VARIANT OF OPTIMALITY CRITERIA METHOD FOR MULTIPLE STATE OPTIMAL DESIGN PROBLEMS*

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Abstract. We consider multiple state optimal design problems, aiming to find the best arrangement of two given isotropic materials, such that the obtained body has some optimal properties regarding m different right-hand sides. Using the homogenization method as the relaxation tool, the standard variational techniques lead to necessary conditions of optimality. These conditions are the basis for the optimality criteria method, a commonly used numerical (iterative) method for optimal design problems. In Vrdoljak (2010), one variant of this method is presented, which is suitable for the energy maximization problems. We study another variant of the method, which works well for energy minimization problems. The explicit calculation of the design update is presented, which makes the implementation simple and similar to the case of single state equation. The method is tested on examples, showing that exact solutions are well approximated with the obtained numerical solutions.

Keywords. stationary diffusion; optimal design; homogenization; optimality criteria method.

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1. Introduction

In optimal design problems the goal is to find the best arrangement of given materials within the body which optimizes its properties with respect to some optimality criteria. We consider such problems in the context of the stationary diffusion equation

$$\begin{cases} -\mathsf{div}(\mathbf{A}\nabla u) = f \\ u \in \mathrm{H}_0^1(\Omega) \end{cases}. \tag{1.1}$$

In this case, function u represents the temperature (or the potential in electrostatics) uniquely determined by external heat (or electric charge) density $f \in \mathrm{H}^{-1}(\Omega)$, while $\mathbf{A} \in \mathrm{L}^\infty(\Omega; \mathrm{M}_d(\mathbf{R}))$ represents thermal (or electrical) conductivity of a material. We are dealing with multiple state optimal design problems, where one can have several different regimes effecting on the observed body, which leads to several state equations.

Here, the body is represented by a bounded and open set $\Omega \subset \mathbf{R}^d$ and we assume that it is filled by two isotropic materials with conductivities α and β ($0 < \alpha < \beta$).

The conductivity matrix is then given by

$$\mathbf{A} = \chi \alpha \mathbf{I} + (1-\chi)\beta \mathbf{I},$$

where $\chi \in \mathrm{L}^\infty(\Omega; \{0,1\})$ is a characteristic function of the part of the domain Ω occupied by the first material. If we assume that the volume of the first material is prescribed: $\int_\Omega \chi(\mathbf{x})\, d\mathbf{x} = q_\alpha$, where $0 < q_\alpha < |\Omega|$ is given, then the classical multiple state optimal design problem consists of minimizing the functional

$$\int_\Omega (\chi(\mathbf{x}) g_\alpha(\mathbf{x}, \mathsf{u}) + (1-\chi(\mathbf{x})) g_\beta(\mathbf{x}, \mathsf{u}))\, d\mathbf{x}, \tag{1.2}$$

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over the set of all measurable characteristic functions on Ω satisfying the volume constraint. Here, g_α and g_β are given, while $\mathsf{u} = (u_1, \ldots, u_m)$ denotes the state function: for each $i \in \{1, \ldots, m\}$, temperature u_i is the solution of (1.1) with given right-hand side f_i and $\mathbf{A} = \chi \alpha \mathbf{I} + (1 - \chi) \beta \mathbf{I}$. The volume constraint of the first material is handled by introducing Lagrange multiplier l, leading to an unconstrained minimization problem

$$\begin{cases} J(\chi) = \int_\Omega (\chi(\mathbf{x}) g_\alpha(\mathbf{x}, \mathsf{u}) + (1 - \chi(\mathbf{x})) g_\beta(\mathbf{x}, \mathsf{u})) \, d\mathbf{x} + l \int_\Omega \chi(\mathbf{x}) \, d\mathbf{x} \longrightarrow \min \\ \chi \in L^\infty(\Omega; \{0, 1\}). \end{cases} \tag{1.3}$$

The proposed optimal design problem usually does not admit a solution, thus it is natural to consider an appropriate relaxation of the original problem. Murat and Tartar's relaxation by the homogenization method [13] uses a couple $(\theta, \mathbf{A})$, called a generalized design referring to a fine mixture of original materials, where $\theta \in \mathrm{L}^\infty(\Omega; [0, 1])$ represents a local fraction of the first material in a mixture, while $\mathbf{A}$ is a homogenized conductivity matrix containing information on how materials are mixed. G-closure problem deals with the question of characterizing the set $\mathcal{K}(\theta)$ of all possible homogenized conductivities which can be obtained with the prescribed local fraction θ. It is solved in case of mixing two isotropic materials [12,16]: for given $\theta \in [0, 1]$, the set $\mathcal{K}(\theta)$ consists of all symmetric matrices with eigenvalues $\lambda_1, \ldots, \lambda_d$ satisfying the inequalities

$$\lambda_\theta^- \leq \lambda_j \leq \lambda_\theta^+, \quad j = 1, \ldots, d, \tag{1.4}$$

$$\sum_{j=1}^d \frac{1}{\lambda_j - \alpha} \leq \frac{1}{\lambda_\theta^- - \alpha} + \frac{d - 1}{\lambda_\theta^+ - \alpha}, \tag{1.5}$$

$$\sum_{j=1}^d \frac{1}{\beta - \lambda_j} \leq \frac{1}{\beta - \lambda_\theta^-} + \frac{d - 1}{\beta - \lambda_\theta^+}, \tag{1.6}$$

where $\lambda_\theta^- = \left(\frac{\theta}{\alpha} + \frac{1 - \theta}{\beta} \right)^{-1}$ and $\lambda_\theta^+ = \theta \alpha + (1 - \theta) \beta$. Inequalities $\lambda_\theta^- \leq \lambda_j$ can be omitted from the above description of the set $\mathcal{K}(\theta)$, as they follow from other inequalities. The set of all such d-tuples $(\lambda_1, \ldots, \lambda_d)$ is denoted by $\Lambda(\alpha, \beta; \theta)$.

Finally, the relaxation of problem (1.3) reads

$$\begin{cases} J(\theta, \mathbf{A}) = \int_\Omega (\theta(\mathbf{x}) g_\alpha(\mathbf{x}, \mathsf{u}) + (1 - \theta(\mathbf{x})) g_\beta(\mathbf{x}, \mathsf{u})) \, d\mathbf{x} + l \int_\Omega \theta(\mathbf{x}) \, d\mathbf{x} \longrightarrow \min \\ (\theta, \mathbf{A}) \in \mathcal{A} = \{ (\theta, \mathbf{A}) \in L^\infty(\Omega; [0, 1] \times \mathrm{M}_d(\mathbf{R})) : \mathbf{A}(\mathbf{x}) \in \mathcal{K}(\theta(\mathbf{x})) \, \mathrm{a.e.}\, \mathbf{x} \in \Omega \} \end{cases} \tag{1.7}$$

and it is a true relaxation of the original problem, under suitable conditions on g_α and g_β. More information about homogenization theory and applications in optimal design can be found in [1, 13, 14, 18, 19].

Recently, problem (1.7) was solved analytically [5, 6, 21] for some simple domains like ball or annulus and a functional corresponding to a conic sum of energies obtained for each state equation where $g_\alpha = g_\beta = \sum_{i=1}^m \mu_i f_i u_i$ (for single state problems, see also [7, 13]). For more complicated domains (or functionals), it is quite unlikely to find an analytic solution [10], which imposes a need for various numerical methods. One of them is optimality criteria method, an iterative method based on optimality conditions of the relaxed formulation, which produces good results in shape optimization [4, 15]. For the case of a single state equation, the method is described in [1]. Actually, two variants of the method are introduced: already in [13] it was noticed that in the case

of energy functional, two different approaches to optimality conditions are needed; one for the minimization and the other for the maximization of energy.

Regarding multiple state problems, in [20], an optimality criteria method is introduced, based on the optimality conditions derived in [1]. It appears that this method works properly for maximization of a conic sum of energies, but fails for the minimization of the same functional. In this work, we present another variant of the optimality criteria method which is suitable for minimization of a conic sum of energies.

The paper is organized as follows: in the second section we derive the necessary condition of optimality for the relaxed minimization problem and present calculations essential for the implementation of the optimality criteria method for the two and three-dimensional cases. In the last section, an implementation of the optimality criteria method is described and some numerical results are presented.

2. Optimality criteria method

Let us denote by $(\theta^*, \mathbf{A}^*)$ a local minimum of the relaxed problem (1.7) and consider an admissible smooth path $\varepsilon \mapsto (\theta^\varepsilon, \mathbf{A}^\varepsilon) \in \mathcal{A}$ given by

$$(\theta^\varepsilon, \mathbf{A}^\varepsilon) = (\theta^*, \mathbf{A}^*) + \varepsilon(\delta\theta, \delta\mathbf{A}) + o(\varepsilon), \quad \lim_{\varepsilon \searrow 0} \frac{\|o(\varepsilon)\|_{\mathrm{L}^\infty}}{\varepsilon} = 0.$$

Then, for any admissible variation $(\delta\theta, \delta\mathbf{A}) = \frac{d}{d\epsilon}(\theta^\epsilon, \mathbf{A}^\epsilon)\upharpoonright_{\epsilon=0^+}$, the first order variation of J is given by ([1, Sect. 3.2.3])

$$\delta J = \int_\Omega (g_\alpha(\mathbf{x}, \mathsf{u}(\mathbf{x})) - g_\beta(\mathbf{x}, \mathsf{u}(\mathbf{x})) + l)\, \delta\theta(\mathbf{x})\, d\mathbf{x} - \int_\Omega \sum_{i=1}^m \delta\mathbf{A}(\mathbf{x})\nabla u_i(\mathbf{x}) \cdot \nabla p_i(\mathbf{x})\, d\mathbf{x}, \quad (2.1)$$

where the *adjoint states* $p_1, \ldots, p_m$ are unique solutions of adjoint boundary value problems

$$\begin{cases} -\mathsf{div}\,(\mathbf{A}\nabla p_i) = \theta \dfrac{\partial g_\alpha}{\partial u_i}(\cdot, \mathsf{u}) + (1-\theta)\dfrac{\partial g_\beta}{\partial u_i}(\cdot, \mathsf{u}) \\ p_i \in \mathrm{H}_0^1(\Omega) \end{cases} \qquad i = 1, \ldots, m. \qquad (2.2)$$

The necessary condition of optimality states that $\delta J \geq 0$, for any admissible variation $(\delta\theta, \delta\mathbf{A})$ of the optimal design $(\theta^*, \mathbf{A}^*)$. The main difficulty in analysing this optimality condition is that variations in θ and $\mathbf{A}$ are not independent. Therefore, we use an analogous technique to that presented in [1, 13, 17, 18]. As the first step let us consider variations only in $\mathbf{A}$, taking $\delta\theta$ to be 0. As noticed in [1, Remark 2.2.16], the condition $\mathbf{A} \in \mathcal{K}(\theta)$ can be equivalently expressed as $\mathbf{A}^{-1} \in \tilde{\mathcal{K}}(\theta)$, where $\tilde{\mathcal{K}}(\theta)$ is the set of all matrices with eigenvalues $\nu_j = \frac{1}{\lambda_j}$ (λ_j being the eigenvalues of $\mathbf{A}$) satisfying

$$\nu_\theta^+ \leq \nu_j \leq \nu_\theta^-, \quad j = 1, \ldots, d, \qquad (2.3)$$

$$\sum_{j=1}^d \frac{1}{\alpha^{-1} - \nu_j} \leq \frac{1}{\alpha^{-1} - \nu_\theta^-} + \frac{d-1}{\alpha^{-1} - \nu_\theta^+}, \qquad (2.4)$$

$$\sum_{j=1}^d \frac{1}{\nu_j - \beta^{-1}} \leq \frac{1}{\nu_\theta^- - \beta^{-1}} + \frac{d-1}{\nu_\theta^+ - \beta^{-1}}, \qquad (2.5)$$

for $\nu_\theta^+ = \frac{1}{\lambda_\theta^+}$ and $\nu_\theta^- = \frac{1}{\lambda_\theta^-}$. The set of all $(\nu_1, \ldots, \nu_d)$ satisfying (2.3)-(2.5) is denoted by $\mathcal{V}(\alpha, \beta; \theta)$. As before, inequalities $\nu_j \leq \nu_\theta^-$ can be omitted. Due to the convexity

of $\mathcal{K}(\theta^*)$, it is natural to take a segment in $\mathcal{K}(\theta^*)$ as the admissible path, which leads to the variant of optimality criteria method that appears suitable for maximization problems [1, 20]. Here, we choose another path: since $\tilde{\mathcal{K}}(\theta^*)$ is also convex, we can take the admissible smooth path $\mathbf{A}^\varepsilon = (\varepsilon \mathbf{A}^{-1} + (1-\varepsilon)\mathbf{A}^{*-1})^{-1}$, for some $\mathbf{A} \in \mathcal{K}(\theta^*)$, which represents a segment in $\tilde{\mathcal{K}}(\theta^*)$. Then the admissible variation $\delta \mathbf{A}$ is of the form $\mathbf{A}^*(\mathbf{A}^{*-1} - \mathbf{A}^{-1})\mathbf{A}^*$, and by (2.1), the necessary condition of optimality reads

$$\sum_{i=1}^{m} \mathbf{A}^{-1}\sigma_i^* \cdot \tau_i^* \geq \sum_{i=1}^{m} \mathbf{A}^{*-1}\sigma_i^* \cdot \tau_i^*,$$

almost everywhere on Ω, where $\sigma_i^* = \mathbf{A}^* \nabla u_i^*$ and $\tau_i^* = \mathbf{A}^* \nabla p_i^*$. Therefore, $\mathbf{A}^*$ is a solution of the minimization problem

$$\begin{cases} \sum_{i=1}^{m} \mathbf{A}^{-1}\sigma_i^* \cdot \tau_i^* \to \min \\ \mathbf{A} \in \mathcal{K}(\theta^*), \end{cases} \tag{2.6}$$

which is a constrained minimization of a linear function. By introducing a matrix function $\mathbf{N}^* = \mathrm{Sym} \sum_{i=1}^{m} \sigma_i^* \otimes \tau_i^*$, we have $\sum_{i=1}^{m} \mathbf{A}^{-1}\sigma_i^* \cdot \tau_i^* = \mathbf{A}^{-1} : \mathbf{N}^*$. Here, the symbol $\otimes$ denotes the tensor product of two vectors, while : stands for the matrix inner product. By the classical von Neumann result [11], the optimal $\mathbf{A}$ for the above minimization problem is simultaneously diagonalizable with $\mathbf{N}^*$ and thus the problem (2.6) reduces to

$$\begin{cases} \sum_{j=1}^{d} \nu_j \eta_j^* \longrightarrow \min \\ \nu_j \in \mathcal{V}(\alpha, \beta; \theta^*), \qquad j = 1, \dots, d, \end{cases} \tag{2.7}$$

where $\eta_1^* \geq \eta_2^* \geq \dots \geq \eta_d^*$ are eigenvalues of the symmetric matrix $\mathbf{N}^*$.

Now we take into account variations in θ and consider an admissible smooth path $\varepsilon \mapsto (\theta^\varepsilon, \mathbf{A}^\varepsilon)$ such that almost everywhere on Ω

$$(\mathbf{A}^\varepsilon)^{-1} : \mathbf{N}^* = g(\theta^\varepsilon, \mathbf{N}^*),$$

where function $g : [0, 1] \times \mathrm{Sym}_d \to \mathbf{R}$ is defined by

$$g(\theta, \mathbf{N}) = \min_{\mathbf{A} \in \mathcal{K}(\theta)} (\mathbf{A}^{-1} : \mathbf{N}).$$

Since $\theta \mapsto g(\theta, \mathbf{N})$ is differentiable, as we shall see later, using variations $(\delta\theta, \delta\mathbf{A})$ generated by this smooth path, the necessary condition of optimality leads us to the following result.

THEOREM 2.1.   *Let* $(\theta^*, \mathbf{A}^*)$ *be a local minimizer for the relaxation problem (1.7) with corresponding states* u_i^* *and adjoint states* p_i^*. *We introduce symmetric matrix*

$$\mathbf{N}^* = \mathrm{Sym} \sum_{i=1}^{m} \sigma_i^* \otimes \tau_i^*,$$

for $\sigma_i^* = \mathbf{A}^* \nabla u_i^*, \tau_i^* = \mathbf{A}^* \nabla p_i^*$, *and function*

$$R^*(\mathbf{x}) := g_\alpha(\mathbf{x}, \mathsf{u}^*(\mathbf{x})) - g_\beta(\mathbf{x}, \mathsf{u}^*(\mathbf{x})) + l + \frac{\partial g}{\partial \theta}(\theta^*(\mathbf{x}), \mathbf{N}^*(x)), \quad a.e. \ \mathbf{x} \in \Omega.$$

Then the optimal θ^* satisfies (almost everywhere on Ω)

$$\theta^*(\mathbf{x}) = 0 \implies R^*(\mathbf{x}) \geq 0,$$
$$\theta^*(\mathbf{x}) = 1 \implies R^*(\mathbf{x}) \leq 0,$$
$$0 < \theta^*(\mathbf{x}) < 1 \implies R^*(\mathbf{x}) = 0,$$

or equivalently

$$R^*(\mathbf{x}) > 0 \implies \theta^*(\mathbf{x}) = 0,$$
$$R^*(\mathbf{x}) < 0 \implies \theta^*(\mathbf{x}) = 1.$$

Proof. The theorem can be proved analogously as Theorem 3.2.14. in [1]. $\square$

For single state optimal design problems, function g attains a minimum in a simple laminate which is easily expressed in terms of σ^* and τ^*. This fact makes a calculation of the partial derivative $\frac{\partial g}{\partial \theta}$ straightforward. Furthermore, this calculation enables an explicit update of the design variables $(\theta^k, \mathbf{A}^k)$ in the optimality criteria method. Let us describe a strict analogue of this method applied to multiple state problems.

ALGORITHM 2.1.   *Take some initial θ^0 and $\mathbf{A}^0$. For k from 0 to N:*
(1) Calculate u_i^k, $i = 1, \ldots, m$, the solution of

$$\begin{cases} -\mathsf{div}\,(\mathbf{A}^k \nabla u_i) = f_i \\ u_i \in \mathrm{H}_0^1(\Omega) \end{cases}.$$

(2) Calculate p_i^k, $i = 1, \ldots, m$, the solution of

$$\begin{cases} -\mathsf{div}\,(\mathbf{A}^k \nabla p_i) = \theta^k \dfrac{\partial g_\alpha}{\partial u_i}(\cdot, \mathsf{u}^k) + (1 - \theta^k) \dfrac{\partial g_\beta}{\partial u_i}(\cdot, \mathsf{u}^k) \\ \qquad p_i \in \mathrm{H}_0^1(\Omega), \mathsf{u}^k = (u_1^k, \ldots, u_m^k) \end{cases}$$

and define $\sigma_i^k := \mathbf{A}^k \nabla u_i^k, \tau_i^k := \mathbf{A}^k \nabla u_i^k$ and $\mathbf{N}^k := \mathrm{Sym} \sum\limits_{i=1}^{m} (\sigma_i^k \otimes \tau_i^k)$.
(3) For $\mathbf{x} \in \Omega$ let $\theta^{k+1}(\mathbf{x}) \in [0,1]$ be a zero of the function

$$\theta \mapsto R^k(\theta, \mathbf{x}) := g_\alpha(\mathbf{x}, \mathsf{u}^k(\mathbf{x})) - g_\beta(\mathbf{x}, \mathsf{u}^k(\mathbf{x})) + l + \frac{\partial g}{\partial \theta}(\theta, \mathbf{N}^k(\mathbf{x})), \qquad (2.8)$$

and if a zero doesn't exist, take 0 (or 1) if the function is positive (or negative) on $[0,1]$.
(4) Let $\mathbf{A}^{k+1}(\mathbf{x})$ be the minimizer in the definition of $g(\theta^{k+1}(\mathbf{x}), \mathbf{N}^k(\mathbf{x}))$.

In the rest of the paper, we shall present explicit formulae for the partial derivative $\frac{\partial g}{\partial \theta}$ for the general (multi-state) case. As mentioned in the Introduction, the first variant of the optimality criteria method is presented in [20], but it does not converge for examples presented in Section 3. On the other hand, that variant behaves well for the question of maximization of the same functionals instead of minimization. This kind of behaviour is expected for a class of self-adjoint problems, since already, the single state self-adjoint problems exhibit a similar effect [1, 13].

Let us first consider the two-dimensional case. As commented, the minimization over $\mathcal{K}(\theta)$ in the definition of function g can be expressed equivalently by minimization

over eigenvalues:

$$g(\theta, \mathbf{N}) = \min_{\boldsymbol{\nu} \in \mathcal{V}(\alpha,\beta;\theta)} \sum_{j=1}^{d} \nu_j \eta_j,$$

where η_j are the eigenvalues of the symmetric matrix $\mathbf{N}$.

In the two-dimensional case one can easily show that the set $\mathcal{V}(\alpha,\beta;\theta)$ equals to the set $\Lambda\left(\frac{1}{\beta}, \frac{1}{\alpha}; 1-\theta\right)$. This remark can be used to calculate g and its partial derivative over θ on the basis of [1, Lemma 3.2.17], as presented in the next theorem.

THEOREM 2.2.

For the case $d=2$, for given $\theta \in [0,1]$ and a symmetric matrix $\mathbf{N}$ with eigenvalues $\eta_1 \geq \eta_2$, we have

A. *If $\eta_2 > 0$ and $\theta^A := \left(\alpha \dfrac{\sqrt{\eta_1}}{\sqrt{\eta_2}} - \beta\right) \dfrac{1}{\alpha - \beta}$, then*

$$\frac{\partial g}{\partial \theta}(\theta, \mathbf{N}) = \begin{cases} \dfrac{1}{\beta}\left(\beta^2 - \alpha^2\right)\left(\dfrac{\sqrt{\eta_1} + \sqrt{\eta_2}}{\theta(\alpha - \beta) + \beta + \alpha}\right)^2, & \theta < \theta^A \\[2ex] \dfrac{(\beta - \alpha)\eta_1}{(\theta(\alpha - \beta) + \beta)^2} + \eta_2\left(\dfrac{1}{\alpha} - \dfrac{1}{\beta}\right), & \theta \geq \theta^A \end{cases}.$$

B. *If $\eta_1 < 0$ and $\theta^B := \left(\dfrac{\sqrt{-\eta_1}}{\sqrt{-\eta_2}} - 1\right) \dfrac{\beta}{\alpha - \beta}$, then*

$$\frac{\partial g}{\partial \theta}(\theta, \mathbf{N}) = \begin{cases} -\dfrac{1}{\alpha}\left(\beta^2 - \alpha^2\right)\left(\dfrac{\sqrt{-\eta_1} + \sqrt{-\eta_2}}{\theta(\alpha - \beta) + 2\beta}\right)^2, & \theta > \theta^B \\[2ex] \dfrac{(\beta - \alpha)\eta_1}{(\theta(\alpha - \beta) + \beta)^2} + \eta_2\left(\dfrac{1}{\alpha} - \dfrac{1}{\beta}\right), & \theta \leq \theta^B \end{cases}.$$

C. *If $\eta_1 \geq 0$ and $\eta_2 \leq 0$, then*

$$\frac{\partial g}{\partial \theta}(\theta, \mathbf{N}) = \frac{(\beta - \alpha)\eta_1}{(\theta(\alpha - \beta) + \beta)^2} + \eta_2\left(\frac{1}{\alpha} - \frac{1}{\beta}\right).$$

Proof. In the proof we emphasize parameters α and β in the set $\mathcal{K}(\theta)$ by denoting it by $\mathcal{K}(\alpha,\beta;\theta)$, for given $\theta \in [0,1]$. For dimension $d=2$, condition $\mathbf{A} \in \mathcal{K}(\alpha,\beta;\theta)$ can be equivalently expressed as $\mathbf{A}^{-1} \in \mathcal{K}\left(\frac{1}{\beta}, \frac{1}{\alpha}; 1-\theta\right)$. Now it follows

$$g(\theta, \mathbf{N}) = \min_{\mathbf{A} \in \mathcal{K}(\alpha,\beta;\theta)} \mathbf{A}^{-1} : \mathbf{N} = -\max_{\mathbf{A}^{-1} \in \mathcal{K}\left(\frac{1}{\beta}, \frac{1}{\alpha}; 1-\theta\right)} \mathbf{A}^{-1} : (-\mathbf{N}) = -f_{1/\beta}^{1/\alpha}(1-\theta, -\mathbf{N}),$$

where, for $0 < \gamma < \delta$, function $f_\gamma^\delta : [0,1] \times \mathrm{Sym}_d \longrightarrow \mathbf{R}$ is defined as in [1, Theorem 3.2.14], i. e.

$$f_\gamma^\delta(\theta, \mathbf{M}) = \max_{\mathbf{A} \in \mathcal{K}(\gamma,\delta;\theta)} \mathbf{A} : \mathbf{M}.$$

Furthermore,

$$\frac{\partial g}{\partial \theta}(\theta, \mathbf{N}) = \frac{\partial f_{1/\beta}^{1/\alpha}}{\partial \theta}(1-\theta, -\mathbf{N}).$$

Therefore, one can use the formula for f_α^β given in [1, Lemma 3.2.17] to obtain $\frac{\partial g}{\partial \theta}$. □

In this case ($d=2$), the function $\theta \mapsto R^k(\theta, \mathbf{x})$ introduced in (2.8) is monotone for almost every $\mathbf{x} \in \Omega$, so its zero point (if it exists) is unique. Moreover, by formulae presented in Theorem 2.2, the zero point can be calculated explicitly, as a zero of a quadratic equation. For example, if the eigenvalues of matrix $\mathbf{N}^k$ fits the case A above, then the function $\theta \mapsto R^k(\theta, \mathbf{x})$ is strictly increasing. Therefore, one should simply check signs of $R^k(\theta, \mathbf{x})$ for $\theta \in \{0, 1\}$ (and $\theta = \theta_A$, if $0 < \theta^A < 1$) to locate the zero point (if it exists), and solve the corresponding quadratic equation for θ.

In the three-dimensional case, the situation is more tedious, and we shall begin by solving the minimization problem (2.7).

THEOREM 2.3 ($d=3$). *Let $0 < \theta < 1$ and $\eta_1 \geq \eta_2 \geq \eta_3$ be given. Then the minimization problem*

$$\begin{cases} \nu_1\eta_1 + \nu_2\eta_2 + \nu_3\eta_3 \longrightarrow \min \\ (\nu_1, \nu_2, \nu_3) \in \mathcal{V}(\alpha, \beta; \theta), \end{cases} \tag{2.9}$$

has a solution ν^* as follows:

I. *If $\left(\eta_3 < 0 \text{ and } \eta_2 \geq \eta_3 \left(\frac{1-\alpha\nu_\theta^-}{1-\alpha\nu_\theta^+}\right)^2\right)$ or $\left(\eta_3 \geq 0 \text{ and } \eta_2 \geq \eta_3 \left(\frac{\beta\nu_\theta^- - 1}{\beta\nu_\theta^+ - 1}\right)^2\right)$, then $\nu^* = \left(\nu_\theta^+, \nu_\theta^+, \nu_\theta^-\right)$ is optimal.*

II. *Let $\eta_2 < \eta_3 \left(\frac{1-\alpha\nu_\theta^-}{1-\alpha\nu_\theta^+}\right)^2$ (this is possible only if $\eta_2 < 0$).*

   (1) If $\eta_1 \geq 0$ or else if $\sqrt{-\eta_2} + \sqrt{-\eta_3} \geq \sqrt{-\eta_1}\left(1 + \frac{1-\alpha\nu_\theta^+}{1-\alpha\nu_\theta^-}\right)$ then $\nu^* = \left(\nu_\theta^+, \nu_2, \nu_3\right)$ is optimal, where

$$\nu_i = \frac{1}{\alpha} - \frac{1}{\sqrt{-\eta_i}} \frac{\sqrt{-\eta_2} + \sqrt{-\eta_3}}{c_1(\theta)}, \qquad i = 2,3; \tag{2.10}$$

   with $c_1(\theta) = \frac{1}{\alpha^{-1} - \nu_\theta^-} + \frac{1}{\alpha^{-1} - \nu_\theta^+}$.

   (2) Otherwise, if $\eta_1 < 0$ and $\sqrt{-\eta_2} + \sqrt{-\eta_3} < \sqrt{-\eta_1}\left(1 + \frac{1-\alpha\nu_\theta^+}{1-\alpha\nu_\theta^-}\right)$ then $\nu^* = (\nu_1, \nu_2, \nu_3)$ is optimal, where

$$\nu_i = \frac{1}{\alpha} - \frac{1}{\sqrt{-\eta_i}} \frac{\sqrt{-\eta_1} + \sqrt{-\eta_2} + \sqrt{-\eta_3}}{c_2(\theta)}, \qquad i = 1,2,3; \tag{2.11}$$

   with $c_2(\theta) = \frac{1}{\alpha^{-1} - \nu_\theta^-} + \frac{2}{\alpha^{-1} - \nu_\theta^+}$.

III. *Let $\eta_2 < \eta_3 \left(\frac{\beta\nu_\theta^- - 1}{\beta\nu_\theta^+ - 1}\right)^2$ (this is possible only if $\eta_3 > 0$).*

   (1) If $\sqrt{\eta_2} + \sqrt{\eta_3} \leq \sqrt{\eta_1}\left(1 + \frac{\beta\nu_\theta^+ - 1}{\beta\nu_\theta^- - 1}\right)$ then $\nu^* = \left(\nu_\theta^+, \nu_2, \nu_3\right)$ is optimal, where

$$\nu_i = \frac{1}{\beta} + \frac{1}{\sqrt{\eta_i}} \frac{\sqrt{\eta_2} + \sqrt{\eta_3}}{d_1(\theta)}, \qquad i = 2,3; \tag{2.12}$$

   with $d_1(\theta) = \frac{1}{\nu_\theta^- - \beta^{-1}} + \frac{1}{\nu_\theta^+ - \beta^{-1}}$.

   (2) If $\sqrt{\eta_2} + \sqrt{\eta_3} > \sqrt{\eta_1}\left(1 + \frac{\beta\nu_\theta^+ - 1}{\beta\nu_\theta^- - 1}\right)$ then $\nu^* = (\nu_1, \nu_2, \nu_3)$ is optimal, where

$$\nu_i = \frac{1}{\beta} + \frac{1}{\sqrt{\eta_i}} \frac{\sqrt{\eta_1} + \sqrt{\eta_2} + \sqrt{\eta_3}}{d_2(\theta)}, \qquad i = 1,2,3; \tag{2.13}$$

with $d_2(\theta) = \frac{1}{\nu_\theta^- - \beta^{-1}} + \frac{2}{\nu_\theta^+ - \beta^{-1}}$.

Proof. Note that due to the symmetry of the set $\mathcal{V}(\alpha, \beta; \theta)$ in ν_1, ν_2, ν_3, we can conclude that a minimum point satisfies $\nu_\theta^+ \le \nu_1 \le \nu_2 \le \nu_3$. Moreover, by observing that we are minimizing a linear function over a convex set, the optimal point belongs to the boundary of the set $\mathcal{V}(\alpha, \beta; \theta)$ and conversely, every boundary point of $\mathcal{V}(\alpha, \beta; \theta)$ can be obtained as a solution of (2.9) for some η_1, η_2 and η_3. In addition, if $\eta_1 \ge 0$ and $\eta_2 = \eta_3 = 0$, the problem (2.9) has a non-unique solution, one of them being simple laminate $\nu^* = (\nu_\theta^+, \nu_\theta^+, \nu_\theta^-)$. Otherwise, there is a unique minimizer which we find by solving the Karush-Kuhn-Tucker (KKT) system. We already eliminated flat parts of the boundary of the set $\mathcal{V}(\alpha, \beta; \theta)$ (non-uniqueness of the solution appears here), so we have to analyze the rest of the boundary consisting precisely of: simple laminates, second and third order sequential laminates with matrix material α, and second and third order sequential laminates with matrix material β. These five cases correspond exactly to cases I, II.1, II.2, III.1, and III.2 of Theorem 2.3.

Here we only prove part II.1 of the theorem, while others follow similarly. Suppose that the minimizer $\nu^* = (\nu_1, \nu_2, \nu_3)$ belongs to the part of boundary of $\mathcal{V}(\alpha, \beta; \theta)$ corresponding to second order sequential laminates with matrix material α, described by

$$\nu_1 = \nu_\theta^+, \tag{2.14}$$

$$\nu_2, \nu_3 > \nu_\theta^+, \tag{2.15}$$

$$\sum_{j=1}^{3} \frac{1}{\alpha^{-1} - \nu_j} = \frac{1}{\alpha^{-1} - \nu_\theta^-} + \frac{2}{\alpha^{-1} - \nu_\theta^+}, \tag{2.16}$$

$$\sum_{j=1}^{3} \frac{1}{\nu_j - \beta^{-1}} < \frac{1}{\nu_\theta^- - \beta^{-1}} + \frac{2}{\nu_\theta^+ - \beta^{-1}}. \tag{2.17}$$

We shall derive conditions on η_1, η_2 and η_3 which ensure that optimal ν^* belongs to this part of the boundary, and calculate the optimal ν^* in terms of η_1, η_2 and η_3. In this case, the KKT system reads:

$$\eta_1 = \frac{-a_1}{(\alpha^{-1} - \nu_1)^2} + a_3$$

$$\eta_2 = \frac{-a_1}{(\alpha^{-1} - \nu_2)^2}$$

$$\eta_3 = \frac{-a_1}{(\alpha^{-1} - \nu_3)^2},$$

for some nonnegative multipliers a_1 and a_3. From the argument made at the beginning of the proof, we conclude $a_1 > 0$, implying that $\eta_2, \eta_3 < 0$ and

$$\frac{1}{\alpha^{-1} - \nu_i} = \sqrt{\frac{-\eta_i}{a_1}}, \qquad i = 2, 3, \tag{2.18}$$

which together with (2.16) gives

$$\sqrt{a_1} = \frac{\sqrt{-\eta_2} + \sqrt{-\eta_3}}{c_1(\theta)}, \quad \text{where } c_1(\theta) = \frac{1}{\alpha^{-1} - \nu_\theta^-} + \frac{1}{\alpha^{-1} - \nu_\theta^+}. \tag{2.19}$$

Inserting this into (2.18), one obtains formula (2.10). It remains to identify under which conditions on η_1, η_2 and η_3, the condition (2.15) is satisfied, with $\eta_1 = \frac{-a_1}{(\alpha^{-1} - \nu_1)^2} + a_3$,

for $a_1, a_3 \geq 0$. A simple calculation gives that condition $\nu_\theta^+ < \nu_2$ is equivalent to

$$\sqrt{-\eta_3} < \sqrt{-\eta_2} \frac{1 - \alpha \nu_\theta^+}{1 - \alpha \nu_\theta^-}, \tag{2.20}$$

while condition $a_3 \geq 0$ leads to

$$\eta_1 + \frac{a_1}{(\alpha^{-1} - \nu_1)^2} \geq 0.$$

The above inequality is trivially satisfied if $\eta_1 \geq 0$, while if $\eta_1 < 0$, then from (2.19), using (2.14), it is equivalent to the inequality

$$\sqrt{-\eta_2} + \sqrt{-\eta_3} \geq \sqrt{-\eta_1} \left(1 + \frac{1 - \alpha \nu_\theta^+}{1 - \alpha \nu_\theta^-} \right). \tag{2.21}$$

$$\square$$

Before providing the function $g(\theta, \mathbf{N})$ and its derivatives, let us rewrite the statement of Theorem 2.3 in a more convenient way for implementation on a computer.

COROLLARY 2.1 ($d = 3$).   *Given $\eta_1 \geq \eta_2 \geq \eta_3$ and $0 < \theta < 1$ one can calculate the minimum point $\nu^* = (\nu_1, \nu_2, \nu_3)$ for (2.9) in the following way:*

   If $\eta_3 = 0$, then the optimal point is $\nu^* = (\nu_\theta^+, \nu_\theta^+, \nu_\theta^-)$.

   Else if $\eta_3 > 0$, then calculate ν_1 by formula (2.13).

      If $\nu_\theta^+ < \nu_1$, then both ν_2 and ν_3 are given by (2.13).

      Else, calculate ν_2 by formula (2.12).

         If $\nu_\theta^+ < \nu_2$, then $\nu_1 = \nu_\theta^+$ and ν_3 is given by (2.12).

         Else $\nu^* = (\nu_\theta^+, \nu_\theta^+, \nu_\theta^-)$.

   Else ($\eta_3 < 0$)

      If $\eta_1 \geq 0$, then

         if $\eta_2 \geq \eta_3 \left(\frac{1 - \alpha \nu_\theta^-}{1 - \alpha \nu_\theta^+} \right)^2$ then $\nu^* = (\nu_\theta^+, \nu_\theta^+, \nu_\theta^-)$.

         Else $\nu^* = (\nu_\theta^+, \nu_2, \nu_3)$, where ν_2 and ν_3 are given by (2.10).

      Else ($\eta_1 < 0$) calculate ν_1 by formula (2.11).

         If $\nu_\theta^+ < \nu_1$, then both ν_2 and ν_3 are given by (2.11).

         Else, calculate ν_2 by formula (2.10).

            If $\nu_\theta^+ < \nu_2$,, then $\nu_1 = \nu_\theta^+$ and ν_3 is given by (2.10).

            Else $\nu^* = (\nu_\theta^+, \nu_\theta^+, \nu_\theta^-)$.

Once the optimal solution $\nu^* = (\nu_1, \nu_2, \nu_3)$ for (2.9) is determined, one can easily calculate the function $g(\theta, \mathbf{N}) = \nu_1 \eta_1 + \nu_2 \eta_2 + \nu_3 \eta_3$, as well as its partial derivative over θ. Partial derivatives of the function g are given below.

THEOREM 2.4.   *For $d = 3$, given $\theta \in [0,1]$ and matrix $\mathbf{N}$ with eigenvalues $\eta_1 \geq \eta_2 \geq \eta_3$, we have*

   A. If $\eta_3 = 0$ then $\dfrac{\partial g}{\partial \theta}(\theta, \mathbf{N}) = \dfrac{\beta - \alpha}{(\theta \alpha + (1 - \theta)\beta)^2}(\eta_1 + \eta_2)$.

B. If $\eta_3 > 0$ and additionally $\sqrt{\eta_2} + \sqrt{\eta_3} - \sqrt{\eta_1} > 0$, it holds that

$$\frac{\partial g}{\partial \theta}(\theta, \mathbf{N}) = \begin{cases} \dfrac{(\beta - \alpha)(\alpha + 2\beta)}{\beta}\left(\dfrac{\sqrt{\eta_1} + \sqrt{\eta_2} + \sqrt{\eta_3}}{2\theta(\alpha - \beta) + \alpha + 2\beta}\right)^2, & \theta < \theta_1^B, \\[3mm] \dfrac{\beta^2 - \alpha^2}{\beta}\left(\dfrac{\sqrt{\eta_2} + \sqrt{\eta_3}}{\theta(\alpha - \beta) + \alpha + \beta}\right)^2 + \dfrac{(\beta - \alpha)\eta_1}{(\theta\alpha + (1 - \theta)\beta)^2}, & \theta_1^B \leq \theta < \theta_2^B, \\[3mm] \dfrac{(\beta - \alpha)\eta_3}{\alpha\beta} + \dfrac{\beta - \alpha}{(\theta\alpha + (1 - \theta)\beta)^2}(\eta_1 + \eta_2), & \theta \geq \theta_2^B, \end{cases}$$

where $\theta_1^B = 1 - \dfrac{\alpha(2\sqrt{\eta_1} - \sqrt{\eta_2} - \sqrt{\eta_3})}{(\beta - \alpha)(\sqrt{\eta_2} + \sqrt{\eta_3} - \sqrt{\eta_1})}$ and $\theta_2^B = 1 - \dfrac{\alpha(\sqrt{\eta_2} - \sqrt{\eta_3})}{(\beta - \alpha)\sqrt{\eta_3}}$.

If $\sqrt{\eta_2} + \sqrt{\eta_3} - \sqrt{\eta_1} \leq 0$ then we omit the first case in the above formula.

C. If $\eta_3 < 0$ then, if η_2 and η_1 are negative as well, we have

$$\frac{\partial g}{\partial \theta}(\theta, \mathbf{N}) = \begin{cases} -\dfrac{(\beta - \alpha)(2\alpha + \beta)}{\alpha}\left(\dfrac{\sqrt{-\eta_1} + \sqrt{-\eta_2} + \sqrt{-\eta_3}}{2\theta(\alpha - \beta) + 3\beta}\right)^2, & \theta > \theta_1^C, \\[3mm] -\dfrac{\beta^2 - \alpha^2}{\alpha}\left(\dfrac{\sqrt{-\eta_2} + \sqrt{-\eta_3}}{\theta(\alpha - \beta) + 2\beta}\right)^2 + \dfrac{(\beta - \alpha)\eta_1}{(\theta\alpha + (1 - \theta)\beta)^2}, & \theta_2^C < \theta \leq \theta_1^C, \\[3mm] \dfrac{(\beta - \alpha)\eta_3}{\alpha\beta} + \dfrac{\beta - \alpha}{(\theta\alpha + (1 - \theta)\beta)^2}(\eta_1 + \eta_2), & \theta \leq \theta_2^C, \end{cases}$$

(2.22)

where $\theta_1^C = \dfrac{\beta(\sqrt{-\eta_2} + \sqrt{-\eta_3} - 2\sqrt{-\eta_1})}{(\beta - \alpha)(\sqrt{-\eta_2} + \sqrt{-\eta_3} - \sqrt{-\eta_1})}$ and $\theta_2^C = \dfrac{\beta(\sqrt{-\eta_3} - \sqrt{-\eta_2})}{(\beta - \alpha)\sqrt{-\eta_3}}$.

If $\eta_2 < 0$ and $\eta_1 \geq 0$ then θ_1^C is not defined and we can express $\frac{\partial g}{\partial \theta}(\theta, \mathbf{N})$ by the second and the third term in (2.22), omitting the assumption $\theta \leq \theta_1^C$ in the second case.

If $\eta_2 \geq 0$ then both θ_1^C and θ_2^C are not defined and $\frac{\partial g}{\partial \theta}$ is given by the formula in the third case of (2.22), for any $\theta \in [0, 1]$.

Proof.   Let us first remark that $\theta_1^B \leq \theta_2^B \leq 1$ and $0 \leq \theta_2^C \leq \theta_1^C$. We are going to present only the proof of case C, as other cases can be proved analogously. If $\eta_1 < 0$ and the optimal (ν_1, ν_2, ν_3) is given by the formula (2.11), from

$$g(\theta, \mathbf{N}) = \eta_1\nu_1 + \eta_2\nu_2 + \eta_3\nu_3$$

an easy calculation gives us the formula which corresponds to the first term of the function $\frac{\partial g}{\partial \theta}$ in the case C. Here, the condition $\nu_\theta^+ < \nu_1$ is equivalent to $\theta > \theta_1^C$. If $\nu_1 = \nu_\theta^+$ (or equivalently, $\theta \leq \theta_1^C$) and ν_2 and ν_3 are given by (2.10), then one gets the second formula in case C. This occurs if $\nu_\theta^+ < \nu_2$ or equivalently $\theta > \theta_2^C$. Finally, the last term in case C is easily reconstructed since in this case $(\nu_\theta^+, \nu_\theta^+, \nu_\theta^-)$ is optimal for the minimization problem in definition of function g.   □

It is important to notice that function $\theta \mapsto g_\alpha(\mathbf{x}, \mathbf{u}^k(\mathbf{x})) - g_\beta(\mathbf{x}, \mathbf{u}^k(\mathbf{x})) + l + \frac{\partial g}{\partial \theta}(\theta, \mathbf{N}^k(\mathbf{x}))$ is continuous in the three-dimensional case, due to the continuity of the function $\theta \mapsto \frac{\partial g}{\partial \theta}$, but not necessarily monotone as it was in the two-dimensional case. The possible lack of monotonicity can occur in case C, when $\eta_1 \geq 0$, $\eta_2 < 0$, and for some choices of α, β, η_1, η_2, η_3. In this case, one can get two possible zeros of this function on $[0, 1]$, and then we simply take the smaller one for the next iteration of θ. However, in all examples that we considered, this situation never actually occurred. In all other cases, the function (2.8) is monotone and its zero is explicitly calculated by solving quadratic (or quartic) equation.

3. Numerical examples

In this section, we apply Algorithm 2.1 on several problems of optimal design. The state and adjoint equations are solved by the finite element method in deal.II library [3] using Lagrange elements on a fine mesh, while a design $(\theta, \mathbf{A})$ is discretized on a (possibly different) mesh [8], by piecewise constant elements. Lagrange multiplier l is recalculated at each step in a way that θ^{k+1} satisfies the volume constraint, which is done quite effectively by the bisection method. All problems are treated for various volume fractions $\eta := \frac{q_\alpha}{|\Omega|}$ of the first phase (with conductivity α). For the initial design we take constant $\theta^0 = \eta$, while $\mathbf{A}^0$ is taken to be a simple laminate ($\mathbf{A}^0 = \mathrm{diag}(\lambda_\theta^-, \lambda_\theta^+)$ if $d = 2$ or $\mathbf{A}^0 = \mathrm{diag}(\lambda_\theta^-, \lambda_\theta^+, \lambda_\theta^+)$ if $d = 3$). In all examples we calculate 20 iterations of Algorithm 2.1, but it appears that optimal design is well approximated already by the first several iterations.

The first three examples deal with a self-adjoint case, which is addressed already in [1,2,9,13]. For a numerical point of view and the question of convergence, in the case of single state problems, see e.g. [1, Section 5.1.3]. Theorems 3.2.30 and 3.2.31 in [1] (see also [2,9]) show that the relaxed problem (1.7) can be expressed as a minimization problem in terms of complementary energy

$$\inf_{(\theta, \mathbf{A}) \in \mathcal{A}} \int_\Omega \left(\sum_{i=1}^m f_i u_i + l\theta \right) d\mathbf{x} = \inf_{\substack{\boldsymbol{\tau} \in \mathrm{L}^2(\Omega; \mathbf{R}^{dm}) \\ -\mathsf{div}\, \boldsymbol{\tau}_i = f_i}} \int_\Omega QF(\boldsymbol{\tau}),$$

where $QF(\boldsymbol{\tau}) = \min_{0 \le \theta \le 1}(g(\theta, \boldsymbol{\tau}^\tau \boldsymbol{\tau}) + l\theta)$ is a quasiconvex integrand. More precisely, it can be understood as a quasiconvex envelope of the integrand which appears in the original (unrelaxed) problem, which gives another view to its relaxation.

3.1. Two-state problem on a ball. In the first example we consider two-dimensional problem of weighted energy minimization

$$J(\theta, \mathbf{A}) = 2 \int_\Omega f_1 u_1 \, d\mathbf{x} + \int_\Omega f_2 u_2 \, d\mathbf{x} \longrightarrow \min,$$

where $\Omega \subseteq \mathbf{R}^2$ is a ball $B(\mathbf{0}, 2)$, $\alpha = 1$, $\beta = 2$, while u_1 and u_2 are state functions for

$$\begin{cases} -\mathsf{div}\,(\mathbf{A}\nabla u_i) = f_i, \\ u_i \in \mathrm{H}_0^1(\Omega) \end{cases}, \quad i = 1, 2, \tag{3.1}$$

where we take $f_1 = \chi_{B(\mathbf{0}, 1)}$ and $f_2 \equiv 1$ for right-hand sides. This problem is explicitly solved in [6] so we can compare our numerical solution to the exact one. The comparison is done with respect to mesh refinement: the original triangulation of the domain is refined up to 8 times, where each refinement introduces four times finer mesh [3].

The L^1 error between the numerical and exact solutions is presented on Figure 3.1 for various choices of η, and, as it can be seen, the numerical solution aproximates well the exact one.

For $\eta = 0.25$, the numerical solution is presented in Figure 3.2. Let us recall that $\theta = 0$ corresponds to the material with conductivity β, $\theta = 1$ corresponds to the material with conductivity α, while $\theta \in \langle 0, 1 \rangle$ corresponds to a fine mixture of the original phases. Convergence history is presented in Figure 3.3.

3.2. Single state problem on an annulus. Let us now consider energy minimization problem

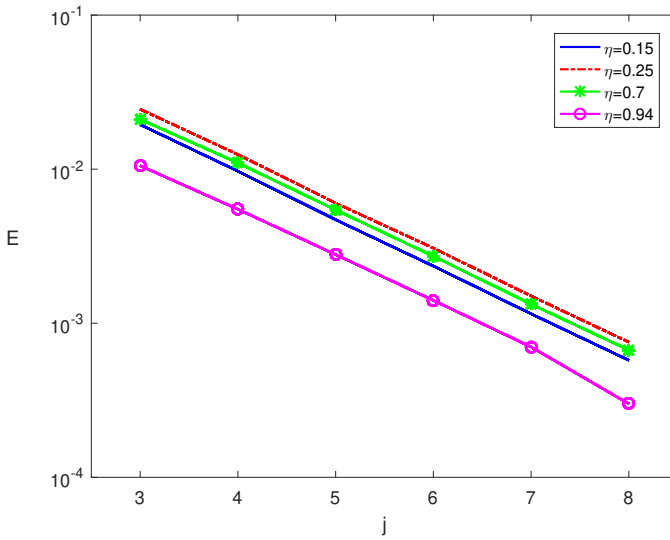$$J(\theta, \mathbf{A}) = \int_\Omega f u \, d\mathbf{x} \longrightarrow \min,$$

Fig. 3.1: L^1 *norm E of difference between numerical and exact solution with respect to mesh refine-ment (each refinement introduces four times finer mesh) for various choices of volume fractions η of the first phase (Subsection 3.1).*
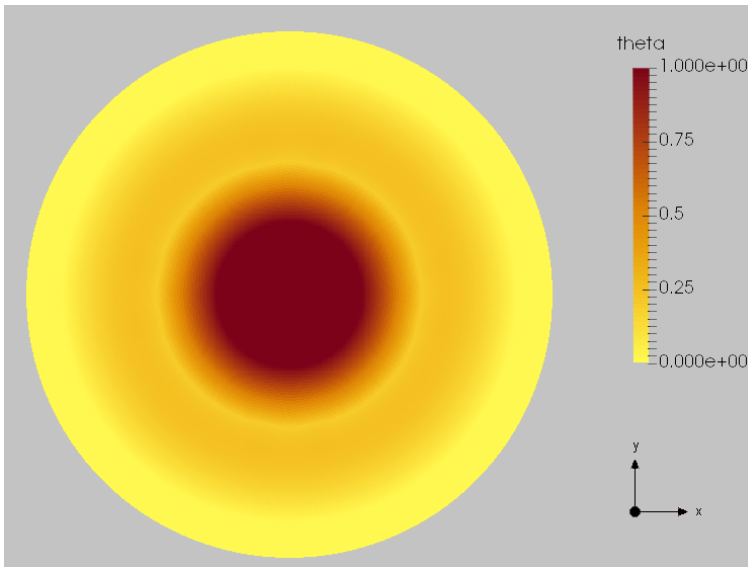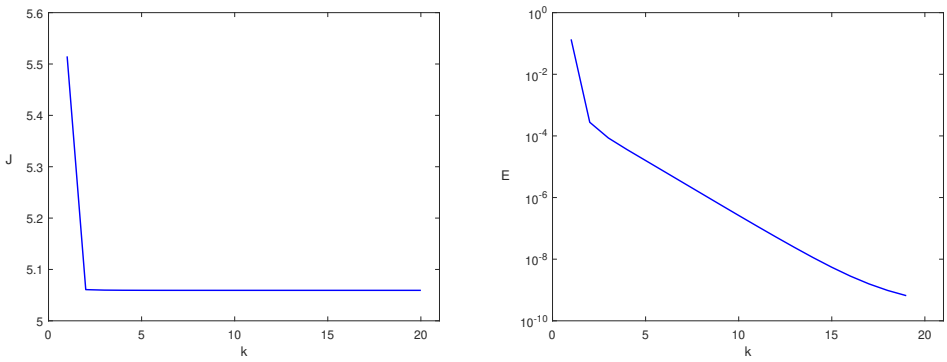

Fig. 3.2: *Optimal distribution of materials with volume fraction $\eta = 0.25$ of the first phase – Subsection 3.1.*

within an annulus $B(\mathbf{0};1,2) \subseteq \mathbf{R}^2$, with inner radius 1 and outer radius 2 and the state equation

$$\begin{cases} -\mathsf{div}\,(\mathbf{A}\nabla u) = 1 \\ u \in \mathrm{H}_0^1(\Omega). \end{cases} \tag{3.2}$$

(a) Cost functional J in terms of the iteration number k.

(b) $E = \|\theta^k - \theta^{k+1}\|_{L^2}^2$ in terms of the iteration number k.

Fig. 3.3: *Convergence history with volume fraction $\eta = 0.25$ of the first phase – Subsection 3.1.*
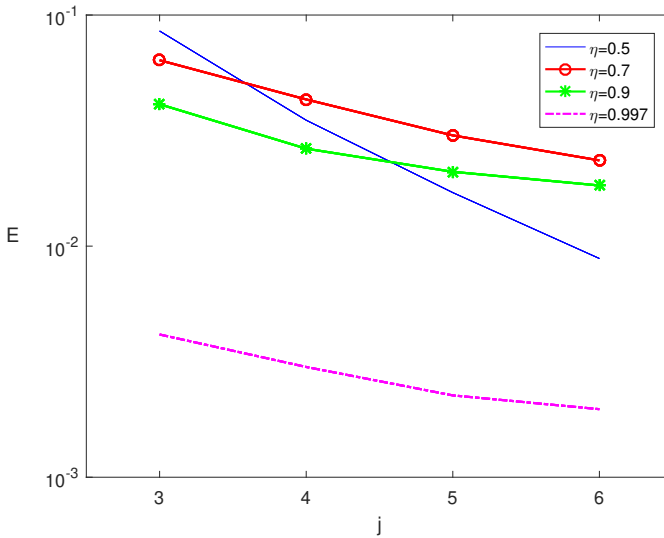
Fig. 3.4: *L^1 norm E of difference between numerical and exact solution with respect to mesh refinement (each refinement introduces four times finer mesh) for various choices of volume fraction η of the first phase (Subsection 3.2).*

Exact solution for this example is calculated in [5], which allows us to compare our numerical solution to the exact one. The L^1 error between the numerical and exact solutions is given in Figure 3.4 for various $0 < \eta < 1$ and it is again a decreasing function with respect to mesh refinement.

Optimal distribution with 50% of the first material is shown in Figure 3.5, while convergence histories of the cost functional and the approximation error are illustrated in Figure 3.6.
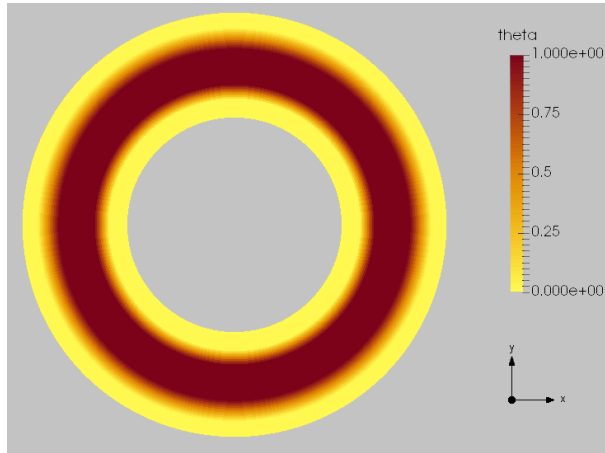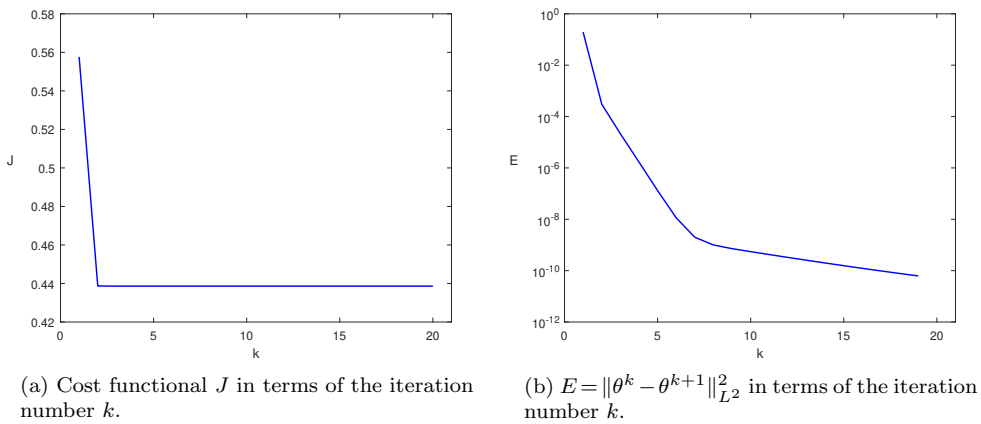
Fig. 3.5: *Optimal distribution of materials with volume fraction $\eta = 0.5$ of the first phase – Subsection 3.2.*

(a) Cost functional J in terms of the iteration number k.

(b) $E = \|\theta^k - \theta^{k+1}\|_{L^2}^2$ in terms of the iteration number k.

Fig. 3.6: *Convergence history with volume fraction $\eta = 0.5$ of the first phase – Subsection 3.2.*

We can conclude from both examples that the optimality criteria method proposed in Section 2 gives a good approximation of the exact solution.

3.3. Two-state problem on a cube. The third example is the three-dimensional energy minimization problem

$$J(\theta, \mathbf{A}) = \int_\Omega (f_1 u_1 + f_2 u_2) \, d\mathbf{x} \longrightarrow \min,$$

with $\alpha = 1$, $\beta = 2$ and two state equations

$$\begin{cases} -\mathsf{div}\,(\mathbf{A}\nabla u_i) = f_i, \\ u_i \in \mathrm{H}_0^1(\Omega) \end{cases}, \quad i = 1, 2. \tag{3.3}$$

(a) Outer look.

(b) Intersection of the cube with $x=0$ plane.
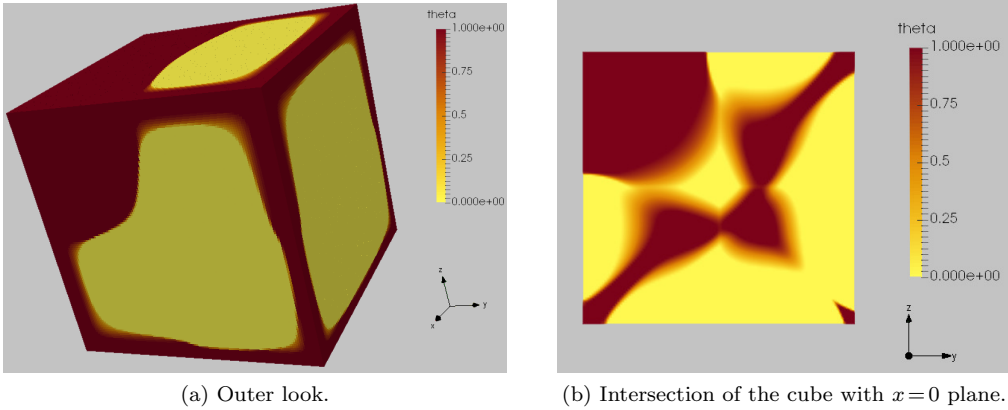
Fig. 3.7: *Numerical solution for Subsection 3.3 with volume fraction $\eta=0.5$ of the first phase.*

(a) Cost functional J in terms of the iteration number k.

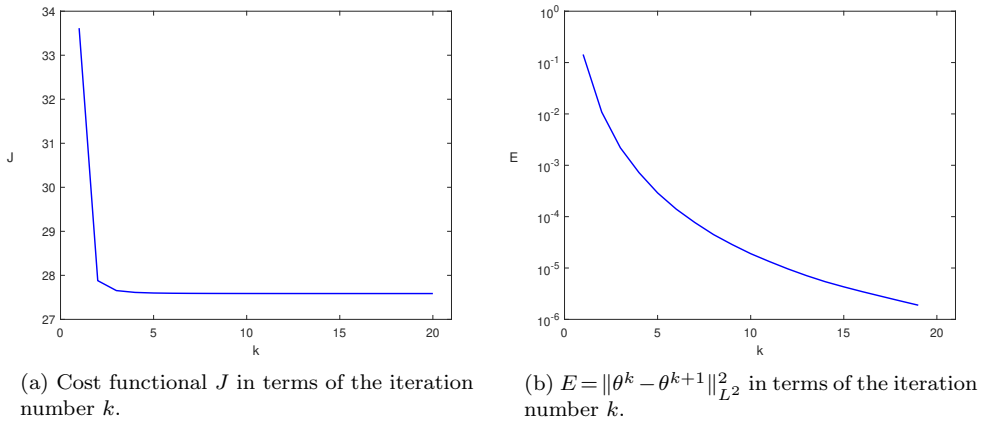(b) $E=\|\theta^k-\theta^{k+1}\|_{L^2}^2$ in terms of the iteration number k.

Fig. 3.8: *Convergence history with volume fraction $\eta=0.5$ of the first phase - Subsection 3.3.*

We take a cube $\Omega=[-1,1]^3$ as the domain and set function f_1 to be zero on the upper half ($z>0$) and 10 on the lower half of the cube, while function f_2 to be zero on the left half ($y<0$) and 10 on the right half of the cube. Optimal design of the 20-th iteration of the Algorithm 2.1 with volume fraction $\eta=0.5$ of the first material is shown in Figure 3.7a. Material with greater conductivity is placed at the center of the cube and on the sides, which can be seen in Figure 3.7b. Most of the upper left part of the cube is occupied by the material with smaller conductivity, which is expected because there is no external source on this part of the domain. Convergence history of the cost functional and the residual are given in Figure 3.8.

3.4. Non self-adjoint problem on a cube. Let us now consider a non self-adjoint two-state minimization problem, where the cost functional is given by

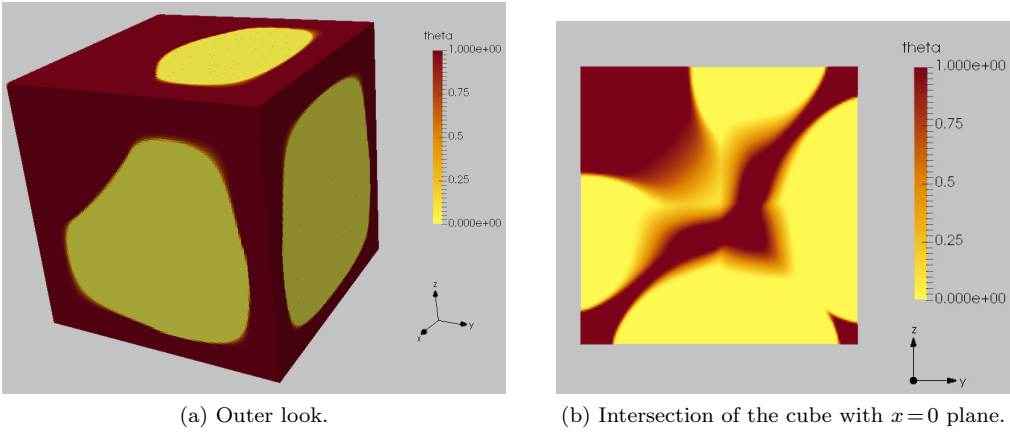$$J(\theta,\mathbf{A})=\int_\Omega (u_1^2+u_2^2)\,d\mathbf{x}.$$

(a) Outer look.

(b) Intersection of the cube with $x=0$ plane.

Fig. 3.9: *Numerical solution for Subsection 3.4 with volume fraction $\eta=0.5$ of the first phase.*

(a) Cost functional J in terms of the iteration number k.

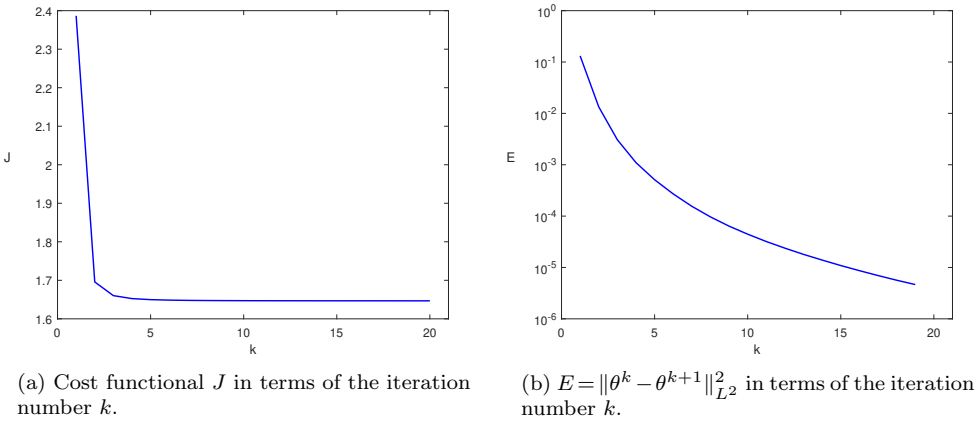(b) $E = \|\theta^k - \theta^{k+1}\|_{L^2}^2$ in terms of the iteration number k.

Fig. 3.10: *Convergence history with volume fraction $\eta=0.5$ of the first phase - Subsection 3.4.*

We take state equations (3.3) and domain $\Omega = [-1,1]^3$, with f_1 and f_2 being similar as in Subsection 3.3. In this case, the adjoint equations are given by

$$\begin{cases} -\mathrm{div}\,(\mathbf{A}\nabla p_i) = 2u_i \\ p_i \in \mathrm{H}_0^1(\Omega) \end{cases}, \quad i=1,2. \tag{3.4}$$

Optimal distribution of materials with conductivites $\alpha=1$ and $\beta=2$ is presented in Figure 3.9a, while intersection of the domain with the $x=0$ plane is given in Figure 3.9b. Convergence history is given in Figure 3.10.

4. Conclusion

In this paper, we were dealing with multiple state optimal design problems for stationary diffusion equation. We derived another variant of the optimality criteria method for (two- and three-dimensional) optimal design problems. Although the method relies on complicated formulae, it can be implemented quite effectively with almost explicit

update formulae for the design variables. As tested on many examples, this numerical method shows good convergence properties revealing an optimal design in very few iterations. Moreover, the convergence seems indifferent to the initial design, and behaves well on mesh refinement.

The method is written for general functionals, and it appears to suit well for problems of minimizing a conic sum of energies, contrary to the variant presented in [20]. In more complicated situations, it is expected that a combination of these two variants would be the right choice.

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