

Two-material Topology Optimization for the Design of Passive Thermal Control Structures

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Abstract

A sandwich-panel structure that exhibits effective variable thermal conductivity through its thickness would find applications in spacecraft thermal control. Topology optimization is considered as a means to guide the design of a compliant-cell core that deforms in response to a temperature gradient, alternately creating and breaking heat conduction paths. Topology optimization is a mathematical tool that generates a material distribution to achieve the best performance as defined by an objective function. This paper explores a topology optimization method for the design of two-material structures that must operate under mechanical and thermal loads. 2D compliant mechanisms that are simultaneously subjected to both prescribed temperature and heat flux boundary conditions are of particular interest. The isotropic materials considered may have different stiffnesses, thermal conductivity, and coefficients of thermal expansion. The design domain is filled by two isotropic material phases and a void phase. The presence of one phase in preference to another at each location in the domain is determined using a Solid Isotropic Material Penalization (SIMP) approach. Mechanical and thermal behavior is coupled via material coefficients of thermal expansion; finite element models are used to predict both uncoupled and coupled behavior. Optimization of the mechanical compliance under uncoupled conditions yields results that agree with those in the literature; the coupled results are novel. The volume fraction of individual materials is typically prescribed. However, coupled multi-physics analysis with multiple materials can yield interesting and useful designs when only the amount of void is constrained and the algorithm is free to choose which combination of materials to use. This design freedom is especially important in problems for which thermal conduction is critical, and it produces designs in which the best thermal properties are exploited. This topology optimization approach, when combined with appropriate contact models, should find application to the development of a passive thermal control interface for spacecraft thermal control.

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1. INTRODUCTION

Topology optimization techniques frequently generate non-intuitive structural designs. As discussed by Sigmund and Maute [1], several mathematical schemes exist for the formulation of topology optimization problems, and the technique has been successfully applied in the fields of aerodynamics [2] [3], electrostatics [4], fluid dynamics [5] or modal analysis [6]. For the design of single-material structures, density approach methods such as Solid Isotropic Material Penalization (SIMP) are quite popular. A matlab algorithm for optimizing mechanical compliance was developed by Sigmund [7], and was improved later into an 88-line code [8]. These codes use a SIMP interpolation scheme of the material properties and filtering techniques to reduce mesh-dependent designs that can arise with finite element formulations. Other methods such as the Finite Volume Method (FVM) [9] [10] or mesh-less techniques [11] have also been investigated in thermal optimization problems, and simulations produced results similar to those of finite element approaches, though not identical.

Minimizing the mechanical compliance of a structure is often a good objective for structural design, and in particular for compliant mechanisms. Mehta *et al.* [12] studied a method for the design of cellular compliant mechanisms in high-strain configurations. These were modified to include internal contact.

Thermal optimization problems usually focus exclusively on thermal conduction effects. Following the SIMP approach, one phase corresponds to material and the other to void (with quasi-null conductivity). The effects of heat convection further complicate the physical model and the optimization process, and are usually not considered [13]. A typical objective for thermal conduction problems involves finding the best material distribution such that the average temperature over the domain is minimized. For a limited amount of conductive material, a uniformly heated domain with a combination of fixed-temperature and insulated boundaries can provide interesting geometries [9] [10].

Thermo-mechanical optimization usually seeks to minimize the mechanical compliance of a structure. In most cases, these problems consider a uniform temperature offset from a reference temperature at which the thermal strains are considered null; the thermal governing equations are not solved. Rubio *et al.* [14] developed a method to optimize an output displacement while minimizing the thermal effects. The thermal compensations introduced in this paper preserved the functionality of initial non-compensated mechanisms and enhanced the reliability of operation at higher temperatures. Other studies investigated the effect of thermal expansion on a single-material design [15]. Rodrigues and Fernandes [16] demonstrated that a uniform temperature offset could severely modify the optimal geometry and, in some cases, could improve the mechanical compliance.

Topology optimization methods are well-developed for one-material (two-phase) design. The physical assumptions are usually adequate to accurately represent the behavior of a single-material structure, and optimization of the mechanical compliance can be realized efficiently using a heuristic fixed-point method [7] [8]. However, extension of the optimization process to accommodate a third phase is not trivial, requiring modification of the SIMP interpolation scheme as well as a more sophisticated method for updating the design variables. Tavakoli and Mohseni [17] recently proposed an active-phase algorithm based on the work of Sigmund [7] and Andreassen [8] for multi-phase topology optimization.

A topology optimization technique for two-material designs using a thermo-mechanical model was developed by Sigmund and Torquato [18]. Using two materials having positive coefficients of thermal expansion (CTE), they showed that it was possible to generate a structure that exhibits effective negative thermal expansion. Also, Sigmund developed a multi-physics topology optimization method for the design of one-material micro-electromechanical actuators [19], which was extended to a two-material model [20] that allows for the possibility of not specifying individual volume fractions.

The approach in this paper generally follows the work of Sigmund. However, heat flux forcing is considered in addition to prescribed temperatures, both the thermal and mechanical governing equations are solved (using a 2D finite element formulation) and the objective function to be minimized is the mechanical compliance. Furthermore, the effect of thermo-mechanical couplings on the optimum design is

emphasized, in the context of a two-material model. Following the SIMP method for the interpolation of the material densities, the Method of Moving Asymptotes (MMA) developed by Svanberg [21] is used as a marching scheme to update the design variables. The aims are to evaluate the influence of the material properties on the final design, and to assess the efficiency of the method for optimizing the design of thermo-elastic compliant mechanisms.

2 TOPOLOGY OPTIMIZATION METHOD

In this section, both, mechanical and thermal systems of equations are derived in a two-dimensional analysis. The materials are assumed to be isotropic, and contact is not considered. For additional details, refer to Thurier [22].

2.1 The Solid Isotropic Material Penalization (SIMP) Method

The domain is discretized into elements, within which uniform material properties are defined. The element material properties considered in this paper are the moduli of elasticity (E), the thermal conductivity (k) and the coefficient of thermal expansion (α). These are defined over the domain using the Solid Isotropic Material Penalization (SIMP) approach [23]. They are functions of the properties of the two materials that compose the structure, *material 1* and *material 2*. The SIMP approach consists of introducing continuous design variables $(\rho_0, \rho_1) \in [0,1]$ that define the amount of material within each element. $\rho_0 = 0$ indicates the presence of void, while $\rho_0 = 1$ indicates material. Similarly, in a non-void element, $\rho_1 = 0$ indicates the presence of material 1, while $\rho_1 = 1$ indicates the presence of material 2. Following this model, the material properties follow the SIMP method as in Sigmund's approach [20]:

$$E(\rho_0, \rho_1) = \rho_0^{p_0} (\rho_1^{p_1} E_1 + (1 - \rho_1)^{p_1} E_2) \quad (1)$$

$$k(\rho_0, \rho_1) = \rho_0^{p_0} (\rho_1^{p_1} k_1 + (1 - \rho_1)^{p_1} k_2) \quad (2)$$

$$\alpha(\rho_0, \rho_1) = \rho_1^{p_1} \alpha_1 + (1 - \rho_1)^{p_1} \alpha_2 \quad (3)$$

Where (p_0, p_1) are penalty terms. Typically, the experience shows that the value $p_0 = 3$ provides reliable optimum results [23]. The value $p_1 = 1$ is chosen so that the material properties within an element correspond to a weighted average of the material properties of the two materials, weighted by the design variable ρ_1 . The role of the penalty terms is to penalize possible intermediate densities that can appear during the optimization steps, and therefore to avoid properties having little physical significance. (E_i, k_i, α_i) represent the material properties of material $i = \{1,2\}$. The materials are assumed to be isotropic and their properties do not depend on temperature. Finally, the amount of each material to be used in the domain is prescribed. The objective of the optimization process is to realize the best performance by distributing the available material(s) in the best locations.

2.2 Governing Equations

A two-dimensional four-noded square element formulation is used to solve both the mechanical and thermal systems of equations. The model assumes that the systems are in equilibrium / at steady-state (no time dependence). The mechanical system is coupled with the thermal system of equations through the

coefficient of thermal expansion (CTE) of the materials. Therefore, the temperature field T must be determined before solving for the displacement field d .

After formulating the heat equation element-wise, the global thermal system of equations can be written as:

$$K_{th}T = F_{th} \quad (4)$$

where the conductivity matrix K_{th} is given by the assembly of the element stiffness matrix:

$$K_{th} = \sum_{e=1}^N K_{th}^e(\rho_0, \rho_1) \quad (5)$$

F_{th} is the load vector (in W/m^2) which characterizes the heat flux at the boundary and internal heat generation terms, N the number of elements in the domain. Solving equation (4) provides the temperature field, and the additional stresses and strains due to thermal expansion can then be determined. These depend also on the reference temperature T_{ref} at which the thermal strain effects are considered null. With the notation $\rho = (\rho_0, \rho_1)$ for the design variables, the (unconstrained) thermal strain is modeled as:

$$\epsilon_0^e = \alpha(\rho)[N(x, y)T^e - T_{ref}][1 \ 1 \ 0]^T \quad (6)$$

where $N(x, y)$ is the vector of linear shape functions used in the finite element formulation. As a result, the internal strain energy in an element is given by:

$$\phi = \frac{1}{2} \iint (\epsilon^T - \epsilon_0^T) D(\rho) (\epsilon - \epsilon_0) t \, dx \, dy \quad (7)$$

with D the matrix derived from the strain-stress relations in plain stress, and t the thickness of an element. The mechanical system of equations is then derived as:

$$K_m d = F_p + F_\epsilon \quad (8)$$

where F_p represents the mechanical load vector and F_ϵ the thermal expansion effects. F_ϵ is obtained by assembling the element vectors:

$$F_\epsilon^e = \iint B^T D \epsilon_0 \, t \, dx \, dy \quad (9)$$

with B the matrix of the derivatives of the linear shape functions in the finite element formulation. Similarly as in equation (5) for the thermal system, the global stiffness matrix is found by assembly of the element stiffness matrices. Finally, the system of equations to be solved sequentially can be written as:

$$\begin{cases} K_{th}T = F_{th} \\ K_m d = F_p + F_\epsilon(T) \end{cases} \quad (10)$$

Using this formulation, the sensitivity analysis is then performed.

2.3 Sensitivity Analysis and Updating Scheme

Using the solutions of the governing equations, the sensitivity analysis determines the direction of descent for the optimization process. Using an adjoint method, the optimization problem can be written as:

$$\begin{aligned} \text{Minimize}_{\boldsymbol{\rho}} \quad & L(\boldsymbol{\rho}) = c_0(\boldsymbol{\rho}) + \boldsymbol{\lambda}_{th}^T (\mathbf{K}_{th} \mathbf{T} - \mathbf{F}_{th}) + \boldsymbol{\lambda}_m^T (\mathbf{K}_m \mathbf{d} - \mathbf{F}_p - \mathbf{F}_\epsilon(\mathbf{T})) \\ \text{subject to} \quad & c_i(\boldsymbol{\rho}) \leq 0, \quad i = 1, \dots, l. \end{aligned} \quad (11)$$

where c_0 is the objective function, $(\boldsymbol{\lambda}_m, \boldsymbol{\lambda}_{th})$ the set of adjoint vectors to be determined, and c_i the constraints, which represent essentially the volume fraction constraints. Solving the adjoint problem consists of finding $(\boldsymbol{\lambda}_m, \boldsymbol{\lambda}_{th})$ such that the derivatives of the field variables with respect to the design variables verify $\partial \mathbf{d} / \partial \boldsymbol{\rho} = 0$ and $\partial \mathbf{T} / \partial \boldsymbol{\rho} = 0$. Carrying out the derivations, the adjoint equations to be solved are written as follow:

$$\begin{cases} \frac{\partial c_0}{\partial \mathbf{d}} + \boldsymbol{\lambda}_m^T \mathbf{K}_m = 0 \\ \frac{\partial c_0}{\partial \mathbf{T}} + \boldsymbol{\lambda}_{th}^T \mathbf{K}_{th} - \boldsymbol{\lambda}_m^T \frac{\partial \mathbf{F}_\epsilon}{\partial \mathbf{T}} = 0 \end{cases} \quad (12)$$

Therefore, the derivatives of the Lagrangian within each element e are determined explicitly as:

$$\frac{\partial L}{\partial \rho_i^e}(\rho_0^e, \rho_1^e) = \frac{\partial c_0}{\partial \rho_i^e} + \boldsymbol{\lambda}_{th}^T \left(\frac{\partial \mathbf{K}_{th}}{\partial \rho_i^e} \mathbf{T} - \frac{\partial \mathbf{F}_{th}}{\partial \rho_i^e} \right) + \boldsymbol{\lambda}_m^T \left(\frac{\partial \mathbf{K}_m}{\partial \rho_i^e} \mathbf{d} - \frac{\partial \mathbf{F}_m}{\partial \rho_i^e} \right) \quad (13)$$

The constraints c_i consist of the volume fraction of each phase that can be used in the domain. In the context of two-material optimization, the volume constraints of each phase can be described as:

$$\begin{aligned} \text{Void:} \quad & 1 - \frac{V^e}{V(1-f_0)} \sum_{e=1}^N (1 - \rho_0^e) \leq 0 \\ \text{Material 1:} \quad & 1 - \frac{V^e}{V f_0 f_1} \sum_{e=1}^N \rho_0^e \rho_1^e \leq 0 \\ \text{Material 2:} \quad & 1 - \frac{V^e}{V f_0 (1-f_1)} \sum_{e=1}^N \rho_0^e (1 - \rho_1^e) \leq 0 \end{aligned} \quad (14)$$

where V^e denotes the element volume, V the total volume of the domain, f_0 the volume fraction of material to be used (over the entire domain), and f_1 regulates the trade-off between the presence of material 1 and material 2. This way, the fraction of void over the domain is $1 - f_0$, while the fraction of material 1 is $f_0 \times f_1$. Note that these constraints are not linearly independent since it is possible to express one constraint as a function of the other two.

For the first iteration of the optimization process, an initial material distribution must be defined. Conventionally, each element in the domain is assumed to contain a mixture of all the phases (materials and void) that respect the overall volume constraints. Therefore, unless otherwise stated, the domain consists initially of a uniform mixture containing the prescribed amount of each phase.

2.4 Filtering and Update of the Design Variables

The next step of the optimization process consists of *filtering* the Lagrangian's sensitivities in each element. As suggested by Sigmund [20], the filtering technique reduces the mesh-dependence of designs arising from the finite element formulation, and avoids checkerboard problems to provide more reliable and realistic results. The technique used in the algorithms is the same as the one used by Andreassen *et al.* [8], adapted to two-material designs using Sigmund's method [20]. The derivatives with respect to ρ_0 are transformed into a weighted average considering the sensitivities in neighboring elements. The derivatives with respect to ρ_1 are treated similarly, although weighting is not required.

These filtered sensitivities are then used in the update of the design variables. According to Sigmund [19], the Method of Moving Asymptotes (MMA) developed by Svanberg [21] used in this paper present the advantage to be quite stable and computationally efficient compared to other methods such as Sequential Linear Programming (SLP). For further information about the numerical implementation of the technique, the interested reader is referred to Svanberg [21].

Finally, the optimization process consists of iteration, with the following steps:

- (i) Solve the governing equations
- (ii) Perform sensitivity analysis and filtering
- (iii) Update the design variables
- (iv) If a stopping criterion based on changes in the design variables is met, stop the optimization. Otherwise, go back to step (i), using the new design variables.

The stopping criterion corresponds to the amount of change in the design variables between two iterations. If the maximum change in all the element design variables is less than 1%, the optimum is considered to be reached.

3. VALIDATION

Unless otherwise stated, the mechanical compliance of the structure is the objective function considered, as given in equation (15). This has the advantage of generating the stiffest design with respect to the loads and boundary conditions. It is also a global criterion which complies with the numerical treatment of the optimization.

$$c_0 = \mathbf{d}^T \mathbf{K}_m \mathbf{d} \quad (15)$$

3.1 Validity of the Algorithm.

The validity of the algorithm was tested on problems available in the literature, first for the uncoupled mechanical and thermal systems of equations. Using a mechanical system of equations only, the algorithm successfully reproduced mechanical compliance optimization results presented in the work of Sigmund [7] and Andreassen *et al.* [8]. The performance of the algorithm was also tested on thermal compliance optimization, as performed by Liang *et al.* [9] and Gersborg-Hansen [10]. In these cases, the objective function was to minimize the global heat over the domain while the domain was heated uniformly, defined by $c_0 = \mathbf{T}^T \mathbf{K}_{th} \mathbf{T}$; mechanical aspects were not considered. The algorithm reproduced shapes similar to those presented in the papers, though extended to two-material designs, as shown in

Figure 1. As expected, the material with the highest conductivity (shown in red on Figure 1) is placed in the most critical locations.

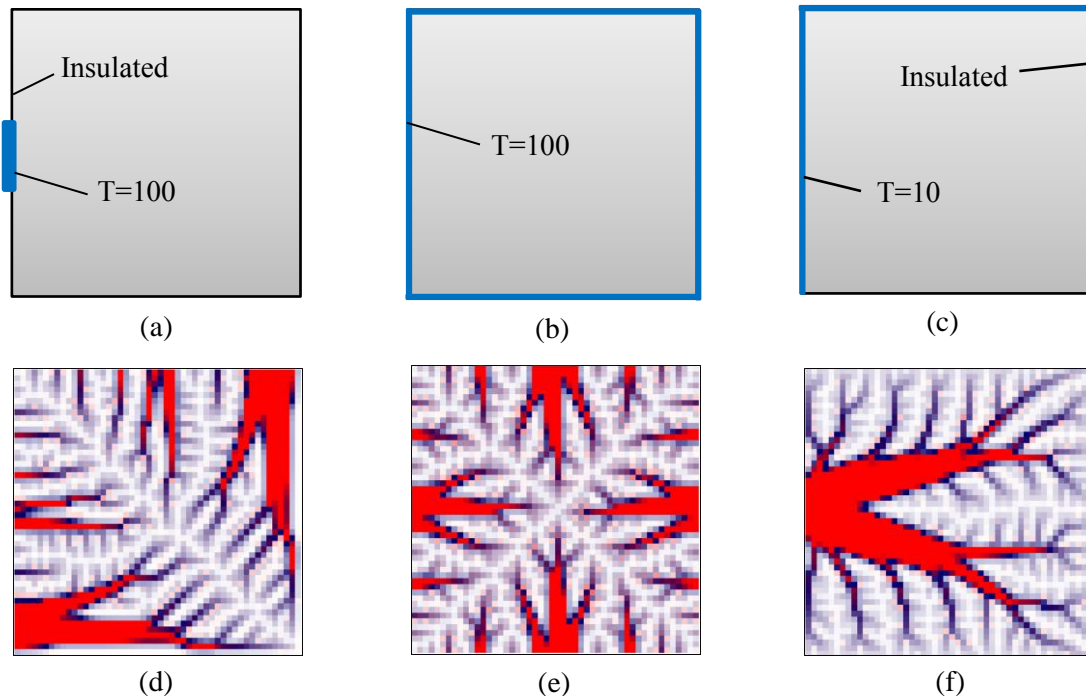


Figure 1. Validation of the algorithm for thermal compliance optimization using two materials. (a), (b) and (c) present the boundary condition used to generate of the designs (d), (e) and (f) respectively. Colors: material 1 is in red, material 2 is in blue.

Table 1 shows the values of the parameters used in these cases. Note that nominal units are used.

Conductivity of material 1	k_1	1
Conductivity of material 2	k_2	2
Volume fraction of material	f_0	0.4
Trade-off material 1/material 2	f_1	0.5
Filter's radius [8]	r_{min}	1.2
Mesh Resolution	$n_x \times n_y$	50×50

Table 1. Parameters value for the thermal simulations.

3.2 Thermo-mechanical System with Heat Flux Boundary Conditions.

Mechanical compliance optimization was performed using the thermo-mechanical system of equations presented in Section 2.2. The algorithm was initially tested using a uniform temperature field over the domain. Designs similar to those of Rodrigues and Fernandes [16]. were obtained. However, the introduction of heat flux boundary conditions revealed some numerical instabilities.

Figure 2 (a) and (b) represent respectively the mechanical and thermal boundary conditions used in the other simulations presented in this paper. In particular, the thermal boundary conditions consist of a heat flux input at the top boundary, a sink temperature T_{sink} at the bottom, and insulated sides. In the

presence of a non-zero heat flux input, the algorithm did not converge because elements near the top boundary alternated between material and void from one iteration to the next. The difficulty is that heat flux into the domain cannot be effectively transmitted by the void elements that can appear during optimization. These elements present very low thermal conductivity, and therefore extremely high temperatures can be reached. The numerical issues for sensitivity analysis are significant, as illustrated by the design in Figure 2 (c). To avoid these numerical issues, a high conductivity layer, simulating a conductive structural face sheet, was introduced at the top of the domain. This layer serves to distribute the input heat efficiently into the structure and an optimum design can be found, as shown in Figure 2 (d).

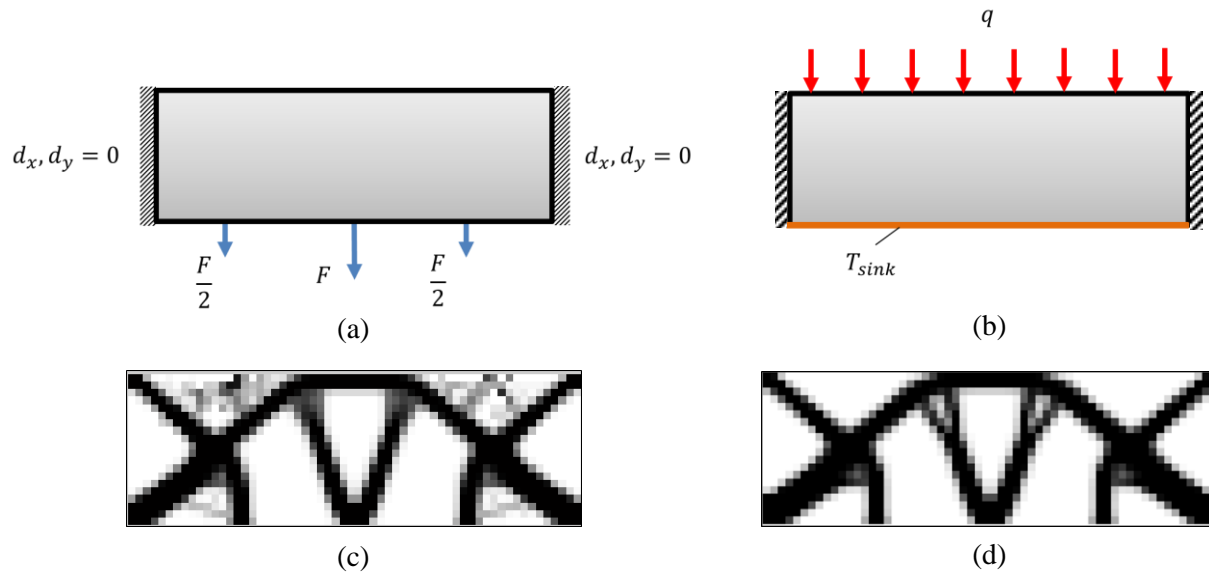


Figure 2. One-material mechanical compliance optimization using the thermo-mechanical model. (a) and (b): Boundary conditions. (c) Typical design obtained when no high conductivity layer is used; isolated elements near the top boundary alternate between void and material. (d) Optimum result using a high conductivity layer at the top of the domain.

3.3 Two-material Designs for Thermo-mechanical Models.

Two-material designs were generated using this added high conductivity layer, and the effects of the thermo-mechanical gradients on the shape of the structure were evaluated.

Table 2 summarizes the standard values of the parameters used in the simulations. In Figure 3 and Figure 4, the amount of material is constrained such that void occupies 60% of the domain, and each material occupies an equal amount of 20% each. Material 1 is the stiffest material, and is represented in red.

For a structure maintained at the reference temperature, the stiffest material is placed in critical locations to stiffen the structure, as shown in Figure 3(a): near the clamped ends and the point of application of the forces. An optimal heated structure can present a different shape: in Figure 3(b), thermal expansion increases the effective compliance of the structure.

In Figure 4, the ratio of the CTEs of the two materials is modified from Figure 4(a) to Figure 4(b). While this change does not substantially modify the shape of the structure, the material with the smallest CTE tends to be placed in the top corners and in the middle of the structure. The structure seems to use thermal expansion of the materials to reinforce the “bridge” configuration to resist the forces pulling downwards.

Modulus of elasticity of material 1	E_1	2
Modulus of elasticity of material 2	E_2	1
Conductivity of material 1	k_1	2
Conductivity of material 2	k_2	1
CTE of material 1	α_1	5×10^{-4}
CTE of material 2	α_2	2×10^{-4}
Poisson ratio	ν	0.3
Reference Temperature	T_{ref}	0
Sink Temperature	T_{sink}	0
Heat flux input	q	1.5
Force input	F	-1
Volume fraction of material	f_0	0.4
Trade-off material 1/material 2	f_1	0.5
Filter's radius [8]	r_{min}	1.2
Mesh Resolution	$n_x \times n_y$	60×20

Table 2. Parameters value for the thermo-mechanical simulations of Section 3.3.

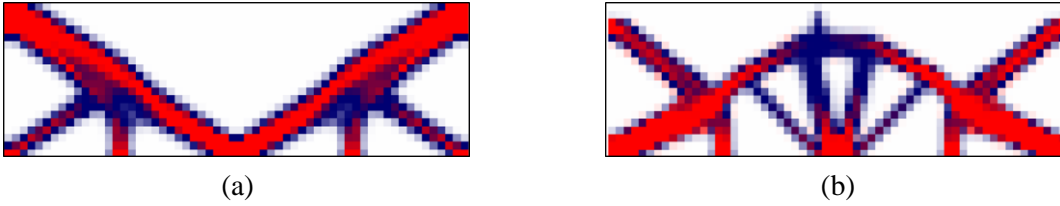


Figure 3. Influence of the heat flux on a two-material topology optimization structure using a thermo-mechanical model. (a) Optimal structure at reference temperature ($q = 0$). Objective function final value: $c_0 = 17.35$. (b) Optimal structure of a heated structure ($q = 2$). Objective function final value: $c_0 = 22.98$. Colors: material 1 is in red, material 2 is in blue.

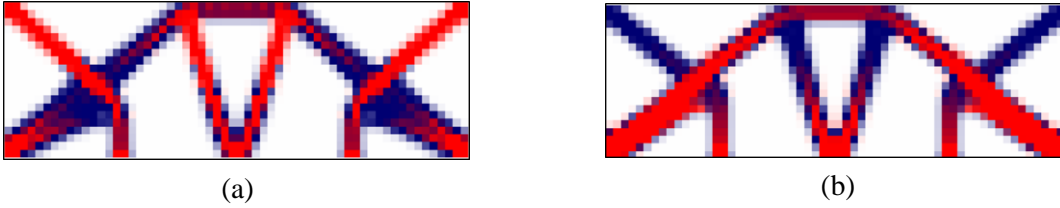


Figure 4. Influence of the CTE on a two-material topology optimization structure using a thermo-mechanical model. (a) $\alpha_2 = 2.5 \alpha_1 = 2 \times 10^{-4}$. Objective function final value: $c_0 = 21.89$. (b) $\alpha_2 = 0.4 \alpha_1 = 5 \times 10^{-4}$. Objective function final value: $c_0 = 21.82$. Material 1 is in red, material 2 is in blue.

In the preceding simulations, the volume fractions of the individual materials used are constrained. However, for a two-material, multi-physics problem, it could be useful to relax some of the constraints. Indeed, with respect to the compliance minimization problem, the amount of void is generally prescribed to avoid trivial solutions that consist of filling the entire domain with material. However, the quantities of individual materials do not need to be prescribed: the decision of how much of each material to use can be left to the optimization process. Considering the mechanical system only, the obvious choice is that the material with the highest modulus of elasticity is chosen, leaving the other material unused, as shown in Figure 5(a).

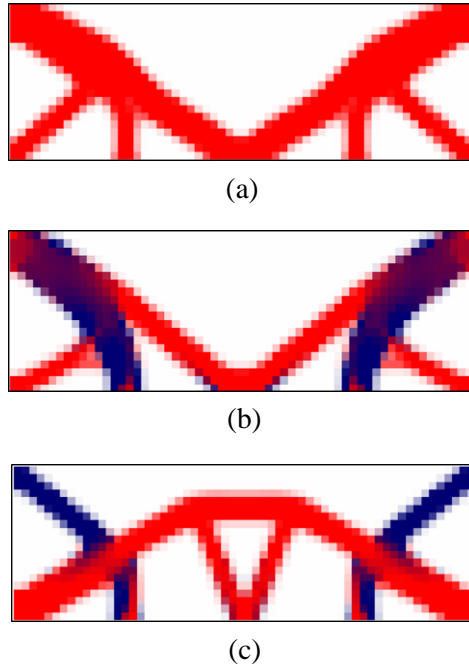


Figure 5. Partially constrained optimization of the mechanical compliance of a two-material structure. Conductivities of the materials: $k_1 = 1$, $k_2 = 5$. (a) Non heated structure ($q = 0$). Objective function final value: $c_0 = 14.27$. (b) Heated structure with $q = 1$. Objective function final value: $c_0 = 20.82$. (c) Heated structure with $q = 1.5$. Objective function final value: $c_0 = 20.35$. Material 1 is in red, material 2 is in blue.

Nevertheless, some heated configurations such as those shown in Figure 5(b) and Figure 5(c) suggest introducing the other material in some specific locations to minimize the compliance. Therefore, the thermal properties of the two materials do influence the optimal results, despite the objective function focusing on mechanical aspects. In these examples, an initially equal amount of each material was assumed in the domain, and the optimal solutions did not seem to depend highly on these initial values.

4. CONCLUSION

Based on previous algorithms and techniques mainly used for one-material structural optimization problems, a two-material thermo-mechanical topology optimization algorithm was developed and tested on mechanical compliance minimization problems with input heat fluxes. The two-material model was tested on thermal problems that successfully reproduced the shape of existing one-material designs from the literature. A high conductivity layer was introduced to improve the distribution of heat input to the structure. Also, material thermal expansion properties were found to affect the optimal structures in problems with input heat fluxes. Finally, partially constrained problems in which the volume fractions of individual materials are not prescribed were found to be useful.

This method can be improved. Nondimensionalization and subsequent extension to specific design problems of interest should be addressed. The use of more rigorous bounds for the material properties, such as the Hashin-Shtrikman bounds [20] [23], could also be considered to ensure feasible, manufacturable solutions. Finally, the use of a commercial finite element code might improve the accuracy of the analysis for domains having more complex geometry, and allow further development of this work.

Finally, thermo-mechanical systems of this type are of interest for passive spacecraft thermal control systems on spacecraft [24]. Based on mismatch of thermal expansion of two materials, mechanical and thermal contact could be created or broken in order to modify heat conduction paths between electronic “black boxes” and a thermal bus. The goal would be to maintain the electronics within an allowable range of temperature. Important features of this problem include heat flux boundary conditions. Under low heat loads, the contacts should be open and the effective conductivity should be low to prevent the electronics from getting too cold. Under high heat load, the contacts should close to increase the effective conductivity and prevent the electronics from getting too hot. Topology optimization with contact should provide a means to guide the design of a compliant-cell sandwich-panel core that exhibits variable thermal conductivity.

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