Simultaneous material and topology optimization

von

J. Greifenstein & M. Stingl
Simultaneous material and topology optimization

Jannis Greifenstein · Michael Stingl

October 21, 2014

Abstract The problem of parametrized material and simultaneous topology optimization of an elastic continuum is considered. To ensure existence of solutions and to be able to impose a deliberate maximal material grading, pointwise bounds on design variable gradients are imposed, or a filtering technique based on a convolution product is applied. For the topology optimization, the parametrized material is multiplied with a penalized continuous density variable. A finite element discretization of the problem is suggested and a proof of convergence of the finite element solutions to solutions of the continuous problem is given. The convergence proof also implies the absence of checkerboards. The concepts are demonstrated by means of numerical examples using a number of different material parametrizations and comparing the results to global lower bounds.

Keywords material optimization · topology optimization · slope constraints · density filters

1 Introduction

In this paper, we investigate an approach for the optimization of the local material properties of a loaded body, where the material parameters in each point are described by (nonlinear) functions of the design variables. In the material optimization literature, two main streams can be identified: the so-called free material optimization approach (Ringertz (1993); Bendsøe et al (1994)) and optimization of microstructures in a two-scale optimization (Bendsøe and Kikuchi (1988)). While FMO allows for all physically admissible material tensors in the optimization problem, in the two-scale approach macroscopic material properties are represented through microstructures made up of a given material, possibly periodically homogenized. Considering the former ansatz, FMO has the advantage that the formulation allows for a global solution of compliance minimization problems, providing lower bounds for parametrized material optimization problems, given that design constraints are imposed in a compatible manner. On the other hand, even though material tensors resulting from FMO may be represented through microstructures (Schury et al (2012)), this approach is complicated and the material use of the microstructures will usually not be altogether efficient. We would like to study material parametrizations that are closer to a physical interpretation, while still allowing for a comparison to the lower bounds provided by FMO. Going back to the two-scale approach, in terms of manufacturability this brings with it the problem of joining two different microstructures together. Similarly to Schury et al (2012), we want to deal with this by limiting the extent, material parameters may vary from one cell to the next. In contrast to Schury et al (2012), however, we want to do this directly for the design parameters as e.g. homogenization parameters like laminate volume fraction or cell rotation angle. Consequently, we refrain from globalized methods such as perimeter control (see e.g. Ambrosio and Buttazzo (1993); Haber et al (1996)). Instead we will use two different regularization approaches: slope constraints and density filtering. Slope constraints have been established by Petersson and Sigurdsson (1998), while density filters were
introduced in Bruns and Tortorelli (2001) and Bourdin (2001). An existence and convergence proof for compliance minimization in topology optimization for slope constraints and density filters was also given in Petersson and Sigmund (1998) and Bourdin (2001), respectively. In this work, both regularization approaches will be combined and used in a more general material optimization framework with additional constraints, instead of a pure topology optimization with a volume constraint as in the mentioned papers and an existence and convergence proof will be given. Furthermore, we will show that density filters may be used for a rigorous gradient control as well and give estimations of the maximal gradient of filtered design variables.

The most straightforward approach to introduce a rigorous gradient control would be to use slope constraints for all design variables. However, the slope constraints introduce a large number of constraints up to $2n_e d$ per design variable, where $n_e$ denotes the number of elements in an appropriate finite element discretization and $d$ the space dimension. This means, the used optimization algorithm needs to be suitable for treating problems with a large number of constraints. In order to cope with this, we will use SNOPT (Gill et al (2005)), an SQP code adept at solving problems with a large number of sparse constraints, for the numerical solution of the design problems addressed in this paper. Nevertheless, using slope constraints on a number of different design variables will lead to too many constraints as to allow for an efficient solution of the optimization problem. Thus, we will also use density filters as an alternative means of regularization. We will estimate the maximum slope of a filtered design variable depending on the used filter kernel. However for too tight bounds on the slopes of the design variables, this requires large filter radii, which slows down the computation of the filter. Note that this slow computation time of the filter might be circumvented by means of filtering methods based on partial differential equations recently introduced in Lazarov and Sigmund (2011), however using large filters together with local constraints (using only the design variables defined on one element), we still lose the sparsity of the constraints resulting in a vast increase in computation time. Hence we choose to use slope constraints when the filter radius needed to obtain the desired maximal design gradients is too large. Finally, a number of numerical results will be presented.

### 2 Problem statement

#### 2.1 General problem statement

All problems are treated in the two dimensional case, the extension to three dimensions is straightforward. Let $\Omega \subset \mathbb{R}^2$ be a bounded and open Lipschitz domain. We introduce the standard Sobolev spaces $W^{k,p}(\Omega)$ and denote the corresponding norms by $\| \cdot \|_{m,p,\Omega}$. For $p = 2$ we write $H^m(\Omega) = W^{m,2}(\Omega)$, $H^m(\Omega)^2 = (H^m(\Omega))^2$ and for $m = 0$, $L^p(\Omega) = W^{0,p}(\Omega)$. We use the following abbreviations for the norms: $\| \cdot \|_m = \| \cdot \|_{m,2,\Omega}$, while the corresponding seminorms are denoted by $| \cdot |_m$; an analogous notation is used for the norms in $(W^{k,p})^2$.

For a more comprehensive description of the spaces and norms we refer to Adams (1975). The norm in euclidean space will be denoted by $\| \cdot \|$.

Let $V$ be the space of kinematically admissible displacements,

$$ V = \{ v \in H^1(\Omega) : v_i = 0 \text{ on } \Gamma_0 \ (i = 1, 2) \}, $$

with $\Gamma_0$ the part of $\partial \Omega$ with zero-prescribed displacements.

For the definition of the physical problem of linear elasticity in the weak form, we introduce the elasticity tensor $E_{ijkl}$ and the energy bilinear form

$$ a_E(u, v) = \int_{\Omega} E_{ijkl}(x) \varepsilon_{ij}(u) \varepsilon_{kl}(v) \, dx, $$

where $\varepsilon_{ij}(u)$ denote linearized strains, $\varepsilon_{ij}(u) = \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$ and the summation convention is used, i.e. two repeated indices denote a summation from 1 to 2. Furthermore we define the external load linear form $\ell : V \to \mathbb{R}$, which is assumed to be bounded in the operator norm,

$$ \| \ell \|_{\text{op}} = \sup_{\phi \neq v \in V} \frac{| \ell(v) |}{\| v \|_1} < \infty. $$

It may take e.g. the form

$$ \ell(v) = \int_{\Gamma_t} t \cdot v \, ds + \int_{\Omega} f \cdot v \, dx, \tag{1} $$

where $f$ are the body forces and $t$ are the tractions on the traction part of the boundary $\Gamma_t \subset \partial \Omega$.

Now we can define a general material and topology optimization problem as finding the optimal elasticity tensor $E_{ijkl}(x)$ over the domain $\Omega$ w.r.t. a given lower semicontinuous cost functional $J(u)$:

$$ \text{(P)} \begin{cases} \min_{E \in E_{\text{ad}}} J(u) \\ a_E(u, v) = \ell(v) \quad \forall v \in V \end{cases} $$

such that
In the following, we will use a parametrized material formulation for this set of admissible material tensors, i.e. $E$ will be a function depending on a number of design variables. For this sake, we introduce two design spaces $\mathcal{G}$ and $\mathcal{H}$ for filtered and slope constrained design variables, respectively:

$$\mathcal{G} = \{ \rho \in L^\infty(\mathbb{R}^2) : \rho \leq \rho_0 \text{ a.e. in } \Omega, \rho_0 \equiv 0 \text{ a.e. in } \mathbb{R}^2 \setminus \Omega \}$$

$$\mathcal{H} = \{ \vartheta \in W^{1,\infty}(\Omega) : \vartheta \leq \vartheta_0 \leq \vartheta, \frac{\partial \vartheta}{\partial x_i} \leq c^S (i = 1, 2) \text{ a.e. in } \Omega \}$$

For the slope constrained design variables, this regularization ansatz is straightforward, as it requires the design to have bounded weak derivatives. For the filtered design variables, a convolution product with a filter kernel is used to smoothen the design. The filter kernel $F$ is assumed to fulfill the following properties:

$$F \in W^{1,1}(\mathbb{R}^2)$$
$$\text{supp}(F) \subset B_R(0)$$
$$F \geq 0 \text{ a.e. in } B_R(0)$$
$$\int_{B_R(0)} F(x) \, dx = 1,$$

where $R > 0$ is called the characteristic radius of $F$ and $B_R(0)$ is the open ball with center 0 and radius $R$. The filtered design then becomes for $\rho \in \mathcal{G}$

$$(F \ast \rho)(x) := \int_{\mathbb{R}^2} F(x - y) \rho(y) \, dy.$$

The properties of the convolution transform yield (see e.g. Kees (1982))

$$\nabla(F \ast \rho) = (\nabla F) \ast \rho$$

and thus

$$F \ast \rho \in W^{1,\infty}(\mathbb{R}^2) \quad \forall \rho \in L^\infty(\mathbb{R}^2).$$  \hspace{1cm} (2)

The design used in the optimization problem is then normalized again to lie in $[\rho, \bar{\rho}]$ \footnote{The alternative would be to define $\rho \in [\rho, \bar{\rho}]$ outside of $\Omega$, which should be done by means of symmetries and translations of the known design values.} and we denote this operation by $\ast_\Omega$ for $\rho \in \mathcal{G}$:

$$(F \ast_\Omega \rho)(x) := \int_{\mathbb{R}^2} F(x - y) \rho(y) \, dy \int_{B_R(0)} F(x - y) \, dy = \int_{B_R(0)} F(x - y) \rho(y) \, dy \int_{B_R(0)} F(x - y) \, dy.$$

For this normalized filtering we further assume that $\int_{\Omega} F(x - y) \, dy \geq C_{F_R} > 0 \forall x \in \Omega$ for some positive constant $C_{F_R}$. This ensures $F \ast_\Omega \rho \in W^{1,\infty}(\Omega)$. In fact, the filtered and normalized design variables satisfy a similar property to the slope constraints dependent on the derivative of the filter kernel:

$$\left| \frac{\partial}{\partial x_i} (F \ast_\Omega \rho)(x) \right| = \left| \frac{\partial}{\partial x_i} \left( \frac{(F \ast \rho)(x)}{\int_{\Omega} F(x - y) \, dy} \right) \right|$$

$$= \frac{\partial}{\partial x_i} F(x - y) \frac{(F \ast \rho)(x)}{\int_{\Omega} F(x - y) \, dy} \int_{\Omega} F(x - y) \, dy^2$$

$$= \int_{\Omega} \frac{\partial}{\partial x_i} F(x - y) \rho(y) \, dy$$

$$= \frac{(F \ast \rho)(x)}{\int_{\Omega} F(x - y) \, dy} \int_{\Omega} F(x - y) \, dy$$

$$= \int_{\Omega} \frac{\partial}{\partial x_i} F(x - y) \rho(y) \, dy \int_{\Omega} F(x - y) \, dy$$

For some constant $c^F$ only dependent on the chosen filter kernel $F$, the fixed design bounds and $C_{F_R} := \min_{x \in \Omega} \int_{\Omega} F(x - y) \, dy$. From these estimates and (2), it follows immediately that $\ast_\Omega$ fulfills the same regularization property in $\Omega$ as $\ast \in \mathbb{R}^2$.

Generally the estimates for the maximum slope far from and close to the boundary will be similar. E.g. for a rectangular domain and a radially symmetric filter kernel $C_{F_R}$ is $\frac{1}{4}$, however this value is attained in the corner, where the integral in the numerator is reduced to $\frac{1}{2}$ as well.

To give an example of the bound, for the common filter kernel $F(x) := \frac{1}{\pi R^2} \max(0, 1 - \sqrt{x^2 + y^2}/R)$, a radially decreasing hat function in 2D with radius $R$, the estimate far from the boundary is:

$$\left| \frac{\partial}{\partial x_i} (F \ast_\Omega \rho)(x) \right| \leq \left| \frac{\rho - \rho_i}{B_R(0)} \right| \int_{B_R(0)} \frac{3}{\pi R^2} \frac{x_i}{\sqrt{x_i^2 + x_j^2} R} \, dx_i$$

$$= \frac{3\left| \rho - \rho_i \right|}{\pi R^2} \int_0^R \int_{-\pi}^\pi \frac{r \sin \phi}{r R} \, r \, dr \, d\phi$$

$$= \frac{6\left| \rho - \rho_i \right|}{\pi R} \text{ a.e. in } \Omega.$$
i.e. the maximum slope decreases linearly with the filter radius.

In the following, the vector containing all design variables will be denoted as $(\rho, \vartheta) \in G^n \times \mathcal{M}^m$, i.e. the first $n$ design variables are filtered and the last $m$ design variables have weak derivatives bounded by $cS$. Note that for each design variable $\rho_i$, $i = 1, \ldots, n$ a different filter kernel and for each design variable $\vartheta_j$, $j = 1, \ldots, m$ a different slope bound may be used. However in the following, it is assumed without loss of generality, that there is only one filter kernel and one bound $c^2$. Moreover, $n$ or $m$ may be 0.

In the parametrization, the filtered design variables will be used, which we abbreviate as $(\tilde{\rho}, \tilde{\vartheta}) := (F \ast \rho_1, \ldots, F \ast \rho_n, \vartheta_1, \ldots, \vartheta_m)$. The elasticity bilinear form for a given $(\rho, \vartheta)$ is then defined as

$$a_{i,j,k,l}(u, v) = \int_{\Omega} E_{ijkl}(\tilde{\rho}, \tilde{\vartheta}) \varepsilon_{ij}(u) \varepsilon_{kl}(v) \, dx,$$

The parametrization $E_{ijkl}$ maps $\mathbb{R}^{n+m}$ to $\mathbb{R}$ for $i,j,k,l = 1, 2$ and represents, at least up to a scaling, elasticity constants.

We introduce functions $g^+ : (L^\infty(\Omega))^n \rightarrow \mathbb{R}^{n \times n}$, which are used to model resource constraints such as a volume constraint and $g^- : \mathbb{R}^{n+m} \rightarrow \mathbb{R}^{n \times r}$, which for given $x \in \Omega$ represent local stiffness and/or feasibility constraints. Furthermore, let $f((\tilde{\rho}, \tilde{\vartheta}), u(\tilde{\rho}, \tilde{\vartheta}))$ a lower semi-continuous cost functional (weakly l.s.c. in $u$), e.g. the compliance functional. With this, we may now define the parametrized optimization problem

$$\min_{\rho, \vartheta \in G^n \times \mathcal{M}^m} J((\tilde{\rho}, \tilde{\vartheta}), u(\tilde{\rho}, \tilde{\vartheta})) \text{ such that }$$

$$\begin{cases}
\begin{align*}
a_{i,j}(u, v) &= \ell(v) \quad \forall v \in V, \\
g^+(\tilde{\rho}, \tilde{\vartheta}) &\leq 0, \\
g^-(\tilde{\rho}(x), \vartheta(x)) &\leq 0 \quad \text{a.e. in } \Omega.
\end{align*}
\end{cases}
\right.$$  

We define the sets of admissible design variables and design values admissible to the parametrization as

$$S := \{ (\rho, \vartheta) \in G^n \times \mathcal{M}^m, g^+(\tilde{\rho}, \tilde{\vartheta}) \leq 0, \ g^-(\tilde{\rho}(x), \vartheta(x)) \leq 0 \quad \text{a.e. in } \Omega \},$$

$$\tilde{S} := \{ p \in \mathbb{R}^{n+m} : g^+(p) \leq 0 \}. $$

As the chosen design spaces might not directly imply symmetric and positive definite elasticity tensors, it is assumed that for all $p \in \tilde{S}$, the tensor $(E_{ijkl}(p))_{ijkl}$ is symmetric and positive definite with uniform lower and upper bounds. These assumptions grant the following properties of the bilinear form:

(5) \quad \exists M > 0 : |a_{i,j}(p, v)| \leq M \|v\|_1 \|v\|_1 \quad \forall v \in V, \quad \forall p \in \tilde{S}

(6) \quad \exists \beta > 0 : a_{i,j}(p, v) \geq \beta \|v\|_1^2 \quad \forall v \in V, \quad p \in \tilde{S}

Furthermore, we assume continuity of $E_{ijkl}$, $i,j,k,l = 1, 2$ on $\tilde{S}$, Hölder continuity of $g^+$ on $\tilde{S}$ and Hölder continuity of $g^-$ on $\tilde{S}$ with the smallest Hölder coefficient of $g^+$ and $g^-$ denoted by $\alpha$. Note that, using Sobolev’s embedding theorem, $\tilde{S}$ is actually a set of continuous functions.

A simple example for this setting is the well known SIMP model, where $E_{ijkl}(\tilde{\rho}) = \eta(\tilde{\rho}) E_{ijkl}^{0}, g(\tilde{\rho}) = \int_{\Omega} \tilde{\rho} \, dx - V \leq 0$, while the resulting tensor is always positive definite and no feasibility constraints are required.

### 3 Existence of solutions

In order to show the existence of solutions to (P), we first show the compactness of the set of admissible design variables $\tilde{S}$. Let $(\rho, \vartheta)_k, u_k) \in S \times V$ be a minimizing sequence of (P). According to the uniform boundedness and ellipticity assumptions of the parametrization we get

$$\beta \|u_k\|_1^2 \leq a_{i,j}(\rho, \vartheta)(u_k, u_k) = \ell(u_k) \leq \|\ell\|_{L^1} \|u_k\|_0 \leq C \|u_k\|_1.$$  

Hence $\{u_k\}$ is uniformly bounded and we obtain

$$\exists u \in V \text{ and a subsequence } u_k, \text{ s.t. } u_k \rightharpoonup u,$$  

where $\rightharpoonup$ denotes weak convergence.

Concerning the design variables, the compactness of $\mathcal{M}$ may be found e.g. in Petersson and Sigmund (1998), where in fact for $\{\rho_k\} \subset \mathcal{M}$ uniform convergence (up to a subsequence extraction) to a $p \in \mathcal{M}$ is shown. As we did not impose any additional regularity conditions in $G$, we only get weak star compactness here. For $\{\rho_k\} \subset G$ we have $\|\rho_k\|_{L^\infty} \leq \max(\|\rho\|_{L^\infty}, \|\rho\|_{H^1})$ and by Banach-Alaoglu’s theorem there exists a subsequence, again denoted by $\rho_k$, and some $p \in L^\infty(\Omega)$, s.t. $\rho_k \rightharpoonup p$. For a filter kernel $F$ we thus have

$$W^{1, \infty}(\Omega) \ni F \ast \rho_k \rightharpoonup F \ast \rho \in W^{1, \infty}(\Omega) \quad \text{pointwise.}$$
On the other hand, \( F \ast \Omega \rho_k \in W^{1, \infty}(\Omega) \) and using the same arguments referred to for \( \mathcal{H} \) in the last paragraph, we get (up to another subsequence extraction) \( F \ast \Omega \rho_k \to \hat{\rho} \) uniformly for some \( \hat{\rho} \in W^{1, \infty}(\Omega) \). Since these limits have to be the same, we get \( \hat{\rho} = F \ast \Omega \rho \) and thus

\[
F \ast \Omega \rho_k \to F \ast \Omega \rho \quad \text{uniformly.} \tag{9}
\]

Assuming now \( \rho \notin \mathcal{G} \), then there exists a compact \( \omega \subset \Omega \) which is not a set of measure zero, with \( \rho < \hat{\rho} \) (or analogously \( \rho > \hat{\rho} \) on \( \omega \)). Thus for the characteristic function on \( \omega \), \( \chi_\omega \in L^1(\mathbb{R}^2) \):

\[
0 \leq \int \chi_\omega (\rho_k - \rho) \, dx \to \int \chi_\omega (\rho - \rho) < 0
\]

and we have a contradiction.

Putting things together, there exists a \((\rho, \vartheta) \in \mathcal{G}^n \times \mathcal{H}^m \), s.t. up to a subsequence

\[
(\tilde{\rho}, \tilde{\vartheta})_k \to (\tilde{\rho}, \tilde{\vartheta}) \quad \text{uniformly in } \Omega. \tag{10}
\]

It is now easy to verify, that the inequality constraints in \((P)\) are satisfied using the continuity assumptions on the constraints:

\[
g_k^l(\tilde{\rho}, \tilde{\vartheta}) = g_k^l((\tilde{\rho}, \tilde{\vartheta})_k) + g_k^l((\tilde{\rho}, \tilde{\vartheta})_k) \leq 0,
\]

as the first term converges uniformly to 0, \( i = 1, \ldots, n_c \), and similarly for \( g^l \). This yields the compactness of the set \( \bar{S} \).

It remains to show, that any limit as in \((8), (10)\) satisfies the state problem. Due to the compactness of \( \bar{S} \), the functions \( E_{ijkl}, i, j, k, l = 1, 2 \) are uniformly continuous and we obtain from \((10)\)

\[
E_{ijkl}(\tilde{\rho}, \tilde{\vartheta}_k) \to E_{ijkl}(\tilde{\rho}, \tilde{\vartheta}) \quad \text{uniformly, } i, j, l, k = 1, 2.
\]

It follows

\[
\begin{align*}
|a(\tilde{\rho}, \vartheta)(u_k, v) - a(\tilde{\rho}, \vartheta)(u, v)| &
\leq |a(\tilde{\rho}, \vartheta)(u_k, v) - a(\tilde{\rho}, \vartheta)(u_k, v)| \\
&+ |a(\tilde{\rho}, \vartheta)(u_k, v) - u_k, v)| \\
&= \int_{\Omega} \left| E_{ijkl}(\tilde{\rho}, \tilde{\vartheta}_k) - E_{ijkl}(\tilde{\rho}, \tilde{\vartheta}) \right| \varepsilon_{ij}(u_k) \varepsilon_{kl}(v) \, dx
\end{align*}
\]

\[
\quad \to 0 \quad \forall v \in V
\]

\[
\Rightarrow a(\tilde{\rho}, \vartheta)(u_k, v) \to a(\tilde{\rho}, \vartheta)(u, v) \quad \forall v \in V.
\]

This proves that \( u \) solves the state problem, while the lower (semi)continuity assumptions on \( \mathcal{G} \) give optimality.

4 Finite element discretization

From now on, we assume that \( \Omega \) is a rectangular domain partitioned into \( n_c = n_x n_y \) mutually disjoint squared finite elements of equal size, i.e. \( n_c \) finite elements in the horizontal direction and \( n_y \) in the vertical. Although these restrictions might seem severe, they are only made to simplify the notation and the results obtained are expected to hold in much more general settings. Denote the (open) squares \( \Omega_{jk} \) with \( j = 1, \ldots, n_x \) and \( k = 1, \ldots, n_y \). These squares are mutually disjoint and satisfy \( \bar{\Omega} = \bigcup_{j=1}^{n_x} \bigcup_{k=1}^{n_y} \Omega_{jk} \). From now on, \( \forall j, k \) will mean \( \forall(j, k) \in \{1, \ldots, n_x \} \times \{1, \ldots, n_y \} \).

Using piecewise linear approximations for the displacements, the discretized equivalent to \( V \) is

\[
V_h = \{ v : v_i \in C^0(\bar{\Omega}), v_i|_{\Omega_{jk}} \in P_i(\Omega_{jk}) \forall (i = 1, 2) \}
\]

\[
\cap V,
\]

where \( P_i(\Omega_{jk}) \) denotes the space of bilinear functions and constant functions on \( \Omega_{jk} \) for \( l = 1 \) and \( l = 0 \), respectively. It is well known from the literature (see e.g. Ciarlet (1978)), that the space \( C^\infty(\bar{\Omega}) \cap V \) is dense in \( V \) and that there exists an interpolation operator \( \pi_h \) and a constant \( C > 0 \) s.t.

\[
\| u - \pi_h u \|_1 \leq C h^l \| u \|_2,
\]

which in turn implies

\[
\pi_h u \to u \quad \text{strongly in } V, \quad \text{as } h \to 0, \forall u \in C^\infty(\bar{\Omega}) \cap V.
\]

Furthermore we choose piecewise linear approximations for all design variables and impose the following oscillation conditions for the slope constrained design variables:

\[
|\vartheta_{j+1,k} - \vartheta_{j,k}| \leq c_h, \quad j = 1, \ldots, n_x - 1, \quad k = 1, \ldots, n_y \quad \text{(12)}
\]

and

\[
|\vartheta_{j,k+1} - \vartheta_{j,k}| \leq c_h, \quad j = 1, \ldots, n_x, \quad k = 1, \ldots, n_y - 1, \quad \text{(13)}
\]

where \( \vartheta_{jk} \) denotes the value on \( \Omega_{jk} \) for any piecewise constant function \( \vartheta \). With this, the discrete design variable spaces are defined as

\[
\mathcal{G}_h = \{ \vartheta \in \mathcal{G} : \vartheta_{ij} \in P_0(\Omega_{jk}) \forall (i, j), \vartheta \leq \rho \leq \bar{\rho} \}
\]

and

\[
\mathcal{H}_h = \{ \vartheta \in \mathcal{H} : \vartheta_{ij} \in P_0(\Omega_{jk}) \forall (i, j), \vartheta \leq \bar{\theta} \leq \bar{\bar{\theta}}, \quad \text{(12) and (13)} \}.
\]
The corresponding projection operator is defined as
\[ \Pi_h : \mathcal{G} \rightarrow \mathcal{G}_h, \rho \mapsto \rho_h \quad \text{s.t.} \quad \rho_h|_{\Omega_h} = \frac{1}{|\Omega_j|} \int_{\Omega_j} \rho(x) \, dx \]
and identically defined as \( \Pi_h : \mathcal{H} \rightarrow \mathcal{H}_h \). However as a filtered design variable is an outer approximation of the design variables it is needed as in the problem formulation an outer approximation of the design variables is an outer approximation of the design variables is an outer approximation of the design variables.


\[
(\hat{\Pi}_h F|_{\Omega_j}) := F|_{\Omega_j} \rho(c_{jk}),
\]
with \( c_{jk} \) the center of \( \Omega_j \). Note that using \( \Pi_h \) again works as well, but would be inconsistent with the discrete filter approximation used later in Section 6. Clearly \( V_h \subset V \) and using an appropriate extension \( \mathcal{G}_h \subset \mathcal{G} \), but \( \mathcal{H}_h \not\subset \mathcal{H} \), i.e. for the displacements and filtered design variables an inner or conforming approximation is used, while the approximation of the slope constrained design variables is an outer approximation.

The fully discretized optimization problem thus becomes

\[
(\mathbf{P}_h) \quad \left\{ \begin{array}{l}
\min_{(\rho_h, \vartheta_h) \in \mathcal{G}_h \times \mathcal{H}_h} f((\hat{\Pi}_h \rho_h, \vartheta_h), \Pi_h (\hat{\Pi}_h \rho_h, \vartheta_h)) \\
a_{(\hat{\Pi}_h \rho_h, \vartheta_h)}(u_h, v_h) = \ell(v_h) \quad \forall v_h \in V_h, \\
g^\ell((\hat{\Pi}_h \rho_h, \vartheta_h)) \leq h^q, \\
g^{\ell}(\Pi_h (\hat{\Pi}_h \rho_h, \vartheta_h)|_{\Omega_j}) \leq h^q \quad \forall j, k
\end{array} \right.
\]
for some fixed \( q \in (0, \alpha) \).

Analogous to the continuous case, we define the sets
\[
\hat{S}_h = \{ p \in \mathbb{R}^{n+m} : g^\ell(p) \leq \varepsilon \}, \\
S_h := \{ (\rho, \vartheta) \in \mathcal{G}_h \times \mathcal{H}_h : g^\ell(\rho, \vartheta) \leq \varepsilon, \\
g^{\ell}(\Pi_h (\hat{\Pi}_h \rho_h, \vartheta_h)|_{\Omega_j}) \leq \varepsilon \quad \forall j, k \}
\]
for some small constant \( \varepsilon > 0 \). For problem \( (\mathbf{P}_h) \) to be well-posed for \( h \) sufficiently small, we need to extend the continuity assumptions on \( g^\ell \) to \( \hat{S} \cup \hat{S}_h \) and on \( E_{ijkl} \), \( i, j, k, l = 1, 2 \) and \( g^{\ell} \) to \( \hat{S}_h \). Furthermore, we assume the parametrization to yield a uniformly bounded and uniformly elliptic elasticity tensor on this set as before. In practice, however, this is a reasonable assumption, as the feasibility constraints need to imply strictly positive eigenvalues of the elasticity tensor \( E \) and hence generally allow for an additional \( \varepsilon \) gap of feasibility. This relaxation is needed, as in the problem formulation an outer approximation of the design variables is used and we otherwise could not in general guarantee the discrete approximations to fulfill the constraints.

4.1 Convergence result

The rest of this section follows the proof given in Petersson and Sigmund (1998) and extends it for the filtered design variables and the inequality constraints. We show the convergence of the solutions of the discretized optimization problems to the solution of the continuous problem. To this end, we show the following steps:

1. Each sequence of finite element solutions has a weakly convergent subsequence as \( h \rightarrow 0 \) with some limit elements.
2. Each such limit fulfills the equilibrium equation.
3. The deformations even converge strongly.
4. The approximated design set is “close” to the original continuous set.
5. Each limit from 1. solves the discretized minimization problem.

4.1.1 Weak compactness

Let \( ((\hat{\Pi}_h \rho_h, \vartheta_h), u_h((\hat{\Pi}_h \rho_h, \vartheta_h))) \) be a sequence of finite element solutions. As \( u_h \) and \( \rho_h \) are inner approximations, we get a weakly convergent subsequence of \( u_h \) and a uniformly convergent subsequence of \( \rho_h \) as in Section 3. The continuity of the latter functions subsequently gives \( \hat{\Pi}_h \rho \rightarrow \rho \) uniformly in \( \Omega \). For the slope constrained design variables \( \vartheta_h \), we refer to the proof in Petersson and Sigmund (1998) and also obtain \( \vartheta_h \rightarrow \vartheta \) uniformly in \( \Omega \), with the limit satisfying the slope constraints. Finally, the uniform convergence of the design variables with the continuity assumptions on the constraints gives analogously to the continuous case, that the inequality constraints are fulfilled in the limit. Thus we have

\[
u_h \rightharpoonup u \in V, \quad (\hat{\Pi}_h \rho_h, \vartheta_h) \rightarrow (\rho, \vartheta) \quad \text{uniformly in } \Omega \text{ for some } (\rho, \vartheta) \text{ admissible to } (\mathbf{P}).
\]

This holds in particular for the solutions to \( (\mathbf{P}_h) \): \( u_h^* \rightharpoonup u^* \in V, \quad (\hat{\Pi}_h \rho_h, \vartheta_h)^* \rightarrow (\rho, \vartheta)^* \quad \text{uniformly in } \Omega \text{ for some } (\rho, \vartheta)^* \text{ admissible to } (\mathbf{P}) \).

4.1.2 Limit solves the state problem

We have to show, that each limit pair \( ((\rho, \vartheta), u) \) as in (17) again solves the state equation, i.e.

\[
a(\rho, \vartheta)(u, v) = \ell(v) \quad \forall v \in V.
\]

The density of \( C^\infty(\hat{\Omega}) \cap V \) in \( V \) and (11) imply the existence of a sequence \( v_h \in V_h \), such that \( v_h \rightarrow v \).

From \( a(\hat{\Pi}_h \rho_h, \vartheta_h)(u_h, v_h) = \ell(v_h) \) we get

\[
a(\hat{\Pi}_h \rho_h, \vartheta_h)(u_h, v_h - v) + a(\hat{\Pi}_h \rho_h, \vartheta_h)(u_h, v) = \ell(v_h).
\]
4.1.3 Strong convergence of the displacements

We already have weak convergence (of subsequences) of the displacement. Together with the equilibrium coupling in the discrete setting, we can even obtain strong convergence. Using the uniform ellipticity, we have

\[
\beta \|u_h^* - u^*\|^2 \leq a(u_h^*, \tilde{\varphi}) - a(u_h, \tilde{\varphi}) - a(u_h^*, \tilde{\varphi}) - a(u_h, \tilde{\varphi}) = a(u_h^*, u_h^*) - a(u_h, u_h),
\]

where the first term converges to zero, the second to \(\ell(u^*)\) and the last one, \(a(u_h^*, \tilde{\varphi})\), to \(a(\tilde{u}^*, \tilde{\varphi})\). This term again equals \(\ell(u^*)\) by (19), and we obtain

\[u_h^* \to u^*\text{ strongly in } V.\]

4.1.4 Density of the design approximation

We need to show, that any variable of the continuous problem can be sufficiently well approximated by its discrete counterpart. For the displacement, this is apparent by (11) and the density of \(C^\infty(\bar{\Omega})\cap V\) in \(V\). We now prove that for every \((\rho, \vartheta) \in S\) there exists a sequence \((\rho_h, \vartheta_h) \in S_h\) such that \((\Pi_h \rho_h, \Pi_h \vartheta_h)\) converges uniformly to \((\tilde{\rho}, \tilde{\vartheta})\).

Even though an exterior approximation for the slope \(\vartheta_h\) is not available in general. Hence, we approximate \(\vartheta_h\) by \(\vartheta_i\), \(i = 1, \ldots, m\) implies the existence of an \(\hat{x} \in \Omega_h\), s.t. \(\vartheta_i(\hat{x}) = \Pi_h \vartheta_i(x)\). This gives

\[\Pi_h \vartheta_i(x) - \vartheta_i(x) = |\vartheta_i(\hat{x}) - \vartheta_i(x)| \leq \sqrt{2e^5} \|\hat{x} - x\| \leq 2e^5 h, \quad i = 1, \ldots, m.\]

It follows, that \((\Pi_h F * \Omega \Pi_h \rho, \Pi_h \vartheta)\) converges to \((\tilde{\rho}, \tilde{\vartheta})\) uniformly as \(h \to 0\). It remains to show, that the constructed sequence satisfies the inequality constraints. This can be seen applying the Hölder continuity:

\[
g_i^*(\hat{x}) = \|\hat{x} - x\| \leq 2e^5 h, \quad i = 1, \ldots, m.
\]

Defining \(\hat{F}(y) := F(x - y) \in L^1(\Omega) \forall x \in \Omega\), the proof in the appendix gives

\[
\int_{\Omega}(\Pi_h \rho)(y) \hat{F}(y) \, dy = \int_{\Omega} \rho(y) \hat{F}(y) \, dy = H^q /
\]

Then

\[
x^* = \left| \int_{\Omega} \rho(y) (\Pi_h \rho)(y) \hat{F}(y) \, dy \right| \\
= \left\| \Pi_h \rho \right\|_{L^1(B_{R+d}(x) \cap \Omega)} \left( \|\hat{F}\|_{L^1(B_{R+d}(x) \cap \Omega)} \right) \\
\leq \|\Pi_h \rho \|_{L^1(B_{R+d}(x) \cap \Omega)} \|\hat{F}\|_{L^1(B_{R+d}(x) \cap \Omega)} \\
\leq C_D h \|\hat{F}\|_{L^1(B_{R+d}(x) \cap \Omega)} / dist(x, \partial\Omega) < R \]

as both \(\Pi_h \rho \) and \(F(x - y)\) are constant zero outside the ball \(B_{R+d}(x)\) for a small fixed number \(d > 0\) and \(h\) small enough \((\sqrt{2}h \leq \delta)\). \(C\) is a constant only depending on the shape of the finite elements and \(C_{FG}\) is defined as in (3).

Finally, let \(x\) be arbitrary in \(\Omega\). Then \(x\) belongs to some \(\Omega_{jk}\). Using (3) and (20), we obtain

\[
|\hat{F}(y) - \Pi_h \rho(y)(x)| \\
= \left| (\Pi_h \rho)(y)(x) - (\Pi_h \rho)(x) \right| \\
= \left| (\Pi_h \rho)(y)(x) - (\Pi_h \rho)(x) \right| \\
= \left| \int_{\Omega} (\Pi_h \rho)(y) \hat{F}(y) \, dy - (\Pi_h \rho)(x) \right| \\
= \left| \int_{\Omega} (\Pi_h \rho)(y) \hat{F}(y) \, dy \right| \\
\leq \left| \int_{\Omega} \rho(y) \hat{F}(y) \, dy \right| \\
\leq C_D h \|\hat{F}\|_{L^1(B_{R+d}(x) \cap \Omega)} / dist(x, \partial\Omega) < R
\]

Furthermore, the continuity of \(\vartheta_i\), \(i = 1, \ldots, m\) implies the existence of an \(\hat{x} \in \Omega_{jk}\), s.t. \(\vartheta_i(\hat{x}) = \Pi_h \vartheta_i(x)\). This gives

\[
|\Pi_h \vartheta_i(x) - \vartheta_i(x)| = |\vartheta_i(\hat{x}) - \vartheta_i(x)| \leq \sqrt{2e^5} \|\hat{x} - x\| \leq 2e^5 h, \quad i = 1, \ldots, m.
\]

The continuity of \(\dot{\vartheta}_i\), \(i = 1, \ldots, m\) implies the existence of an \(\hat{x} \in \Omega_{jk}\), s.t. \(\dot{\vartheta}_i(\hat{x}) = \Pi_h \dot{\vartheta}_i(x)\). This gives

\[
|\Pi_h \vartheta_i(x) - \vartheta_i(x)| = |\vartheta_i(\hat{x}) - \vartheta_i(x)| \leq \sqrt{2e^5} \|\hat{x} - x\| \leq 2e^5 h, \quad i = 1, \ldots, m.
\]
for \( h \) small enough and \( i = 1, \ldots, n_c \). Analogously, we can show 
\[
\mathbf{g}^{\mathcal{M}} ((\tilde{\Pi}_h F \ast \rho, \Pi_h \bar{\vartheta}, \Pi_h \bar{\vartheta})) \leq h^d \forall j, k.
\]
Thus, for \( h \) small enough, \( \Pi_h \) maps \( \mathcal{G}^m \times \mathcal{H}^m \) into \( \mathcal{G}_h^m \times \mathcal{H}_h^m \) and the projection is admissible for \((\bar{\rho}, \bar{\vartheta})\).

Furthermore, \((\tilde{\Pi}_h F \ast \rho, \Pi_h \bar{\vartheta})\) converges uniformly to \((\bar{\rho}, \bar{\vartheta})\) as \( h \downarrow 0 \).

### 4.1.5 Optimality for a pair of cluster points

We need to prove, that any pair of cluster points \(((\bar{\rho}, \bar{\vartheta})^*, \mathbf{u}^*)\) to a sequence of solutions to \((\Phi_h)\) solves \((\Phi)\). In order to do this, we show
\[
\mathcal{J}((\bar{\rho}, \bar{\vartheta})^*, \mathbf{u}^*) \leq \mathcal{J}((\bar{\rho}, \bar{\vartheta}), \mathbf{u}) \tag{21}
\]

for any pair \(((\rho, \vartheta), \mathbf{u})\) admissible to \((\Phi)\).

From the section above, we can choose elements \((\rho_h, \vartheta_h) \in \mathcal{G}_h^m \times \mathcal{H}_h^m\) admissible to \((\Phi_h)\), s.t. \((\tilde{\Pi}_h F \ast \rho, \Pi_h \vartheta_h)\) converges uniformly to \((\bar{\rho}, \bar{\vartheta})\). Let \( \mathbf{u}_h \) be the solution to (19) for this \((\rho_h, \vartheta_h)\). Since \(((\rho_h, \vartheta_h), \mathbf{u}_h)\) is an admissible pair to \((\Phi_h)\),
\[
\mathcal{J}((\tilde{\Pi}_h \rho_h, \Pi_h \vartheta_h)^*, \mathbf{u}_h) \leq \mathcal{J}((\tilde{\Pi}_h \rho_h, \Pi_h \vartheta_h), \mathbf{u}_h) \tag{22}
\]
holds true. From Section 4.1.1 we get an element \( \tilde{\mathbf{u}} \in \mathbf{V} \) such that \( \mathbf{u}_h \to \tilde{\mathbf{u}} \) in \( \mathbf{V} \) for some subsequence. Section 4.1.2 shows that \( \tilde{\mathbf{u}} \) solves the state problem for \(((\rho, \vartheta), \mathbf{u})\), as well as \( \mathbf{u} \) by assumption. As the solution corresponding to a design is unique, one arrives at \( \mathbf{u} = \mathbf{u}_h \).

Finally, passing to the limit in (22) (for an appropriate subsequence), yields (21).

### 5. Parametrization models

In this Section, we describe a number of different possible tensor parametrizations, we will use later in the numerical examples. In order to be closer to a physical interpretation of the material properties, we focus on orthotropic material.

In the following, we use the Voigt notation to denote the fourth-order stiffness tensor \( E_{ijkl} \) by a symmetric \( 3 \times 3 \)-matrix and the strains and stresses by a vector:
\[
\mathbf{E} = \begin{pmatrix}
E_{1111} & E_{1122} & \sqrt{2}E_{1112} \\
E_{2222} & \sqrt{2}E_{2212} & 2E_{1212} \\
\end{pmatrix}
\]
\[
\mathbf{\varepsilon} = \begin{pmatrix}
\varepsilon_{11} \\
\varepsilon_{22} \\
\sqrt{2}\varepsilon_{12}
\end{pmatrix}, \quad \mathbf{\sigma} = \begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sqrt{2}\sigma_{12}
\end{pmatrix}
\]

#### 5.1 Topology optimization

In order to combine a material optimization scheme with topology optimization, we introduce a penalized pseudodensity variable \( \rho \) as in the well known SIMP model (see e.g. Bendsoe and Sigmund (2003)) and multiply it with the material parametrization:
\[
E(\kappa, \bar{\rho}, \bar{\vartheta}) = \kappa^p E(\bar{\rho}, \bar{\vartheta}),
\]
where \( p > 1 \) is a fixed penalty parameter. The regularization used for this pseudodensity is usually a filter with small radius and \( \kappa \) is replaced by \( \tilde{\kappa} \).

#### 5.2 Material parametrizations

As example parametrizations we choose different orthotropic material formulations ranging from an abstract formulation via a formulation governed by more interpretable engineering constants to rank-2 laminates.

##### 5.2.1 Orthotropic material

This abstract parametrization represents an orthotropic material with given lower eigenvalue bound \( c \):
\[
E(a, b, c, G_{xy}) = \begin{pmatrix}
c & 0 & 0 \\
0 & \kappa & 0 \\
0 & 0 & 0
\end{pmatrix}
\]

So far the symmetry axes of the orthotropic material are aligned with the coordinate axes. In order to achieve an arbitrary orthotropic material formulation, we introduce a 2D rotation matrix \( \Phi \) as
\[
\Phi(\phi) = \begin{pmatrix}
\cos(\phi)^2 & \sin(\phi)^2 & -\sqrt{2}/2 \sin(2\phi) \\
\sin(\phi)^2 & \cos(\phi)^2 & \sqrt{2}/2 \sin(2\phi) \\
\sqrt{2}/2 \sin(2\phi) & -\sqrt{2}/2 \sin(2\phi) & \cos(\phi)
\end{pmatrix}
\]

With this, the rotation angle \( \phi \) of the material becomes an additional design variable:
\[
E(\phi, a, b, c, G_{xy}) = \Phi(\phi)^T E(a, b, c, G_{xy}) \Phi(\phi) \tag{23}
\]

##### 5.2.2 Orthotropic material based on engineering constants

In order to be closer to a physical interpretation of the material, we directly use engineering constants as design parametrization of the orthotropic material. Applying the symmetry condition directly, the plane stress stiffness tensor is (see e.g. Halpin (1992))
\[
E(E_{xx}, E_{yy}, G_{xy}, \nu_{yx}) = \begin{pmatrix}
E_{xx} & E_{yy} & G_{xy} \\
E_{yy} & E_{xx} & G_{xy} \\
G_{xy} & G_{xy} & 2G_{xy}
\end{pmatrix}
\]
where \( E_x, E_y \) denote the Young's moduli in the respective directions \( x \) and \( y \), \( G_{xy} \) the shear modulus and Poisson's ratio \( \nu_{yx} \). The positive definiteness conditions now translate to

\[
E_x, E_y, G_{xy} > 0, \quad E_y - \nu_{yx}^2 E_x > 0
\]

These feasibility constraints can be linearized by substituting the design variable \( \theta := \nu_{yx}^2 \frac{E_y}{E_x} = \nu_{yx} \nu_{xy} \). This does, however, exclude negative Poisson’s ratios, as we apply \( \nu_{yx} = \sqrt{\theta E_y/E_x} \). We have:

\[
E(E_x, E_y, G_{xy}, \theta) = \begin{pmatrix}
\frac{E_x}{1-\theta} & \frac{\sqrt{\theta E_x E_y}}{1-\theta} & 0 \\
\frac{\sqrt{\theta E_x E_y}}{1-\theta} & \frac{E_y}{1-\theta} & 0 \\
0 & 0 & 2G_{xy}
\end{pmatrix}
\]

where \( E_x, E_y, G_{xy} > 0, \ 0 \leq \theta < 1 \).

As in the last subsection, the matrix \( \Phi \) is used to rotate the material:

\[
E(\phi, E_x, E_y, G_{xy}, \theta) = \Phi(\phi)^\top E(E_x, E_y, G_{xy}, \theta) \Phi(\phi)
\]

(24)

Note that without the substitution of \( \theta \) this parametrization could represent an orthogonal anisotropic (2D) stiffness tensor with the substitution only excluding negative Poisson’s ratios.

Furthermore, we will consider a special case of this parametrization, namely an orthotropic material with Poisson’s ratio 0:

\[
E(E_x, E_y, G_{xy}) = \Phi(\phi)^\top \begin{pmatrix}
E_x & 0 & 0 \\
0 & E_y & 0 \\
0 & 0 & 2G_{xy}
\end{pmatrix} \Phi(\phi)
\]

(25)

5.2.3 Layered material

In order to have a direct representation of the orthotropic material as a microstructure, we consider rank-2 sequential laminates with perpendicular layers (see Fig. 1). Using void as one material phase and a given isotropic material with Young’s modulus \( E \) and Poisson’s ratio \( \nu \), we have explicit homogenization formulæ given, e.g., in Bendsoe and Sigmund (2003):

\[
E_{11} = \frac{\gamma E}{\mu(1-\nu^2) + (1-\mu)} \quad E_{22} = \mu E + \mu^2 \nu^2 E_{11} \quad E_{33} = 0,
\]

where \( \mu \) denotes the density of the primary layering in 2-direction and \( \nu \) the density of the secondary layering in direction 1. The resulting total density in the unit cell is

\[
\rho = \mu + (1-\mu) \gamma = \mu + \gamma - \mu \gamma
\]

As in the last section, we allow the structures to be rotated by means of rotation matrices \( \Phi \) and introduce a topological design variable \( \rho \):

\[
E(\rho, \phi, \mu, \gamma, E, \nu) = \rho \Phi(\phi)^\top E(\mu, \gamma, E, \nu) \Phi(\phi)
\]

(26)

Fig. 1 Illustration of a rank-2 sequential laminate rotated by 45°

5.2.4 Free material optimization

The so-called free material optimization (FMO, see e.g. Kočvara et al (2008)) uses the tensor entries directly as optimization variables. Thus, apart from the specific constraints added to the optimization problem, every physically admissible tensor is allowed. The used structure allows for the global solution of compliance problems as a semidefinite program and while the problem may also be treated in the presented setting, we use it as a comparison to a global optimum obtained using a semidefinite solver. Moreover, in most examples we will use the global solution of an FMO problem with the same resource constraints to generate a starting value.

6 Numerical procedure

In this section, we describe the numerical procedure for solving \( (P_h) \) and outline the sensitivity analysis. In order to keep the notation as simple as possible, we will do this for a density filter and a single discrete design vector \( p_\rho \) containing the design values on the finite elements. Moreover, we denote the finite elements \( \Omega_{ij} \) by a single letter now and write \( p_\rho \) for the design value on element \( e \). The generalization to more design variables is straightforward and the problem setting for a non-filtered design variable has already been covered.
ness matrices are local stiffness matrices \( K_i \) of points.

\[
(F * h \rho)_e = \frac{\sum_{j \in V(e)} \rho_j \int_j F(x - c_e) \, dx}{\sum_{j \in V(e)} \int_j F(x - c_e) \, dx}
= \frac{\sum_{j \in V(e)} \rho_j F_{ij}}{\sum_{j \in V(e)} F_{ij}},
\]

where by \(*_h\) we denote the operator with discrete coefficients equivalent to \( \rho \) for a design vector. The state problem \((P_h)\) then takes the form

\[
K(F * h \rho)u = f
\]

where \( f \) is the numerically integrated load form, \( u \) the displacement vector (containing the nodal values of \( u_i \)) and \( K \) is the global stiffness matrix assembled by the local stiffness matrices \( K = \sum_{i \in E} K_i \). The local stiffness matrices are

\[
K_i(F * h \rho) = \sum_{i \in V(e)} B_{il} E \left( \sum_{j \in V(i)} \rho_j F_{ij} \right) B_{il},
\]

where \( B_{il}, \ l = 1, \ldots, n_{ig} \) denote standard strain displacement matrices and \( n_{ig} \) the number of integration points.

Thus, the sensitivity of the stiffness matrix is

\[
\frac{\partial}{\partial \rho_e} K = \sum_{i \in V(e)} \frac{\partial}{\partial \rho_e} \sum_{l=1}^{n_{ig}} B_{il} E' \left( \sum_{j \in V(i)} \rho_j F_{ij} \right) B_{il}
= \sum_{i \in V(e)} \sum_{j \in V(i)} B_{ij} E' \left( (F * h \rho)_j \right) F_{ie} \sum_{j \in V(i)} F_{ij} B_{el}
= \sum_{i \in V(e)} \left[ K_i'(F * h \rho)F_{ie} / (\sum_{j \in V(i)} F_{ij}) \right],
\]

where \((\cdot)'\) denotes the differentiation w.r.t. the primary variable. The sensitivities of the constraints are computed analogously. Note that, far from the boundary \((\sum_{j \in V(i)} F_{ij} \equiv 1)\) and for a radially symmetric filter kernel, (28) can be written as

\[
\frac{\partial}{\partial \rho_e} K = (F * h (K_i'(F * h \rho)))_{i \in E} e.
\]

In the following, the cost functional \( J \) will be the compliance

\[
J(u(\rho)) = \int_{\Gamma_t} t \cdot u \, ds + \int_{\Omega} f \cdot u \, dx
\]

with the sensitivity computed by the adjoint method

\[
\frac{\partial}{\partial \rho_e} J(u(\rho)) = -u^T \frac{\partial}{\partial \rho_e} Ku.
\]

6.1 Numerical experiments

For the numerical demonstration of the model, we use two standard examples from literature. The setups used are shown in Fig. 2 and consist of one single load case and one multi-load case. The domains of Setup 1 and 2 are discretized by 50 × 50 and 100 × 50 rectangular finite elements, respectively. All problems are solved using the SQP solver SNOPT. As the filter kernel \( F \), we use the radially decreasing hat function \( F(x) := \frac{3}{\pi R^2} \max(0, 1 - \sqrt{x_1^2 + x_2^2}/R) \). Using a single integration point in the center of the element in (27) this gives

\[
(F * h \rho)_e = \frac{\sum_{j \in V(e)} (R - \| c_j - c_e \|) \rho_j}{\sum_{j \in V(e)} (R - \| c_j - c_e \|)}.
\]

6.1.1 Material optimization

The aim of this section is the comparison of the different parametrizations for orthotropic material from Section 5 to each other as well as to global lower material optimization bounds obtained from FMO. Furthermore, we investigate the behavior of stronger and weaker regularization values. Here, weaker regularization will mean a filter radius of 1 and stronger regularization slope constraints of 10 degrees on the rotation angle from one element to the next and a filter radius of 7.

Fig. 2 Exemplary setups

For the numerical demonstration of the model, we use two standard examples from literature. The setups used are shown in Fig 2 and consist of one single load case and one multi-load case. The domains of Setup 1 and 2 are discretized by 50 × 50 and 100 × 50 rectangular finite elements, respectively. All problems are solved using the SQP solver SNOPT. As the filter kernel \( F \), we use the radially decreasing hat function \( F(x) := \frac{3}{\pi R^2} \max(0, 1 - \sqrt{x_1^2 + x_2^2}/R) \). Using a single integration point in the center of the element in (27) this gives

\[
(F * h \rho)_e = \frac{\sum_{j \in V(e)} (R - \| c_j - c_e \|) \rho_j}{\sum_{j \in V(e)} (R - \| c_j - c_e \|)}.
\]

6.1.1 Material optimization

The aim of this section is the comparison of the different parametrizations for orthotropic material from Section 5 to each other as well as to global lower material optimization bounds obtained from FMO. Furthermore, we investigate the behavior of stronger and weaker regularization values. Here, weaker regularization will mean a filter radius of 1.5 element lengths on all design variables, stronger regularization slope constraints of 10 degrees on the rotation angle from one element to the next and a filter radius of 7.0 element lengths on the remaining design variables. The resource constraints are in all examples an upper maximum tensor trace of 15 in each element and a relative maximum sum of all element traces of 7.5 (i.e. a total volume of 15 in the two-load case), while the forces in the different examples are each set to 1. The design variable bounds
for the different parametrizations are chosen s.t. on the diagonal of the stiffness tensor values between 0.01 and 15 can be reached. Starting values are generated solving the corresponding FMO problem with a semidefinite solver and adapting the optimal material entries to the respective parametrization. A visualization of some of the computed results can be found in Figs. 3 and 4. For the single load example we can see in Table 1, that the resulting compliance values for the weaker regularized most general orthotropic parametrization and FMO are close. As the FMO compliance value constitutes a global lower bound, this means that the algorithm converged to a minimum very close to the global one. Apparently this is achieved by use of negative Poisson’s ratios in parts of the optimal structure, which cannot be employed by the other parametrizations and as a result their optimal values do not come as close to this global lower bound. We want to emphasize, however, that we actually are not able to judge if the gap between both solutions is caused only by this or the fact that the solver is trapped in a different local optimum. Imposing the stronger regularization and thus a noticeable restriction in the admissible material grading, the compliance values apparently get worse again. In every investigated material optimization problem we could observe an extensive use of the shear modulus only in parts of the domain, mostly in joints of different bar-like structures or when the regularization did not allow for a “locally optimal” rotation angle.

6.1.2 Simultaneous material and topology optimization

For the simultaneous topology optimization we use the ansatz presented in Section 5.1. As we now have a distinct topology, we will focus on the more physically interpretable parametrizations, namely the formulation in engineering constants and laminates. We use stronger regularization values as defined in Section 6.1.1, but with a filter radius of 2.5 element lengths for the pseudodensity $\kappa$.

The volume constraint for the pseudodensity $\kappa$ is calculated as $V = \sum_{e} \kappa_e$ and we use a penalty parameter

Table 1 Compliance values and relative loss w.r.t. FMO value

<table>
<thead>
<tr>
<th>Setup 1</th>
<th>Setup 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Regularization</td>
<td>weaker</td>
</tr>
<tr>
<td>ortho (see (23))</td>
<td>1.325</td>
</tr>
<tr>
<td>eng (see (24))</td>
<td>1.524</td>
</tr>
<tr>
<td>diag (see 25))</td>
<td>1.538</td>
</tr>
<tr>
<td>FMO</td>
<td>1.322</td>
</tr>
</tbody>
</table>

Fig. 4 Optimal result for parametrization in engineering constants (24) and Setup 2, strong regularization. Right side omitted due to symmetry.
Fig. 5 Simultaneous material and topology optimization with strong regularization

Table 2 Compliance values with topology variable and relative loss w.r.t. FMO value

<table>
<thead>
<tr>
<th>Topology</th>
<th>Setup 1</th>
<th></th>
<th>Setup 2</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>yes</td>
<td>no</td>
<td>yes</td>
<td>no</td>
</tr>
<tr>
<td>eng (see (24))</td>
<td>1.889</td>
<td>31%</td>
<td>1.812</td>
<td>26%</td>
</tr>
<tr>
<td>FMO</td>
<td>-</td>
<td>-</td>
<td>1.437</td>
<td>0%</td>
</tr>
<tr>
<td>Volume</td>
<td>0.4343</td>
<td>6.515</td>
<td>1.004</td>
<td>15.06</td>
</tr>
<tr>
<td>laminates (see (26))</td>
<td>2.311</td>
<td>60%</td>
<td>2.251</td>
<td>56%</td>
</tr>
<tr>
<td>FMO</td>
<td>-</td>
<td>-</td>
<td>1.443</td>
<td>0%</td>
</tr>
<tr>
<td>Volume</td>
<td>0.4345</td>
<td>0.2172</td>
<td>0.9670</td>
<td>0.4835</td>
</tr>
</tbody>
</table>
of $p = 5$. In Table 2 we give the resulting physical volume that is also used to calculate an equivalent resource constraint for a comparison to material optimization problems. For both FMO problems, the integral of the physical tensor trace is used as the reference volume.

For the first parametrization and the FMO problem the maximal local trace before multiplication with the density variable is again 15. Evaluating the physical trace in the constraint would result in a resource ambiguity, as values of the density variable lower than 1 could still lead to maximum tensor traces (through higher values of the other design variables), however use up less volume. The isotropic base material of the laminates has an elastic modulus of 25 and a Poisson’s ratio of 0.3 and we use an upper bound of the local volume $\mu + \gamma - \mu\gamma$ of 0.5. The upper local trace bound of the FMO problem is chosen as the maximal trace occurring in the compared optimal result. We use strong regularization values analogous to the ones described in the previous examples.

Some of the results are visualized in Fig. 5. The first observation in Table 2 is, that the results of the layered material formulation are a great deal worse than the still abstract orthotropic material. Our interpretation is that the tradeoff is due to the fact that the laminate material arises from an underlying microstructure and the stiffness cannot be used as efficiently as in the case of the more artificial orthotropic parametrizations. Most of the loss can probably attributed to the fact that the laminate formulae always result in zero shear modulus material, which might be circumvented by allowing fully solid material as well. The next observation is that the gap between the regularized material optimization results and FMO (quite obviously) is rather large, while the simultaneous topology optimization is in comparison pretty close to the material optimization. Interestingly in one case, the topology problem even results in a slightly better compliance. This can be explained by the strong regularization, that prevents fast drops from full material to no material in pure material optimization, while the additional topology variable in conjunction with the penalization allow this. We remark that the laminates formulation turned out to be very numerically demanding so we discontinued using the filtered design variables in the local constraints, which led to a huge speedup while still yielding reasonable results.

7 Conclusions

In this paper we have provided a general setting for simultaneous material and topology optimization with rigorous local gradient constraints achieved either directly through slope constraints or using a convolution
product with a filter kernel. We have shown that the described problems are well-posed in that the existence of solutions is guaranteed and the solutions of a finite element approximation converge uniformly to the set of exact solutions when refining the mesh. The numerical results suggest, that all treated problems could be solved satisfactorily. The presented ansatz of multiplying a SIMP-type topology variable to the material tensor seems to work rather well.

A drawback of the presented setting is the computational speed. Using slope constraints for any of the used design variables, we need to choose a solver suitable to dealing with the large amount of constraints such as SNOPT. The use of the filtered design variables in local constraints slowed the computations down even more than the slope constraints, as the sparsity property got basically lost. Even though this was required in the existence proof, numerical evidence suggests a better performance using the non-filtered quantities in the framework of the local constraints.

As for the computational time of the filter calculation itself, partial differential equation based filters as described in Lazarov and Sigmund (2011) might be a viable alternative. Note that in the presented theory, the filter kernel would then be replaced by the Green’s function of the differential equation, which does not satisfy the bounded support assumption stated in this work. However, considering design variables with bounded support, the developed theory is still expected to hold.

8 Appendix

We use the following definitions:

\[ \rho \in L^\infty(\Omega), \bigcup_{jk} \Omega_{jk} = \Omega, \Pi_h \rho|_{\Omega_{jk}} = \frac{1}{h^2} \int_{\Omega_{jk}} \rho(z) \, dz \]

In order to show \( \Pi_h \rho \xrightarrow{\Delta} \rho \) in \( \Omega \), let \( g \in L^1(\Omega) \) be arbitrary. Then

\[
\int_{\Omega} (\Pi_h \rho)g \, dx = \int_{\Omega} \sum_{j,k} \frac{1}{h^2} \int_{\Omega_{jk}} \rho(z) \chi_{\Omega_{jk}}(x) g(x) \, dx = \sum_{l,m} \int_{\Omega_{lm}} \frac{1}{h^2} \sum_{j,k} \rho(z) \chi_{\Omega_{jk}}(x) g(x) \, dz \, dx = \sum_{j,k} \int_{\Omega_{jk}} \int_{\Omega_{lm}} \frac{1}{h^2} \chi_{\Omega_{jk}}(x) g(x) \, dx \rho(z) \, dz \]

and applying

\[
\int_{\Omega_{lm}} \chi_{\Omega_{jk}}(x) g(x) \, dx = \begin{cases} 0 & \Omega_{jk} \neq \Omega_{lm}, \\
\int_{\Omega_{lm}} g(x) \, dx & \Omega_{jk} = \Omega_{lm}, \\
\int_{\Omega_{lm}} g(x) \, dx & \Omega_{jk} \ni z \notin \Omega_{lm}, \\
\int_{\Omega_{lm}} g(x) \, dx & \Omega_{jk} \ni z \in \Omega_{lm}, \end{cases}
\]

we have

\[
* = \sum_{j,k} \sum_{l,m} \frac{1}{h^2} \int_{\Omega_{jk}} \int_{\Omega_{lm}} g(x) \, dx \chi_{\Omega_{lm}}(z) \rho(z) \, dz
\]

\[
= \sum_{j,k} \int_{\Omega_{jk}} (\Pi_h g)(z) \rho(z) \, dz
\]

\[
= \int_{\Omega} \rho \Pi_h g \, dz \xrightarrow{h \to 0} \int_{\Omega} \rho g \, dz,
\]

which concludes the proof.

Acknowledgements The authors would like to thank the German Research Foundation (DFG) for funding this research work within Collaborative Research Centre 814, subproject C2.

References


366 J. Jahn: Vectorization in set optimization (06.03.2013)
368 R. Becker, M. Bittl, D. Kuzmin: Analysis of a combined CG1-DG2 method for the transport equation (12.09.2013)
370 C. Basting, D. Kuzmin: Optimal control for mass conservative level set methods (01.10.2013)
371 H.S. Mahato: A homogenization approach to a system of semilinear diffusion-reaction equations in a porous medium (01.10.2013)
372 H.S. Mahato, M. Böhm: An existence result for a system of coupled semilinear diffusion-reaction equations with flux boundary conditions (01.10.2013)
373 M. Herz, P. Knabner: Including van der Waals forces in diffusion-convection equations - modeling, analysis, and numerical simulations (17.10.2013)
374 S. Weller: Variational time discretization for free surface flows (20.11.2013)
376 F. Frank, P. Knabner: Convergence analysis of a BDF2 / mixed finite element discretization of a Darcy-Nernst-Planck-Poisson system (17.01.2014)
377 J. Jahn: A derivative-free descent method in set optimization (08.04.2014)
378 E. Köbis: Variable ordering structures in set optimization (06.05.2014)
379 O. Krehel, A. Muntean, P. Knabner: Multiscale modeling of colloidal dynamics in porous media: capturing aggregation and deposition effects (08.05.2014)
381 M. Herz, P. Knabner: Global existence of weak solutions of a model for electrolyte solutions – Part 2: Multicomponent case (16.05.2014)
382 M. Herz, P. Knabner: Modeling and simulation of coagulation according to DVLO-theory in a continuum model for electrolyte solutions (16.05.2014)
383 M. Herz, P. Knabner: A thermodynamically consistent model for multicomponent electrolyte solutions (02.06.2014)
384 M. Gahn, P. Knabner, M. Neuss-Radu: Homogenization of reaction-diffusion processes in a two-component porous medium with a nonlinear flux condition at the interface, and application to metabolic processes in cells (09.07.2014)
385 J. Jahn: Directional derivatives in set optimization with the set less order relation (08.08.2014)
386 N. Ray, P. Knabner: Upscaling flow and transport in an evolving porous medium with general interaction potentials (06.10.2014)
387 J. Greifenstein, M. Stingl: Simultaneous material and topology optimization (21.10.2014)