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Material interpolation schemes in topology optimization

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Summary In topology optimization of structures, materials and mechanisms, parametrization of geometry is often performed by a grey-scale density-like interpolation function. In this paper we analyze and compare the various approaches to this concept in the light of variational bounds on effective properties of composite materials. This allows us to derive simple necessary conditions for the possible realization of grey-scale via composites, leading to a physical interpretation of all feasible designs as well as the optimal design. Thus it is shown that the so-called artificial interpolation model in many circumstances actually falls within the framework of microstructurally based models. Single material and multi-material structural design in elasticity as well as in multi-physics problems is discussed.

Key words topology optimization, multi-material designs, effective property, interpolation scheme, micro-mechanics

1
Introduction

The area of computational variable-topology shape design of continuum structures is presently dominated by methods which employ a material distribution approach for a fixed reference domain in the spirit of the so-called 'homogenization method' for topology design, [1]. That is, the geometric representation of a structure is similar to a grey-scale rendering of an image, in discrete form corresponding to a raster representation of the geometry. This concept has proven very powerful, but it does involve a number of difficulties. One is the issue of existence of solutions, another the issue of solution method. Here, the notion of physical models for 'grey' material is of great importance, and it is these interpolation schemes and their relation to characterizations of composite materials which are the themes in the following.

In many applications, the optimal topology of a structure should consist solely of a macroscopic variation of one material and void, meaning that the density of the structure is given by a "0–1" integer parametrization (often called a black-and-white design). Unfortunately, this class of optimal design problems is ill-posed in that, for example, nonconvergent, minimizing sequences of admissible designs with finer and finer geometrical details can be found, see [2, 3]. Existence of black-and-white solutions can be achieved by confining the solution space to limit the complexity of the admissible designs, making the designs dependent on the choice of parameters in the geometrical constraint. Such a restriction of the design space can be accomplished in a number of ways, e.g. by enforcing an upper bound on the perimeter of the

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structure [4–6], one can introduce a filtering function that effectively limits the minimum width of a member, [7]; see also [8] for an overview; or one can impose constraints on slopes on the parameters defining the geometry, [9–12].

For reasonable raster representations of the "0–1" black-and-white design, the solution of the resulting large-scale integer programming problem becomes a major challenge. Recently, dual methods have been shown to be effective, in the absence of local constraints, [13]. However, the most commonly used approach is to replace the integer variables with continuous variables, and then introduce some form of penalty that steers the solution to discrete 0–1 values. A key part of these methods is the introduction of an interpolation function that expresses various physical quantities, e.g. material stiffness, cost, etc., as a function of continuous variables. The continuous variables are often interpreted as material densities, as in the so-called penalized, proportional 'fictitious material' model. Inspired by the relaxed formulations that introduce composites (see below), some methods use interpolations derived from employing composite materials of some given form together with penalizations of intermediate densities of material.

Existence of solutions can also be achieved through relaxation, leaving the concept of a black-and-white design. Relaxation is sometimes attained by expanding the solution space to include microstructures and using homogenized properties to describe their behaviour, as seen in [1, 14]. In these formulations, the design is allowed to exhibit high-frequency oscillations at an indeterminate, microscopic length scale. Alternatively, we may describe these nonconventional designs through mathematical relaxation, e.g., quasi-convexification, etc. [15, 16]. In general, these approaches lead to designs that can only be realized by incorporating microstructure; however, there is no definite length scale associated with the microstructure. Relaxed formulations provide an appropriate basis for direct synthesis where composite materials are allowed to constitute part of the final design, simply because microstructure is admissible. Indeed, the demand for "ultimate" performance can lead one to consider all possible materials in the design formulation, [17, 18]. In general, relaxation yields a set of continuously variable design fields to be optimized over a fixed domain, so the algorithmic problems associated with the discrete 0–1 format of the basic problem statement are circumvented; this was one of the main motivations for the initial use of the relaxation concept. Sometimes, a subset of the design fields is optimized analytically, leaving a reduced problem for numerical optimization, [19, 20].

It should be emphasized that the continuum relaxation approach can be very involved theoretically. As of today, it has been mathematically fully worked for minimum compliance design of structures only (for both single and multiple loads) and for a broader class of problems involving the Laplace operator [15, 19, 21–24].

While this paper has some of the features of a survey paper, it is not our purpose here to cover all contributions to the area. The interested reader is instead referred to more comprehensive surveys which can be found in [8, 9, 25–30].

In the subsequent section we will study the various interpolation schemes used in black-and-white topology design, as seen from a micromechanical point of view. That is, the interpolation schemes will be compared to variational bounds for effective material parameters of mixtures of materials (e.g. the Hashin-Shtrikman bounds), and it will be shown how the interpolations can be realized using composites. Among other things, this implies that the commonly used label 'fictitious material model' is actually misleading. This investigation is first done for single material topology design (material and void structures) in elasticity, then for multiple materials, ending with a discussion of techniques for problems involving several material characteristics, for example in multiple physics problems.

It is important to point out that this comparison of interpolation schemes with micromechanical models is significant mainly for the benefit of understanding the nature of such computational measures. If a numerical scheme leads to black-and-white designs, one can in essence choose to ignore the physical relevance of intermediate steps which may include 'grey'. However, the question of physical relevance is often raised, especially as most computational schemes involving interpolations do give rise to designs which are not completely clear of 'grey'. Also, the physical realization of all feasible designs plays a role when interpreting results from a premature termination of an optimization algorithm.

2
Basic problem statement

The continuum topology design problems considered are defined on a fixed reference domain Ω in R^2 or R^3. In this domain, we seek the optimal distribution of material, with the term 'optimal' being defined through choice of objective and constraint functions, and through choice of design parametrization. The objective and constraint functions involve some kind of physical modelling that provides a measure of efficiency within the framework of a given area of applications, for example structural mechanics.

The basis for our discussion is the minimum compliance problem for a linearly elastic structure in 2-*D* (or 3-*D*, when specified as an example only; the micromechanical considerations in the sequel are not restricted to this setting). We thus consider a mechanical element as a body occupying a domain Ω^m which is part of a the reference domain Ω, on which applied loads and boundary conditions are defined Fig. 1. This reference domain is often referred to as the ground-structure, in analogy with terminology in truss topology design, [26]. Referring to the reference domain Ω we can define the optimal topology-shape design problem as a minimization of force times displacement, over admissible designs and displacement fields satisfying equilibrium

$$\begin{aligned}
&\underset{u \in U,\, \Theta}{\text{minimize}} \quad \int_\Omega pu \,\mathrm{d}\Omega + \int_{\Gamma_T} tu \,\mathrm{d}s, \\
&\text{subject to:} \\
&\int_\Omega C_{ijkl}(x)\, \varepsilon_{ij}(u)\varepsilon_{kl}(v)\mathrm{d}\Omega = \int_\Omega pv \,\mathrm{d}\Omega + \int_{\Gamma_T} tv \,\mathrm{d}s, \ \text{for all } v \in U, \\
&C_{ijkl}(x) = \Theta(x) C^0_{ijkl}, \\
&\Theta(x) = \begin{cases} 1 & \text{if } x \in \Omega^m, \\ 0 & \text{if } x \in \Omega\backslash\Omega^m, \end{cases} \\
&\mathrm{Vol}(\Omega^m) = \int_\Omega \Theta(x)\mathrm{d}\Omega \le V, \\
&\mathrm{Geo}(\,\Omega^m) \le \mathrm{K}\ .
\end{aligned} \tag{1}$$

Here, the equilibrium equation is written in its weak, variational form, with U denoting the space of kinematically admissible displacement fields, u the equilibrium displacement, p the body forces, t boundary tractions and $\varepsilon(u)$ linearized strains. Moreover, $\mathrm{Geo}(\,\Omega^m)$ denotes a constraint function limiting the geometric complexity of the domain Ω^m, imposed here to obtain a well-posed problem.

In problem (1), C^0_{ijkl} denotes the stiffness tensor of a given elastic material from which the structure is to be manufactured, with a total amount of material V; $\Theta(x)$ denotes the pointwise volume fraction of this material, and for a black-and-white design this can only attain the values zero or one.

Problem (1) is a discrete optimization problem, and for many applications it is useful to consider reformulations in terms of continuous variables, with the goal of using derivative based mathematical programming algorithms. This means that one changes the model for material properties, i.e., the relations defined in (1) as

$$C_{ijkl} = \Theta\, C^0_{ijkl} = \begin{cases} \text{either} & C^0_{ijkl}, \\ \text{or} & 0\ , \end{cases} \tag{2}$$

to a situation where the volume fraction is allowed any value between zero and one. It may also involve finding an appropriate method for limiting geometric complexity, for example, exchanging the total variation of a density for the perimeter of a domain.

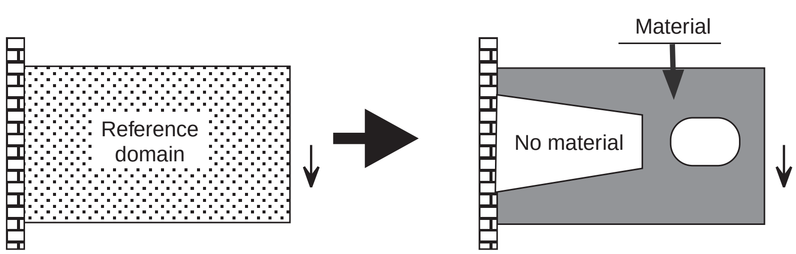

Fig. 1. The generalized shape design problem of finding the optimal material distribution

In the subsequent sections we will concentrate solely on the interpolation models for the material properties, and will not address in further detail other aspects of the modelling and solution procedures connected with various choices of objective and constraint functions, physical modelling, discretization schemes, and optimization algorithms.

3
Isotropic models for solid-void interpolation in elasticity

3.1
The SIMP model

In order to set the scene for our discussions of the various popular interpolation schemes we will begin by studying the so-called penalized, proportional 'fictitious material' model, also names as the solid isotropic material with penalization model (SIMP), [31–34]. Here, a continuous variable ρ, $0 \leq \rho \leq 1$ is introduced, resembling a density of material by the fact that the volume of the structure is evaluated as

$$\mathrm{Vol} = \int_{\Omega} \rho(x) \mathrm{d}\Omega \quad . \tag{3}$$

In computations, a small lower bound, $0 < \rho_{\min} \leq \rho$, is usually imposed, in order to avoid a singular FEM problem, when solving for equilibrium in the full domain Ω.

The relation between this density and the material tensor $C_{ijkl}(x)$ in the equilibrium analysis is written as

$$C_{ijkl}(\rho) = \rho^p \, C^0_{ijkl} \quad , \tag{4}$$

where the given material is isotropic, i.e. C^0_{ijkl} is characterized by just two variables, here chosen as the Young' s modulus E^0 and the Poisson ratio ν^0. The interpolation (4) satisfies that

$$C_{ijkl}(0) = 0, \quad C_{ijkl}(1) = C^0_{ijkl} \quad . \tag{5}$$

This means that if a final design has density zero or one in all points, this design is a black-and-white design for which the performance has been evaluated with a correct physical model. For problems where the volume constraint is active, experience shows that optimization does actually result in such designs if one chooses p sufficiently big (in order to obtain true '0–1' designs, $p \geq 3$ is usually required). The reason is that, for such a choice, intermediate densities are penalized; volume is proportional to ρ, but stiffness is less than proportional.

3.2
Microstructures realizing the SIMP-model

For the SIMP interpolation (4), it is not immediately apparent that areas of grey can be interpreted in physical terms. However, it turns out that, under fairly simple conditions on p, any stiffness used in the SIMP model can be realized as the stiffness of a composite made of void and an amount of the base material corresponding to the relevant density. Thus using the term 'density' for the interpolation function ρ is quite natural.

The stiffness tensor $C_{ijkl}(\rho)$ of the SIMP model is isotropic, with a Young's modulus varying with ρ and a constant Poisson ratio, independent of ρ. If this tensor is to correspond to a composite material constructed from void and the given material at a real density ρ, the bulk modulus κ and the shear modulus μ of the tensor $C_{ijkl}(\rho)$ should satisfy the Hashin-Shtrikman bounds for two-phase materials, [35], written here for plane elasticity and for the limit of one phase being void

$$0 \leq \kappa \leq \frac{\rho \kappa^0 \mu^0}{(1-\rho)\kappa^0 + \mu^0}, \quad 0 \leq \mu \leq \frac{\rho \kappa^0 \mu^0}{(1-\rho)(\kappa^0 + 2\mu^0) + \kappa^0} \quad (\text{in 2-}D) \quad . \tag{6}$$

Here κ^0, μ^0 are the bulk and shear moduli, respectively, of the base material. This implies that the Young modulus should satisfy [36]

$$0 \le E \le E^* = \frac{\rho E^0}{3-2\rho} \quad (\text{in 2-}D) \ . \tag{7}$$

From (7), the SIMP model should satisfy

$$\rho^p E^0 \le \frac{\rho E^0}{3-2\rho} \quad \text{for all} \ \ 0 \le \rho \le 1 \ , \tag{8}$$

which is true if and only if $p \ge 3$. However, the SIMP model presumes that the Poisson's ratio is independent of the density, and this leads to a stronger condition. From the relationship

$$\kappa^0 = \frac{E^0}{2(1-\nu^0)}, \quad \mu = \frac{E^0}{2(1+\nu^0)} \ (\text{in 2-}D) \ , \tag{9}$$

the condition (6) for the SIMP model can be written for all $0 \le \rho \le 1$ as

$$\begin{aligned} 0 &\le \frac{\rho^p E^0}{2(1-\nu^0)} \le \frac{\rho E^0}{4-2(1+\nu^0)\rho}, \\ 0 &\le \frac{\rho^p E^0}{2(1+\nu^0)} \le \frac{\rho E^0}{2(1-\rho)(3-\nu^0)+2(1+\nu^0)} \ . \end{aligned} \tag{10}$$

After some algebra, this leads to a condition on the power p in the form

$$p \ge p^*(\nu^0) = \max\left\{\frac{2}{1-\nu^0}, \frac{4}{1+\nu^0}\right\} \quad (\text{in 2-}D) \ , \tag{11}$$

which in itself implies $p \ge 3$. The inequality $p \ge 2/(1-\nu^0)$ comes from the bulk modulus bound, while the inequality $p \ge 4/(1+\nu^0)$ is due to the shear modulus bound. Example values of p^* are

$$\begin{aligned} &p^*(\nu^0 = \tfrac{1}{3}) = 3; \quad p^*(\nu^0 = \tfrac{1}{2}) = 4; \quad p^*(\nu^0 = 0) = 4; \quad p^*(\nu^0 = 1) = \infty; \\ &p^*(\nu^0 = -1) = \infty \ (\text{in 2-}D) \ , \end{aligned} \tag{12}$$

and $p^* = 3$ holds only for $\nu^0 = 1/3$.

It is important to note that the condition (11) implies that the SIMP model can be made to satisfy the Hashin-Shtrikman bounds, so that it makes sense to look for composites which realize the stiffness tensor for the model. The form of this composite can be computed through a design process, where the desired material properties of a periodic medium are obtained by an inverse homogenization process, [7, 39, 40]. The geometry of the composite may depend on the density, and one can normally not expect to obtain the wanted properties by analytical methods.

It is still an open problem if all material parameters satisfying the bounds also can be realized as composites of the given materials. For two materials, one infinitely stiff, one infinitely soft, it is shown in [37] that composites can be build for any positive definite material tensor. However, in topology design the stiffness is restricted and the density specified.

In order to illustrate the realization of the SIMP model we use an example with a base material with $\nu^0 = 1/3$. For this case the requirement on the power p is $p \ge 3$, and the bulk and shear bounds as well as the Young's modulus bound (8) all give rise to this condition. As the Young's modulus bound (8) is achieved by a composite for which both the maximum bulk and shear modulus is attained, and as this material will also have Poisson ratio $\nu = 1/3$, independent of density, we can compare the bounds and the SIMP model in one diagram which shows the values of Young's modulus as a function of density, Figs. 2 and 3. In these figures we also show the geometry of the base cell of a periodic medium that realize the relevant corresponding Young's moduli and $\nu = 1/3$. These geometries are obtained through the methodology of inverse homogenization (material design) described in [7, 39–41]. An illustration of typical microstructures which realize the SIMP model with $p = 4$ and for Poisson's ratio $\nu = 0$ and $\nu = 1/2$ are shown in Fig. 4.

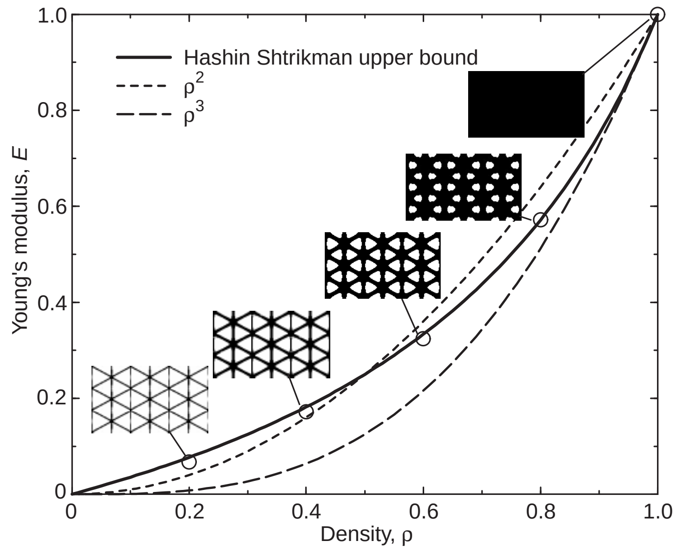

Fig. 2. A comparison of the SIMP model and the Hashin-Strikhman upper bound for an isotropic material with Poisson ratio 1/3 mixed with void. For the H-S upper bound, microstructures with properties almost attaining the bounds are also shown

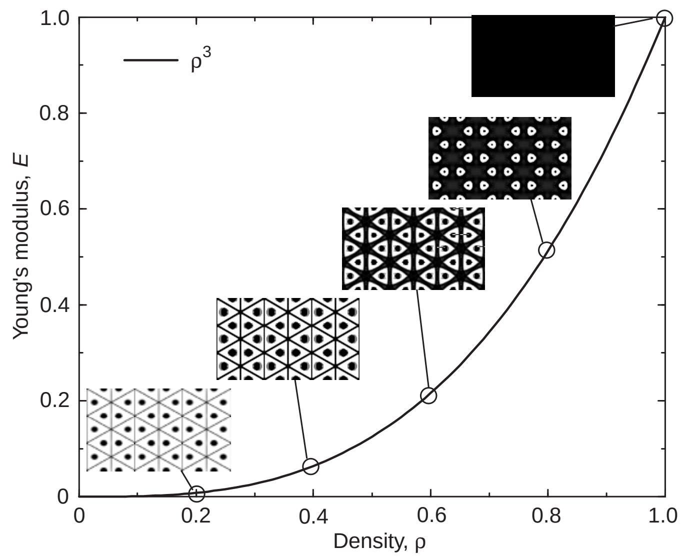

Fig. 3. Microstructures of material and void realizing the material properties of the SIMP model with $p = 3$ Eq. (11), for a base material with Poisson's ratio $\nu = 1/3$. As stiffer material microstructures can be constructed from the given densities, non-structural areas are seen at the cell centers

The discussion above holds for planar problems. In 3-*D*, there is, in a sense, more geometric freedom to construct microstructures, and here the Hashin-Shtrikman bounds lead to the condition

$$p \geq \max\left\{15\frac{1-\nu^0}{7-5\nu^0}, \frac{3}{2}\frac{1-\nu^0}{1-2\nu^0}\right\} \quad (\text{in 3-}D) , \tag{13}$$

on the power p in the SIMP model. This condition can be derived as outlined above, but as the algebra is rather lengthy this is omitted here. Example bounds are here

$$\begin{aligned} &p \geq 3 \quad \text{for} \quad \nu^0 = \tfrac{1}{3}; \quad p \geq 2 \quad \text{for} \quad \nu^0 = \tfrac{1}{5}; \quad p \geq \tfrac{15}{7} \quad \text{for} \quad \nu^0 = 0; \\ &p \geq \tfrac{5}{2} \quad \text{for} \quad \nu^0 \to -1; \quad p \to \infty \quad \text{for} \quad \nu^0 \to \tfrac{1}{2} \ (\text{in 3-}D) , \end{aligned} \tag{14}$$

so some lower values of p are possible in dimension three. Note, however, that for $\nu = 1/3$ we have the same bounds in 2-*D* and in 3-*D*.

3.3
Variable thickness sheets – the Voigt bound

Design of variable thickness sheets allows for a physical given linear interpolation of stiffness through the thickness variable of the sheet

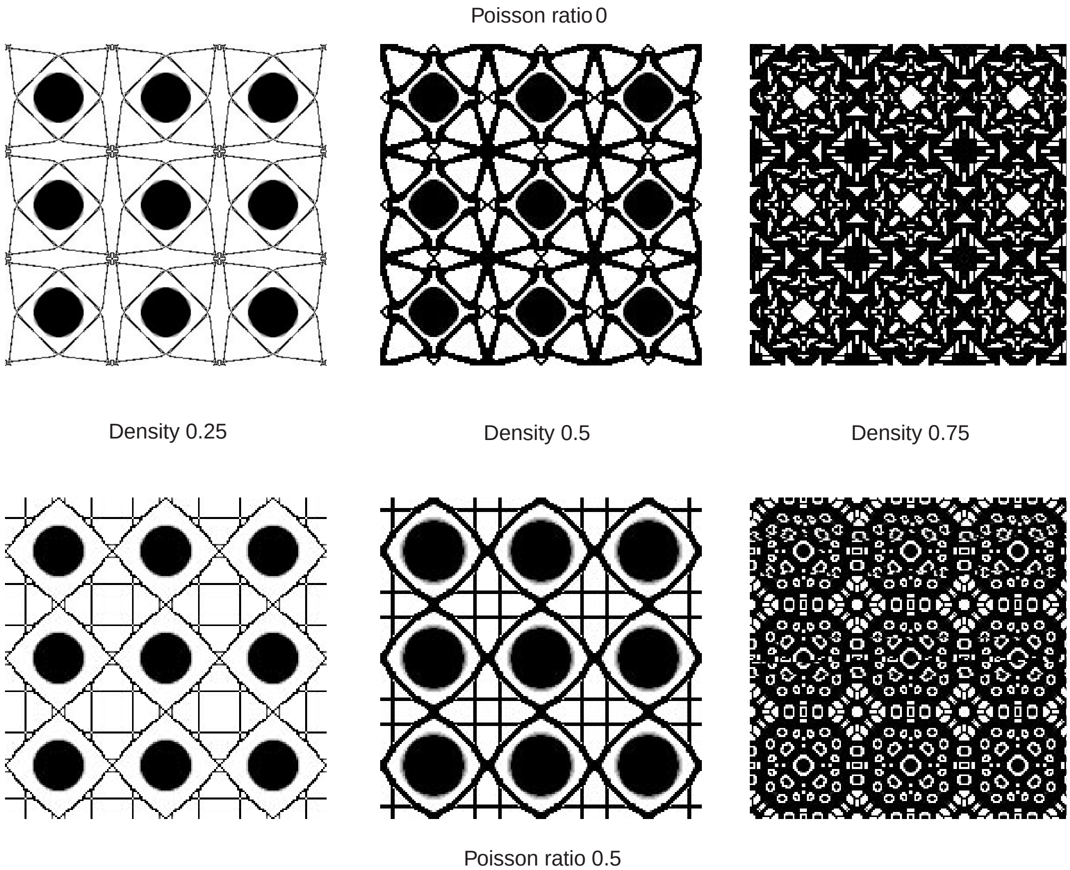

Fig. 4. Microstructures of material and void realizing the material properties of the SIMP model with $p = 4$, Eq. (11), for a base material with Poisson's ratio $\nu = 0$ and $\nu = 0.5$, respectively. As in Fig. 3, nonstructural areas are seen at the centers of the cells

$$C_{ijkl} = h\, C^0_{ijkl}, \quad 0 \le h(x) \le 1, \;\; x \in \Omega \subset R^2, \mathrm{Vol} = \int_\Omega h(x)\mathrm{d}\Omega \;\; . \tag{15}$$

Here, the maximal thickness is set equal to one, in order to maintain the setting of an interpolation scheme, cf. (2). This problem was first studied in [42] as a basis for computational topology design. Mathematically, the linear dependence of stiffness and volume on the thickness h leads to the existence of solutions for the compliance problem also in the case where geometric constraints are not imposed, see [43] and references therein. Optimal designs within this framework of variable thickness sheets customarily possess large areas of intermediate thickness, but topology may also be identified from areas with $h = 0$. The discrete computational form of the variable thickness problem is analogous to what is seen in optimal truss topology design, and very efficient algorithms can be devised, [44]. Of other recent numerical studies we mention [45, 46].

The variable thickness sheet problem is in essence a problem in "dimension $2\frac{1}{2}$" . For purely planar and purely three dimensional problems, an interpolation of the form

$$C_{ijkl} = \rho\, C^0_{ijkl}\,, \quad 0 \le \rho(x) \le 1, \mathrm{Vol} = \int_\Omega \rho(x)\mathrm{d}\Omega, \tag{16}$$

where ρ is a density of material, corresponds to using the Voigt upper bound on stiffness, which cannot be realized by composites of material and void. The use of the Voigt upper-bound interpolation for general topology optimization is nevertheless fairly popular, especially in the so-called evolutionary design methods, [47, 48]. Also note that striving for black-and-white designs requires some form of penalization of 'grey', and such measures necessitates the reintroduction of geometric constraints in order to obtain a well-posed problem.

It is worth noting that the variable-thickness sheet problem plays an important role as an equivalent subproblem in the design labelled 'free-material optimization', [17, 18]. Here, the design problem is defined over all possible material tensors, with a generalized, linear cost expressed in terms of tensor invariants. This setting has also been used for black-and-white topology design in [49], by posing a sequence of well-posed, free material design problems.

3.4
The Hashin-Shtrikman bound

In light of the importance of the Hashin-Shtrikman bounds for the realization of intermediate densities and noting that the bounds have a similar penalization of intermediate density as does the SIMP model, it is rather surprising that these bounds have so far not been used as interpolation functions for topology design. Using these bounds one will have an interpolation of Young's modulus and of Poisson's ratio in the form

$$E(\rho) = \frac{\rho E^0}{3 - 2\rho}, \qquad \nu(\rho) = \frac{1 - \rho\,(1 - \nu^0)}{3 - 2\rho} \quad , \tag{17}$$

where not only Young's modulus, but also Poisson's ratio, depends on density. Observe that independent of the Poisson ratio of the base material, the low volume fraction limit has a Poisson ratio equal to 1/3. The interpolation (17) corresponds to the material parameters of a composite that achieves simultaneously the Hashin-Shtrikman upper bounds on bulk and shear moduli, and such a material can be realized by, for example, an isotropic rank-3 lamination (see [40] for a recent overview).

3.5
Other models

The Voigt upper-bound model (16) has been combined in a number of papers [50–52] with the Reuss lower bound for mixtures of materials in order to obtain alternative schemes. For a mixture of void and material, the Reuss lower bound is zero, and in this case the interpolation (called the Reuss-Voigt interpolation in the sequel) reads

$$C_{ijkl}(\rho) = \begin{cases} \alpha\rho C^0_{ijkl} & \text{if } \rho < 1, \\ C^0_{ijkl} & \text{if } \rho = 1, \end{cases} \qquad \mathrm{Vol} = \int_\Omega \rho(x)\mathrm{d}\Omega \quad . \tag{18}$$

Here, α is a parameter which weighs the contribution by the Voigt and Reuss bounds. The interpolation introduces a jump at $\rho = 1$ (a potential problem in computations), but this is not the case when void is exchanged with a material with higher stiffness (see below).

Similarly to the analysis for the SIMP model above, one can check the range of the parameter α for which the Hashin-Shtrikman bounds are satisfied. For 2-*D* elasticity this leads to the condition

$$\alpha \le \alpha^*(\nu^0) = \min\left\{\frac{1-\nu^0}{2}, \frac{1+\nu^0}{4}\right\} \quad . \tag{19}$$

The largest value of α is thus $1/3$, and this is only possible if $\nu^0 = 1/3$. For comparison, the Young's modulus of the Hashin-Shtrikman bounds, the Reuss-Voigt interpolation and the Voigt bound, as a function of density, is illustrated in Fig. 5; for consistence we choose $\nu^0 = 1/3$, as this results in a constant Poisson ratio of $\nu = 1/3$ for all three cases.

Finally, we note that an isotropic interpolation model based on the 3-*D* effective properties of a statistically isotropic medium with spherical inclusions has been proposed in [53, 54]. The Young's modulus and Poisson's ratio of this model has also been used for planar problems. However, it is worth noting that for this interpolation scheme the 2-*D* Hashin-Shtrikman bounds are violated, a feature stemming from the incompatibility of planar elasticity and spherical inclusions.

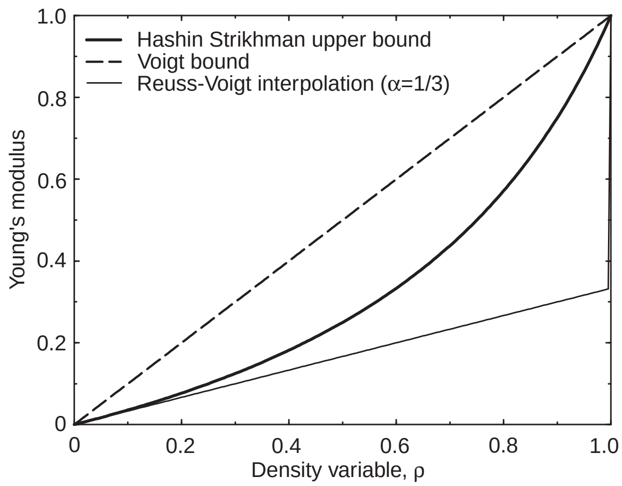

Fig. 5. A comparison of the Voigt upper bound, the Hashin-Strikhman upper bound and the Reuss-Voigt interpolation for a mixture of material and void (Poisson's ratio $\nu = 1/3$)

3.6
Example designs

The interpolation schemes described above are, in essence, computational approximations to the black-and-white 0–1 problem. As the problems are different in form, the results obtained with the various methods are, as expected, not the same. Conceptually, there are strong similarities, but the differences in detail can be quite significant. This is not a major problem when employing the techniques in a design context, as long as these differences are understood and acknowledged.

In implementations of topology design schemes based on density interpolation it is often seen that a too severe penalization of intermediate density can lead to designs which are local minima, and which are very sensitive to the choice of the initial design for the iterative optimization procedure. Thus, a continuation method is often advisable, which, for example, for the SIMP method means that the power p is slowly raised through the computations, until the final design is arrived at for a power satisfying (11) or (13). This procedure is thus a compromise, since initial designs will be analysed using an interpolation which is not realizable as a composite structure.

Figure 6 shows examplary optimal designs for a simple, planar, minimum-compliance design problem using the Voigt upper-bound interpolation, the Hashin-Shtrikman upper-bound interpolation and SIMP for various powers of p. For the latter cases, the power is maintained fixed in the iterative optimization scheme, except in one situation. Note that the Voigt upper-bound interpolation does not satisfy our goal of finding a black-and-white design. The com-

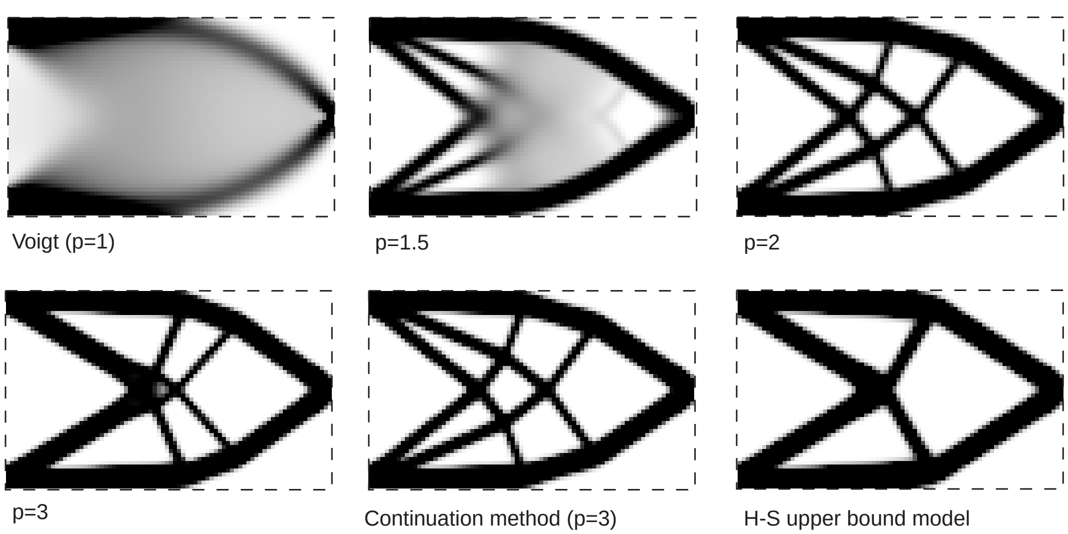

Fig. 6. Optimal design results for material and void, using various powers p in the SIMP interpolation scheme, and using the Hashin-Shtrikman upper bound. Problem definition as in Fig. 1

putations for all cases were here carried out with a filter technique for maintaining a limited geometric resolution, and in order to avoid checkerboard-like areas in the solution (see [8] for further details on these aspects).

4
Homogenization models with anisotropy

The initial work on numerical methods for topology design of continuum structures used composite materials as the basis for describing varying material properties in space, [1]. This approach was strongly inspired by theoretical studies on generalized shape design in conduction and torsion problems, and by numerical and theoretical work related to plate design, [2, 3, 14, 15]. Initially, composites consisting of square or rectangular holes in periodically repeated square cells were used for planar problems. Later so-called ranked laminates (layers) have become popular, both because analytical expressions of their effective properties can be given and because investigations proved the optimality of such composites, in the sense of bounds on effective properties, (see [55–57] and references therein). Also, with layered materials existence of solutions to the minimum compliance problem for both single and multiple load cases is obtained, without any need for additional constraints on the design space e.g. without constraints on the geometric complexity. For all the models mentioned here, homogenization techniques for computing effective moduli of materials play a central role. Hence the use of the phrase 'the homogenization method' for topology design for procedures involving this type of modelling.

The homogenization method for topology design involves working with orthotropic or anisotropic materials. This adds to the requirements of the finite element analysis code, but the main additional complication are the extra design variables required to describe the structure. Thus, a microstructure with rectangular holes in square cells requires three distributed variables, as the material properties at each point of the structure will depend on two size-variables characterizing the hole and one variable characterizing the angle of rotation of the material axes (the axes of the cell).

In topology design based on homogenization of periodic media, one always works with microstructures of a given type, so the realization of the interpolation is not an issue. However, a key question also in this case is a comparison of the stiffness parameters of the microstructure at hand with bounds on such parameters. For anisotropic materials, such bounds are expressed in terms of strain or complementary energies.

For planar problems, any composite, constructed from void and an isotropic, linearly elastic material with Young's modulus E^0 and Poisson ratio ν^0, has an elasticity tensor $\mathbf{C}$ which satisfies the lower complementary energy bound, [57],

$$\frac{1}{2}\left[C^{-1}\right]_{ijkl}\sigma_{ij}\sigma_{kl} \geq \begin{cases} \frac{1}{2E^0\rho}\ \left[\sigma_I^2+\sigma_{II}^2-2(1-\rho+\rho\nu^0)\sigma_I\sigma_{II}\right] & \text{if } \sigma_I\sigma_{II}\leq 0, \\ \frac{1}{2E^0\rho}\ \left[\sigma_I^2+\sigma_{II}^2+2(1-\rho-\rho\nu^0)\sigma_I\sigma_{II}\right] & \text{if } \sigma_I\sigma_{II}\geq 0\ , \end{cases} \tag{20}$$

for any stress tensor $\boldsymbol{\sigma}$ with principal stresses σ_I, σ_{II}. The inequalities (20) express an upper bound on the stiffness of the composite. This bound can also be expressed in terms of strain energy, [20],

$$\frac{1}{2}C_{ijkl}\varepsilon_{ij}\varepsilon_{kl} \leq \begin{cases} \frac{E\left[\varepsilon_I^2+\varepsilon_{II}^2+2(1-\rho+\rho\nu)\varepsilon_I\varepsilon_{II}\right]}{2(1-\nu)(2-\rho+\nu\rho)} & \text{if } \frac{\varepsilon_I+\varepsilon_{II}}{(1-\nu)\varepsilon_I}<\rho, \\ \frac{E\left[\varepsilon_I^2+\varepsilon_{II}^2-2(1-\rho-\rho\nu)\varepsilon_I\varepsilon_{II}\right]}{2(1+\nu)(2-\rho-\nu\rho)} & \text{if } \frac{\varepsilon_I-\varepsilon_{II}}{(1+\nu)\varepsilon_I}<\rho, \\ \frac{\rho E\varepsilon_I^2}{2} & \text{otherwise}\ . \end{cases} \tag{21}$$

This holds for any strain tensor $\boldsymbol{\varepsilon}$ with principal strains $\varepsilon_I, \varepsilon_{II}$ ordered such that $|\varepsilon_I| \leq |\varepsilon_{II}|$. As void is allowed, the lower bound on stiffness is zero.

The bounds (20) and (21) can be attained by so-called rank-2 laminates, consisting of a layering at two length scales and with the layers (and axes of orthotropy) directed along the principal strain or principal stress axes (they coalesce). For stresses with $\sigma_I\sigma_{II} \geq 0$, single-scale, single inclusion microstructures (named after Vidgergauz) which attain the bounds, have been presented in [58, 59]. In a recent study, [60], it is shown that for $\sigma_I\sigma_{II} < 0$ no single-scale periodic composite obtain the bounds, and any composite obtaining the bound (in 2-D) must be degenerate (i.e. has a singular stiffness tensor). For illustration, Fig. 7 shows a range of single inclusion Vigdergauz-like microstructures for a range of positive as well as negative values of σ_{II}/σ_I; these structures have been computed by the inverse homogenization methodology (see above for references).

For their use in optimal topology design it is useful to compare energies attainable by other microstructures and interpolation schemes with the bound (20). Figure 8 thus shows a comparison of the optimal bound for $\rho = 0.5$, achievable by the ranked layered materials, with the range of minimal complementary energies which can be obtained by the SIMP interpolation, by microstructures with square holes, by microstructures with rectangular holes, and by the Vigdergauz microstructures. What is noticeable, is how close the various energies are for stress fields close to pure dilation, while shearing stress fields demonstrate a considerable difference. In the latter case, the microstructural based models are considerably stiffer than the SIMP model, an effect which can to a large extent be attributed to the possibility of rotation for the orthotropic microstructures. Moreover, the microstructure with square holes is notably less stiff for uniaxial stresses compared to the other microstructures, since the imposed symmetry of this microstructure here hinders an efficient use of material.

The plots of the complementary energy explain many features of computational experience with various interpolation schemes. For compliance optimization, the complementary energy should be minimized. As ranked laminates are efficient also at intermediate densities, optimal

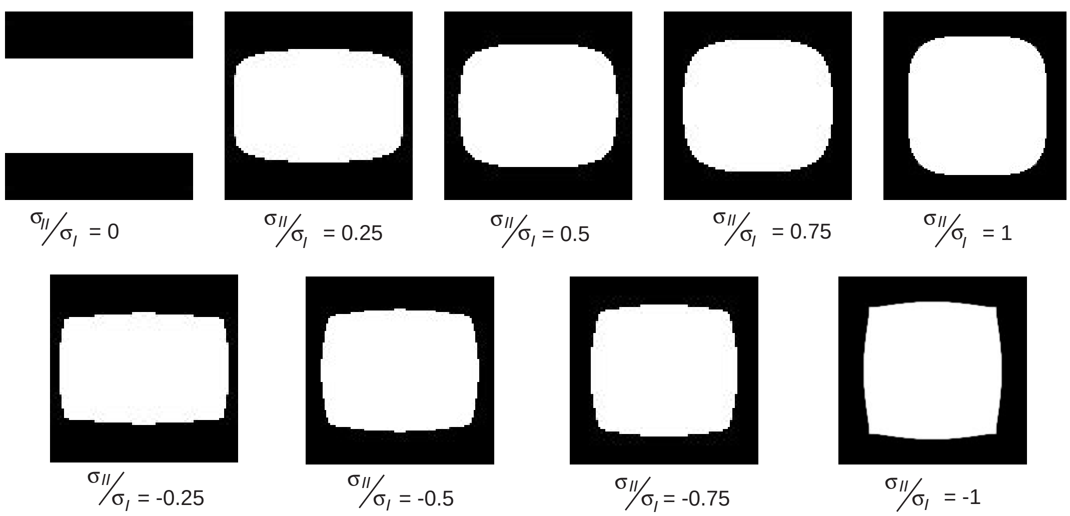

Fig. 7. The shape of single inclusions of void in a cell of a homogenized, periodic medium minimizing complementary energy (Vigdergauz-like structures for $\nu = 1/3$ and a density $\rho = 0.5$). Results for a range of principal stress ratios of a macroscopic stress field

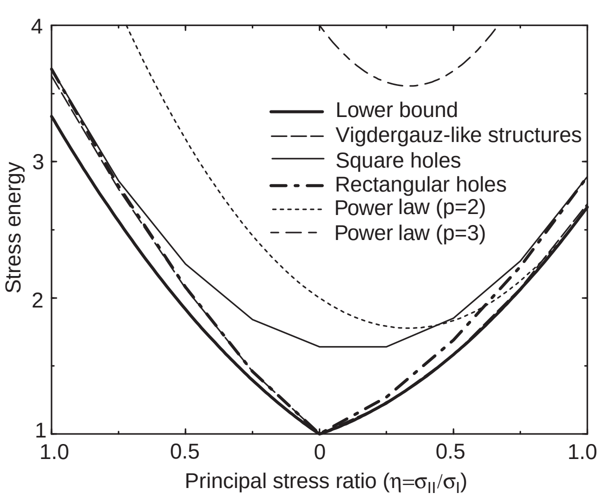

Fig. 8. Comparison of the optimal (minimal) complementary energy as a function of the ratio of the principal stresses, for a density $\rho = 0.5$, and for various types of microstructures and interpolation schemes (material and void mixtures). The Vidgergauz-like structures are shown in Fig. 7

design with this material model leads to designs with typically rather large areas of intermediate density. This is also the case when using the microstructures with rectangular holes and the Vigdergauz microstructures. Thus if such materials are used for obtaining black-and-white designs, some other form of penalization of intermediate density has to be introduced, [5, 61]. One possibility is adding a term $K\int_\Omega \rho(x)\,(1-\rho(x))\mathrm{d}\Omega$ to the objective function (with K large). On the other hand, the SIMP model and the microstructure with square holes usually lead to designs with very little 'grey', as intermediate values of density tend to give poor performance in comparison with cost.

We close this section by noticing that the 'homogenization method', based on interpolation with composites, has constituted the basis for studies ranging over a wide area of design problems, encompassing vibration and buckling problems, design of compliant mechanisms, design of materials etc. We refer to the surveys mentioned in the introduction for further details.

5 Multiple materials in elasticity

5.1 Two materials with non-vanishing stiffness

For a topology design problem, where we seek the optimal distribution of two isotropic, linearly elastic materials with nonvanishing stiffness, the stiffness tensor of the problem (1) takes the form

$$C_{ijkl} = \Theta\, C^1_{ijkl} + (1-\Theta)C^2_{ijkl} = \begin{cases} \text{either} & C^1_{ijkl} \\ \text{or} & C^2_{ijkl} \end{cases} \tag{22}$$

where the two materials are characterized by the stiffness tensors C^1_{ijkl}, C^2_{ijkl}. Here we assume that material 1 is the stiffer, i.e., $C^1_{ijkl}\varepsilon_{ij}\varepsilon_{kl} \geq C^2_{ijkl}\varepsilon_{ij}\varepsilon_{kl}$ for any strain $\boldsymbol{\varepsilon}$. Note that the volume constraint now signifies the amount of material 1 which can be used, as the total amount of material amounts to the total volume of the domain Ω.

The two-material problem has been the focal point of theoretical works on generalized shape design problems, as the possible singularity of stiffness is not an issue. Computational studies are scarcer, with early numerical work concentrating on conduction problems, [14, 15], but this variant of the topology design problem has gained recent interest, mainly as a method for generating microstructures with interesting (and extreme) behaviour, [40, 41, 62].

An analysis of various interpolation schemes can follow exactly the same lines as above, as the bounds on effective properties used there are actually just special cases of the general results for mixtures of any two materials. The 'special' case was here treated first, as the material-void problems is the most studied for topology design applications. Moreover, the algebra for this case is more transparent.

For the two-material problem, the SIMP model can be expressed, as suggested in [41];

$$\begin{aligned} &C_{ijkl}(\rho) = \rho^p\, C^1_{ijkl} + (1-\rho^p)C^2_{ijkl}, \\ &\mathrm{Vol}\,(\text{material } 1) = \int_\Omega \rho(x)\mathrm{d}\Omega\ , \end{aligned} \tag{23}$$

while the Reuss-Voigt interpolation model takes the form, [50–52],

$$\begin{aligned} &C_{ijkl}(\rho) = \alpha[\rho\, C^1_{ijkl} + (1-\rho)C^2_{ijkl}] + (1-\alpha)[\rho\,\left(C^1\right)^{-1} + (1-\rho)\left(C^2\right)^{-1}]^{-1}_{ijkl}, \\ &\mathrm{Vol}\,(\text{material } 1) = \int_\Omega \rho(x)\mathrm{d}\Omega\ . \end{aligned} \tag{24}$$

For the two-material problem, the lower Hashin-Shtrikman bound for isotropic composites is non-zero, so here a goal of realization with microstructures means that both lower and upper bounds will impose constraints on the interpolation models. In order to clarify the fundamental effects of these bounds, the discussion here will be limited to the 2-D case, where both base materials as well as the interpolations have Poisson's ratio equal to 1/3.

In this case, the Hashin-Shtrikman bounds on the bulk and shear moduli for isotropic composites reduce to one and the same condition, which can be expressed as a condition on the Young's modulus

$$\frac{(2+\rho)E_1+(1-\rho)E_2}{2(1-\rho)E_1+(1+2\rho)E_2}E_2 \leq E(\rho) \leq \frac{\rho E_1+(3-\rho)E_2}{(3-2\rho)E_1+2\rho E_2}E_1 \quad (\text{in 2-}D) \ , \tag{25}$$

where E_1, E_2 denotes the Young's moduli of the two materials, for which $E_1 \geq E_2$.

The derivative at zero density of the lower bound in (25) is positive. Thus, condition (25) implies that a SIMP model in the form (23) will never satisfy the Hashin-Shtrikman bounds for all densities. However, it is possible to keep the SIMP model fairly close to the behaviour governed by these bounds, see Fig. 9. Moreover, it can be shown that the Reuss-Voigt interpolation model (with $\nu = 1/3$) satisfies the bounds if and only if $\alpha = 1/3$. As also noted in Sec. 4, the Hashin-Shtrikman bounds in themselves constitute sensible interpolations, and here one can choose between the upper and the lower bound. For comparison of the various models we also include here results for the short 'cantilever' problem treated in Sec. 4, Fig. 10.

5.2
Three-materials design

Topology design involving void and two materials with non-vanishing stiffness has so far been used for design of sandwich-like structures (using layered microstructures, [63]) and for design of multi-phase composites with extreme behaviour [41, 62].

In this case isotropic interpolation schemes can be compared to the multiphase Hashin-Shtrikman bounds for isotropic composites, [35]. As above, this is done here in the case of Poisson's ratio equal to 1/3 for all phases as well as the interpolation scheme. As one phase is zero, the bounds, expressed in terms of Young's modulus are (again we assume $E_1 \geq E_2$)

$$0 \leq E(\rho_1,\rho_2) \leq \frac{\rho_1 E_1(\rho_2 E_1+(3-\rho_2)E_2)}{(3-2\rho_1\rho_2)E_1+(6-6\rho_1+2\rho_1\rho_2)E_2} \quad \text{if } \rho_1 < 1 \quad (\text{in 2-}D) \ . \tag{26}$$

Here $\rho_1,\ 0 \leq \rho_1 \leq 1$ is the density of the mixture of the two materials with stiffness, and $\rho_2,\ 0 \leq \rho_2 \leq 1$ is the density of material 1 in this mixture, such that

$$\text{Vol (material 1)} = \int_\Omega \rho_1(x)\ \rho_2(x)\mathrm{d}\Omega, \quad \text{Vol (material 2)} = \int_\Omega \rho_1(x)\ (1-\rho_2(x))\mathrm{d}\Omega,$$

$$\text{Total volume of material} = \int_\Omega \rho_1(x)\mathrm{d}\Omega \ . \tag{27}$$

For a SIMP-like interpolation model, it is most convenient to interpolate first between the two nonzero phases and then between this 'material' and void. The resulting model is

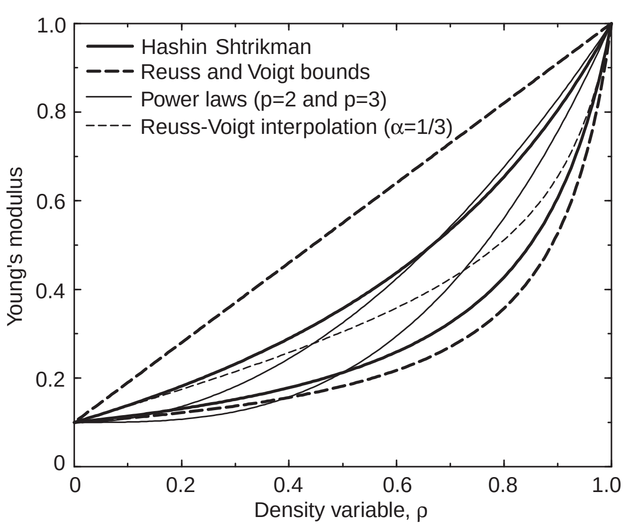

Fig. 9. A comparison of the Voigt upper and the Reuss lower bound, the Hashin-Strikhman upper and lower bound, SIMP models, and the Reuss-Voigt interpolation for mixtures of two material with equal Poisson's ratio $\nu = 1/3$, and with Young's moduli $E_1 = 1$ and $E_2 = 0.1$

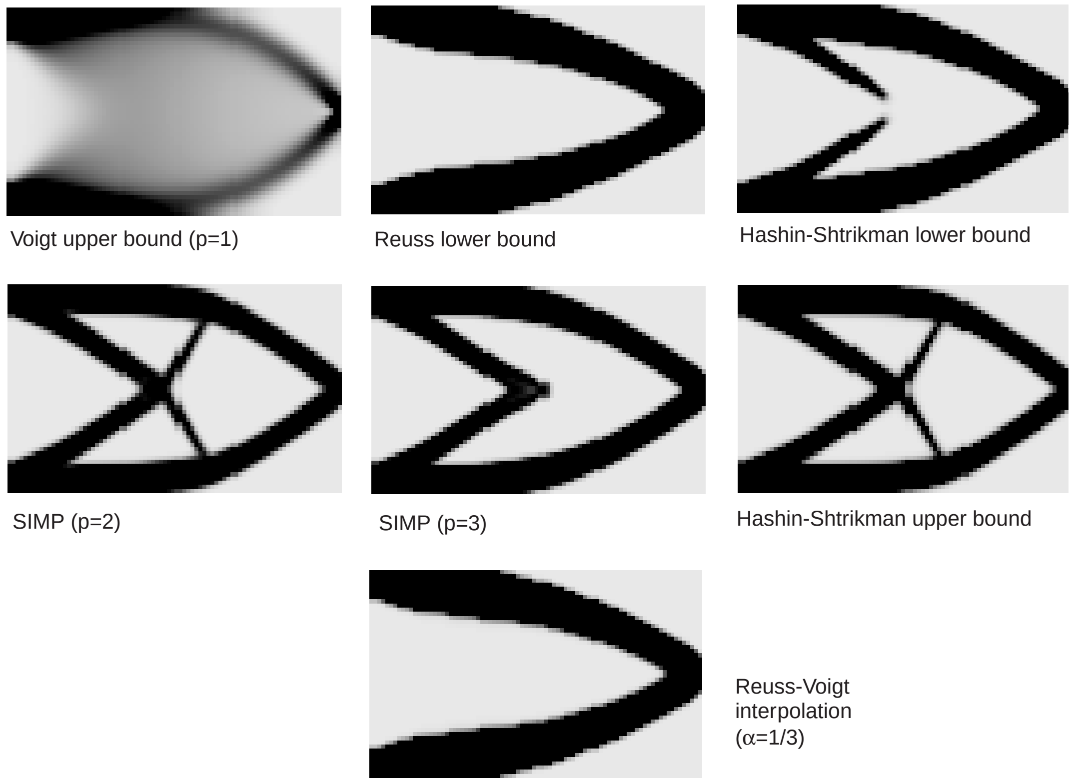

Fig. 10. Optimal design results for two-materials design (for $E_1 = 1$, $E_2 = 0.1$, and $\nu_1 = \nu_2 = 1/3$), using various interpolation schemes. The geometry and loading of the problem as in Fig. 1, comp. Fig. 6. The compliances of the designs lie within a few percent of one another

$$E = \rho_1^{p_1}\left[\rho_2^{p_2}E_1 + \left(1 - \rho_2^{p_2}\right)E_2\right] \quad , \tag{28}$$

which for example for $p_1 = p_2 = 3$ is compatible with (26), i.e., for $\nu_1 = \nu_2 = 1/3$. Note, however, that for $\rho_1 = 1$ the bounds (25) should be satisfied, and there is a (natural) singularity in the conditions when shifting from a solid mixture to a mixture involving void. Designs obtained using (28) are shown in Fig. 11.

6
Multiple physics, nonlinear problems and anisotropic phases

6.1
Multiple physics

The phrase 'multiple physics' is used here to cover topology design where several physical phenomena are involved in the problem statement, thus covering situations where for example elastic, thermal and electromagnetic analyses are involved.

When modelling such situations, the basic concept of the homogenization method for topology design provides a general framework for computing interpolation schemes. As the theory and computational framework of homogenization of composite media is not limited to elasticity, choosing a specific class of composites and computing effective elastic, thermal and electromagnetic properties will lead to the required relationships between intermediate density and material properties. An example of this approach for thermo-elastic problems can be found in [64]. However, direct links between specific classes of composites and proofs of existence for such coupled problems have yet to be discovered.

The reduced complexity of the design description achieved by the SIMP approach has also lead to the development of such interpolation schemes for multiple physics problems. In [41], microstructures with extreme thermal expansion are designed by combining the three-materials interpolation of (28) for the elastic properties with an interpolation of the thermal expansion coefficients in the form

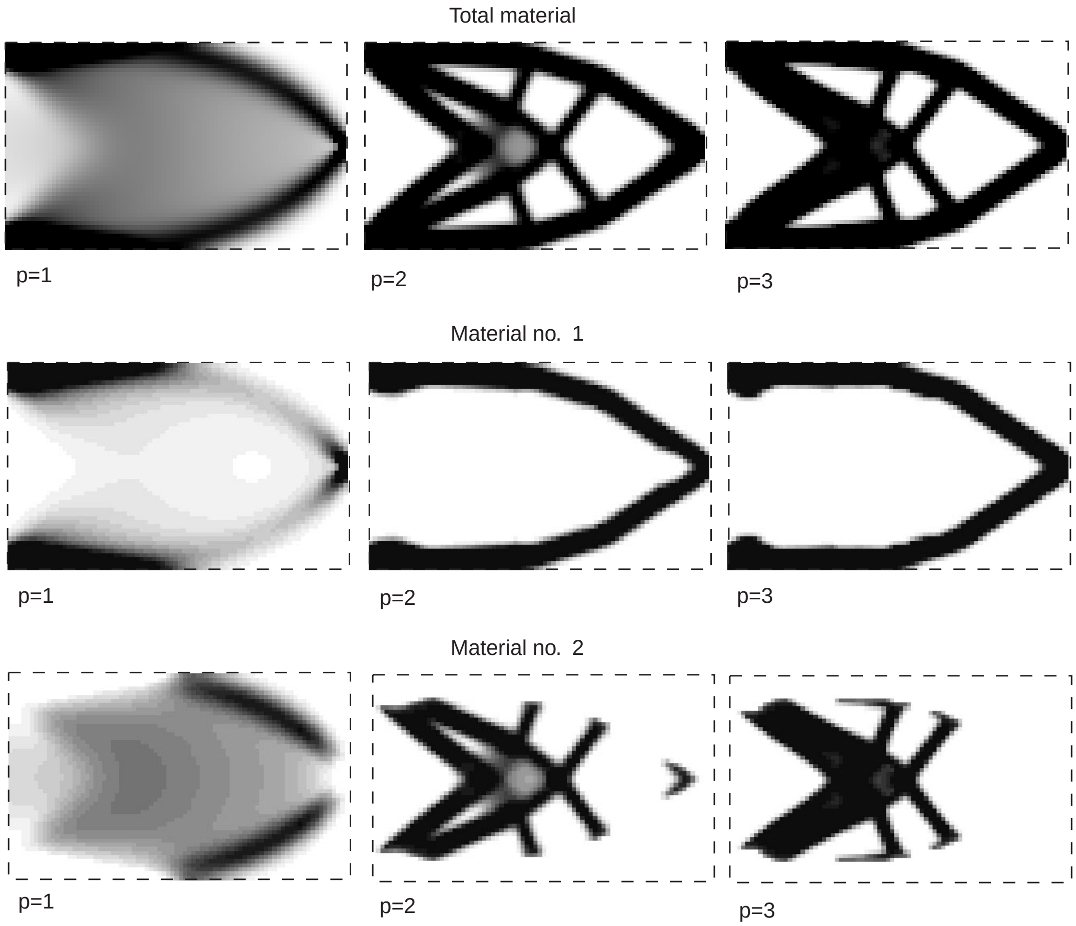

Fig. 11. Optimal design results for three-materials design (two materials with $v_1 = v_2 = 1/3$ and with stiffness $E_1 = 1$, $E_2 = 0.1$, and void), using various powers p in the interpolation scheme (28). The geometry and loading of the problem as in Fig. 1. Compare with Figs. 6 and 10

$$\alpha_{ij} = (1 - \rho_2^p)\alpha_{ij}^1 + \rho_2^p \alpha_{ij}^2 \tag{29}$$

Here α_{ij} is the thermal strain tensor which does not depend on the total density ρ_1 of the mixture of the two materials 1 and 2. In recent work on topology design of thermo-electro-mechanical actuators, an interpolation of isotropic, thermal as well as electric conduction properties (with d^0 denoting the conductivity of the solid material)

$$\mathrm{d}(\rho) = \rho^p d^0 \ , \tag{30}$$

has with success been combined with the basic SIMP interpolation (4), [65]. It is here worth noting that for this combination of interpolations, the condition (11) for the power p is sufficient for compatibility also with the Hashin-Shtrikman bounds for conduction

$$\mathrm{d}(\rho) \leq \frac{\rho}{2-\rho}\ d^0 \ , \tag{31}$$

as well as the cross-property bounds [36, 66],

$$\frac{\kappa^0}{\kappa} - 1 \geq \frac{\kappa^0 + \mu^0}{2\mu^0}\left[\frac{d^0}{d} - 1\right]; \quad \frac{\mu^0}{\mu} - 1 \geq \frac{\kappa^0 + \mu^0}{\kappa^0}\left[\frac{d^0}{d} - 1\right] \ . \tag{32}$$

Topology design methods have also been implemented for the design of piezo-electric composites, which involves a coupled electrostatic and elastic analysis. Here, material interpolation has been performed using a homogenized medium, [67], as well as by a Voigt-type interpolation of the stiffness tensor, the piezoelectric tensor and the dielectric tensor, with a separate penalization of intermediate density, [68].

6.2 Nonlinear problems

For nonlinear problems (elasto-plasticity etc.) both the 'homogenization method' and the SIMP approach to topology design provide an even greater theoretical challenge, mainly due to the less developed and more involved theory of homogenization and to difficulties in deriving bounding theorems for such problems. It is here important to underline that micromechanical considerations should always play a role in the development of interpolation schemes, as experience shows that the computational feasibility of such schemes can be closely related to how faithfully the interpolations mimic physical reality.

For geometrically nonlinear problems, the constitutive laws remain linear so it is here natural to use the interpolation schemes developed for the linear problems. This has been done for large displacement problems in [69, 70], using the SIMP model to design structures and compliant mechanisms.

For materially nonlinear problems, references [71] and [72] use numerical analysis of the homogenized elasto-plastic behaviour of a microstructure of rectangular holes in square cells as the basis for topology design for elasto-plastic problems (beams and shells), while the SIMP approach has been implemented in [73]. A fundamental question in these problems, among others, is a reasonable description (interpolation) of the yield limit at intermediate densities, a problem that also is to be addressed for stress-constrained design problems. The stress-constrained problem is treated in the linear elastic domain. In [74], a micromechanical study of rank-2 laminates together with numerical experiments lead to a SIMP interpolation of the stiffness and stress limit in the form

$$E(\rho) = \rho^p E_0, \quad \sigma^Y(\rho) = \rho^p \sigma_0^Y \ . \tag{33}$$

It is here convenient to interpret (33) as an interpolation between physical properties, which are relevant if material is present, and which should vanish when material is not present, and in order not to introduce bias, all properties are based on the same interpolation. For topology design involving damage models, [75], a similar scheme is to express the linear and nonlinear strain energies in a form

$$\Psi(\rho) = \rho^p \Psi_0, \quad \Psi^D(\rho) = \rho^p \Psi_0^D \ , \tag{34}$$

which is consistent for a black-and-white design (an index zero indicates the energy expression valid at density 1).

6.3 Anisotropic phases

It is straightforward to extend the SIMP model to encompass also topology design with anisotropic materials, but for such cases the rotation of the base material should also be included as a design variable, [76]. The design of laminates (as stacks of plies of fiber-reinforced materials) can be seen as a topology design problem, where a combination of the Voigt bound (for the membrane stiffness), SIMP with $p = 2$ (coupling stiffness) and SIMP with $p = 3$ (bending stiffness) describes the design. This analogy allows for the application of a range of the theoretical tools developed for the homogenization method for topology design [77].

7 The significance of void

The discussion in this paper on interpolation models all refer to an approach to topology design where material is distributed in a fixed domain. A pivotal aspect of this idea in computational implementations is the use of a fixed FEM mesh for the domain. This is not an inherent requirement, but is useful for computational efficiency. Recently, adaptive strategies have been implemented in order to improve geometric resolution, [73]. If the topology of material and void is the goal of the design process, this will imply that low density areas are also included in the analysis for each feasible design. For certain settings this leads to difficulties both in the formulation of the problem as well as in the numerical treatment.

For stress-constrained problems, the so-called stress singularity phenomenon, [78, 79], means that it is crucial that the design formulation only imposes the stress constraint in areas of nonzero density. This is, from a mathematical programming point of view, a complicated type of constraint which, as it turns out, requires use of constraint-relaxation techniques (not to be misinterpreted in terms of the variational relaxation discussed elsewhere in this paper), [74].

A somewhat more subtle problem arising from the basic design representation in topology design appears in situations involving stability and vibration criteria. The relevant criteria are here the eigenvalues of the structurally relevant parts of the structure, i.e., the buckling loads and the vibration frequencies of the 'black' part of a black-and-white design. In a true black-and-white design, this are the nonzero eigenvalues, but at intermediate steps of an iterative optimization method implemented with interpolation schemes it can become unclear what are the relevant values to consider. Examples of this are localized modes which appear in low density regions and which should be filtered out in order that the optimization deals with the structurally interesting modes. Such a procedure is demonstrated in [80] for buckling problems, solved using homogenized material properties. For vibration problems two-materials design (labelled 'reinforcement problems') is usually reported (see [81] for a survey), but in vibration problems for black-and-white design local modes are also seen and require similar attention, [82].

8
Conclusions and perspectives

The analyses presented here demonstrates that various approaches to black-and-white topology design can in many situations all be interpreted within the framework of micromechanically based models, thus clarifying a long ongoing discussion in the structural optimization community regarding the physical relevance of different interpolation schemes. However, it remains an important issue to examine models in relation to micromechanics, and to be fully aware of limitations or approximations used in the numerical schemes which are devised for solving topology design problems. Moreover, it is in this context crucial to recognize if a topology design study is supposed to lead to black-and-white designs or if composites can constitute part of the solution, (see [30] for further discussion on this). It should again be emphasized that, if a numerical method leads to black-and-white designs, one can, in essence, choose to ignore the physical relevance of 'grey', and in many situations a better computational scheme can be obtained if one allows for a violation of the bounds on properties of composites. This is especially the case where the bounds do not allow for a high enough penalization of intermediate density. The alternative is to introduce an explicit penalization of the density, cf. Sec. 4.

It is also evident from an overview of current methodologies that despite the abundance of results, here are still complicated theoretical and practical questions to overcome. Thus, the precise relationship between relaxation, microstructures, and existence of solutions is open for most classes of problems, and closely related to this are questions of bounds on properties for coupled and nonlinear problems. From a practical point of view, the most pressing question is no doubt the development of a general framework for devising interpolation schemes for coupled and nonlinear problems.

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