3i}^T \otimes \mathbf{b}_{3i}) \right), \quad (44)$$

where $\mathbf{b}_{ji}$ corresponds to i -th integration point and denotes the j -th row of a $\mathbf{B}_i$ matrix containing the derivatives of element shape functions. Corresponding numerical code is

presented in Appendix A, e.g. the composite solution in Fig. 8b is obtained by executing

`tophomog4(200, 100, 0.5),`

where the parameters respectively denote the number of elements in the horizontal and vertical directions and the solid fraction of the design area.

5.3 Comments on the GRAMP approach

Approximate function U_{GRAMP} is smooth, see Figs. 2 and 3 hence it is invertible in the whole range of ζ . For the purpose of this paper, two MATLAB implementations of the GRAMP scheme were coded. The difference between them lies in the method of element stiffness matrix integration and in the number of points in which strains and stresses are computed. This, in turn, leads to the difference in obtained solutions. Application of the first code results in composite designs and it is similar to the code based on the homogenization approach. Slight modifications are detailed in Appendix A. This implementation of the GRAMP scheme, used for mimicking the composite solution of `tophomog4`, is illustrated in Fig. 8c and obtained by executing

`topgramp4(200, 100, 0.5, 1),`

where the last parameter stands for the GRAMP penalization factor $q = 1$.

In the second code, presented in Appendix B, the element stiffness matrix $\mathbf{K}_e$ is calculated as

$$\mathbf{K}_e = 2k_{\text{GRAMP}} \mathbf{K}_1 + 2\mu_{\text{GRAMP}} \mathbf{K}_2 \quad (45)$$

where

$$\mathbf{K}_1 = \int_{\Omega_e} \mathbf{b}_1^T \otimes \mathbf{b}_1, \quad \mathbf{K}_2 = \int_{\Omega_e} (\mathbf{b}_2^T \otimes \mathbf{b}_2 + \mathbf{b}_3^T \otimes \mathbf{b}_3) \quad (46)$$

and

$$k_{\text{GRAMP}} = \frac{E(\theta)}{2(1 - \nu(\theta))}, \quad \mu_{\text{GRAMP}} = \frac{E(\theta)}{2(1 + \nu(\theta))}, \quad (47)$$

see (11) and (28). Strains and stresses are calculated in the middle of each element. The updated distribution of material is determined by making use of (36).

5.4 Comments on the filtered designs

For practical purposes it is desirable that the intermediate densities are filtered out from the final design. Application of such filter allows not only for obtaining nearly black-and-white material layouts but also helps in avoiding the checkerboard instability of numerical calculations. Roughly speaking, filtering the density $\theta(x)$ at given $x \in \Omega$ works by averaging it over the neighborhood of given radius r . By this, the tendency to reproduce the fine-scale arrangement of solid and void is bypassed and composite regions are introduced in Ω . In turn, these regions are penalized by proper parameter adjustment in the material interpolation formula. As a result, the topology of final design becomes nearly “0-1” and the width of transition between void and solid areas depends on the filtering radius r .

According to e.g. Bendsøe and Sigmund (2003), implementing a filtering technique in the formulation of optimal design problem at hand does not impose any additional limit on the space $L^\infty(\Omega, [0, 1])$, i.e. the space of material distribution functions. Density filter can be applied at each $x \in \Omega$ independently as a part of the material redistribution procedure.

Numerous filtering methods are reviewed in Sigmund (2007) and some issues related to the programming in MATLAB are tackled in Bendsøe and Sigmund (2003) and Andreassen et al. (2011). In the present paper we make use of the built-in MATLAB convolution function `conv2`, see MathWorks (2011), adjusted to the cone-shaped density filter of Bruns and Tortorelli (2001) and Bourdin (2001).

For simplicity, assume that the design area Ω is mimicked by a $k \times l$ regular mesh of square elements with unit side length. Let the indices (i, j) respectively determine the horizontal and vertical location of the element and write $\theta_{(i,j)}$ for the material density. Density $\theta_{(i,j)}^{\text{mod}}$ modified by making use of `conv2` function is computed as the weighted average

$$\theta_{(i,j)}^{\text{mod}} = \frac{\sum_{m,n} h_{(m,n)} \theta_{(i+m,j+n)}}{\sum_{m,n} h_{(m,n)}},$$

$$m \in \{-i+1, -i+2, \dots, -1, 0, 1, \dots, k-i\},$$

$$n \in \{-j+1, -j+2, \dots, -1, 0, 1, \dots, l-j\} \quad (48)$$

where

$$h_{(m,n)} = \max\{0, r_{\min} - d_{(m,n)}\} \quad (49)$$

and $d_{(m,n)}$ denotes the distance between the centers of given element (i, j) and the one located at $(i+m, j+n)$ while $r_{\min}$ stands for the filtering radius.

The exemplary solution in Fig. 8e is acquired by calling

```
topgramp1(200, 100, 0.5, 3, 1.5, 1),
```

where the last three parameters respectively stand for the value of the GRAMP penalization factor, the filtering radius and a flag for filter application. It is worth noting that by setting $r_{\min} = 1.5$ the material density in given element is calculated as a weighted average over all adjacent ones.

For the layouts related to the original RAMP and SIMP schemes, shown in Fig. 8d, f, the `topgramp1` code requires slight modifications whose summary is given in Appendix B.

6 Conclusions

Considering the formula $W_{\text{opt}}(N, \theta)$ for stress energy of a material-void mixture as a reference expression in a research for its approximation is motivated by the non-smoothness of W_{opt} for $\det N = 0$. Consequently, a differentiable, two-parameter estimate $W_{\text{app}}(N, \theta)$ is obtained. Additional requirement of approximation uniformity for different signs of $\det N$ and arbitrary $\theta \in [0, 1]$ leads to the simplified variant of a scheme. It is nicknamed GRAMP, as it justifies and generalizes the RAMP model of Stolpe and Svanberg (2001b) in a simple way, easy to implement in numerical subroutines. Moreover, besides the simplified composite solutions to the minimal compliance problem, GRAMP is able to produce the almost “0-1” layouts of basic material as a result of the continuation method possibly combined with certain design smoothing routines. However, application of these techniques are dealt with in this paper only in limited scope.

Exact formulae determining material distribution functions are explicitly derived for various interpolation models, like SIMP, original RAMP and the one based on the Hashin-Shtrikman requirement of macrostructural isotropy of a composite material. By this, the heuristic material density updating schemes may be avoided in the development of numerical codes solving the compliance minimization problem.

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Appendix A The MATLAB code for composite solutions

A.1 The homogenization-based approach

```

1  %%%          Topology optimization code for minimal compliance          %%%
2  %%% with the material interpolation scheme based on the exact solution %%%
3  function tophomog4(nelx,nely,volfrac)
4  %% pure material properties
5  E0 = 1; nu0 = 1/3;
6  k0 = E0/(2*(1-nu0)); mu0 = E0/(2*(1+nu0));
7  %% FEA preparation
8  % B matrices at integration points
9  a = 3; b = sqrt(3);
10 B1 = sqrt(2)/12*[-a-b -a-b  a+b -a+b  a-b  a-b -a+b  a+b;
11                  -a-b  a+b  a+b  a-b  a-b -a+b -a+b -a-b;
12                  -a-b -a-b -a+b  a+b  a-b  a-b  a+b -a+b];
13 B2 = sqrt(2)/12*[-a-b -a+b  a+b -a-b  a-b  a+b -a+b  a-b;
14                  -a-b  a-b  a+b  a+b  a-b -a-b -a+b -a+b;
15                  -a+b -a-b -a-b  a+b  a+b  a-b  a-b -a+b];
16 B3 = sqrt(2)/12*[-a+b -a+b  a-b -a-b  a+b  a+b -a-b  a-b;
17                  -a+b  a-b  a-b  a+b  a+b -a-b -a-b -a+b;
18                  -a+b -a+b -a-b  a-b  a+b  a+b  a-b -a-b];
19 B4 = sqrt(2)/12*[-a+b -a-b  a-b -a+b  a+b  a-b -a-b  a+b;
20                  -a+b  a+b  a-b  a-b  a+b -a+b -a-b -a-b;
21                  -a-b -a+b -a+b  a-b  a-b  a+b  a+b -a-b];
22 % B(i,:)'*B(i,:) matrices at integration points
23 B1B11 = B1(1,:)'*B1(1,:); B2B21 = B1(2,:)'*B1(2,:); B3B31 = B1(3,:)'*B1(3,:);
24 B1B12 = B2(1,:)'*B2(1,:); B2B22 = B2(2,:)'*B2(2,:); B3B32 = B2(3,:)'*B2(3,:);
25 B1B13 = B3(1,:)'*B3(1,:); B2B23 = B3(2,:)'*B3(2,:); B3B33 = B3(3,:)'*B3(3,:);
26 B1B14 = B4(1,:)'*B4(1,:); B2B24 = B4(2,:)'*B4(2,:); B3B34 = B4(3,:)'*B4(3,:);
27 % auxiliary algebraic objects
28 nodenrs = reshape(1:(1+nelx)*(1+nely),1+nely,1+nelx);
29 edofVec = reshape(2*nodenrs(1:end-1,1:end-1)+1,nelx*nely,1);
30 edofMat = repmat(edofVec,1,8)+repmat([0 1 2*nely+[2 3 0 1] -2 -1],nelx*nely,1);
31 iK = reshape(kron(edofMat,ones(8,1))',64*nelx*nely,1);
32 jK = reshape(kron(edofMat,ones(1,8))',64*nelx*nely,1);
33 %% loads and supports
34 U = zeros(2*(nely+1)*(nelx+1),1);
35 alldofs = [1:2*(nely+1)*(nelx+1)];
36 % half mbb beam
37 F = sparse(2,1,-1,2*(nely+1)*(nelx+1),1);
38 fixeddofs = union([1:2:2*(nely+1)], [2*(nelx+1)*(nely+1)]);
39 freeddofs = setdiff(alldofs,fixeddofs);
40 %% optimization loop preparation
41 % initial composite material properties at integration points
42 xgauss = repmat(volfrac,nely*nelx,4);
43 k = (k0*mu0*xgauss)./(mu0+k0*(1-xgauss));
44 mu = mu0*ones(nely*nelx,4);
45 % initial values for optimization loop
46 x = sum(xgauss,2)/4;

```



```

47 loop = 0;
48 change = 1;
49 %% optimization loop
50 while (change > 1e-2)
51     loop = loop + 1;
52     %% Finite Element Analysis
53     sK1 = 2*(B1B11(:)*k(:,1)' + (B2B21(:)+B3B31(:))*mu(:,1)');
54     sK2 = 2*(B1B12(:)*k(:,2)' + (B2B22(:)+B3B32(:))*mu(:,2)');
55     sK3 = 2*(B1B13(:)*k(:,3)' + (B2B23(:)+B3B33(:))*mu(:,3)');
56     sK4 = 2*(B1B14(:)*k(:,4)' + (B2B24(:)+B3B34(:))*mu(:,4)');
57     sK = reshape(0.25*(sK1+sK2+sK3+sK4),64*nely*nely,1);
58     K = sparse(iK,jK,sK); K = (K+K')/2;
59     U(freedofs) = K(freedofs,freedofs)\F(freedofs);
60     %% compliance
61     J = U'*K*U;
62     %% calculation of strains and stresses
63     EPS1 = U(edofMat)*B1';
64     EPS1(:,1) = sign(EPS1(:,1)).*max(1e-9,abs(EPS1(:,1))); % to avoid numerical errors
65     EPS2 = U(edofMat)*B2';
66     EPS2(:,1) = sign(EPS2(:,1)).*max(1e-9,abs(EPS2(:,1))); % as above
67     EPS3 = U(edofMat)*B3';
68     EPS3(:,1) = sign(EPS3(:,1)).*max(1e-9,abs(EPS3(:,1))); % as above
69     EPS4 = U(edofMat)*B4';
70     EPS4(:,1) = sign(EPS4(:,1)).*max(1e-9,abs(EPS4(:,1))); % as above
71     STR1 = 2*[k(:,1) mu(:,1) mu(:,1)].*EPS1;
72     STR2 = 2*[k(:,2) mu(:,2) mu(:,2)].*EPS2;
73     STR3 = 2*[k(:,3) mu(:,3) mu(:,3)].*EPS3;
74     STR4 = 2*[k(:,4) mu(:,4) mu(:,4)].*EPS4;
75     N1new(:,1) = 1/sqrt(2)*(STR1(:,1)+sqrt(STR1(:,2).^2+STR1(:,3).^2));
76     N1new(:,2) = 1/sqrt(2)*(STR2(:,1)+sqrt(STR2(:,2).^2+STR2(:,3).^2));
77     N1new(:,3) = 1/sqrt(2)*(STR3(:,1)+sqrt(STR3(:,2).^2+STR3(:,3).^2));
78     N1new(:,4) = 1/sqrt(2)*(STR4(:,1)+sqrt(STR4(:,2).^2+STR4(:,3).^2));
79     N2new(:,1) = 1/sqrt(2)*(STR1(:,1)-sqrt(STR1(:,2).^2+STR1(:,3).^2));
80     N2new(:,2) = 1/sqrt(2)*(STR2(:,1)-sqrt(STR2(:,2).^2+STR2(:,3).^2));
81     N2new(:,3) = 1/sqrt(2)*(STR3(:,1)-sqrt(STR3(:,2).^2+STR3(:,3).^2));
82     N2new(:,4) = 1/sqrt(2)*(STR4(:,1)-sqrt(STR4(:,2).^2+STR4(:,3).^2));
83     %% convergence criterion
84     if loop > 1
85         change = sqrt(sum(sum((N1new-N1).^2))+sum(sum((N2new-N2).^2)));
86     end
87     N1 = N1new;
88     N2 = N2new;
89     %% design variables update
90     l1 = 0; l2 = 1e9;
91     while (l2-l1)/(l1+l2) > 1e-3
92         lmid = 0.5*(l2+l1);
93         xgauss = min(1,1/sqrt(lmid*E0)*(abs(N1)+abs(N2)));
94         xgauss = max(1e-6,xgauss); % to avoid numerical errors
95         xnew = reshape(sum(xgauss,2)/4,nely,nely);
96         if sum(xnew(:)) > volfrac*nely*nely, l1 = lmid; else l2 = lmid; end
97     end
98     %% print of results
99     fprintf(' It.:%5i Obj.:%11.4f Vol.:%7.3f ch.:%7.3f\n',loop,J,mean(xnew(:)),change);
100    %% plot of densities
101    colormap(gray); imagesc(1-xnew); caxis([0 1]); axis equal; axis off; drawnow;
102    %% material properties update
103    x=xnew;
104    zeta(:,1) = abs(sqrt(EPS1(:,2).^2+EPS1(:,3).^2)./EPS1(:,1));

```

```

105 zeta(:,2) = abs(sqrt(EPS2(:,2).^2+EPS2(:,3).^2)./EPS2(:,1));
106 zeta(:,3) = abs(sqrt(EPS3(:,2).^2+EPS3(:,3).^2)./EPS3(:,1));
107 zeta(:,4) = abs(sqrt(EPS4(:,2).^2+EPS4(:,3).^2)./EPS4(:,1));
108 z1 = (k0+(1-xgauss)*mu0)./(xgauss*mu0);
109 z2 = (xgauss*k0)./(mu0+(1-xgauss)*k0);
110 k = 0.5*(1+sign(z2-zeta)).*(xgauss*k0*mu0)./(mu0+(1-xgauss)*k0) + ...
111     0.5*(sign(zeta-z2)+sign(z1-zeta)).*(k0*mu0*xgauss.*(1+zeta))./(k0+mu0) + ...
112     0.5*(sign(zeta-z1)+1)*k0;
113 mu = 0.5*(1+sign(z2-zeta))*mu0 + ...
114     0.5*(sign(zeta-z2)+sign(z1-zeta)).*(k0*mu0*xgauss.*(1+1./zeta))./(k0+mu0) + ...
115     0.5*(sign(zeta-z1)+1).*(xgauss*k0*mu0)./(k0+(1-xgauss)*mu0);
116 end

```

A.2 Modifications of `tophomog4` leading to the GRAMP scheme for composite solutions

```

...
3 function topgramp4(nelx,nely,volfrac,penal)
...
43 k = k0*ones(nely*nelx,4);
...
93 xgauss = min(1,1/sqrt(lmid*E0).*sqrt((1+penal)*(N1.^2+N2.^2)));
...
REMOVE LINES 104–116 AND ADD THE LINES BELOW
104 k = E0*xgauss./(2*(1+penal*(1-xgauss)-nu0*xgauss));
105 mu = E0*xgauss./(2*(1+penal*(1-xgauss)+nu0*xgauss));
106 end

```

Appendix B The MATLAB code for nearly “0-1” solutions

B.1 The GRAMP scheme

```

1  %%% Topology optimization code for minimal compliance %%%
2  %%%           with the GRAMP interpolation scheme           %%%
3  function topgramp1(nelx,nely,volfrac,penal,rmin,ft)
4  %% pure material properties
5  E0 = 1; nu0 = 1/3;
6  k0 = E0/(2*(1-nu0)); mu0 = E0/(2*(1+nu0));
7  %% FEA preparation
8  % B matrix in the middle of the element and preintegrated matrices K1, K2
9  B = sqrt(2)/4*[-1 -1 1 -1 1 1 -1 1;
10                -1 1 1 1 1 -1 -1 -1;
11                -1 -1 -1 1 1 1 1 -1];
12 K1 = 1/24*[ 4 3 -4 3 -2 -3 2 -3; 3 4 -3 2 -3 -2 3 -4;
13            -4 -3 4 -3 2 3 -2 3; 3 2 -3 4 -3 -4 3 -2;
14            -2 -3 2 -3 4 3 -4 3; -3 -2 3 -4 3 4 -3 2;
15            2 3 -2 3 -4 -3 4 -3; -3 -4 3 -2 3 2 -3 4];
16 K2 = 1/12*[ 4 0 -1 -3 -2 0 -1 3; 0 4 3 -1 0 -2 -3 -1;
17            -1 3 4 0 -1 -3 -2 0; -3 -1 0 4 3 -1 0 -2;
18            -2 0 -1 3 4 0 -1 -3; 0 -2 -3 -1 0 4 3 -1;
19            -1 -3 -2 0 -1 3 4 0; 3 -1 0 -2 -3 -1 0 4];

```

```

20 % auxiliary algebraic objects
21 nodenrs = reshape(1:(1+nelx)*(1+nely),1+nely,1+nelx);
22 edofVec = reshape(2*nodenrs(1:end-1,1:end-1)+1,nelx*nely,1);
23 edofMat = repmat(edofVec,1,8)+repmat([0 1 2*nely+[2 3 0 1] -2 -1],nelx*nely,1);
24 iK = reshape(kron(edofMat,ones(8,1))',64*nelx*nely,1);
25 jK = reshape(kron(edofMat,ones(1,8))',64*nelx*nely,1);
26 %% loads and supports
27 U = zeros(2*(nely+1)*(nelx+1),1);
28 alldofs = [1:2*(nely+1)*(nelx+1)];
29 % half mbb beam
30 F = sparse(2,1,-1,2*(nely+1)*(nelx+1),1);
31 fixeddofs = union([1:2:2*(nely+1)], [2*(nelx+1)*(nely+1)]);
32 freedofs = setdiff(alldofs,fixeddofs);
33 %% density filter preparation (built-in conv2 function)
34 if ft ~= 0
35     [dx,dy] = meshgrid(-ceil(rmin)+1:ceil(rmin)+1,-ceil(rmin)+1:ceil(rmin)-1);
36     h = max(0,rmin-sqrt(dx.^2+dy.^2));
37     Hs = conv2(ones(nely,nelx),h,'same');
38 end
39 %% optimization loop preparation
40 % initial composite material properties in the middle of the element
41 x = repmat(volfrac,nely,nelx);
42 k = k0*x; mu = mu0*x;
43 % initial values for optimization loop
44 loop = 0;
45 change = 1;
46 %% optimization loop
47 while (change > 1e-2)
48     loop = loop + 1;
49     %% Finite Element Analysis
50     sK = reshape(2*(K1(:)*k(:)'+K2(:)*mu(:)'),64*nelx*nely,1);
51     K = sparse(iK,jK,sK); K = (K+K')/2;
52     U(freedofs) = K(freedofs,freedofs)\F(freedofs);
53     %% compliance
54     J = U'*K*U;
55     %% calculation of strains and stresses
56     EPS = U(edofMat)*B';
57     STR = 2*[k(:) mu(:) mu(:)].*EPS;
58     N1new = 1/sqrt(2)*(STR(:,1)+sqrt(STR(:,2).^2+STR(:,3).^2));
59     N2new = 1/sqrt(2)*(STR(:,1)-sqrt(STR(:,2).^2+STR(:,3).^2));
60     N2new = sign(N2new).*max(1e-9,abs(N2new)); % to avoid numerical errors
61     %% convergence criterion
62     if loop > 1
63         change = sqrt(sum((N1new-N1).^2)+sum((N2new-N2).^2));
64     end
65     N1 = N1new;
66     N2 = N2new;
67     zeta = N1./N2;
68     %% design variables update
69     l1 = 0; l2 = 1e9;
70     while (l2-l1)/(l1+l2) > 1e-3
71         lmid = 0.5*(l2+l1);
72         xnew = min(1,abs(N2)./(sqrt(lmid*E0)).*sqrt((1+penal)*(zeta.^2+1)));

```

```

73     xnew = max(1e-3,xnew); % to avoid numerical errors
74     xnew = reshape(xnew,nely,nelx);
75     if ft ~= 0, xnew = conv2(xnew,h,'same')./Hs; end
76     if sum(xnew(:)) > volfrac*nelx*nely, l1 = lmid; else l2 = lmid; end
77 end
78 %% print of results
79 fprintf(' It.:%5i Obj.:%11.4f Vol.:%7.3f ch.:%7.3f\n',loop,J,mean(xnew(:)),change);
80 %% plot of densities
81 colormap(gray); imagesc(1-xnew); caxis([0 1]); axis equal; axis off; drawnow;
82 %% material properties update
83 x=xnew;
84 k = E0*x./(2*(1+penal*(1-x)-nu0*x));
85 mu = E0*x./(2*(1+penal*(1-x)+nu0*x));
86 end

```

B.2 Modifications of topgramp1 leading to the RAMP and SIMP schemes

RAMP

```

...
3 function topgramp1(nelx,nely,volfrac,penal,rmin,ft)
...
72 xnew = min(1,(abs(N2)./(sqrt(lmid*E0)).*sqrt((1+penal)*(zeta.^2-2*nu0*zeta+1))));
...
84 k = E0/(2*(1-nu0))*x./(1+penal*(1-x));
85 mu = E0/(2*(1+nu0))*x./(1+penal*(1-x));
...

```

SIMP

```

...
3 function topsimp1(nelx,nely,volfrac,penal,rmin,ft)
...
72 xnew = min(1,(penal*N2.^2/lmid/E0.*(zeta.^2-2*nu0*zeta+1)).^(1/(1+penal))));
...
84 k = E0/(2*(1-nu0))*x.^penal;
85 mu = E0/(2*(1+nu0))*x.^penal;
...

```

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