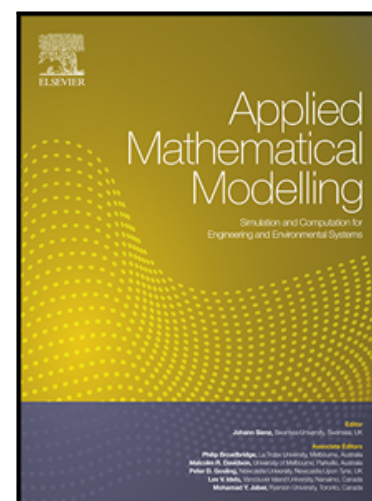


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Juan C. Álvarez Hostos, Víctor D. Fachinotti, Ignacio Peralta

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### Highlights

- Topology optimization-based design of thermo-mechanical metadivices is proposed
- The so-designed devices can be manufactured by using simple isotropic materials
- The devices performance has been analyzed via finite element method simulations
- Such devices exhibit a good performance, when compared to more complex metadivices

# Computational design of thermo-mechanical metadevices using topology optimization

Juan C. Álvarez Hostos<sup>\*,a,b</sup>, Víctor D. Fachinotti<sup>a</sup> and Ignacio Peralta<sup>a,c</sup>

<sup>a</sup>Centro de Investigación de Métodos Computacionales (CIMEC), Universidad Nacional del Litoral (UNL)/Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Predio CCT-CONICET Santa Fe, Argentina.

<sup>b</sup>Department of Chemical Metallurgy, Universidad Central de Venezuela, Ciudad Universitaria, Los Chaguaramos, Caracas, Venezuela.

<sup>c</sup>Laboratorio de Flujometría (FLOW), Facultad Regional Santa Fe (FRSF), Universidad Tecnológica Nacional (UTN), Lavalse 610, 3000, Santa Fe, Argentina.

## Abstract

The present work has been conducted in order to introduce a novel approach for the design of mechanical devices conceived to manipulate the displacements field in linear elastic materials subjected to thermal gradients. Such an approach involves the solution of a topology optimization problem where the objective function defines the error in achieving a prescribed displacement field, and the mechanical device consists of two macroscopically distinguishable isotropic candidate materials. The material distribution is defined as a continuous function by following the solid isotropic microstructure (or material) with penalization (SIMP) method. The so-designed devices are easy to manufacture, since the design variables dictate the candidate materials distribution. Based on such an approach it is not necessary to devise further ways to simultaneously mimicking several thermal and mechanical effective properties, as required by coordinates transformation-based metamaterial design methods. Although the candidate materials are isotropic, the mechanical device behaves as a metamaterial allowing the desired manipulation of the displacements field. As an example, this topology optimization-based approach is applied to the design of an elastostatic cloaking device subjected to thermal gradients, considering also thermo-dependent mechanical properties.

**Keywords:** Topology Optimization, Metadevices, Thermo-mechanical, Cloaking, Sensitivity Analysis, Design Variables

## 1. Introduction

Recent developments in engineered materials has allowed the manipulation of physical fields in outstanding and unprecedented ways, including cloaking [1–6], concentration [2, 4, 6–11], inversion [4, 6–8], shielding [4–6] and channeling [6, 12] in heat conduction, and cloaking in elastostatics [13–16], elastodynamics [17–19] and acoustics [20], among others. These engineered materials are called metamaterials for having effective properties that goes beyond (meta in Greek) those found in nature.

Classically, metamaterials and metadevices (those devices made of or behaving as metamaterials) have been designed via the coordinate transformation approach originally proposed by Leonhardt [21] and Pendry [22] for electromagnetic cloaking. Such an idea was subsequently adapted to the design of metadevices for heat flux manipulation [1–3, 9] and mechanical cloaking [18, 19]. The implementation of such an approach in the design of mechanical metamaterials leads to the need of achieving an invariant form of the linear momentum balance equation, which poses several issues. Norris and Shuvalov [23] demonstrated that the coordinates transformation procedure leads to the anisotropic materials obeying the Willis constitutive equations [24]. Milton et al. [25] achieved a transformation-invariant form of the linear momentum balance for cloaking by including a third-order tensor besides the standard (fourth-order) elasticity tensor, whereas Brun et al. [26] did it by breaking the symmetry of the standard elasticity tensor. Great efforts have been devoted to manufacture the so-conceived mechanical metamaterials [13, 14, 17, 27]. Stenger et al. [17] designed a

circular mechanical cloaking device with radially variable effective elastic properties, in an attempt to emulate the invariant form of the plate equation derived by Farhat et al. [28]. Kadic et al. [27] proposed to use pentamodal materials to emulate any material conceived from coordinates transformation, and such an idea was followed by Bückmann et al. [13] for the manufacture of an elastostatic cloaking device. As an alternative to the coordinates transformation-based procedures, Bückmann et al. [14] proposed the implementation of a direct-lattice transformation technique to design elastostatic cloaking devices. Such an approach is conceived to directly prescribe the geometry of the metamaterial or metadevice to be manufactured from lattices without the need of devising further ways to achieve the inhomogeneous material properties required for the task accomplishment, which is a crucial improvement in comparison with the coordinates transformation-based procedure.

Recently, Peralta et al. [10] introduced the optimization-based metamaterial design (OMD) approach for the design of thermal metamaterials, free from the limitations of coordinates transformation-based procedures. Such a procedure consists in solving a large-scale continuous optimization problem to minimize the error in the accomplishment of a given task, where the parameters describing the metamaterial microstructure (microparameters) are taken as design variables. Examples of design variables are the geometrical parameters defining a biomimetic unit cell of artificial bones [29, 30], the relative thickness of layers and their orientation in laminates [5, 10, 16], and the artificial density [31, 32] in material distribution problems. Like the direct-lattice technique [14], the OMD approach directly prescribes how

to manufacture the metamaterial or metadvice. Additionally, it allows the design of any metadvice having a quantitatively characterizable microstructure, including lattices as particular cases. Another noteworthy advantage of the OMD approach lies on the possibility of designing metadvice conceived to perform any heat flux manipulation task (including concentration, shielding, reversion, and cloaking), by using a unique objective function to avoid the need of a different formulation for each task [4]. The OMD versatility was demonstrated when it was extended to the design of metadvice for elastostatic cloaking under given boundary traction [15] and thermal gradients [16].

Although OMD dictates how to manufacture the metamaterial at each point, the achievement of such a precise inhomogeneous metamaterial is still a critical issue that precludes real applications. In further efforts towards manufacturability, the well known topology optimization method [33] was used in the design of thermal [4, 11], mechanical [15], and thermo-mechanical [31, 32, 34–38] metadvice. Topology optimization was originally formulated for structural problems [39–41], where the design variables define the presence of material at a point. According to the possibility of achieving a discrete material distribution in terms of continuous design variables, this technique has been successfully extended to heat transfer [42, 43], electro-mechanical [44], fluid flow [45], dynamic fatigue [46, 47], thermo-mechanical [48, 49] and even electro-thermo-mechanical [50] applications. Regarding the design of metamaterials and metadvice, the design variables are rather used to choose between materials with highly contrasting properties. Topology optimization-based metamaterial design (TOMD) has changed the mainstream belief that it is imperative to use anisotropic inhomogeneous metamaterials for the manipulation of macroscopic fields [7, 14, 18, 51]. For instance, Fachinotti et al. [4] applied the well-known solid isotropic microstructure (or material) with penalization (SIMP) [33] approach in the framework of TOMD in order to design an easy-to-make heat flux inversion metadvice, which consisted of two piecewise macroscopically distinguishable homogeneous materials with very different isotropic thermal conductivities. Such a device was actually significantly simpler, easier to make and more efficient than the coordinates transformation-based inverter designed by Narayana and Sato [51]. Sigmund and Torquato [31, 32] used TOMD with a SIMP-like approach involving three phases (two solids, one void) to optimize both the topology and material distribution in each base cell of metamaterials for extreme thermal expansion responses, whereas Wang et al. [34, 36, 37] used a multiphase level-set method for such a purpose. The possibility of manufacturing such thermo-mechanical metamaterials obtained by TOMD has been demonstrated by Takezawa et al. [35], who have succeeded in implementing additive manufacturing techniques to obtain an extreme thermal expansion metamaterial designed via a SIMP-based multiphase topology optimization procedure [31, 32] coupled to a phase field method [52].

Later, Peralta et al. [11] adapted a multiphase topology optimization method known as discrete material optimization (DMO) [53] to the design of thermal metadvice made of any number of homogeneous candidate materials, either isotropic or not. By this way, these authors designed a heat flux concentrator made of laminates of copper and polydimethylsiloxane in different orientations. As a further demonstration of its versatility, this approach was applied by Fachinotti et al. [15] for the design of mechanical metadvice, showing an elastostatic cloaking device as example.

Regarding all the previously mentioned TOMD-based thermo-mechanical metamaterials for extreme thermal expansion [31, 32, 34–38], it is worth to mention that such metamaterials were conceived under the assumption that the temperature is homogeneous throughout the metamaterial without being affected by the material distribution. Such an excessively restrictive hypothesis is actually appropriate only when a unique temperature is prescribed on all the device boundaries and there are no internal heat sources, given the usually high conductivity contrast within metamaterials. The sensitivity of coupled temperature and displacement fields to microstructural changes [54] has been recently accounted for Álvarez-Hostos et al. [16] in the design of thermo-mechanical metamaterials, which involves the coupled solution of heat transfer and mechanical problems throughout the entire optimization process. These authors used the OMD approach, hence suffering from manufacturability issues.

In agreement with the aforementioned aspects, the present work is focused on extending the TOMD approach (and its advantages regarding manufacturability) to the design of thermo-mechanical metadvice accounting for the coupling between displacement and temperature fields. In this case, the objective function representing the mechanical task (e.g., elastostatic cloaking) will depend on displacement, which in turn depends on temperature. Accordingly, the performance of such metadvice will be dictated by the spatial distribution of both mechanical (elastic moduli and thermal expansion) and transport (conductivity) properties, which are dependent on the design variables defining the material distribution in the optimization problem. So, the computation of the objective function at each one of the iterations (usually, hundreds to thousands) during the optimization process requires the fully coupled solution of the linear momentum and thermal energy balance equations, making this thermo-mechanical problem considerably more expensive to solve when compared to that in which a homogeneous temperature field is directly prescribed [31, 32, 34–38].

The current TOMD is conducted under the classical SIMP approach [33] for the design of thermo-mechanical metadvice, which consist of two piecewise macroscopically distinguishable homogeneous materials with very different mechanical (elastic moduli and thermal expansion coefficient) and thermal (conductivity) properties. As a

further contribution unprecedented in the design of thermo-mechanical metamaterials and metadvice, the dependence of elastic moduli with the temperature is allowed.

Finally, a device for cloaking under surface traction and thermal gradients is designed using two isotropic materials (aluminum and polyethylene) in order to highlight the capability of this approach to design easy-to-make thermo-mechanical metadvice. The performance of such a cloaking metadvice of feasible manufacture can actually be compared to that of a metamaterial proposed in a previous communication [16], which is made of laminates based on the same materials. Such metamaterial consists in an inhomogeneous distribution of the relative thickness of the constituent materials and orientation of the laminates, whereby its manufacturability is uncertain.

## 2. Governing equations

The topology optimization-based design of a thermo-mechanical metadvice implies the minimization of an objective function that quantifies the error in accomplishing a given task, which generally depends on displacement and temperature. The evaluation of such an objective function requires to solve both the linear momentum and thermal energy balance equations, which is done in this work via the finite element method (FEM).

### 2.1. Thermo-mechanical problem

The domain  $\Omega$  depicted in Fig. 1 represents a heterogeneous solid body, undergoing a steady state thermo-mechanical loading process. Assuming a linear thermo-elastic behaviour and small strains, the displacement field  $\mathbf{u}$  in  $\Omega$  is governed by the equilibrium equation:

$$\text{div } \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0}, \quad (1)$$

where  $\mathbf{b}$  is the body force, and  $\boldsymbol{\sigma}$  is the Cauchy stress tensor defined by the Duhamel-Neumann law for thermo-elasticity:

$$\boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon} + \mathbf{d} (T - T_{\text{ref}}),$$

being  $\boldsymbol{\varepsilon} = [\text{grad } \mathbf{u} + (\text{grad } \mathbf{u})^T]/2$  the infinitesimal strain tensor,  $\mathbf{C}$  the elastic moduli tensor,  $\mathbf{d}$  the stress increment per unit temperature,  $T$  the temperature and  $T_{\text{ref}}$  the reference temperature for zero thermal strain. The solution of Eq. (1) is subjected to the boundary conditions:

$$\begin{aligned} \mathbf{u} &= \mathbf{u}^{\text{wall}} & \text{in } \Gamma_{\mathbf{u}}, \\ \boldsymbol{\sigma} \cdot \mathbf{n} &= \mathbf{t}^{\text{wall}} & \text{in } \Gamma_{\mathbf{t}}, \end{aligned}$$

where  $\mathbf{n}$  is the unit vector normal to and pointing outwards  $\Gamma$ , whereas  $\mathbf{u}^{\text{wall}}$  and  $\mathbf{t}^{\text{wall}}$  are the displacement and surface traction vectors prescribed on the non overlapping portions  $\Gamma_{\mathbf{u}}$  and  $\Gamma_{\mathbf{t}}$  of  $\Gamma$ , respectively.

The dependence of  $\mathbf{u}$  on  $T$  gives rise to the need of coupling the solution of (1) to the heat conduction equation:

$$-\text{div}(\mathbf{q}) + s = 0, \quad (2)$$

where  $s$  is the internal heat source, and  $\mathbf{q}$  the heat flux vector given by the Fourier's Law.

$$\mathbf{q} = -\mathbf{k} \cdot \text{grad } T,$$

being  $\mathbf{k}$  the thermal conductivity tensor. The solution of Eq. (2) is subjected to the boundary conditions:

$$\begin{aligned} T &= T^{\text{wall}} & \text{in } \Gamma_T, \\ \mathbf{q} \cdot \mathbf{n} &= q^{\text{wall}} & \text{in } \Gamma_q, \end{aligned}$$

where  $T^{\text{wall}}$  and  $q^{\text{wall}}$  are the temperature and heat flux prescribed on the non overlapping portions  $\Gamma_T$  and  $\Gamma_q$  of  $\Gamma$ , respectively.

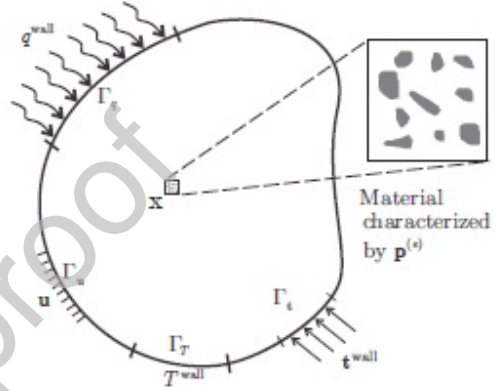


Figure 1: Thermo-mechanical problem in a macroscopic domain where the effective properties depend on a quantitatively characterized microstructure

### 2.2. Finite element formulation

The thermo-mechanical problem described in the previous section will be solved by using the FEM with  $\Omega$  divided in finite elements  $\Omega^{(e)}$ , and approximating the temperature and displacement fields for all  $\mathbf{x} \in \Omega$  as follows:

$$T(\mathbf{x}) = N_i T_i = \mathbf{N}(\mathbf{x}) \mathbf{T}, \quad (3)$$

$$\mathbf{u}(\mathbf{x}) = N_i \mathbf{u}_i = \mathbf{N}^m(\mathbf{x}) \mathbf{U}, \quad (4)$$

where  $T_i$  and  $\mathbf{u}_i$  are the temperature and displacement unknown at each node  $\mathbf{x}_i$  of the finite element mesh, and  $N_i$  is the shape function associated to this node, for which  $N_i(\mathbf{x}_j) = \delta_{ij}$  with  $\delta_{ij}$  denoting the Kronecker delta.  $T_i$  and  $\mathbf{u}_i$  are grouped in vectors  $\mathbf{T}$  and  $\mathbf{U}$ , respectively. The shape functions  $N_i$  are grouped either in the row vector  $\mathbf{N}$  and matrix  $\mathbf{N}^m$  for the thermal and mechanical analysis, respectively. The substitution of Eq. (3) in the Bubnov-Galerkin weak-form of the thermal problem leads to:

$$\mathbf{K} \mathbf{T} = \mathbf{Q}, \quad (5)$$

with

$$\mathbf{K} = \int_{\Omega} \mathbf{B}^T \mathbf{k} \mathbf{B} d\Omega, \quad (6)$$

$$\mathbf{Q} = \underbrace{\int_{\Omega} \mathbf{N}^T s d\Omega}_{\mathbf{Q}^s} - \underbrace{\int_{\Gamma_q} \mathbf{N}^T q^{\text{wall}} d\Gamma_q}_{\mathbf{Q}^q} \quad (7)$$



where  $\mathbf{B}$  is the matrix of shape functions gradient with components  $B_{ij} = \partial N_i / \partial X_j$ . Similarly, the following system of equations is obtained after substituting Eq. (4) in the Bubnov-Galerkin weak-form of the mechanical problem:

$$\mathbf{K}^m \mathbf{U} = \mathbf{F}, \quad (8)$$

with

$$\begin{aligned} \mathbf{K}^m &= \int_{\Omega} [\mathbf{B}^m]^T \mathbf{C} \mathbf{B}^m d\Omega, \\ \mathbf{F} &= \underbrace{\int_{\Gamma_t} \mathbf{N}^T \mathbf{t}^{\text{wall}} d\Gamma_t}_{\mathbf{F}^t} + \underbrace{\int_{\Omega} \mathbf{N}^T \mathbf{b} d\Omega}_{\mathbf{F}^b} \\ &\quad - \underbrace{\int_{\Omega} [\mathbf{B}^m]^T \mathbf{d} (T - T_{\text{ref}}) d\Omega}_{\mathbf{F}^{\text{Th}}}, \end{aligned} \quad (9)$$

where  $\mathbf{B}^m$  denotes the strain-displacement matrix. In Eqs. (9) and (10), the elastic moduli  $\mathbf{C}$  and stress increment per unit temperature  $\mathbf{d}$  tensors are given in Voigt notation. Let the microstructure at each finite element  $\Omega^{(e)}$  in a heterogeneous region  $\Omega_{\text{dev}} \subset \Omega$  occupied by a metadvice, be quantitatively characterized by a vector  $\mathbf{p}_e$  of  $M$  microparameters. Accordingly, the effective material properties  $\mathbf{C}$ ,  $\mathbf{d}$  and  $\mathbf{k}$  at each  $\Omega^{(e)} \in \Omega_{\text{dev}}$  are function of  $\mathbf{p}^{(e)}$ . Consequently the global conduction  $\mathbf{K}$  and stiffness  $\mathbf{K}^m$  matrices, and also the global thermal loads vector  $\mathbf{F}^{\text{Th}}$  are function of the microstructure distribution in  $\Omega_{\text{dev}}$ :

$$\mathbf{K} = \mathbf{K}(\mathbf{P}), \quad \mathbf{K}^m = \mathbf{K}^m(\mathbf{P}), \quad \text{and} \quad \mathbf{F}^{\text{Th}} = \mathbf{F}^{\text{Th}}(\mathbf{P}),$$

with

$$\mathbf{P} = [\mathbf{p}^{(1)}, \mathbf{p}^{(2)}, \dots, \mathbf{p}^{(N)}],$$

whereby both the displacement and thermal fields in the whole domain  $\Omega$  depend on  $\mathbf{P}$ , i.e.  $\mathbf{u} = \mathbf{u}(\mathbf{x}, \mathbf{P})$  and  $T = T(\mathbf{x}, \mathbf{P})$  for all  $\mathbf{x} \in \Omega$  [54].

### 2.3. The displacements manipulation problem under thermal loads

The problem of designing a metadvice  $\Omega_{\text{dev}}$  embedded in the body  $\Omega$  to manipulate the displacement inside the region  $\Omega_{\text{task}} \subset \Omega$  subjected to both thermal and mechanical loads, can be stated as follows: to find  $\mathbf{P}$  such that

$$\mathbf{u}(\mathbf{x}, \mathbf{P}) = \bar{\mathbf{u}}(\mathbf{x}), \quad \text{for all } \mathbf{x} \in \Omega_{\text{task}}, \quad (11)$$

where  $\bar{\mathbf{u}}(\mathbf{x})$  is a prescribed displacement field to be achieved in a region  $\Omega_{\text{task}} \subset \Omega$ . Given the link between the thermal and mechanical responses of the domain, the accomplishment of any displacements manipulation task requires to find a proper spatial distribution of both thermal and mechanical material properties. Thus, the fulfillment of such a task will be affected by the dependence of both displacement and temperature on the microparameters distribution.

In order to make feasible the numerical solution of this problem, the task accomplishment is checked at  $H$  points  $\mathbf{x}^{(h)} \in \Omega_{\text{task}}$ . Further, to guarantee the microstructure feasibility, the search of  $\mathbf{P}$  must be constrained to a feasible

design set  $\mathcal{D}$ . Such a constraint precludes the perfect fulfillment of (11), and it is achieved up to a minimum error:

$$f(\mathbf{P}) = \left[ \frac{\sum_{h=1}^H \|\mathbf{u}(\mathbf{x}^{(h)}, \mathbf{P}) - \bar{\mathbf{u}}(\mathbf{x}^{(h)})\|^2}{\sum_{h=1}^H \|\bar{\mathbf{u}}(\mathbf{x}^{(h)})\|^2} \right]^{1/2}, \quad (12)$$

where the relative error  $f$  in the accomplishment of the displacements manipulation task at all the points  $\mathbf{x}^{(h)} \in \Omega_{\text{task}}$  defines the objective function, whereas the microparameters  $P_i$  defining the microstructure distribution in  $\Omega_{\text{dev}}$  are the design variables.

Constraining the search of  $\mathbf{P}$  to a feasible design set  $\mathcal{D}$  precludes the exact accomplishment of (11), which actually represents a near-elastostatic cloaking under thermal gradients. The near-cloaking problem in elastostatic has also recently been addressed by Craster et al. [55] through a different formulation, which is based on the regularized change of variable originally developed by Kohn et al. [56] for electromagnetic cloaking.

The optimization-based procedure proposed in this communication implies to solve the following non-linear constrained optimization problem:

$$\min_{\mathbf{P} \in \mathcal{D}} f(\mathbf{P}) \quad (13)$$

In principle, there are  $M$  design variables per finite element, whereby the optimization problem (13) is usually a large-scale problem. If the feasible design set  $\mathcal{D}$  is rich enough, it would be possible to achieve a perfect design. If not, it is still possible to obtain a design for which (12) reaches a minimum. In a previous communication [16], the optimization-based approach has been successfully implemented in the design of thermo-mechanical metadvice by using a metamaterial consisting of an orthotropic composite laminate made of two materials with very different thermal and mechanical properties. In such study, there were  $M = 2$  design variables (the relative thickness and orientation of the laminate) at each finite element in the metadvice. Such a design has been obtained without introducing manufacturability constraints, which have already been recognized to be crucial for the manufacture of both thermal [4, 11] and mechanical [15] metadvice. Therefore, the optimization-based design of the current thermo-mechanical metadvice will be conducted putting also special emphasis on manufacturability. Such a feature will be assured by following the SIMP approach, which has been widely used in topology optimization problems. In a previous work, such a technique was successfully implemented in the design of easy-to-make heat flux manipulation metadvice [4]. Thus, in this study the effective elastic moduli, stress increment per unit temperature and thermal conductivity at each finite element  $\Omega^{(e)} \in \Omega_{\text{dev}}$ , are defined as:

$$\begin{aligned} \mathbf{C}^{(e)} &= \rho_e^p \mathbf{C}_A + (1 - \rho_e^p) \mathbf{C}_B, \\ \mathbf{d}^{(e)} &= \rho_e^p \mathbf{d}_A + (1 - \rho_e^p) \mathbf{d}_B, \\ \mathbf{k}^{(e)} &= \rho_e^p \mathbf{k}_A + (1 - \rho_e^p) \mathbf{k}_B, \end{aligned}$$

where  $p > 1$ ,  $\rho_e$  is an artificial density with  $0 \leq \rho_e \leq 1$ , whereas subscripts A and B represent two different isotropic

materials. A value of  $p \geq 3$  is high enough for compelling  $\rho_e^p$  to tend either to 0 or 1. Accordingly, the effective properties at each element  $\Omega^{(e)} \in \Omega_{\text{dev}}$  are defined by  $\rho_e \equiv P_e$  as the only design variable ( $M = 1$ ), determining which of the two materials A or B is at the finite element  $\Omega^{(e)}$ .

## 2.4. Sensitivity analysis

The efficient solution of the optimization problem (13), requires the analytical computation of the derivatives of the objective function  $f$  with respect to the design variables  $P_i \equiv \rho_i$ ,  $i = 1, 2, \dots, N$ . For computational efficiency, these derivatives can be computed using the adjoint method. For this purpose, the objective function is rewritten as [57–60]:

$$f(\mathbf{P}) = f(\mathbf{P}) - \boldsymbol{\xi}^T (\mathbf{K}\mathbf{T} - \mathbf{Q}) - \boldsymbol{\lambda}^T (\mathbf{K}^m \mathbf{U} - \mathbf{F}), \quad (14)$$

where the additional terms are null by virtue of the FEM-based equilibrium and heat conduction equations (5) and (8), respectively. The differentiation of (14) with respect to  $P_i$  yields

$$\begin{aligned} \frac{df}{dP_i} = & \left. \frac{\partial f}{\partial P_i} \right|_{\mathbf{U}=\text{const}} + \frac{\partial f}{\partial \mathbf{U}} \frac{d\mathbf{U}}{dP_i} - \boldsymbol{\xi}^T \left( \frac{\partial \mathbf{K}}{\partial P_i} \mathbf{T} + \mathbf{K} \frac{d\mathbf{T}}{dP_i} + \hat{\mathbf{K}} \frac{d\mathbf{T}}{dP_i} \right) \\ & - \boldsymbol{\lambda}^T \left( \frac{\partial \mathbf{K}^m}{\partial P_i} \mathbf{U} + \mathbf{K}^m \frac{d\mathbf{U}}{dP_i} + \hat{\mathbf{K}}^m \frac{d\mathbf{T}}{dP_i} + \frac{\partial \mathbf{F}^{\text{Th}}}{\partial P_i} + \frac{\partial \mathbf{F}^{\text{Th}}}{\partial \mathbf{T}} \frac{d\mathbf{T}}{dP_i} \right), \end{aligned} \quad (15)$$

where  $\hat{\mathbf{K}}$  and  $\hat{\mathbf{K}}^m$  are the matrices with components  $\hat{K}_{jk} = (\partial K_{jl} / \partial T_k) T_l$  and  $\hat{K}_{jk}^m = (\partial K_{jl}^m / \partial T_k) U_l$ , respectively. The matrix  $\hat{\mathbf{K}}$  is non null only if thermal conductivity depends on temperature, and also  $\hat{\mathbf{K}}^m$  is non null only if the elastic moduli depends on temperature. The terms in (15) can be rearranged as follows:

$$\begin{aligned} \frac{df}{dP_i} = & \left. \frac{\partial f}{\partial P_i} \right|_{\mathbf{U}=\text{const}} + \left( \frac{\partial f}{\partial \mathbf{U}} - \boldsymbol{\lambda}^T \mathbf{K}^m \right) \frac{d\mathbf{U}}{dP_i} \\ & - \left[ \boldsymbol{\lambda}^T \left( \frac{\partial \mathbf{F}^{\text{Th}}}{\partial \mathbf{T}} + \hat{\mathbf{K}}^m \right) + \boldsymbol{\xi}^T (\mathbf{K} + \hat{\mathbf{K}}) \right] \frac{d\mathbf{T}}{dP_i} \\ & - \boldsymbol{\lambda}^T \left( \frac{\partial \mathbf{K}^m}{\partial P_i} \mathbf{U} + \frac{\partial \mathbf{F}^{\text{Th}}}{\partial P_i} \right) - \boldsymbol{\xi}^T \frac{\partial \mathbf{K}}{\partial P_i} \mathbf{T}. \end{aligned} \quad (16)$$

In order to avoid the expensive computation of  $d\mathbf{T}/dP_i$  and  $d\mathbf{U}/dP_i$ , the adjoint vectors  $\boldsymbol{\lambda}$  and  $\boldsymbol{\xi}$  are determined such that:

$$\mathbf{K}^m \boldsymbol{\lambda} = \frac{\partial f}{\partial \mathbf{U}}^T, \quad (17)$$

and

$$(\mathbf{K} + \hat{\mathbf{K}})^T \boldsymbol{\xi} = - \left( \frac{\partial \mathbf{F}^{\text{Th}}}{\partial \mathbf{T}} + \hat{\mathbf{K}}^m \right)^T \boldsymbol{\lambda}. \quad (18)$$

Introducing in Eq. (16) the adjoint vectors  $\boldsymbol{\lambda}$  and  $\boldsymbol{\xi}$  obtained from the solution of (17) and (18), allows the computation of  $df/dP_i$  according to:

$$\frac{df}{dP_i} = \left. \frac{\partial f}{\partial P_i} \right|_{\mathbf{U}=\text{const}} - \boldsymbol{\lambda}^T \left( \frac{\partial \mathbf{K}^m}{\partial P_i} \mathbf{U} + \frac{\partial \mathbf{F}^{\text{Th}}}{\partial P_i} \right) - \boldsymbol{\xi}^T \frac{\partial \mathbf{K}}{\partial P_i} \mathbf{T}. \quad (19)$$

It is worth noting that the current objective function (12) does not explicitly depend on  $\mathbf{P}$ , but only implicitly via  $\mathbf{u}(\mathbf{x}^{(h)}, \mathbf{P})$ , whereby  $\partial f / \partial P_i |_{\mathbf{U}=\text{const}} = 0$ .

Similar analyses were performed for the design of functionally graded materials [58], compliant actuators [59] and composites with rectangular inclusions [54], and also in topology optimization thermo-mechanical problems with stress constraints [60]. However, unlike the current study, the work mentioned above have been conducted without considering the dependence of material properties on temperature. Actually, the current sensitivity analysis can be seen as a particular case of the complete formulation developed by Michaleris et al. [57] that includes, besides thermo-dependent material properties, nonlinear and transient effects.

## 3. Design of an elastostatic cloaking device subjected to thermal loads

As an applied example, the current topology optimization-based procedure will be used in the design of a thermo-mechanical cloaking metadvice.

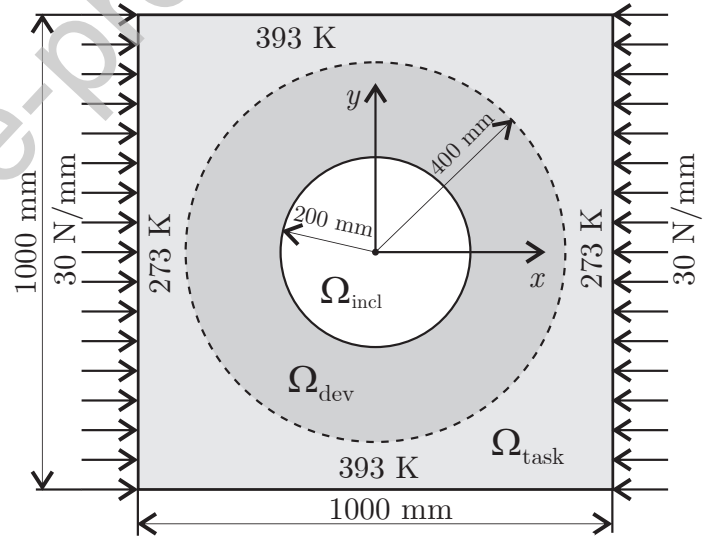


Figure 2: Domain  $\Omega = \Omega_{\text{dev}} \cup \Omega_{\text{incl}} \cup \Omega_{\text{task}}$  and boundary conditions of the thermo-mechanical problem.

Let  $\Omega$  be a full square plate made of nylon (see Table 1 for thermal and mechanical properties) under plane strain conditions, free of internal heat sources and body forces, and subjected to the thermal and mechanical boundary conditions depicted in Fig. 2. Also, let  $\mathbf{u}_0$  be the displacement fields in  $\Omega$  under such conditions. After making a circular hole  $\Omega_{\text{incl}}$  at the center of the plate without altering the boundary conditions mentioned above, the displacements field in  $\Omega$  is significantly affected. For cloaking purposes, a metadvice occupying the annular region around the hole ( $\Omega_{\text{dev}}$ ) will be designed in order to allow the displacement field  $\mathbf{u}$  outside the device ( $\Omega_{\text{task}}$ ) be affected to a minimum extent. To this end, the optimization problem (13) is solved in order to find  $\mathbf{P}$  (the material distribution in  $\Omega_{\text{dev}}$ ) such

that the corresponding displacements  $\mathbf{u}(\mathbf{x}^{(h)}, \mathbf{P})$  matches – up to a minimum error – the displacements  $\mathbf{u}_0(\mathbf{x}^{(h)})$  in the plate before making the hole, at the nodes  $\mathbf{x}^{(h)}$  of the finite elements whose centers lie in the region  $\Omega_{\text{task}}$  of the plate outside the device. Such a device will be designed using aluminum (material A) and polyethylene (material B), whose properties are reported in Table 1. The Young’s modulus of all the materials are temperature-dependent functions, obtained from a nonlinear regression of the data reported in references [61–63]. It should be noted that the single dependence of the Young’s modulus  $E(T)$  on temperature introduces variations in both the elastic moduli  $\mathbf{C}$  and stress increment per unit temperature  $\mathbf{d}$  isotropic tensors, since:

$$\mathbf{C}(T) = \frac{E(T)}{(1+\nu)} \mathbf{I}^{(4)} + \frac{E(T)\nu}{(1+\nu)(1-2\nu)} \mathbf{I}^{(2)} \otimes \mathbf{I}^{(2)},$$

Table 1: Thermal and mechanical properties of nylon, aluminum and polyethylene

Property	Material		
	Nylon	Aluminium	Polyethylene
Thermal conductivity [W(mK) <sup>-1</sup> ]	0.31	$k_A = 205$	$k_B = 0.46$
Young’s modulus [GPa]	$2.33[1.21 - (1 + e^{-0.14 T(\text{K}) + 48.5})^{-1}]$	$E_A = -0.04 T(\text{K}) + 80$	$E_B = 136.16 e^{-0.016 T(\text{K})}$
Poisson ratio	0.4	$\nu_A = 0.33$	$\nu_B = 0.46$
Thermal expansion coefficient [K <sup>-1</sup> ]	$8 \times 10^{-5}$	$\alpha_A = 2.3 \times 10^{-5}$	$\alpha_B = 15 \times 10^{-5}$

### 3.1. Solution procedure of the optimization problem

Given the symmetry of the domain and thermo-mechanical boundary conditions depicted in Fig. 2, the FEM-based solution of the governing equations will be performed only over the upper right quadrant of  $\Omega$  by using an uniform mesh of  $200 \times 200 = 40000$  bilinear finite elements. The thermo-mechanical problem over the plate with the hole is solved with a mesh of 35053 finite elements, which is obtained after discarding the elements whose centers lie in  $\Omega_{\text{incl}}$ . The artificial density  $\rho_e \equiv P_e$  is considered to vary element-wise in  $\Omega_{\text{dev}}$ , which is occupied by 15086 elements. Accordingly, this is a large scale non-linear optimization problem of 15086 design variables subjected to the box constraint  $0 \leq P_e \leq 1$ . As stated so far, the elastostatic cloaking device will be designed by solving the optimization problem (13), with (12) as the objective function to be minimized. The cloaking task is defined by setting  $\bar{\mathbf{u}} = \mathbf{u}_0$  at the nodes  $\mathbf{x}^{(h)}$  of those elements whose centers lie in  $\Omega_{\text{task}}$ .

Finally, such a non-linear large-scale constrained optimization problem is solved using the method of moving asymptotes (MMA) [64]. The checkerboard-type instabilities that usually affect this kind of materials distribution problems [33], will be overcome by using the density filtering technique proposed by Bruns and Tortorelli [65]. Such a strategy has already been proven to be well suited for the design of thermal [4, 5, 10, 11], mechanical [15] and thermo-mechanical [16] metadvicees. Additionally, Heaviside filtering [66, 67] is implemented in order to reduce the “gray” zones (those elements where  $0 < P_e < 1$ , i.e. the material is neither aluminum or polyethylene, but an unlikely feasible material with intermediate properties). The combination of

and

$$\mathbf{d}(T) = -\mathbf{C}(T) : \mathbf{I}^{(2)} \alpha,$$

where  $\mathbf{I}^{(2)}$  is the second order identity tensor with components  $I_{ij}^{(2)} = \delta_{ij}$ , whereas  $\mathbf{I}^{(4)}$  is the fourth order symmetric identity tensor with components  $I_{ijkl}^{(4)} = (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})/2$ . The remaining material properties  $(k, \alpha, \nu)$  are kept constant, since they do not exhibit significant variations within the temperature range inherent to the thermal boundary conditions depicted in Fig. 2. However, it is worth mentioning that the current methodology allows the possibility of introducing the temperature dependence of any property without further complications.

both filtering strategies leads to the definition of a filtered artificial density

$$\bar{P}_e = 1 - e^{-\beta \bar{P}_e} + \bar{P}_e e^{-\beta} \equiv \tilde{H}(\bar{P}_e, \beta), \quad (20)$$

with

$$\bar{P}_e = \frac{\sum_{i=1}^N \langle r - \Delta_{ei} \rangle P_i}{\sum_{i=1}^N \langle r - \Delta_{ei} \rangle}. \quad (21)$$

The above equation defines the density filter [65], being  $r$  the filter radius (adopted in this work as 7 times the finite element size),  $\Delta_{ei}$  the distance between the centers of the elements  $\Omega^{(e)}$  and  $\Omega^{(i)}$ , and  $\langle x \rangle = xH(x)$  the ramp function with  $H(x)$  denoting the Heaviside step function ( $H(x) = 0$  for  $x < 0$ ,  $H(0) = 1/2$  and  $H(x) = 1$  for  $x > 0$ ). The equation (20) defines the Heaviside projection filtering [68], being  $\tilde{H}(x, \beta)$  a regularization of  $H(x)$ , and  $\beta$  a parameter controlling the curvature of  $\tilde{H}$  such that  $\tilde{H}(x, 0) \equiv x$  (i.e., there is no filtering) and  $\tilde{H}(x, \infty) = H(x)$ .

The filtered density  $\bar{P}_e$  is also called “physical” density, since it determines the material properties at the finite element  $\Omega^{(e)}$ . Consequently, the objective function becomes  $\tilde{f}(\mathbf{P}) \equiv f(\bar{\mathbf{P}})$ , but  $\mathbf{P}$  remains as design variable. Accordingly, the optimization problem (15) is replaced by

$$\min_{\mathbf{P} \in \mathcal{D}} \tilde{f}(\mathbf{P}) \quad \text{subjected to } 0 \leq P_i \leq 1 \quad i = 1, 2, \dots, N, \quad (22)$$

Filtering has to be accounted within the sensitivity analysis. Since equation (19) now actually defines  $d\tilde{f}/d\bar{P}_i$  instead of  $df/dP_i$ , the derivative of the new objective function with respect to the design variable  $P_i$  must be computed using the chain rule:

$$\frac{d\tilde{f}}{dP_i} = \frac{d\tilde{f}}{d\bar{P}_i} \frac{d\bar{P}_i}{dP_i},$$



where  $d\tilde{P}_j/d\tilde{P}_k$  and  $d\tilde{P}_k/dP_i$  can be easily derived from equations (20) and (21), respectively.

To obtain the final design, successive optimization problems are solved by gradually increasing  $\beta$  via the continuation method proposed by Andreassen et al. [67], in order to achieve stable convergence and ensuring differentiability in the course of the optimization procedure[66, 67]. This is schematized in the following flowchart in pseudo code:

- (1) Initialization: set  $s = 0$  and  $\mathbf{P}_0 = [0.5, 0.5, \dots, 0.5]$ .
- (2) Continuation: set  $\beta = 2^s$ ,  $i = 0$  and  $\mathbf{P}^{(i)} = \mathbf{P}_0$ .
  - (a) Thermal FEM:  $\tilde{\mathbf{P}} \rightarrow T(\mathbf{x}, \tilde{\mathbf{P}})$
  - (b) Mechanical FEM:  $(T, \tilde{\mathbf{P}}) \rightarrow \mathbf{u}(\mathbf{x}, \tilde{\mathbf{P}})$
  - (c) Objective function:  $\mathbf{u}(\mathbf{x}, \tilde{\mathbf{P}}) \rightarrow f(\tilde{\mathbf{P}})$
  - (d) Sensitivity:  $(\mathbf{P}^{(i)}, \tilde{\mathbf{P}}, \mathbf{u}, T, \dots) \rightarrow \frac{\partial f}{\partial \tilde{\mathbf{P}}}$
  - (e) Update:  $(\mathbf{P}^{(i)}, \frac{\partial f}{\partial \tilde{\mathbf{P}}}) \rightarrow \mathbf{P}^{(i+1)}$
  - (f) Stop criterion:
    - If  $i < i_{\max}$  and  $\|\mathbf{P}^{(i+1)} - \mathbf{P}^{(i)}\|_{\infty} > \epsilon$ ,  $i \leftarrow i + 1$ , go to (a).
    - Otherwise:
      - If  $\beta < \beta_{\max}$ , set  $s \leftarrow s + 1$  and  $\mathbf{P}_0 = \mathbf{P}^{(i+1)}$ , then go to (2).
      - Otherwise, go to (3).
- (3) Thresholding:  $(\tilde{\mathbf{P}}, w^*) \rightarrow \tilde{\mathbf{P}}^{\text{thr}}$ .

In the above procedure,  $\mathbf{P}_0$  is the initial guess, which is first arbitrarily adopted and then updated after each continuation step  $s$ . The optimization solver at each continuation step  $s$  stops at the iteration  $i_{\max} = 300$  or when the change in variables is less than  $\epsilon = 0.01$ . The curvature of the Heaviside approximation is increased until  $\beta_{\max} = 128$ , since greater  $\beta$  seriously deteriorate the convergence of the optimization problem. Although the gray zones are considerably reduced after the successive optimization steps, there is still need of a final filtering (the so-called thresholding) to obtain a fully binary design  $\tilde{\mathbf{P}}^{\text{thr}}$  with  $w^*$  as the threshold for  $\rho_e^p$ . The thresholding strategy to be implemented in this work has been proposed by Fachinotti et al.[4, 15], and its implementation will be explained later.

## 4. Results

The FEM-based solutions for the displacement and temperature fields in the full nylon plate are depicted in Fig. 3 (a)-(c), whereas those in the holed nylon plate are shown in Fig. 3 (d)-(f). After making the hole in the nylon plate, a new displacements field  $\mathbf{u}^{\text{hol}}$  is achieved. Such displacements differs considerably from the field  $\mathbf{u}_0$  corresponding to the full nylon plate, giving rise to an error  $f^{\text{hol}} = 1.203$  in the fulfillment of the cloaking task. The material distribution achieved by solving successive optimization problems (22) via the continuation procedure described in the previous section, is shown in Fig. 4 (a). The displacements

and temperature fields achieved when a cloaking device with such a material distribution occupies the annular region bounded by the dashed lines, are depicted in Fig. 3 (g)-(i). Using such a device allows the error in the fulfillment of the cloaking task to be minimized up to a value of  $f^{\text{opt}} = 0.01284 = 0.0107 f^{\text{hol}}$ , which represents a 98.93% reduction compared to the error  $f^{\text{hol}}$  corresponding to the holed plate without the device. Even after Heaviside filtering, the optimal solution depicted in Fig. 4 (a) still exhibits gray zones. Such a feature precludes the manufacture of the so-designed thermo-mechanical metadvice, which is a main concern in this work.

In order to suppress the gray zones, recourse can be made to a thresholding strategy proposed in previous work related to the design of both thermal[4] and mechanical[15] easy-to-make metadvice: the material at the element  $\Omega^{(e)} \in \Omega_{\text{dev}}$  is aluminum if  $\tilde{P}_e^{\text{thr}} = 1$  and polyethylene if  $\tilde{P}_e^{\text{thr}} = 0$ , with

$$\tilde{P}_e^{\text{thr}} = H(\tilde{P}_e^p - w^*),$$

where  $w^*$  is the threshold. In classical topology optimization,  $w^*$  is frequently determined in order to fulfill volume constraints [69], although it is frequently conceived as a user-defined parameter [70–75]. In problems without volume constraint like the current one, Fachinotti et al. [4, 15] proposed to determine  $w^*$  such that the performance of the metadvice –that is no longer optimal after thresholding– be affected to a minimum extent. In this sense, the thresholding procedure is conceived to find  $w^* \in (0, 1)$  such that  $f^{\text{thr}} = f(\tilde{\mathbf{P}}^{\text{thr}})$  reaches its minimum. The  $f^{\text{thr}}/f^{\text{opt}}$  ratio for different values of  $w^*$  is plotted in Fig. 5, which exhibits a minimum at  $w^* = 0.12$  where  $f^{\text{thr}} = 0.01454 = 1.1324 f^{\text{opt}} = 0.0120 f^{\text{hol}}$ . Accordingly, using the corresponding discrete device shown in 4 (b) offering the best deal between performance and manufacturability, has allowed a 98.79% reduction compared to the error  $f^{\text{hol}}$  without the device. The corresponding displacement field  $\mathbf{u}^{\text{thr}}$  is depicted in Fig. 3 (j)-(k), whereas the temperature field is shown in Fig. 3 (l). So, losing only 0.14% of the initial displacements field recovery (that of the full nylon plate  $\mathbf{u}_0$ ) in  $\Omega_{\text{task}}$  after the thresholding procedure has allowed the achievement of such a device of feasible manufacture.

The distribution of local relative error  $\epsilon^{\text{hol}} = \|\mathbf{u}^{\text{hol}} - \mathbf{u}_0\|/\|\mathbf{u}_0\|$  for the holed homogeneous plate in the region  $\Omega_{\text{task}}$  –where the cloaking task was prescribed– is depicted in Fig. 6 (a), whereas the distribution of local relative error  $\epsilon^{\text{thr}} = \|\mathbf{u}^{\text{thr}} - \mathbf{u}_0\|/\|\mathbf{u}_0\|$  achieved in the same region when including the thresholded (feasible) cloaking device in  $\Omega_{\text{dev}}$  is depicted in Fig. 6 (b). The good performance of such cloaking device can actually be demonstrated by comparing Fig. 6 (a) and Fig. 6 (b): the maximum  $\epsilon^{\text{thr}}$  is 7.4%, which is less than a half of the minimum  $\epsilon^{\text{hol}}$ . These results are also consistent with the deformed contours depicted in Fig. 7, where the displacement are magnified by a factor of 5 for better visualization.

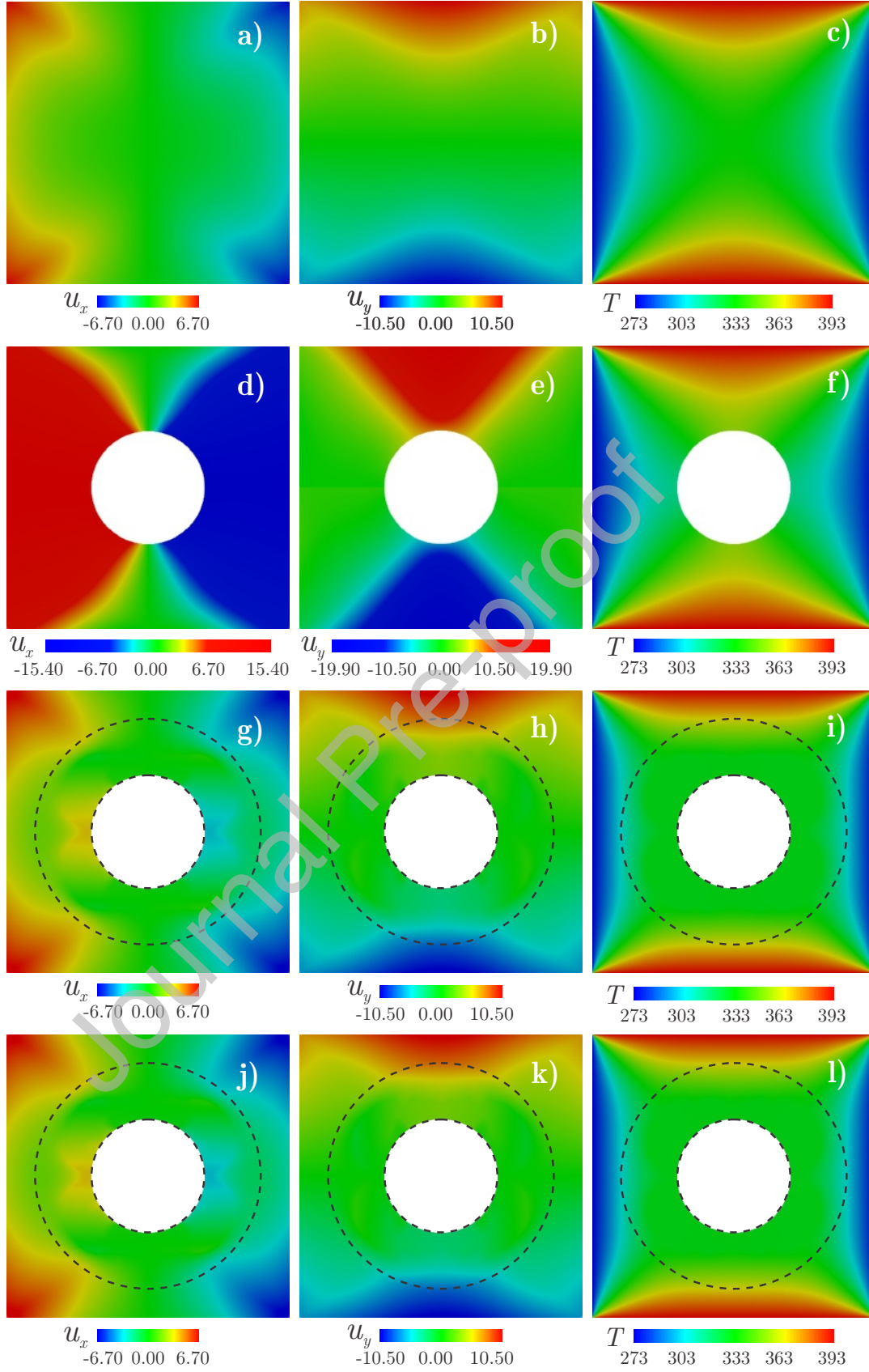


Figure 3: Displacements  $u_x$  (a) and  $u_y$  (b) and temperature  $T$  (c) distributions in the homogeneous plate without hole, the holed homogeneous plate (d-f), the plate with the optimal cloaking device (g-i) and the plate with the fully discrete device (j-l). Displacements and temperature distributions are given in millimeters and Kelvin, respectively.

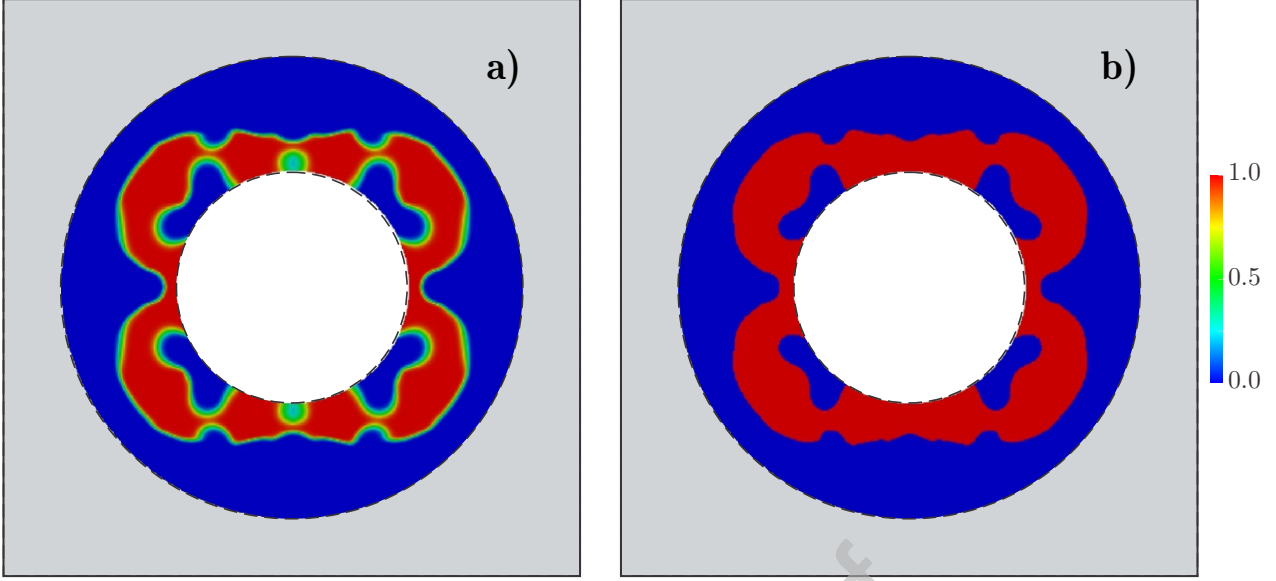


Figure 4: Distribution of aluminum (red) and polyethylene (blue) in the metadvice designed by solving the topology optimization problem. a) Optimal continuous material distribution with gray zones, and b) best discrete material distribution achieved after eliminating the gray zones by thresholding.

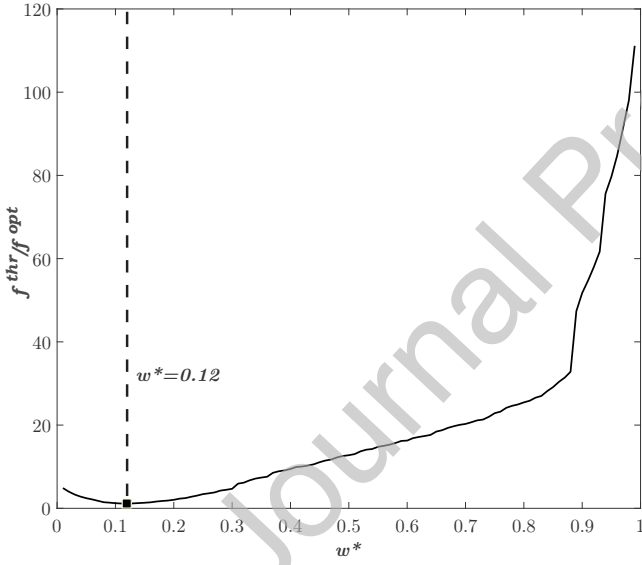


Figure 5: Error in the cloaking task accomplishment by the fully discrete metadvice as a function of the threshold value  $w^*$ .

Such deformed contours involve the points lying on the plate boundaries and also on the diagonal lines throughout it, and the deformed contours of the hole and the metadvice are represented by the dotted lines. This figure depicts the marked differences between the deformed shape of the full plate (black) and the holed plate (red), and also the noteworthy overlapping of the contours corresponding to the holed plate with the metadvice (blue) and the full plate (black) in  $\Omega_{\text{task}}$ . Given the significant reduction of the errors with respect to the target displacements field  $\mathbf{u}_0$  after introducing the metadvice, the deformed contours corresponding to

the full plate and the holed plate with the metadvice are virtually indistinguishable each other in  $\Omega_{\text{task}}$ . These contours also depict how the device works: it is conceived to deform appropriately in order to perform the cloaking task only in  $\Omega_{\text{task}}$ , whereby there is no coincidence of the black and blue contours in the region occupied by such a device (enclosed by the blue dotted lines).

## 5. Discussion

The results reported in the previous section demonstrate the potential of the current topology optimization-based approach to design thermo-mechanical metadvice, providing a simple and feasible manufacture design consisting of two macroscopically distinguishable isotropic materials. The background material (nylon) has intermediate Young's modulus regarding the metadvice constituents (aluminum and polyethylene), which has already been proven to guarantee an efficient design of metadvice for mechanical cloaking [15]. The background material has also intermediate thermal expansion compared to aluminum and polyethylene, which is actually crucial in the design of thermo-mechanical cloaking devices [16].

As shown in the previous section, the performance of the easy-to-make thresholded cloaking device shown in Fig. 4 (b) is highly satisfactory. A richer design set  $\mathcal{D}$  can lead to a metadvice exhibiting even better performance, but that would also be significantly harder to manufacture. For instance, it is possible to design the cloaking device using the same candidate materials, but arranged in laminates of variable relative thickness and orientation.

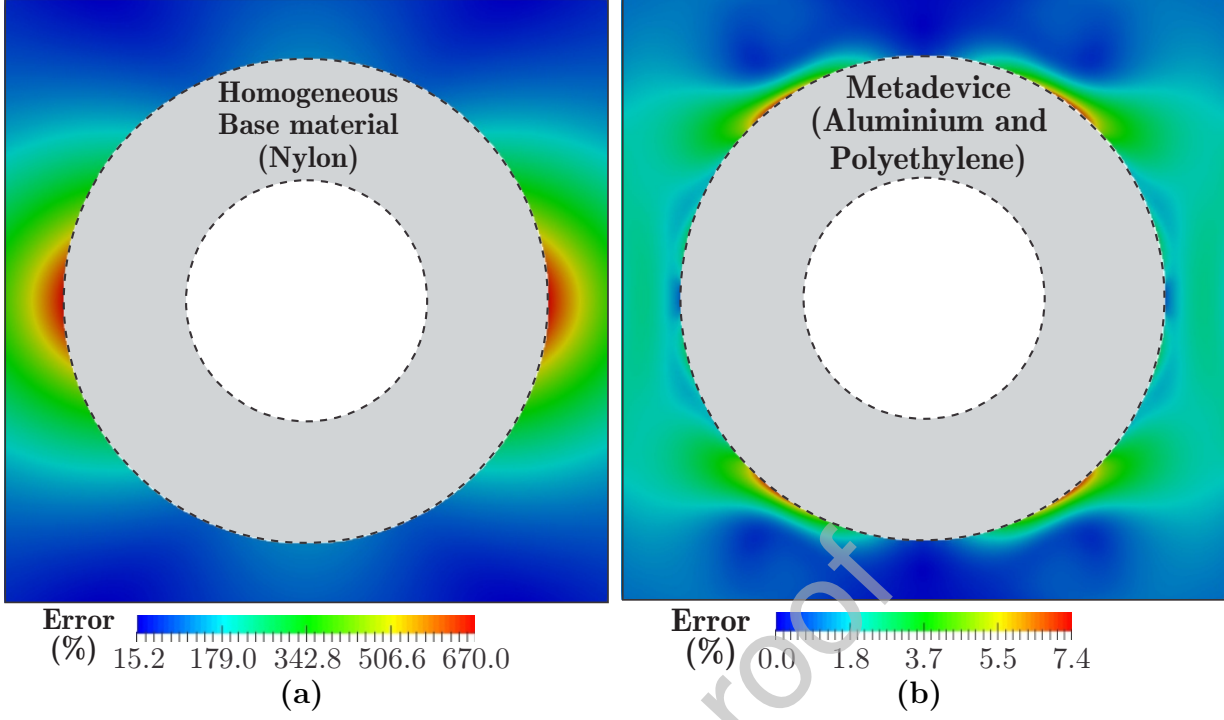


Figure 6: Distribution of local relative error in the cloaking task achievement: (a) Holed homogeneous plate, and (b) Holed plate with the thresholded metadevice.

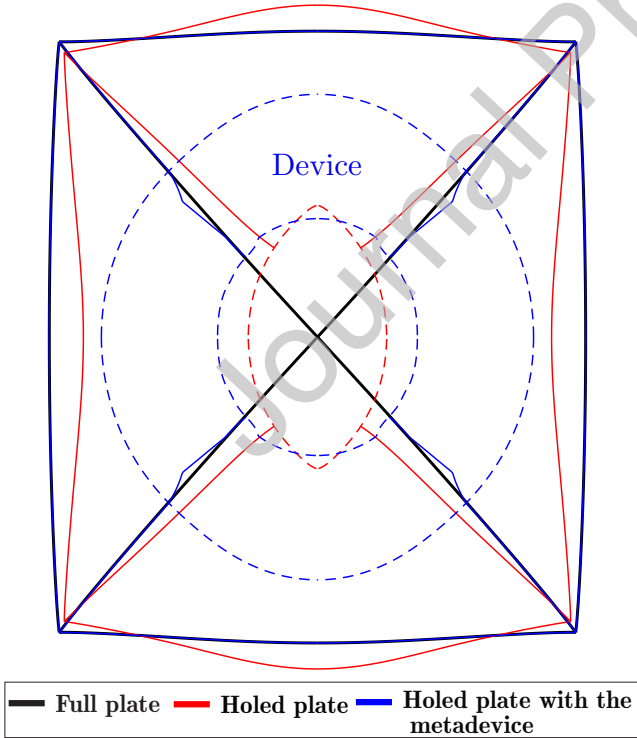


Figure 7: Deformed contours of the internal and external boundaries together to the diagonal lines for the full plate (black), the holed plate (red), and the holed plate with the metadevice (blue).

Such laminates behave as an orthotropic metamaterial, whose properties under plane strain conditions are given in Table 2 [16]. In this case, two design variables are needed to characterize the unit cell at each finite element  $\Omega^{(e)}$ : the orientation  $\theta_e$  of the laminate and the relative thickness  $t_e$  of the aluminum layer. The relative thickness of the polyethylene layer is simply  $1 - t_e$ , whereby it is not a design variable. So, the metamaterial distribution is determined by solving the problem

$$\min_{\mathbf{P} \in \mathbb{R}^{2N}} f(\bar{\mathbf{P}}) \quad \text{subjected to } 0 \leq P_{2i-1} \leq 1 \text{ and } 0 \leq P_{2i} \leq \pi, \quad i = 1, 2, \dots, N, \quad (23)$$

where  $\mathbf{P}$  is the set of design variables  $P_{2i-1} = t_i$  and  $P_{2i} = \theta_i$ , whereas  $\bar{\mathbf{P}}$  is that of density-filtered variables  $\bar{P}_{2i-1} = \bar{t}_i$  and  $\bar{P}_{2i} = \bar{\theta}_i$  defined in terms of their respective design variables by equation (21). The effective properties within such a richer design set support intermediate values between those of aluminum and polyethylene, whereby gray zones are not penalized and there is no Heaviside filtering.

Note that problem (23) has twice as many design variables as (22), becoming considerably more expensive to solve. The solution of (23), once density-filtered, gives rise to the metamaterial distribution shown in Fig. 8. The colormap indicates the relative thickness of the aluminum layers, whereas the black segments represent the laminates orientation.



Table 2: Effective thermal and mechanical properties of a laminate consisting in two layers of materials A and B with respective relative thicknesses  $t_A \equiv t_e$  and  $t_B = 1 - t_e$ , referred to the local Cartesian frame  $\lambda\tau$  ( $\lambda$  in the laminate direction, and  $\tau$  across the laminate).

Thermal conductivity	$k_{\lambda\lambda} = t_A k_A + t_B k_B$ $k_{\tau\tau} = k_A k_B (t_A k_B + t_B k_A)^{-1}$
Elastic moduli	$C_{\lambda\lambda\lambda\lambda} = E_\lambda (1 - \nu_{\lambda\tau} \nu_{\tau\lambda}) [1 - \nu_{\lambda z}^2 - 2\nu_{\lambda\tau} \nu_{\tau\lambda} (1 + \nu_{\lambda z})]^{-1}$ $C_{\tau\tau\tau\tau} = E_\tau (1 - \nu_{\lambda z}) (1 - 2\nu_{\lambda\tau} \nu_{\tau\lambda} - \nu_{\lambda z})^{-1}$ $C_{\lambda\lambda\tau\tau} = E_\tau \nu_{\lambda\tau} (1 - 2\nu_{\lambda\tau} \nu_{\tau\lambda} - \nu_{\lambda z})^{-1}$ $C_{\lambda\tau\lambda\tau} = G_{\lambda\tau}$
Young's moduli	$E_\lambda = [E_A t_A (1 - \nu_A^2)^{-1} + E_B t_B (1 - \nu_B^2)^{-1}] (1 - \nu_{\lambda z}^2)$ $E_\tau = [(1 - 2\nu_A)(1 + \nu_A) t_A (E_A (1 - \nu_A))^{-1} \dots$ $\quad + (1 - 2\nu_B)(1 + \nu_B) t_B (E_B (1 - \nu_B))^{-1} + 2\nu_{\lambda\tau}^2 (E_\lambda (1 - \nu_{\lambda z}))^{-1}]^{-1}$
Poisson ratii	$\nu_{\lambda z} = [E_A t_A \nu_A (1 - \nu_A^2)^{-1} + E_B t_B \nu_B (1 - \nu_B^2)^{-1}] [E_A t_A (1 - \nu_A^2)^{-1} + E_B t_B (1 - \nu_B^2)^{-1}]^{-1}$ $\nu_{\lambda\tau} = [\nu_A t_A (1 - \nu_A)^{-1} + \nu_B t_B (1 - \nu_B)^{-1}] (1 - \nu_{\lambda z})$ $\nu_{\tau\lambda} = \nu_{\lambda\tau} E_\tau E_\lambda^{-1}$
Shear modulus	$G_{\lambda\tau} = G_A G_B (t_A G_B + t_B G_A)^{-1}$
Thermal expansion	$\alpha_{\lambda\lambda} = [\alpha_A E_A t_A (1 - \nu_A)^{-1} + \alpha_B E_B t_B (1 - \nu_B)^{-1}] (1 - \nu_{\lambda z}) E_\lambda^{-1}$ $\alpha_{\tau\tau} = \alpha_A t_A (1 + \nu_A) (1 - \nu_A)^{-1} + \alpha_B t_B (1 + \nu_B) (1 - \nu_B)^{-1} - 2\nu_{\lambda\tau} \alpha_{\lambda\lambda} (1 - \nu_{\lambda z})^{-1}$

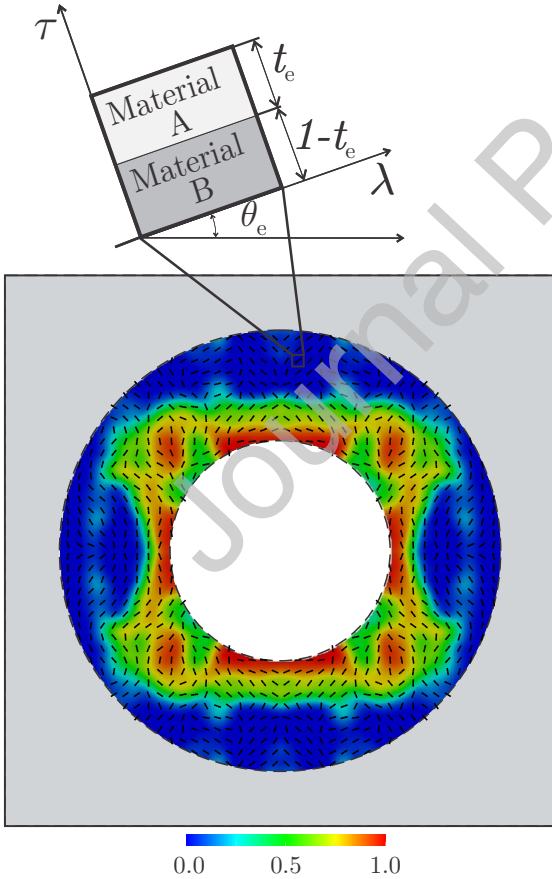


Figure 8: Variable relative thickness of the aluminum layer (colormap) and orientation (black segments) of the optimal heterogeneous metadvice made of laminates of aluminum and polyethylene. On the top, unit cell at a finite element in the metadvice.

Using this completely heterogeneous optimal metadvice allows the error in the fulfillment of the cloaking task to be minimized up to a value of  $f^{\text{het}} = 0.00753 = 0.0063 f^{\text{hol}}$ , which represents a 99.37% reduction compared to the error  $f^{\text{hol}}$  corresponding to the holed plate without the device.

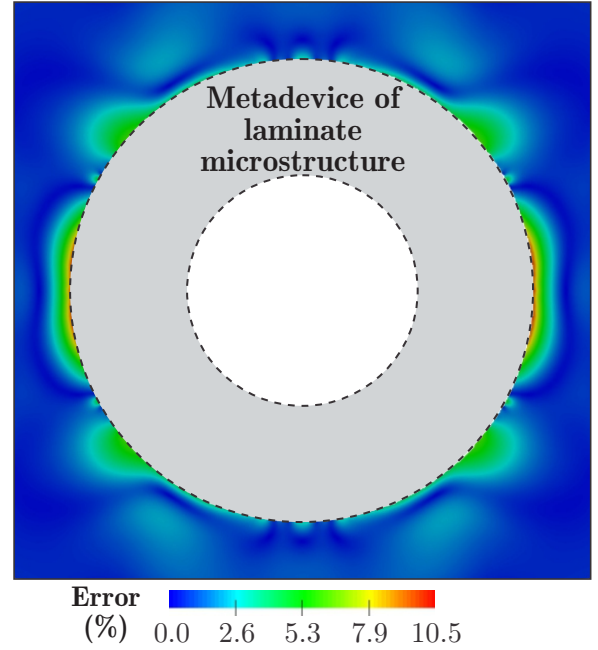


Figure 9: Distribution of local relative error in the cloaking task achievement in the holed plate with the optimal heterogeneous metadvice made of laminates of aluminum and polyethylene.

The distribution of local relative error  $\varepsilon^{\text{het}} = \|\mathbf{u}^{\text{het}} - \mathbf{u}_0\| / \|\mathbf{u}_0\|$  (being  $\mathbf{u}^{\text{het}}$  the displacement field in presence of



this metadvice) in the region  $\Omega_{\text{task}}$  is depicted in Fig. 9, and exhibits a maximum value  $\max \varepsilon^{\text{het}} = 10.5\%$ . Compared to the thresholded metadvice (Fig. 4 (b)), the optimal heterogeneous metadvice (Fig. 8) performs the cloaking task globally better ( $f^{\text{het}} = 0.5179 f^{\text{thr}}$ ) but locally worse ( $\max \varepsilon^{\text{het}} = 1.4189 \max \varepsilon^{\text{thr}}$ ). In conclusion, although it is slightly less efficient to globally accomplish the cloaking task, the thresholded metadvice is largely preferred thanks to its feasibility.

### 5.1. Importance of including temperature-dependent properties

The significance of accounting for the thermal-dependence of material properties in the design of manufacturable thermo-mechanical devices is a feature that – up to the authors’ knowledge – is considered for the first time in this work. Such an aspect can actually be demonstrated by solving again the topology optimization thermo-mechanical problem discussed so far, but neglecting the thermal-dependence of Young’s modulus of all the involved materials. For such a purpose, the Young’s modulus of the materials will be computed at the average value of the temperature range involved in the thermo-mechanical problem ( $T = 333 \text{ K}$ ). Following the procedure described in Section 3.1. in the framework of this thermo-mechanical problem, the thresholded device depicted in Fig. 10 is obtained. Such a metadvice exhibits noteworthy differences in the material distribution with respect to the thresholded device shown in Fig. 4 (b), which was designed taking due account of the thermal-dependence of Young’s moduli.

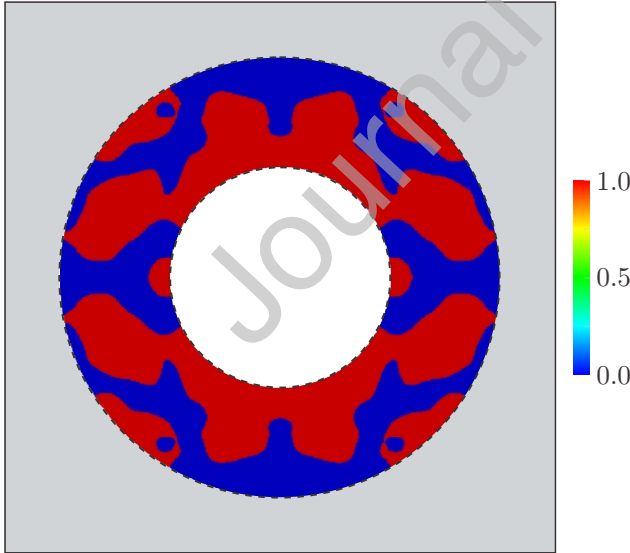


Figure 10: Distribution of aluminum (red) and polyethylene (blue) in the thresholded metadvice obtained after neglecting the thermal-dependence of the Young’s modulus of all the involved materials.

Keeping in mind that the displacement field to be recovered is actually that of the full plate made of nylon with

thermo-dependent Young’s modulus (the field  $\mathbf{u}_0$  shown in Fig. 3 (a) and (b)), the error in the cloaking task achievement using the metadvice shown in Fig. 10 is  $f^{\text{con}} = 0.392 = 26.9601 f^{\text{thr}}$  (much higher than the error  $f^{\text{thr}}$  for thresholded metadvice in the Fig. 4 (b)). The poor performance of this device is a consequence of having been conceived to fulfill the cloaking task under conditions such that the properties of all the materials involved can be considered constant, which is not realistic given that the Young’s modulus of such materials exhibit actually noteworthy variations in the temperature range of the thermo-mechanical problem addressed in this work. In conclusion, neglecting the thermal-dependence of material properties may seriously deteriorate the performance of the metadvice.

### 5.2. Versatility of the topology optimization-based approach

To further highlight the versatility of the current topology optimization-based approach for the design of thermo-mechanical metadvice, the design of a different cloaking device will be carried out under the geometric configuration shown in Fig. 11. This problem is identical to that described in Section 4., but introducing changes in the geometry of both the hole  $\Omega_{\text{incl}}$  and the metadvice  $\Omega_{\text{dev}}$ . The geometry of the hole is changed to a rhombus, whereas the metadvice is now a square surrounding the hole. Such modification in the geometry makes more difficult the search for an invariant form of the conservation equations, when using the classical coordinates transformation-based design approaches [7, 23, 25, 26, 28]. However, when the current topology optimization-based approach is used, the design process is identical to that described in Section 3.1.

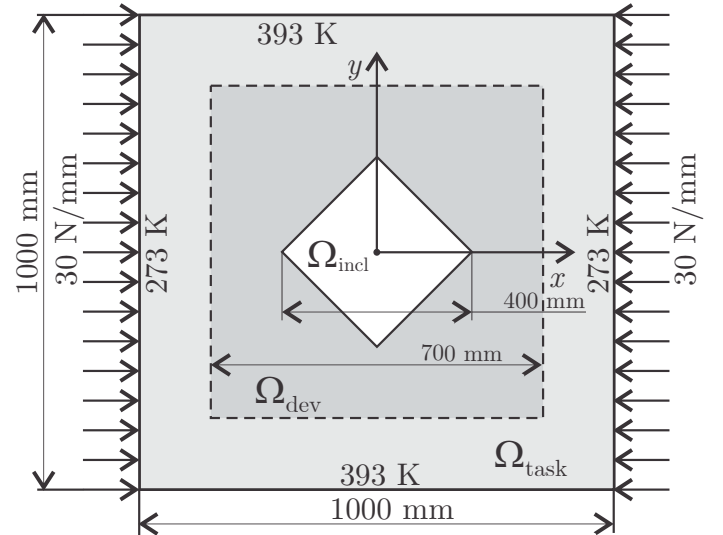


Figure 11: Domain  $\Omega = \Omega_{\text{dev}} \cup \Omega_{\text{incl}} \cup \Omega_{\text{task}}$  and boundary conditions of the thermo-mechanical problem with different geometries for both the hole and the cloaking device.

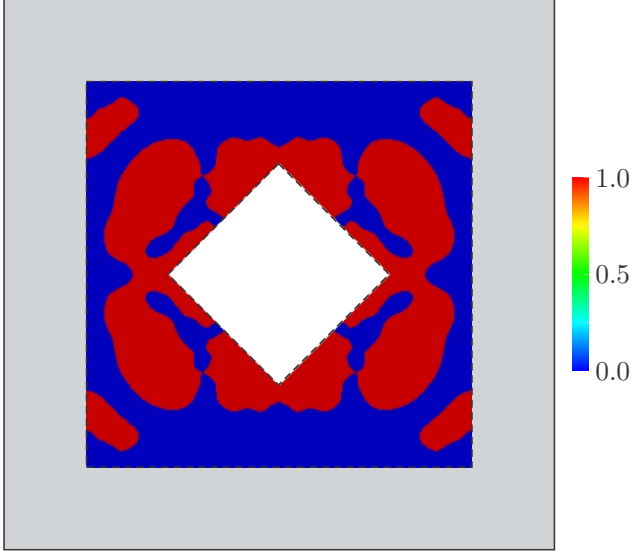


Figure 12: Distribution of aluminum (red) and polyethylene (blue) in the metadvice achieved under the proposed topology optimization-based approach, when considering different geometries for both the hole and the metadvice

After making the rhombic hole in the plate, the changes in the displacements field compared to that of the full plate (the field  $\mathbf{u}_0$  shown in Fig. 3 (a) and (b)) give rise to a global error  $f^{\text{hol}} = 0.89$  in the accomplishment of the cloaking task throughout  $\Omega_{\text{task}}$ . The distribution of local relative error  $\varepsilon^{\text{hol}} = \|\mathbf{u}^{\text{hol}} - \mathbf{u}_0\|/\|\mathbf{u}_0\|$ , with  $\mathbf{u}^{\text{hol}}$  denoting the displacement in this holed plate, is depicted in Fig. 13 (a). Such a distribution exhibits maximum value of  $\max \varepsilon^{\text{hol}} = 616\%$ .

The fully discrete metadvice shown in Fig. 12 has been obtained by following the same steps detailed in section 3.1., finding a threshold of  $w^* = 0.08$  that guarantees the best deal between performance and manufacturability. Using this device reduces the error in the cloaking task up to  $f^{\text{thr}} = 0.0255 = 0.0287f^{\text{hol}}$ , which represents a 97.13% reduction compared to the error  $f^{\text{hol}}$  corresponding to the holed plate without metadvice. Fig. 13 (b) shows the distribution of local relative error  $\varepsilon^{\text{thr}} = \|\mathbf{u}^{\text{thr}} - \mathbf{u}_0\|/\|\mathbf{u}_0\|$ , with  $\mathbf{u}^{\text{thr}}$  denoting the displacement in this holed plate when including in  $\Omega_{\text{dev}}$  the metadvice depicted in Fig. 12.

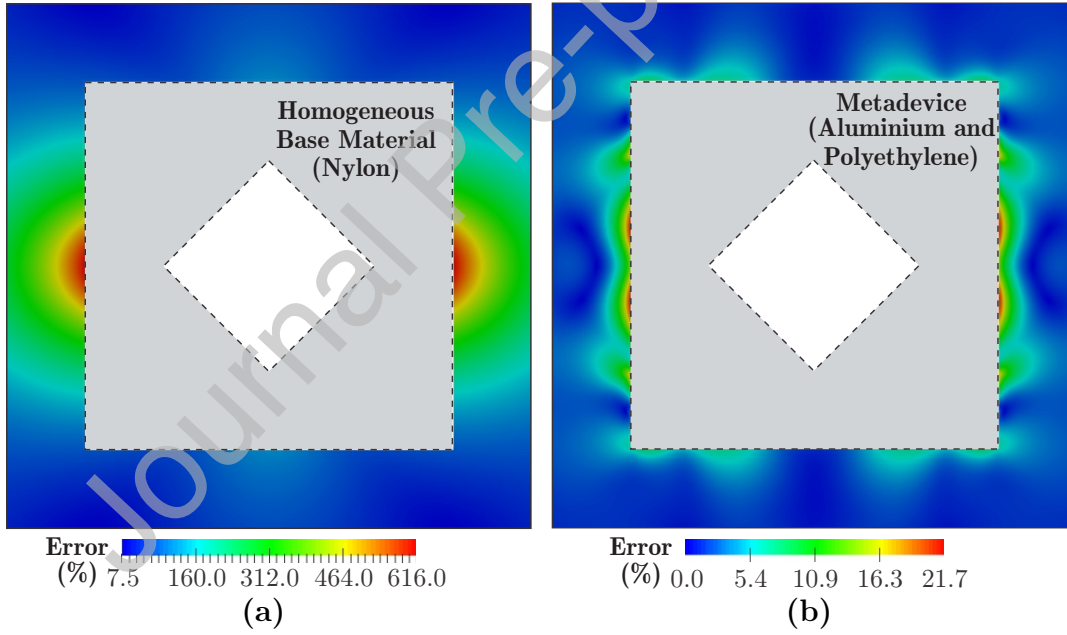


Figure 13: Distribution of local relative error in the cloaking task achievement: (a) Holed homogeneous plate, and (b) Holed plate with the thresholded metadvice.

Note that using this feasible metadvice considerably reduces the maximum local relative error up to  $\max \varepsilon^{\text{thr}} = 21.7\% = 0.0352 \max \varepsilon^{\text{hol}}$ .

Finally, the good performance of this cloaking metadvice is qualitatively appreciated in the deformed contours depicted in Fig. 14 corresponding to the full plate as well as

of the holed plate with and without the metadvice, where the displacements are magnified by a factor of 5 for better visualization. Including the metadvice designed in this alternative case, has also given rise to a noteworthy overlapping of the deformed contours in  $\Omega_{\text{task}}$ . Despite the changes introduced in the problem geometry, the cloaking device still works the way it was intended.

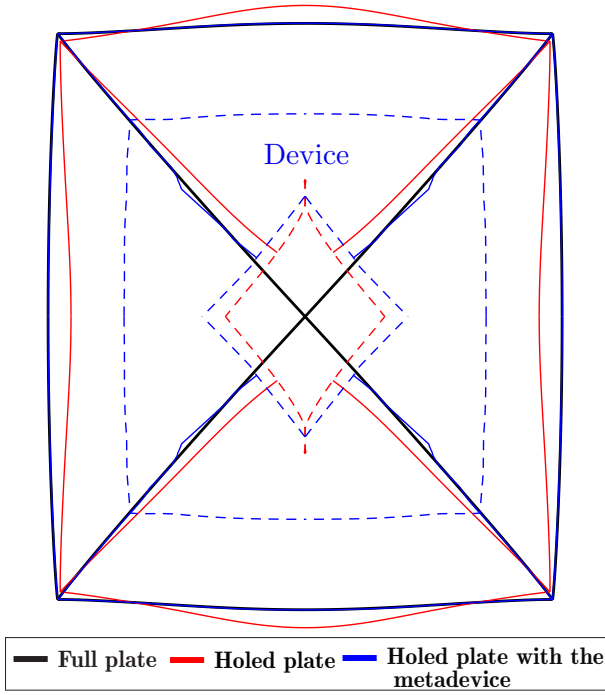


Figure 14: Deformed contours of the internal and external boundaries together to the diagonal lines for the full plate (black), the holed plate (red), and the holed plate with the metadvice (blue).

## 6. Conclusions

A novel approach has been introduced for the computational design of manufacturable thermo-mechanical metadvice, accounting for the coupling between temperature and displacement fields when both are actually influenced by the material distribution. It consists in the solution of a topology optimization problem where the objective function defines the error in the accomplishment of a displacement-dependent task (cloaking, particularly), and the design variables determine the material distribution. This topology optimization problem is solved using the popular solid isotropic microstructure (or material) with penalization (SIMP) interpolation scheme, where the design variable is an artificial density serving to choose between two candidate materials with contrasting thermal and mechanical properties.

Compared to a previous communication also concerning the design of thermo-mechanical devices considering the coupling and design-dependence of temperature and displacement [16], the current work introduces manufacturability as a crucial contribution. Metadvice are made of only two macroscopically distinguishable standard isotropic materials, being easy-to-make, unlike the previously designed heterogeneous metadvice [16] made of orthotropic laminate-based metamaterials.

The thermo-mechanical response of the device is evaluated using the finite element method, allowing fully ar-

bitrary geometries for the device, the domain where it is embedded and its thermal and mechanical boundary conditions, which largely contributes to the high versatility of the currently proposed approach.

The potentiality and versatility of the proposed topology optimization-based approach are demonstrated via its application to the design of a series of elastostatic cloaking metadvice in regions subjected to thermal and mechanical loads, considering either constant or temperature-dependent material properties and different geometries. All the so-designed cloaking metadvice are easy-to-make, exhibiting also a good performance.

Further, in so doing, it was highlighted the importance of the thermal-dependence of material properties on the thermo-mechanical response of the metadvice, and consequently in its final design.

It was also demonstrated that a unique approach serves for different problems.

Based on the obtained results, the following conclusions can be highlighted: (i) the proposed topology optimization-based approach allows the design of manufacturable and high-performance thermo-mechanical metadvice; (ii) the so-designed metadvice can be easily manufactured using two macroscopically distinguishable isotropic materials with contrasting material properties; (iii) the effect of material distribution on temperature was accounted for, which is unprecedented in the design of manufacturable thermo-mechanical metadvice; (iv) by considering the influence of material distribution on temperature, the thermal-dependence of material properties and the coupling of temperature and displacement fields, the current approach allows solving problems that are unaffordable with the classical coordinates transformation-based approach for the design of metamaterials and metadvice; and (v) the material distribution in the thermo-mechanical metadvice is prescribed, which is a crucial advantage with respect to the approaches (like the transformation-based one) that define inhomogeneous and uncertainly feasible material properties.

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