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Optimal material properties for transient problems

S. Turteltaub

Abstract The aim of this article is to analyze the problem of optimizing material properties within the context of a time-dependent problem. The objective is to minimize the difference between the actual values of a field variable and a desired "target" distribution after a prescribed time T. The field variable is related to a transient physical phenomenon with given initial and boundary conditions. The time-independent material properties are taken as the design variables. For simplicity, only the case of transient heat conduction is analyzed, though the method can be naturally extended to elastodynamics. Examples and test cases are solved numerically for different types of boundary conditions and target functions using a scaled-gradient method. The scaling function serves the purpose of satisfying constraints, but can also be used as an implicit penalty formulation to obtain optimal topologies by introducing an additional bias in the scaling. Its performance is compared to the unbiased method.

Key words transient problems, time-dependence, material properties, heat conduction, SIMP method

1 Introduction

The problem of obtaining optimal material properties in the context of a transient phenomenon, such as heat conduction or elastodynamics, can be referred to as a time-dependent optimal design problem, as an optimal control problem, or even as a parameter identification problem. Regardless of its classification, this problem is relevant in structural optimization, in particular in the context of design for crashworthiness. As a model problem for a time-dependent phenomenon, transient heat conduction is considered here, though one can easily extend the formulation for, e.g. impact problems.

The optimal design problem considered here can be described as follows: the purpose is to specify a distribution of material properties within a given domain Ω such that the temperature field at a given time T is as close as possible to a target field $\theta_T = \theta_T(\mathbf{x})$. The minimization in this problem is performed in a least-square sense.

Although optimal control problems have been studied in great detail, typically the "controls" are taken as either variable boundary conditions or body (source) terms, whereas the material properties are considered fixed (see e.g. Carthel *et al.* 1994). In the foregoing analysis, following an approach commonly used in structural optimization, the boundary conditions are assumed to be given (even though they might be time-dependent), whereas the material properties are taken as the design variable.

The optimization of material properties within the context of a transient problem has received attention for high temperature/ high strength applications using functionally graded materials—which essentially are inhomogeneous composite materials (see e.g. Tanaka *et al.* 1996). Optimal distributions of material properties for thermal and mechanical problems, as well as optimal boundary and source control for parabolic and hyperbolic problems are areas of active research. A related problem is the so-called inverse heat conduction problem (see Dorai and Tortorelli 1997).

Functionally graded materials (as well as classical composite materials) can be tailored in order to have varying macroscopic material properties throughout a structure. Depending on the design context, one can use several methods to parameterize the material properties [using, e.g. homogenization theory, a free-material formulation or a solid isotropic material with penalization (SIMP) to name a few (Bendsøe 1995)]. An approach similar to the SIMP method is adopted in the present analysis, where it is assumed that the medium is composed of two homogeneous, isotropic, constitutively linear materials. The penalization, however, is enforced implicitly via a scaled gradient, which also serves the purpose of satisfying some box constraints. It is important to note that,

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even though the target function is defined in terms of the field variable, this approach offers certain flexibility in the sense that related quantitites, such as the gradient of the field variable, can be controlled to a certain extent via a suitable specification of θ_T.

The present communication is organized as follows. Section 2 covers some preliminary topics relevant to the optimization problem, which is subsequently formulated in Sect. 3. Aspects related to a resource constraint and the boundary conditions are also mentioned in that section. The gradient of the objective functional and first-order optimality conditions are developed in Sect. 4. Some remarks about regularization, penalty formulations and scaling of the gradient are included in Sect. 5. Subsequently, an algorithm used to obtain numerical solutions is covered in Sect. 6 while test problems and examples are presented in Sect. 7. Finally, some closing remarks about the method and possible applications are included in the last section.

2 Preliminaries

Consider a simply-connected regular domain Ω, whose boundary $\partial\Omega$ is divided into two disjoint parts: $\partial\Omega_q$, on which *heat flux* is prescribed, and $\partial\Omega_h$, on which heat is exchanged with the environment following a cooling (or heating) law. It is assumed that inside the domain Ω there is an isotropic, heat conducting material that satisfies Fourier's law, i.e.

$$\mathbf{q} = \kappa \nabla\theta \,, \tag{1}$$

where $\mathbf{q} = \mathbf{q}(\mathbf{x}, t)$ is the heat flux vector, $\kappa = \kappa(\mathbf{x})$ is the thermal conductivity field and $\theta = \theta(\mathbf{x}, t)$ is the temperature field. For design purposes, suppose that one disposes of two homogeneous, isotropic, linearly conducting materials with respective conductivities $\overline{\kappa}_1$ and $\overline{\kappa}_2$, mass densities $\overline{\rho}_1$ and $\overline{\rho}_2$ and specific heats at constant deformation $\overline{c}_1$ and $\overline{c}_2$. It is convenient to define the product $\overline{\beta}_i = \overline{\rho}_i \overline{c}_i$, $i = 1, 2$ and to normalize the properties as follows: suppose $\overline{\kappa}_1 \geq \overline{\kappa}_2$ and define

$$\kappa = \frac{\overline{\kappa}}{\overline{\kappa}_1} \,, \quad \beta = \frac{\overline{\beta}}{\overline{\kappa}_1} \,.$$

With this convention, κ now has a (nondimensional) minimum value of $\kappa_2 = \overline{\kappa}_2/\overline{\kappa}_1$ and a maximum value of $\kappa_1 = 1$. The ratio β (inverse of thermal diffusivity) is typically greater in magnitude (numerically) than κ in SI units. Classical linear heat conduction has no intrinsic length scale, although it is common practice to introduce some arbitrary length parameter (often related to the geometry of the domain Ω) and define nondimensional space and time variables. Although this approach will not be used in this analysis, the dimensions of the domain will be chosen on the order of magnitude of unity, hence time and space variables would be numerically similar to nondimensional quantities.

For the purposes of the present analysis, since the main objective is to study a time-dependent physical problem, a simple material parameterization scheme is used. In particular, suppose that at a point $\mathbf{x}$ the thermal properties of a body occupying the region Ω are given in terms of a function $\omega = \omega(\mathbf{x})$ as follows:

$$\kappa(\omega) = \omega\kappa_1 + (1-\omega)\kappa_2 \,, \beta(\omega) = \omega\beta_1 + (1-\omega)\beta_2 \,. \tag{2}$$

Henceforth, the function ω is referred to as the design variable. Some restrictions on the admissible functions ω will be introduced in the next section.

The function ω can have several interpretations. A natural view point is to consider ω as a characteristic function for material 1 defined as $\omega(\mathbf{x}) = 1$ if $\mathbf{x} \in \Omega_1$ and $\omega(\mathbf{x}) = 0$ if $\mathbf{x} \in \Omega_2$, where $\Omega_i \subset \Omega$ (not necessarily simply-connected) correspond to the regions occupied by material $i = 1, 2$ within Ω. A second view point is to consider (2) as an upper bound for effective properties of a statistically isotropic composite, with ω playing the role of a volume fraction of material 1 instead of a characteristic function. In that case, one can consider *continuous* functions ω such that $0 \leq \omega(\mathbf{x}) \leq 1$. In a topology optimization problem, one approach is to approximate a (discontinuous) characteristic function with a continuous function ω and penalize values between 0 and 1 (see Bendsøe and Sigmund 1999, for a review on material interpolation schemes). In the foregoing analysis, ω is assumed to be *continuous*. If one is interested in obtaining a distribution such that ω is close to either 0 or 1, then a penalty scheme should be introduced to drive the design variable to its lower or upper values. To this end, an implicit penalty scheme (similar to the SIMP method) is introduced in Sect. 6 within the context of the numerical implementation of the method.

For a given field ω, the temperature $\theta = \theta(\omega)$ is the solution to the following initial boundary-value problem:

$$\text{(P)} \begin{cases} \operatorname{div} \mathbf{q}(\mathbf{x}, t) - \beta(\mathbf{x})\dot{\theta}(\mathbf{x}, t) = 0 & \text{in } \Omega \times (0, T] \,, \\ \mathbf{q}(\mathbf{x}, t) \cdot \mathbf{n} = q_0(\mathbf{x}, t) & \text{on } \partial\Omega_q \times (0, T] \,, \\ \mathbf{q}(\mathbf{x}, t) \cdot \mathbf{n} = h(\theta^a - \theta(\mathbf{x}, t)) & \text{on } \partial\Omega_h \times (0, T] \,, \\ \theta(\mathbf{x}, 0) = \theta^0(\mathbf{x}) & \text{in } \Omega \,, \end{cases}$$

where $\mathbf{q}$ is given by the constitutive assumption (1), $\kappa(\mathbf{x})$ and $\beta(\mathbf{x}) = \rho(\mathbf{x})c(\mathbf{x})$ are given by (2), $\mathbf{n}$ is the normal outward unit vector to the boundary $\partial\Omega$, $q_0 = q_0(\mathbf{x}, t)$ and $\theta^0 = \theta^0(\mathbf{x})$ are prescribed functions, θ^a is a known ambient temperature and the film coefficient h is assumed to be constant (hence, it is assumed that it does not depend on the temperature, or, for design purposes, on ω).

The same letter θ is used to designate the temperature as a function of position and time as well as when it

is viewed as an implicit function of ω. In particular, $\nabla\theta$ and $\dot{\theta}$ refer to the spacial gradient and time derivative of the temperature as a function of position and time (i.e. these are derivatives of a temperature field θ that corresponds to a fixed field ω) whereas the notation θ_ω will be used for the derivative of θ as a function of ω (i.e. considering different temperature fields that satisfy (P), one for each ω).

3
Formulation of the problem

3.1
Preliminaries

To simplify notation, the function space $L_2(\Omega)$ of square-integrable functions along with its norm $\|\cdot\|_{L_2(\Omega)} \equiv \left\{\int_\Omega (\cdot)^2 \, \mathrm{d}v\right\}^{1/2}$ will be used. Define the objective functional J as

$$J[\omega] = \tfrac{1}{2}\int_\Omega \left[\theta(\mathbf{x},T) - \theta_T(\mathbf{x})\right]^2 \, \mathrm{d}v =$$

$$\tfrac{1}{2}\left\|\theta(\cdot,T) - \theta_T\right\|^2_{L_2(\Omega)} \, . \tag{3}$$

Suppose that ω belongs to some function space X with norm $\|\cdot\|_X$, to be defined later. In view of (2), the values of ω are constrained to lie in the interval $[\omega_m, \omega_M]$, with $\omega_m = 0$, $\omega_M = 1$. Additional restrictions on the design space are necessary to ensure that ω has the required properties. In particular, its X-norm is assumed to lie below some value R, which is chosen from the outset, i.e. the resource constraint is

$$\|\omega\|_X \leq R \, . \tag{4}$$

One function space that will be considered in subsequent sections is $X = H^1(\Omega)$ with corresponding norm $\|\omega\|_{H^1(\Omega)} \equiv \left\{\int_\Omega \left(\omega^2 + \nabla\omega\cdot\nabla\omega\right) \, \mathrm{d}v\right\}^{1/2}$. In this case, the value R serves to bound the amount of material 1 used, but also restricts the gradient of ω. However, other less restrictive choices for X can also be considered.

3.2
Formulation of the problem

In general, define the design space $\mathcal{A}$ as

$$\mathcal{A} = \left\{\, \omega \in X \mid \omega_m \leq \omega \leq \omega_M \, , \; \|\omega\|_X \leq R \right\} \, .$$

The objective functional J given by (3) is seen as a function of ω only since the temperature field at time T is an implicit function of the material properties. With this interpretation, the optimization problem can be expressed as follows:

$$\text{(O)} \begin{cases} \text{find } \omega_0 \in \mathcal{A} \text{ such that} \\ J[\omega_0] \leq J[\omega] \qquad \forall \omega \in \mathcal{A} \, . \end{cases}$$

3.3
Further remarks on the resource constraint

The constraint (4) can be interpreted as a "cost" due to the use of material 1, however, the choice of an "expensive" material is problem-dependent and does not necessarily have the same interpretation as in the minimum compliance problem. Typically, in a structural optimization problem (or in microstructural optimization of material properties of a composite), the stiffer material is assumed to be more expensive. In the foregoing problem, it is not clear from the outset that a better or worse conducting material, or a material with higher or lower specific heat might be more convenient to use. This depends strongly on the initial values, boundary conditions, the choice of a target field and even the time T. The working assumption is that one decides from the outset that one material is more "expensive" than the other. In this case, material 1 (which is chosen to have higher values of its material properties), is assumed to be more expensive. It is possible that this restriction is unnecessary, though this is verified a posteriori; hence it is possible that the constraint on $\|\omega\|_X$ might not be active [a similar situation occurs in a problem with a design-dependent body force analyzed by Turteltaub and Washabaugh (1999)]. In particular, the limit case of an optimal design with pure material 2 ($\omega \equiv 0$) is not excluded. Depending on the choice of the design space, the X-norm of ω can measure the amount of material used, but can also include measures of spacial fluctuations of ω. In particular, if one chooses $X = H^1(\Omega)$, then discontinuities in ω are precluded (though kinks are admissible). Following similar concepts used in topology optimization, very rapid oscillations of ω as a function of position (which could be interpreted as "formation of microstructure") are not allowed to occur if one enforces a restriction such as (4) with a suitably-chosen space X (see also Sigmund and Petersson 1998).

3.4
Boundary conditions and target function

If the source term in the physical problem is zero (as is assumed here), then observe that prescribing temperature only on the boundary can lead to a singular problem. Due to the linearity of the constitutive assumptions, the optimization problem (O) might admit multiple solutions since a prescribed temperature on the boundary does not depend on ω. A simple example to illustrate this point is

as follows: suppose $\beta_1/\kappa_1 = \beta_2/\kappa_2$ and constant temperature is prescribed on $\partial\Omega$ for all $t \in (0,T]$. The temperature field in problem (P) corresponding to $\omega \equiv 0$ is the same as the field corresponding to $\omega \equiv 1$ (with the same initial temperature). This problem does not arise if one prescribes flux or natural convection boundary conditions on, at least, part of the boundary $\partial\Omega$.

In general, one cannot expect to obtain $J = 0$ if the function θ_T does not satisfy certain requirements. In particular, θ_T has to be compatible with the boundary conditions; if, for example, $\theta_T(\mathbf{x}) \equiv$ constant, then $\nabla\theta_T \equiv 0$ and the boundary conditions cannot be satisfied by a temperature field $\theta = \theta_T$ if nonzero flux is prescribed on the boundary. Presumably, a temperature field θ_T has to be achievable for some distribution of material properties, otherwise the procedure can only find the closest distribution of material properties for that target field. Nonetheless, since in practical applications this might be the norm rather than the exception, an example in which the target θ_T is not compatible with the boundary is considered in Sect. 7.

4 Gradient and optimality conditions

As a preliminary step in the implementation of the numerical algorithm used for the solution of problem (O), one needs to compute the gradient of the objective functional with respect to the design variable. The gradient can be obtained via a formal perturbation analysis (see e.g. Glowinski *et al.* 1981; Tortorelli and Haber 1989). To this end, consider a functional L that corresponds to J augmented with the constraint $\|\omega\|_X - R \leq 0$ (the local constraints $\omega_m \leq \omega \leq \omega_M$ will be handled separately). The first variation of L with respect to ω is

$$\delta L[\omega, \Lambda; \delta\omega] =$$

$$\langle \theta(\cdot,T) - \theta_T(\cdot)\,, \theta_\omega(\cdot,T)\delta\omega\rangle_{L_2(\Omega)} + \langle \Lambda\,, \delta\omega\rangle_X\,, \tag{5}$$

where $\delta\theta = \theta_\omega\delta\omega$ is a perturbation of θ induced by $\delta\omega$, θ_ω is the derivative of θ with respect to the design variable and Λ is a Lagrange multiplier related to the resource constraint. To actually obtain the gradient, one has to express the first term in (5) in the form $\langle G\,, \delta\omega\rangle_X$ (i.e. using the scalar product of the design space $\mathcal{A}$). This is accomplished in two steps. The first step is to determine $\delta\theta(\cdot,T) = \theta_\omega(\cdot,T)\delta\omega$ (the Fréchet derivative in the direction of $\delta\omega$) in terms of the solution η of an adjoint problem. The second step is to identify G, which, in view of (5), corresponds to $\theta^*_\omega(\cdot,T)e$, where θ^*_ω is the adjoint of $\theta_\omega(\cdot,T)$ with respect to the X-norm and $e \equiv \theta(\cdot,T) - \theta_T(\cdot)$ (observe that these are functions of position only and are evaluated at a specific ω). The function e measures the pointwise error between the actual field and the target at time T.

A formal perturbation in (P) provides the following initial-boundary value problem satisfied by $\delta\theta(\mathbf{x},t)$ i.e.

$$\left.\begin{aligned} &\operatorname{div}\delta\mathbf{q} = \delta(\beta\dot\theta) && \text{in } \Omega\times(0,T]\,,\\ &\delta\mathbf{q}\cdot\mathbf{n} = 0 && \text{on } \partial\Omega_q\times(0,T]\,,\\ &\delta\mathbf{q}\cdot\mathbf{n} = -h\delta\theta && \text{on } \partial\Omega_h\times(0,T]\,,\\ &\delta\theta(\mathbf{x},0) = 0 && \text{on } \Omega\,, \end{aligned}\right\} \tag{6}$$

where

$$\delta(\beta\dot\theta) = (\beta_\omega\delta\omega)\dot\theta + \beta\delta\dot\theta\,, \quad \delta\mathbf{q} = \kappa_\omega\delta\omega\nabla\theta + \kappa\nabla\delta\theta\,, \tag{7}$$

and, from (2), $\kappa_\omega = (\kappa_1 - \kappa_2)$ and $\beta_\omega = (\beta_1 - \beta_2)$. Let η be a scalar-valued function defined in $\Omega\times[0,T]$. Consider the integral in $\Omega\times[0,T]$ of the governing equation in (6) multiplied by η. Integrating by parts, and in view of (7) and the initial and boundary conditions in (6), one has, after rearranging some terms,

$$\begin{aligned} &\int_\Omega\left[\int_0^T\left(\kappa_\omega\nabla\eta\cdot\nabla\theta + \beta_\omega\eta\dot\theta\right)\,\mathrm{d}t\right]\delta\omega\,\mathrm{d}v =\\ &-\int_0^T\int_{\partial\Omega_h}(h\eta + \kappa\nabla\eta\cdot\mathbf{n})\,\delta\theta\,\mathrm{d}a\,\mathrm{d}t -\\ &\int_0^T\int_{\partial\Omega_q}(\kappa\nabla\eta\cdot\mathbf{n})\delta\theta\,\mathrm{d}a\,\mathrm{d}t +\\ &\int_0^T\int_\Omega(\operatorname{div}(\kappa\nabla\eta) + \beta\dot\eta)\,\delta\theta\,\mathrm{d}v\,\mathrm{d}t -\\ &\int_\Omega\beta\eta(\mathbf{x},T)\delta\theta(\mathbf{x},T)\,\mathrm{d}v\,. \end{aligned} \tag{8}$$

Choose η such that it corresponds to the weak solution of the following adjoint[1] problem, i.e.

$$(\mathrm{P}')\quad\begin{cases} \operatorname{div}(\kappa\nabla\eta) + \beta\dot\eta = 0\,, & \text{in } \Omega\times(T,0]\,,\\ \kappa\nabla\eta\cdot\mathbf{n} = 0 & \text{on } \partial\Omega_q\times(T,0]\,,\\ \kappa\nabla\eta\cdot\mathbf{n} = -h\eta & \text{on } \partial\Omega_h\times(T,0]\,,\\ \beta\eta(\mathbf{x},T) = e(\mathbf{x}) & \text{in } \Omega\,. \end{cases}$$

In particular, choosing $e(\mathbf{x}) = \theta(\mathbf{x},T) - \theta_T(\mathbf{x})$ as an "initial" condition will be useful in the computation of the gradient of the objective functional, as shown below. Observe that problem (P′) is solved from time $T > 0$ to time 0. It is well-posed since the sign in front of $\dot\eta$ is positive[2] If

[1] The word adjoint is used here in the context of the differential operator $L(\cdot) = \operatorname{div}(\kappa\nabla(\cdot)) - \beta\partial(\cdot)/\partial t$ that governs the parabolic heat conduction problem. The adjoint is $L^*(\cdot) = \operatorname{div}(\kappa\nabla(\cdot)) + \beta\partial(\cdot)/\partial t$ and is obtained in a different context than the adjoint of θ_ω referred to earlier. However, as shown below, η is related to the adjoint of θ_ω acting on a function e.

[2] This equation can be seen as a "backwards" equation, though it is different from the backward heat conduction problem, which is intrinsically unstable.

η satisfies problem (P′) with $e(\mathbf{x}) = \theta(\mathbf{x}, T) - \theta_T(\mathbf{x})$, then, from (8),

$$\int_\Omega e\delta\theta(\cdot, T)\,\mathrm{d}v =$$
$$-\int_\Omega \left[\int_0^T \left(\kappa_\omega \nabla\eta\cdot\nabla\theta + \beta_\omega \eta\dot{\theta}\right)\,\mathrm{d}t\right]\delta\omega\,\mathrm{d}v\,.$$

In view of (5) and the previous relation, the first variation of L can be written as

$$\delta L[\omega, \Lambda; \delta\omega] = \langle g\,, \delta\omega\rangle_{L_2(\Omega)} + \langle \Lambda\,, \delta\omega\rangle_X\,, \tag{9}$$

where

$$g(\mathbf{x}) = -\int_0^T \left(\kappa_\omega \nabla\eta\cdot\nabla\theta + \beta_\omega \eta\dot{\theta}\right)\,\mathrm{d}t\,. \tag{10}$$

4.1
Transition to X-topology

The function g can be used to determine the (unconstrained) gradient. The local constraints on ω are $(\omega_m - \omega) \le 0$ and $(\omega - \omega_M) \le 0$ (with $\omega_m = 0$ and $\omega_M = 1$ in this case). If, as it might be expected, some of the constraints are active (satisfied as equalities during an iterative solution process of problem (O) and/or for the solution ω_0), one can introduce Lagrange multipliers $\lambda_m(\mathbf{x}) \ge 0$ and $\lambda_M(\mathbf{x}) \ge 0$ associated with local lower and upper bounds for ω. For points $\mathbf{x}$ where the constraints are not active, $\lambda_M = \lambda_m = 0$. In general, one has to add the term $(\lambda_M - \lambda_m)$ to g in order to take the constraints into account. In the numerical algorithm presented below, however, only the constraint $\|\omega\|_X \le R$ is incorporated explicitly in the gradient. The pointwise constraints will be handled separately, both by using a scaling factor on the gradient and by enforcing them explicitly throughout the solution process.

In order to put (9) in the form $\langle G\,, \delta\omega\rangle_X$, define G as the solution to the following problem: given g (as in (10), or modified to incorporate local Lagrange multipliers if necessary), find G such that

$$\langle G\,, v\rangle_X = \langle g\,, v\rangle_{L_2(\Omega)}\,, \quad \forall v \in X\,. \tag{11}$$

Observe that if $X = L_2(\Omega)$, then this last step is not required since $G = g$, though in principle this function space might not be suitable for an optimal topology problem. If, on the other hand, one uses $X = H^1(\Omega)$, then G corresponds to the (weak) solution of

$$-\Delta G + G = g \quad \text{in}\,\Omega\,, \quad \nabla G\cdot\mathbf{n} = 0 \quad \text{on}\,\partial\Omega\,.$$

In general, since $\delta L[\omega, \Lambda; \delta\omega] = \langle G + \Lambda\,, \delta\omega\rangle_X$ for all $\delta\omega$, then the gradient of the objective functional can be written as

$$L' = G + \Lambda\,.$$

4.2
Optimality conditions

For the optimal distribution of material properties ω_0, the optimality condition (first-order Karush-Kuhn-Tucker condition) can be expressed as

$$\lambda_m \ge 0, \quad \lambda_M \ge 0, \quad \Lambda \ge 0\,,$$
$$\lambda_m(\omega_m - \omega_0) \le 0, \quad \lambda_M(\omega_0 - \omega_M) \le 0\,,$$
$$\Lambda\,\{\|\omega_0\|_X - R\} \le 0\,,$$

and

$$\begin{aligned}
&\text{if } \omega_0(\mathbf{x}) = \omega_m = 0 \quad \Rightarrow \quad G(\mathbf{x}) + \Lambda \ge 0\,,\\
&\text{if } \omega_m < \omega_0(\mathbf{x}) < \omega_M = 1 \quad \Rightarrow \quad G(\mathbf{x}) + \Lambda = 0\,,\\
&\text{if } \omega_0(\mathbf{x}) = \omega_M = 1 \quad \Rightarrow \quad G(\mathbf{x}) + \Lambda \le 0\,.
\end{aligned} \tag{12}$$

In the previous relations, all quantities are evaluated using the fields θ and η that correspond to the solutions of problems (P) and (P′) with $\omega = \omega_0$.

5
Scaling and penalty formulations

In view of (12) and using an approach similar to the one proposed by Coleman and Li (1996) (see also Ulbrich *et al.* 1999), the first-order KKT conditions can also be expressed in a single expression using a scaling S such that

$$S(\mathbf{x}) \begin{cases} = 0 & \text{if } \omega(\mathbf{x}) = \omega_m \text{ and } G + \Lambda \ge 0\,,\\ > 0 & \text{if } \omega_m < \omega(\mathbf{x}) < \omega_M\,,\\ = 0 & \text{if } \omega(\mathbf{x}) = \omega_M \text{ and } G + \Lambda \le 0\,. \end{cases}$$

With this scaling, the optimality conditions can be combined into a single relation, i.e. $S(G + \Lambda) = 0$. One possible choice for S is as follows:

$$S(\mathbf{x}) = \begin{cases} (\omega_M - \omega(\mathbf{x}))^{1/p} & \text{if } G + \Lambda < 0\\ (\omega(\mathbf{x}) - \omega_m)^{1/p} & \text{if } G + \Lambda \ge 0\,, \end{cases} \tag{13}$$

with $p \ge 1$. The purpose of this scaling is to handle the local constraints $\omega_m \le \omega$ and $\omega \le \omega_M$. In a gradient-based iterative numerical method, if at some iteration k the current approximation $\omega^{(k)}$ lies inside the "box" $\omega_m \le \omega \le \omega_M$, the next iterate $\omega^{(k+1)}$ tends to remain in the interior or on the boundary of the box. This occurs because the scaling function gradually tends to zero for values of ω close to the lower and upper values (nonetheless, one has to additionally enforce the local constraints explicitly). In principle this introduces a bias, though for some well-chosen values of p this bias is negligible and the method shows an improved behaviour compared to the unscaled case (see Ulbrich *et al.* 1999). Nonetheless, other scaling functions will be considered in Sect. 7 where the bias is important.

5.1
Regularization and norm constraint

It is worth pointing out that a regularizing term such as $\frac{1}{2}\epsilon^2 \|\omega\|_X^2$ is often added to the objective functional to avoid instabilities with respect to perturbations of the target function. The parameter ϵ typically has to be chosen on the order of magnitude of the perturbations. In that case, the gradient contains the additional term $\epsilon\omega$. Observe that this term plays a similar role compared to the Lagrange multiplier Λ (see also Heinkenschloss 1993, 1998). One important difference, however, is that the regularization term $\epsilon\omega$ in the gradient is generally nonzero even if the constraint $\|\omega\|_X \leq R$ is satisfied as a strict inequality, whereas the term Λ associated to the norm constraint would be zero. Nonetheless, numerical experiments with and without the regularization term $\frac{1}{2}\epsilon^2 \|\omega\|_X^2$ showed that even when Λ was zero, this additional term was not essential from a practical point of view.

5.2
Penalty formulations and scaling

If one would like to obtain the so-called optimal topology ("solutions" where ω is either equal to $\omega_m(=0)$ or $\omega_M(=1)$), then some type of penalty formulation should be used to force ω towards its lower and upper values. Ideally, a penalty formulation should have a minimal effect on the main ingredient of the objective functional (in this case J). Often, a penalty term such as $\epsilon \|(\omega-\omega_m)(\omega_M-\omega)\|_X$ is added to J, hence the gradient is augmented by a term $\epsilon[(\omega_m+\omega_M)-2\omega]$ which is negative if $\omega > (\omega_m+\omega_M)/2$ and positive otherwise. This additional term modifies the gradient such that in an iterative gradient-based numerical method, an intermediate $\omega^{(k)}$ at iteration k tends to increase if it is above the mean value $(\omega_m+\omega_M)/2$ and decrease otherwise. Unfortunately, such penalty terms only have a weak coupling with the actual objective functional. One has to find some reasonable balance between two competing terms (i.e. J and $\epsilon \|(\omega-\omega_m)(\omega_M-\omega)\|_X$) by choosing an appropriate value for ϵ. This task is sometimes nontrivial and often fairly arbitrary.

Other penalty formulations, such as the SIMP method, are based on a multiplicative coupling between the objective functional J and the penalty formulation. This is achieved by replacing ω by ω^n, n being a penalty power. Therefore, in view of (2), the unconstrained gradient is scaled in the SIMP method by a factor $n\omega^{n-1}$. This approach has proven more reasonable in the sense that the optimal topology is obtained via a stronger coupling with the main design objective (i.e. J). Observe, however, that this penalty formulation should not be used directly if one implements a scaling function such as (13) unless the sign of the gradient is taken into account.

For the present problem, an approach that combines the scaling function (13) with a penalty formulation similar to the SIMP method is implemented. In particular, the penalty is introduced implicitly via a strong bias in the scaling function S. The basic idea is to choose a function S such that at every iteration of the numerical procedure (shown in Sect. 6), the updated ω follows the direction of a biased gradient, which is amplified for values of ω farther away from the lower or upper values (0 or 1). This can be accomplished by defining a new scaling function S^* as follows:

$$S^*(\mathbf{x}) = \begin{cases} 1 & \text{if } G+\Lambda < 0 \quad \text{and } \omega < \overline{\omega}\,, \\ \overline{f}(\omega) & \text{if } G+\Lambda < 0 \quad \text{and } \omega \geq \overline{\omega}\,, \\ 1 & \text{if } G+\Lambda \geq 0 \quad \text{and } \omega > \underline{\omega}\,, \\ \underline{f}(\omega) & \text{if } G+\Lambda \geq 0 \quad \text{and } \omega \leq \underline{\omega}\,, \end{cases} \tag{14}$$

where $\overline{f}$ and $\underline{f}$ are convex (biased) functions [as opposed to concave functions used in (12)] that satisfy $\overline{f}(\overline{\omega}) = \underline{f}(\underline{\omega}) = 1$ and $\overline{f}(1) = \underline{f}(0) = 0$. The constants $\overline{\omega}$ and $\underline{\omega}$ can be chosen close to 1 and 0 respectively. This scaling modifies the gradient $G+\Lambda$ such that updates of ω in the algorithm of Sect. 6 are amplified for values of ω which are farther away from 0 or 1. The term "biased" is used here to distinguish S^* from S. The rationale is that in an iterative procedure, at a given iteration k, a decrease of the objective functional is obtained at the preferential expense of values of $\omega^{(k)}$ farther away from 0 and 1 due to the choice of the functions $\overline{f}$ and $\underline{f}$. The method, however, updates $\omega^{(k)}$ taking into account the sign of the gradient at every iteration and stops when no further reduction of J is possible. An example is given in Sect. 7 though, as it is often the case, the "solution" depends on the penalty method.

6
Numerical implementation

The algorithm used for the solution of problem (O) is straight forward.

1. Initialization. Take an arbitrary $\omega = \omega^{(0)}(\mathbf{x})$ such that the global and local constraints are satisfied (either as equality or strict inequality). Choose an arbitrary initial value $\Lambda^{(0)}$ for the Lagrange multiplier.
2. Main loop. From iteration k to iteration $k+1$:
   2.1 Using $\omega = \omega^{(k)}$, solve forward problem (P) and backward problem (P′) to get $\theta^{(k)}$ and $\eta^{(k)}$.
   2.2 Compute $g^{(k)}$ from (10) and $G^{(k)}$ from (11).
   2.3 Update ω as follows:

$$\omega^{(k+1)} = \begin{cases} \omega_m & \text{if } \overline{\omega} \leq \omega_m\,, \\ \overline{\omega} & \text{if } \omega_m < \overline{\omega} < \omega_M\,, \\ \omega_M & \text{if } \overline{\omega} \geq \omega_M\,, \end{cases}$$

   where $\overline{\omega} = \omega^{(k)} - \alpha^{(k)} S\left(G^{(k)} + \Lambda^{(k)}\right)$. The step size $\alpha^{(k)}$ is chosen at every iteration via a line search. The value of $\Lambda^{(k)}$ is computed iteratively

so as to satisfy the constraint (4) (the algorithm allows for $\Lambda^{(k)} = 0$ at any iteration); $\omega^{(k+1)}$ corresponds to the final value in an internal loop to compute $\Lambda^{(k)}$.

3. Convergence test: if $|J^{(k+1)} - J^{(k)}|/J^{(k)} <$ tolerance, then stop, otherwise repeat step 2.

Note that during the solution process, if ω reaches its lower or upper values, the scaling function vanishes and ω remains at that value *only if the gradient is favourable*. If, e.g. $\omega = \omega_m$, then $S = 0$ only if $G + \Lambda \geq 0$, otherwise S jumps to a nonzero value. The nonsmooth behaviour of the scaling function is in fact desirable in order to avoid artificial minima. Other aspects of the numerical implementation are as follows: standard four-node, piecewise linear elements are used for space discretization. Backward Euler integration is used to solve the transient problems with an adaptive scheme. A trapezoidal rule that takes into account the adaptive scheme is used in the discrete version of (10) whereas a 2×2 Gaussian rule is used for all integrals in Ω. A key feature in the numerical implementation is that the field ω was discretized using the same basis functions used for the field variables θ and η. In particular, this means that ω is discretized as a *continuous* function and the capacity and stiffness matrices are computed accordingly.

7 Test cases and examples

In order to verify the method and illustrate its application, two problems are presented in this section. The first one is a test case, which is constructed such that the solution is known a priori. The second one is an example that serves to illustrate two aspects of the problem. Specifically, the target function is chosen so that it is not compatible with the prescribed boundary condition. The same example is used to investigate numerically the use of a biased scaling function.

7.1 Test problem

To construct a solution for a validation problem, one can proceed as follows: choose a specific $\omega = \omega_{\text{test}}$. For example, take

$$\omega_{\text{test}}(\mathbf{x}) = \begin{cases} 0 & \text{if } 0.5 < x_1 < 2.5 \text{ and } 0.5 < x_2 < 1.5\,, \\ 1 & \text{otherwise.} \end{cases}$$

With given initial and boundary conditions, compute the corresponding temperature profile at time T. Next, choose the same profile as the target for a validation problem, i.e. take $\theta_T(\mathbf{x}) \equiv \theta_{\text{test}}(\mathbf{x}, T)$, thus the (known) solution for the validation problem is ω_{test}. In particular, a flux boundary condition on the whole boundary (constant flux q_0 on $\partial\Omega$ was prescribed) together with a uniform initial temperature. An arbitrary initial function ω is chosen to start the optimization procedure. The corresponding (optimal) profile ω_0 is shown in Fig. 1, which agrees well with ω_{test} within the accuracy of the numerical method.

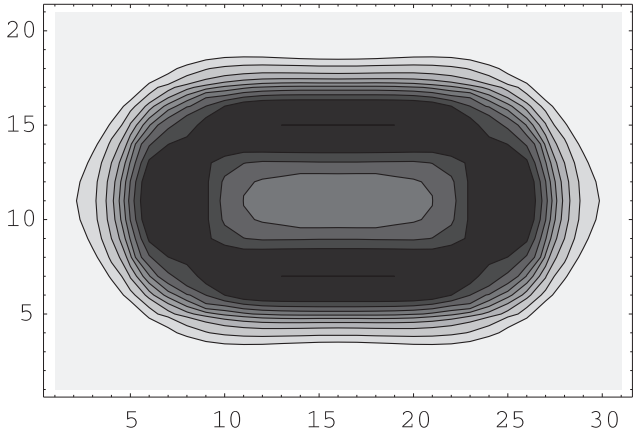

Fig. 1 Optimal distribution of material properties for a test problem using a 30×20 uniform mesh. The lighter areas correspond to higher values of ω_0 (higher conductivity and specific heat)

Other initial functions ω provided similar results. The scaling function used in this test case is (13) with $p = 2$. Both L_2 and H^1 gradients were tested but no significant differences between the two solutions were observed (even though the intermediate steps were in fact different). Nonetheless, using an L_2 gradient and a discretization of ω as a continuous function turned out to be more efficient from a practical point of view, in particular since the transition to a different topology [i.e. problem (11)] was not required. From a theoretical point of view, however, this approach is not consistent since the use of an L_2 gradient calls for an element-wise constant discretization of ω to include discontinuous functions. Nonetheless, the combination of an L_2-gradient and a piecewise linear continuous discretization of ω showed good behaviour in all test cases. The results shown in Fig. 1 were obtained using $q_0 = -10$ (with $\partial\Omega_h = \emptyset$), $T = 10$, $\kappa_1 = 1$, $\kappa_2 = 0.02$, $\beta_1 = 10$, $\beta_2 = 1$ and a uniform initial temperature $\theta^0 = 100$. The domain is a 3×2 rectangle with a 30×20 uniform mesh (the whole domain was discretized; symmetry of the problem was not used). The resource constraint, set at $R = \|\omega_{\text{test}}\|_{L_2(\Omega)}$, was never active throughout the solution process, though $\|\omega_0\|_{L_2(\Omega)}$ was close to R (the initial ω satisfied the constraint as an inequality). Further refinements of the mesh did not modify the solution noticeably.

7.2 Example problem

To investigate the compatibility of the boundary conditions, a noncompatible target function was chosen. In particular, flux is prescribed on the section $1 < x_1 < 2$, $x_2 = 0$ of a 3×2 rectangular domain. Elsewhere on the boundary, natural convection is prescribed. In this example the following data were used: $q_0 = 5$, $h = 1$, $T = 10$, $\kappa_1 = 1$, $\kappa_2 = 0.02$, $\beta_1 = 10$, $\beta_2 = 1$, $\theta^a = 25$ and a uniform initial temperature $\theta^0 = 100$. The domain was discretized using a 60×40 uniform mesh (as in the previous example, the whole domain was discretized). Figure 2 shows the optimal distribution of material properties ω_0 when the target distribution is a constant temperature $\theta_T = 75$. The scaling function used is (13) with $p = 2$. The resource constraint is active with $R = 1$.

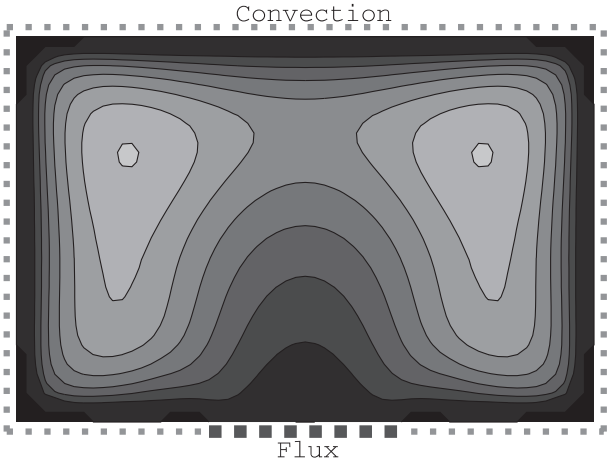

Fig. 2 Optimal distribution of material properties for a constant target function. The lighter areas correspond to higher values of ω_0 (higher conductivity and specific heat)

In order to illustrate the improvement achieved using the optimal distribution ω_0, consider first the difference between the actual temperature field $\theta(\mathbf{x}, T)$ and the target field $\theta_T(\mathbf{x}) = 75$ after a time $T = 10$ when $\omega = 0.25$ for all points, which is an arbitrarily chosen initial distribution of ω in this example. The difference is shown in Fig. 3.

For the optimal distribution ω_0 (shown in Fig. 2), the difference between the actual temperature field $\theta(\mathbf{x}, T)$ and the target field $\theta_T(\mathbf{x}) = 75$ after a time $T = 10$ is shown in Fig. 4. This is an example in which the target field (which corresponds to zero flux on the boundary) is not compatible with the prescribed boundary conditions indicated above. Nonetheless, the procedure minimizes the error $e = \theta(\mathbf{x}, T) - \theta_T(\mathbf{x})$ fairly well for points inside the domain. The greatest deviation occurs on the boundary, which was expected from the outset. In this example, the value of the objective functional for the initial guess is 3740 (i.e. J computed for the field shown in Fig. 3) and

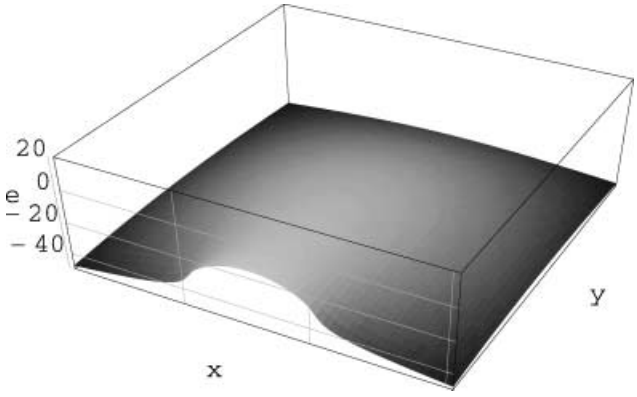

Fig. 3 For initial ω: difference between the actual temperature field at time T and the target field

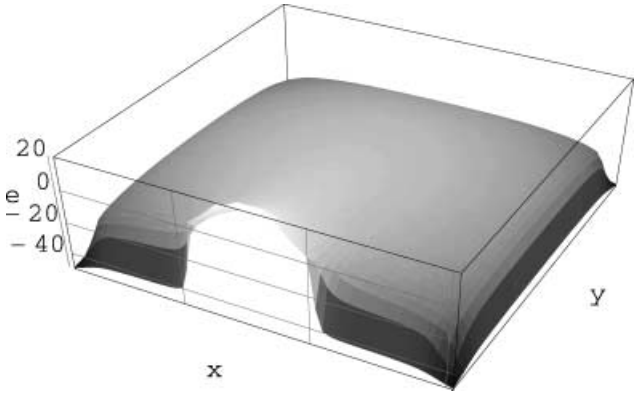

Fig. 4 For optimal ω: difference between the actual temperature field at time T and the target field.

the value for the optimized ω is 630 (i.e. J computed for the field shown in Fig. 4).

7.3 Biased layout

In order to obtain a layout in which ω is closer to its lower and upper values (0 and 1), one can modify the scaling function. Note, however, that this procedure does not provide the "true" minimum, which is the continuous function shown in Fig. 2. Nonetheless, one can force ω to either 0 or 1 by using the scaling function S^* defined in (14). In particular, applying the numerical procedure using (14) instead of (13) (with all other values being the same), results in the layout shown in Fig. 5. The specific values used here are $\underline{\omega} = 0.15$, $\overline{\omega} = 0.85$ and simple concave functions such that the requirements of the scaling functions are satisfied. The bias introduced by the scaling function forces the numerical method to "converge" to a point that, though not being the minimum, has values of ω closer to either 0 or 1. This is typically the case of de-

signs that introduce some penalty to force the function ω towards its lower and upper values.

The difference between the actual temperature and the target function for the biased layout is shown in Fig. 6. Though there is an improvement compared to the initial guess (which is the same as in the nonbiased case), the corresponding value of J is 1400 (as opposed to the optimal value 630).

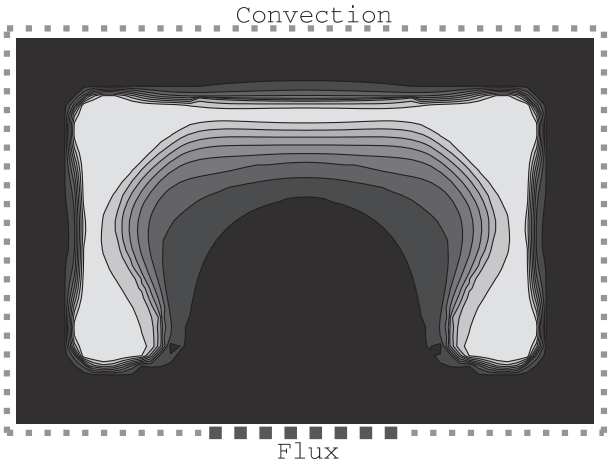

Fig. 5 Layout using a biased gradient. Compare with optimal layout shown in Fig. 2

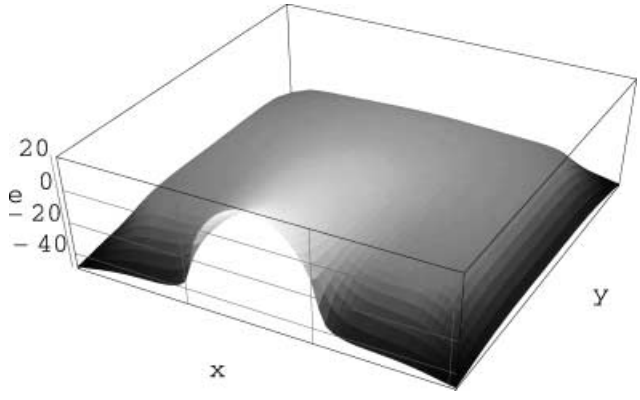

Fig. 6 For biased ω: difference between the actual temperature field at time T and the target field. Compare with the error field at time T for the optimal ω_0 shown in Fig. 4

8 Closing remarks

As shown in this article, the use of optimal topology techniques can be naturally extended for transient physical problems. The limit case of a design with only one material (the second material being "void") is not covered in this analysis, though it is of course of practical interest. However, as opposed to the classical topology optimization problem for minimum compliance, one has to take care of the formation of new boundaries carefully, in particular if a convective boundary condition is used. To this end, a scheme such as the one proposed by Hammer and Olhoff (2000) to keep track of the boundaries can be used. This would permit a simultaneous material and shape optimization. An issue that remains to be addressed is the dependence of the optimal topology on the penalty scheme used, though a detailed analysis of this topic falls outside the scope of this work.

It is worth pointing out that the type of "passive control" covered in this article, though of course not as effective as active or optimal control, has many practical applications. It is an alternative that can be considered in situations in which using an external energy source and complex sensing devices might not be practical or even feasible. Finally, one can note that variants of this problem can be treated similarly. In particular, the minimization of the time *evolution* of the field variable can be addressed using the same method. Similarly, situations in which the material parameterization is not restricted to isotropic materials can be treated analogously. The gradient can be modified accordingly to include a larger material symmetry class.

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