TOPOLOGICAL DERIVATIVE FOR STEADY-STATE ORTHOTROPIC HEAT DIFFUSION PROBLEM

S.M. GIUSTI, A.A. NOVOTNY, AND J. SOKOŁOWSKI

Abstract. The aim of this work is to present the calculation of the topological derivative for the total potential energy associated to the steady-state orthotropic heat diffusion problem, when a circular inclusion is introduced at an arbitrary point of the domain. By a simple change of variables and using the first order Pólya-Szegö polarization tensor, we obtain a closed formula for the topological sensitivity. For the sake of completeness, the analytical expression for the topological derivative is checked numerically using the standard Finite Element Method. Finally, we present two numerical experiments showing the influency of the orthotropy in the topological derivative field and also one example concerning the optimal design of a heat conductor.

1. Introduction

The topological sensitivity analysis gives the topological asymptotic expansion of a shape functional with respect to an infinitesimal singular domain perturbation, like the insertion of holes, inclusions, source-term or cracks. The main term of this expansion, called topological derivative ([12, 31, 10]), is now of common use in numerical procedures of resolution for topology optimization ([4, 22]), image processing ([20, 7, 21]) and inverse problems ([14, 6, 9]). Concerning the theoretical development of the topological asymptotic analysis, the reader may refer to [26], for instance. We refer the reader to [1, 28, 15] and [16], for the numerical methods of shape and topology optimization which include the topological derivatives in the numerical procedure of the *levelset* type.

In order to introduce these concepts, let us consider an open bounded domain $\Omega \subset \mathbb{R}^2$, which is submitted to a non-smooth perturbation in a small region $\omega_\varepsilon(\widehat{\mathbf{x}}) = \varepsilon\omega$ of size ε with center at an arbitrary point $\widehat{\mathbf{x}} \in \Omega$. Thus, we assume that a given shape functional ψ admits the following topological asymptotic expansion

$$\psi(\Omega_\varepsilon) = \psi(\Omega) + f(\varepsilon) D_T(\widehat{\mathbf{x}}) + o(f(\varepsilon)) \ , \tag{1.1}$$

where Ω_ε is the topologically perturbed domain and $f(\varepsilon)$ is a positive function that decreases monotonically such that $f(\varepsilon) \to 0$ when $\varepsilon \to 0$. Then, the term $D_T(\widehat{\mathbf{x}})$ is defined as the topological derivative of ψ. Therefore, this derivative can be seen as a first order correction on $\psi(\Omega)$ to estimate $\psi(\Omega_\varepsilon)$. In addition, from (1.1), we have that the classical definition of the topological derivative is given by

$$D_T(\widehat{\mathbf{x}}) = \lim_{\varepsilon \to 0} \frac{\psi(\Omega_\varepsilon) - \psi(\Omega)}{f(\varepsilon)} \ . \tag{1.2}$$

On the other hand, in the work of [31], the topological sensitivity associated to the nucleation of a hole in a domain characterized by an orthotropic material was calculated. In order to simplify the analysis, the domain was perturbed introducing an elliptical hole oriented in the directions of the orthotropy and with semi-axis proportional to the material properties coefficients in each orthogonal direction. In this paper, we extend the above result considering as perturbation a small circular inclusion of size ε of the same nature as the bulk material (see Fig.1), instead of an elliptical hole. In summary, we present the calculation of the topological derivative for the total potential energy associated to the steady-state orthotropic heat diffusion problem, considering the nucleation of a small circular inclusion.

Key words and phrases. Topological asymptotic analysis, steady-state orthotropic heat diffusion, topological derivative, polarization tensor.

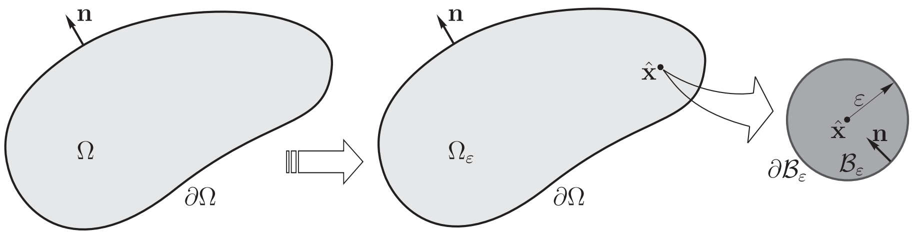


FIGURE 1. Topological derivative concept.

This paper is organized as follows. Section 2 describes the model associated to the steady-state orthotropic heat diffusion problem. The topological sensitivity analysis of the total potential energy associated to the problem under consideration is developed in Section 3, where we present the main result of the paper: a closed formula for the topological derivative. In addition, a simple finite element-based numerical example is also provided for the numerical verification of the analytically derived topological derivative formula. In Section 4 are presented two numerical experiments showing the behavior of the topological sensitivity field for different values of the orthotropic thermal conductivities and also one example concerning the optimal design of heat conductors. The paper ends in Section 5 where concluding remarks are presented.

2. Formulation of the problem

As mentioned in the previous section, the topological asymptotic analysis of the total potential energy associated to the steady-state orthotropic heat diffusion problem is calculated. Thus, the unperturbed shape functional is defined as:

$$\psi(\Omega) := \mathcal{J}_\Omega(u) = \frac{1}{2}\int_\Omega \mathbf{K}\nabla u \cdot \nabla u - \int_\Omega bu + \int_{\Gamma_N} \bar{q}u \ , \tag{2.1}$$

where $\mathbf{K}$ is a symmetric second order thermal conductivity tensor with eigenvalues k_1 and k_2, respectively associated to the orthogonal directions $\mathbf{e}_1$ and $\mathbf{e}_2$, b is a heat source in Ω and u is solution of the following variational problem: find the temperature field $u \in \mathcal{U}(\Omega)$, such that

$$\int_\Omega \mathbf{K}\nabla u \cdot \nabla \eta - \int_\Omega b\eta + \int_{\Gamma_N} \bar{q}\eta = 0 \qquad \forall \eta \in \mathcal{V}(\Omega) \ . \tag{2.2}$$

In the variational problem (2.2) the set of admissible temperature fields, $\mathcal{U}(\Omega)$, and the space of admissible virtual temperature fields, $\mathcal{V}(\Omega)$, are given by

$$\mathcal{U}(\Omega) := \left\{u \in H^1(\Omega) : u|_{\Gamma_D} = \bar{u}\right\} \quad \text{and} \quad \mathcal{V}(\Omega) := \left\{\eta \in H^1(\Omega) : \eta|_{\Gamma_D} = 0\right\} . \tag{2.3}$$

In addition, $\partial\Omega = \Gamma_N \cup \Gamma_D$ with $\Gamma_N \cap \Gamma_D = \varnothing$, where Γ_N and Γ_D are Neumann and Dirichlet boundaries, respectively. Thus, $\bar{u}$ is a Dirichlet data on Γ_D and $\bar{q}$ is a Neumann data on Γ_N, both assumed to be smooth enough, see Fig.2.

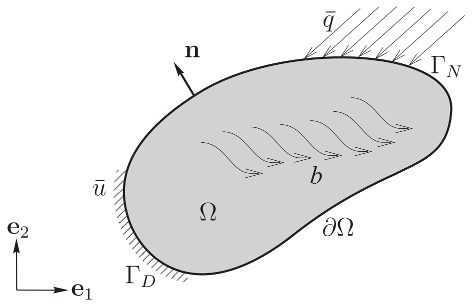


FIGURE 2. Formulation of the problem.

In our particular case, we consider a perturbation on the domain given by the nucleation of a small circular inclusion with thermal conductivity property $\gamma\mathbf{K}$ and heat source δb, where

$\mathbf{K}$ is the thermal conductivity and b is the heat source, both associated to the bulk material, and parameters $\gamma \in [0,\infty)$, $\delta \in [-c,c]$ with c limited, represent the contrasts in the material property and in the heat source, respectively. We assume that there is a small inclusion $\mathcal{B}_\varepsilon(\hat{\mathbf{x}})$ in the region Ω, which leads to the perturbed domain denoted as Ω_ε. If the inclusion becomes a cavity, it is denoted by $\omega_\varepsilon = \mathcal{B}_\varepsilon(\hat{\mathbf{x}})$. The cavity can be obtained from the inclusion by the limit passage $\gamma \to 0$. In the case of inclusion, the region Ω_ε is decomposed into two disjoint parts $\Omega \setminus \overline{\mathcal{B}_\varepsilon(\hat{\mathbf{x}})}$ and $\mathcal{B}_\varepsilon(\hat{\mathbf{x}})$ with different material properties and heat sources, namely $\mathbf{K}$, $\gamma\mathbf{K}$ and b, δb, respectively. The other limit passage with the contrast $\gamma \to \infty$ results in the ideal thermal conductor inclusion $\omega_\varepsilon = \mathcal{B}_\varepsilon(\hat{\mathbf{x}})$.

Now, tacking into account the definition of the perturbed domain Ω_ε and considering an inclusion of the same nature as the bulk material but with contrasts γ and δ, the perturbed shape functional can be written as:

$$\psi(\Omega_\varepsilon) := \mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\Omega_\varepsilon} \gamma_\varepsilon \mathbf{K}\nabla u_\varepsilon \cdot \nabla u_\varepsilon - \int_{\Omega_\varepsilon} \delta_\varepsilon b u_\varepsilon + \int_{\Gamma_N} \bar{q} u_\varepsilon \ , \tag{2.4}$$

where parameters γ_ε and δ_ε are defined as

$$\gamma_\varepsilon := \begin{cases} 1 & \text{if} \quad \mathbf{x} \in \Omega \setminus \overline{\mathcal{B}_\varepsilon(\hat{\mathbf{x}})} \\ \gamma & \text{if} \quad \mathbf{x} \in \mathcal{B}_\varepsilon(\hat{\mathbf{x}}) \end{cases} \quad \text{and} \quad \delta_\varepsilon := \begin{cases} 1 & \text{if} \quad \mathbf{x} \in \Omega \setminus \overline{\mathcal{B}_\varepsilon(\hat{\mathbf{x}})} \\ \delta & \text{if} \quad \mathbf{x} \in \mathcal{B}_\varepsilon(\hat{\mathbf{x}}) \end{cases} . \tag{2.5}$$

In addition, in (2.4) the function u_ε is solution of the following variational problem: find the temperature field $u_\varepsilon \in \mathcal{U}(\Omega_\varepsilon)$, such that

$$\int_{\Omega_\varepsilon} \gamma_\varepsilon \mathbf{K}\nabla u_\varepsilon \cdot \nabla \eta_\varepsilon - \int_{\Omega_\varepsilon} \delta_\varepsilon b \eta_\varepsilon + \int_{\Gamma_N} \bar{q}\eta_\varepsilon = 0 \quad \forall \eta_\varepsilon \in \mathcal{V}(\Omega_\varepsilon) \ , \tag{2.6}$$

and the set $\mathcal{U}(\Omega_\varepsilon)$ and the space $\mathcal{V}(\Omega_\varepsilon)$ are defined as

$$\mathcal{U}(\Omega_\varepsilon) := \left\{u_\varepsilon \in H^1(\Omega_\varepsilon) : u_\varepsilon|_{\Gamma_D} = \bar{u}\right\} \quad \text{and} \quad \mathcal{V}(\Omega_\varepsilon) := \left\{\eta_\varepsilon \in H^1(\Omega_\varepsilon) : \eta_\varepsilon|_{\Gamma_D} = 0\right\} \ . \tag{2.7}$$

Finally, the Euler-Lagrange equation associated to variational problem (2.6) reads: find field u_ε, such that

$$\left\{ \begin{array}{rlll} -\operatorname{div}(\gamma_\varepsilon \mathbf{K}\nabla u_\varepsilon) & = \delta_\varepsilon b & \text{in} & \Omega_\varepsilon \\ u_\varepsilon & = \bar{u} & \text{on} & \Gamma_D \\ -\mathbf{K}\nabla u_\varepsilon \cdot \mathbf{n} & = \bar{q} & \text{on} & \Gamma_N \\ [\![u_\varepsilon]\!] & = 0 & \text{on} & \partial\mathcal{B}_\varepsilon \\ -[\![\gamma_\varepsilon \mathbf{K}\nabla u_\varepsilon]\!] \cdot \mathbf{n} & = 0 & \text{on} & \partial\mathcal{B}_\varepsilon \end{array} \right. . \tag{2.8}$$

In the above expression, we use $[\![(\cdot)]\!]$ to denotes the *jump* of function $(\cdot)$ across the boundary $\partial\mathcal{B}_\varepsilon$:

$$[\![(\cdot)]\!] := (\cdot)|_m - (\cdot)|_i \ , \tag{2.9}$$

with subscripts m and i associated, respectively, with quantity values on the matrix $(\Omega \setminus \overline{\mathcal{B}_\varepsilon(\hat{\mathbf{x}})})$ and inclusion $(\mathcal{B}_\varepsilon(\hat{\mathbf{x}}))$ sides of the interface.

3. Topological sensitivity analysis

Let us state the following result, leading to a constructive method for computing the topological derivatives, [32, 29]:

$$D_T(\hat{\mathbf{x}}) = \lim_{\varepsilon \to 0} \frac{1}{f'(\varepsilon)} \frac{d}{d\varepsilon} \mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon) \ , \tag{3.1}$$

where $f'(\varepsilon)$ is the derivative of the function $f(\varepsilon)$ with respect to the parameter ε and the derivative of the perturbed cost functional $\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon)$ may be seen as the classical sensitivity analysis to the change in shape produced by an uniform expansion of the inclusion.

In fact, considering a direct analogy with the continuum mechanics, see [18], we have that the shape derivative of the cost function $\mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon)$ can be written as

$$\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\Omega_\varepsilon} \mathbf{\Sigma}_\varepsilon \cdot \nabla \mathbf{v} \ , \tag{3.2}$$

where $\mathbf{v}$ is the *shape change velocity field* and tensor $\mathbf{\Sigma}_\varepsilon$ can be interpreted as a generalization of the Eshelby energy-momentum tensor, see [13] and [19], which is given in our particular case by

$$\mathbf{\Sigma}_\varepsilon = \frac{1}{2}\left(\gamma_\varepsilon \mathbf{K}\nabla u_\varepsilon \cdot \nabla u_\varepsilon - 2\delta_\varepsilon b u_\varepsilon\right)\mathbf{I} - \gamma_\varepsilon \mathbf{K}\nabla u_\varepsilon \otimes \nabla u_\varepsilon \ . \tag{3.3}$$

Since u_ε is solution of the state equation (2.8), it is straightforward to verify that, in this particular case, the Eshelby tensor $\mathbf{\Sigma}_\varepsilon$ is a divergence-free field, i.e., $\mathrm{div}\mathbf{\Sigma}_\varepsilon = \mathbf{0}$ in Ω_ε. Integrating (3.2) by parts and applying the divergence theorem, the shape derivative of the cost function $\mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon)$ becomes an integral defined on the boundaries $\partial\Omega$ and $\partial\mathcal{B}_\varepsilon$, that is

$$\frac{d}{d\varepsilon}\mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega} \mathbf{\Sigma}_\varepsilon \mathbf{n}\cdot\mathbf{v} + \int_{\partial\mathcal{B}_\varepsilon} [\![\mathbf{\Sigma}_\varepsilon]\!]\mathbf{n}\cdot\mathbf{v} \ , \tag{3.4}$$

where the normal vector field satisfies $\mathbf{n} := \mathbf{n}|_m = -\mathbf{n}|_i$ on $\partial\mathcal{B}_\varepsilon$. As a consequence, since the velocity field $\mathbf{v}$ is smooth enough in the domain Ω_ε, then the shape sensitivity of the problem only depends on the definition of this field on the boundaries $\partial\Omega$ and $\partial\mathcal{B}_\varepsilon$. However, in our particular case, we observe that only the boundary of the inclusion $\partial\mathcal{B}_\varepsilon$, is submitted to a perturbation (an uniform expansion). Therefore, remembering that $\mathbf{n}$ is the outward normal unit vector (see Fig. 1), the *velocity* $\mathbf{v}$ assumes the following values on the boundaries $\partial\mathcal{B}_\varepsilon$ and $\partial\Omega$

$$\left\{\begin{array}{ll} \mathbf{v} = -\mathbf{n} & \text{on } \partial\mathcal{B}_\varepsilon \\ \mathbf{v} = \mathbf{0} & \text{on } \partial\Omega \end{array}\right. . \tag{3.5}$$

From this last remark and result (3.1), the topological derivative becomes an integral only defined on the boundary of the circular inclusion $\partial\mathcal{B}_\varepsilon$, that is

$$D_T(\widehat{\mathbf{x}}) = -\lim_{\varepsilon\to 0}\frac{1}{f'(\varepsilon)}\int_{\partial\mathcal{B}_\varepsilon} [\![\mathbf{\Sigma}_\varepsilon]\!]\mathbf{n}\cdot\mathbf{n} \ . \tag{3.6}$$

3.1. **Asymptotic analysis .** The problem given by (2.8), eventhough linear, it is not so easy to expand in power of ε. Initially, consider a local coordinate system centered at $\widehat{\mathbf{x}}$ and oriented along the eigenvectors of tensor $\mathbf{K}$. Therefore, let us make the following change of variables

$$x_i = \sqrt{k_i}\, y_i \quad \text{for} \quad i = 1, 2 \quad \Rightarrow \quad \mathbf{x} = \mathbf{K}^{\frac{1}{2}}\mathbf{y}, \tag{3.7}$$

where $\mathbf{x} = (x_1, x_2)$ and $\mathbf{y} = (y_1, y_2)$ are points defined over the domain Ω_ε and transformed domain $\tilde{\Omega}_\varepsilon$, respectively. Thus, the circular inclusion $\mathcal{B}_\varepsilon(\hat{\mathbf{x}})$ is mapped into an ellipse $\tilde{\mathcal{B}}_\varepsilon(\widehat{\mathbf{y}}) = \mathcal{E}_\varepsilon(\widehat{\mathbf{y}})$ with semi-major axis $\alpha = 1/\sqrt{k_1}$, semi-minor axis $\beta = 1/\sqrt{k_2}$ and centered at point $\widehat{\mathbf{y}}$, as can be seen in Fig. 3. The above mapping allows us to rewrite the Euler-Lagrange equation (2.8) as

$$\left\{\begin{array}{rll} -\mathrm{div}\left(\gamma_\varepsilon \nabla u_\varepsilon\right) & = \delta_\varepsilon b & \text{in} \quad \tilde{\Omega}_\varepsilon \\ u_\varepsilon & = \bar{u} & \text{on} \quad \tilde{\Gamma}_D \\ -\frac{\partial u_\varepsilon}{\partial n} & = \bar{q} & \text{on} \quad \tilde{\Gamma}_N \\ [\![u_\varepsilon]\!] & = 0 & \text{on} \quad \partial\tilde{\mathcal{B}}_\varepsilon \\ -[\![\gamma_\varepsilon \frac{\partial u_\varepsilon}{\partial n}]\!] & = 0 & \text{on} \quad \partial\tilde{\mathcal{B}}_\varepsilon \end{array}\right. , \tag{3.8}$$

where for the sake of simplicity we are using the same notation for field u_ε, heat source b and boundary conditions $\bar{q}$ and $\bar{u}$. Then, the following asymptotic expansion of solution $u_\varepsilon(\mathbf{y})$ in $\tilde{\Omega}_\varepsilon$ holds ([11, 23, 2, 27]),

$$u_\varepsilon(\mathbf{y})|_{\tilde{\Omega}\setminus\overline{\mathcal{E}_\varepsilon(\hat{\mathbf{y}})}} = u(\mathbf{y}) + \frac{\varepsilon}{\|\boldsymbol{\zeta}\|^2}\mathbf{P}\nabla u(\widehat{\mathbf{y}})\cdot\boldsymbol{\zeta} + \mathcal{O}(\varepsilon^2), \tag{3.9}$$

$$u_\varepsilon(\mathbf{y})|_{\mathcal{E}_\varepsilon(\hat{\mathbf{y}})} = u(\mathbf{y}) + \varepsilon\mathbf{P}\nabla u(\widehat{\mathbf{y}})\cdot\boldsymbol{\zeta} + \mathcal{O}(\varepsilon^2), \tag{3.10}$$

where $\boldsymbol{\zeta} = (\mathbf{y} - \widehat{\mathbf{y}})/\varepsilon$, $u(\mathbf{y})$ is the solution of the problem in the unperturbed domain $\tilde{\Omega}$, $\nabla u(\widehat{\mathbf{y}})$ is the corresponding gradient evaluated at point $\widehat{\mathbf{y}}$ (the centre of the ellipse) and $\mathbf{P}$ is given by

$$\mathbf{P} = \frac{1}{2}(1-\gamma)\alpha\beta\begin{pmatrix} \frac{\alpha+\beta}{\alpha+\gamma\beta} & 0 \\ 0 & \frac{\alpha+\beta}{\beta+\gamma\alpha} \end{pmatrix}, \tag{3.11}$$

which has been derivated from the polarization tensor for an elliptical inclusion, [30].

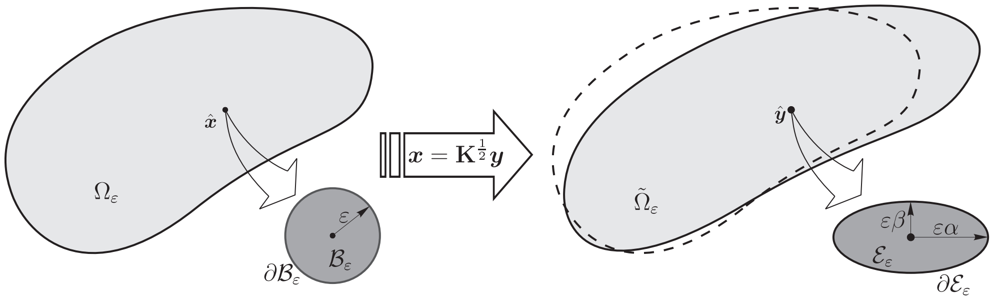


FIGURE 3. Change of variables.

Considering the inverse mapping $\mathbf{y} = \mathbf{J}\mathbf{x}$ in (3.9, 3.10), where $\mathbf{J} := \mathbf{K}^{-\frac{1}{2}}$, we have that the asymptotic expansion for $u_\varepsilon(\mathbf{x})$ in Ω_ε is given by

$$u_\varepsilon(\mathbf{x})|_{\Omega\setminus\overline{\mathcal{B}_\varepsilon(\hat{\mathbf{x}})}} = u(\mathbf{x}) + \frac{\varepsilon}{\|\mathbf{J}\boldsymbol{\xi}\|^2}\mathbf{P}\nabla u(\hat{\mathbf{x}}) \cdot \boldsymbol{\xi} + \mathcal{O}(\varepsilon^2), \tag{3.12}$$

$$u_\varepsilon(\mathbf{x})|_{\mathcal{B}_\varepsilon(\hat{\mathbf{x}})} = u(\mathbf{x}) + \varepsilon\mathbf{P}\nabla u(\hat{\mathbf{x}}) \cdot \boldsymbol{\xi} + \mathcal{O}(\varepsilon^2), \tag{3.13}$$

where $\boldsymbol{\xi} = (\mathbf{x} - \hat{\mathbf{x}})/\varepsilon$. It is well known that the asymptotic expansions can be differentiated term by term ([25, 24]). Thus, by assuming a sufficient regularity of $u(\mathbf{x})$ in Ω and performing its Taylor series expansion around point $\hat{\mathbf{x}}$, we obtain the following expansion for $\nabla u_\varepsilon(\mathbf{x})$ in Ω_ε,

$$\nabla u_\varepsilon(\mathbf{x})|_{\Omega\setminus\overline{\mathcal{B}_\varepsilon(\hat{\mathbf{x}})}} = \nabla u(\hat{\mathbf{x}}) + \frac{1}{\|\mathbf{J}\boldsymbol{\xi}\|^2}\mathbf{S}\mathbf{P}\nabla u(\hat{\mathbf{x}}) + \mathcal{O}(\varepsilon), \tag{3.14}$$

$$\nabla u_\varepsilon(\mathbf{x})|_{\mathcal{B}_\varepsilon(\hat{\mathbf{x}})} = \nabla u(\hat{\mathbf{x}}) + \mathbf{P}\nabla u(\hat{\mathbf{x}}) + \mathcal{O}(\varepsilon), \tag{3.15}$$

with

$$\mathbf{S} := \mathbf{I} - \frac{2}{\|\mathbf{J}\boldsymbol{\xi}\|^2}\mathbf{J}^2\boldsymbol{\xi} \otimes \boldsymbol{\xi} \ . \tag{3.16}$$

3.2. **Topological derivative calculation.** From expansions (3.12-3.15), and using symbolic calculus to solve the integral (3.6) (choosing the function $f(\varepsilon)$ as the size of the perturbation, i.e., $f(\varepsilon) = \pi\varepsilon^2$) we have that the final expression of the topological derivative becomes a scalar function that depends on the solution u associated to the original domain Ω (without inclusion), that is (see also [3]):

$$D_T(\hat{\mathbf{x}}) = -\sqrt{\det \mathbf{K}}\ \mathbf{K}\mathbf{P}\nabla u(\hat{\mathbf{x}}) \cdot \nabla u(\hat{\mathbf{x}}) + (1-\delta)bu(\hat{\mathbf{x}}) \qquad \forall \hat{\mathbf{x}} \in \Omega \ . \tag{3.17}$$

Remark 1. *From the final expression of the topological derivative for the steady-state orthotropic heat diffusion problem (3.17), we can analyze the limits cases of the parameter γ, which are:*

- *ideal thermal insulator ($\gamma \to 0$):*

$$D_T(\hat{\mathbf{x}}) = -\frac{1}{2}\frac{\mathbf{K}}{\sqrt{\det \mathbf{K}}}\left(\sqrt{\det \mathbf{K}}\ \mathbf{I} + \mathbf{K}\right)\nabla u(\hat{\mathbf{x}}) \cdot \nabla u(\hat{\mathbf{x}}) + (1-\delta)bu(\hat{\mathbf{x}}) \qquad \forall \hat{\mathbf{x}} \in \Omega \ , \tag{3.18}$$

- *ideal thermal conductor ($\gamma \to \infty$):*

$$D_T(\hat{\mathbf{x}}) = \frac{1}{2}\left(\sqrt{\det \mathbf{K}}\mathbf{I} + \mathbf{K}\right)\nabla u(\hat{\mathbf{x}}) \cdot \nabla u(\hat{\mathbf{x}}) + (1-\delta)bu(\hat{\mathbf{x}}) \qquad \forall \hat{\mathbf{x}} \in \Omega \ . \tag{3.19}$$

Remark 2. *It is interesting to observe that for isotropic material, we have $k_1 = k_2 = k$ and the final expression for the topological derivative (3.17) degenerates to the classical one given by* [3]*,*

$$D_T(\hat{\mathbf{x}}) = -k\frac{1-\gamma}{1+\gamma}\nabla u(\hat{\mathbf{x}}) \cdot \nabla u(\hat{\mathbf{x}}) + (1-\delta)bu(\hat{\mathbf{x}}) \qquad \forall \hat{\mathbf{x}} \in \Omega \ . \tag{3.20}$$

3.3. **Numerical verification.** In direct analogy with classical finite difference-based methods for the numerical approximation of the derivative of a generic function, a first order *topological finite difference* formula based on (1.2) to approximate numerically the value of $D_T(\widehat{\mathbf{x}})$ at the unperturbed domain can be defined as

$$d_T\mathcal{J} := \frac{\mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon) - \mathcal{J}_\Omega(u)}{f(\varepsilon)} \,, \tag{3.21}$$

with finite ε. The above satisfies

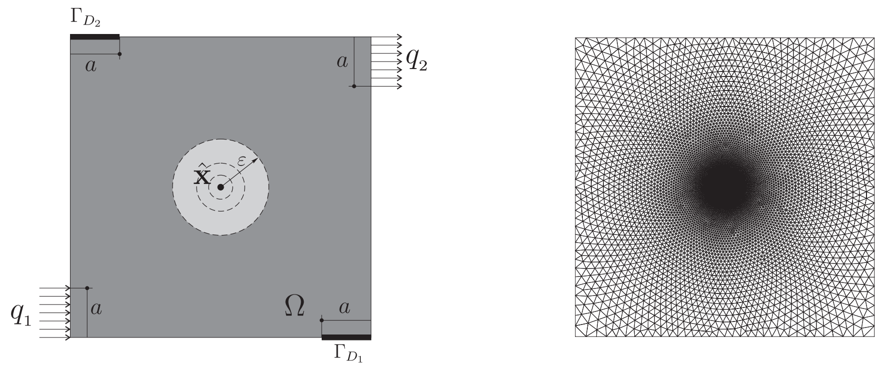
$$\lim_{\varepsilon\to 0} d_T\mathcal{J} = D_T(\widehat{\mathbf{x}}) \,. \tag{3.22}$$

If for a given domain we calculate $\mathcal{J}_\Omega(u)$ and its perturbed counterpart $\mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon)$ for a sequence of decreasing (sufficiently small) inclusion radii ε, the use of formula (3.21) will provide an asymptotic approximation to the analytical value of $D_T(\widehat{\mathbf{x}})$ given by (3.17). Here such a procedure is used to provide a numerical validation of result (3.17). The required values of function $\mathcal{J}_\Omega$ and $\mathcal{J}_{\Omega_\varepsilon}$ are computed numerically by means of the standard Finite Element Method for steady-state orthotropic heat diffusion problems.

For this instance, we have a unit square body without heat source ($b = 0$) and submitted to a temperature $\bar{u} = 0$ on Γ_{D_1} and Γ_{D_2}, a heat flux $q_1 = 1.0$ on Γ_{N_1} and $q_2 = 2.0$ on Γ_{N_2}, as shown in Fig. 4(a), where $a = 0.2$. In addition, the remainder part of the boundary remains insulated. For the computation of the values of $\mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon)$, a sequence of finite element analyses are carried out for perturbed domains obtained by introducing circular inclusions of radii

$$\varepsilon \in \{0.16, 0.08, 0.04, 0.02, 0.01\}, \tag{3.23}$$

centred at $\hat{\mathbf{x}} = (0.5, 0.5)$. The finite element mesh used to discretise the domain Ω_ε was built so that each boundary of radius ε has 120 six-noded (quadratic) triangular isoparametric elements. The obtained mesh contains 50781 nodes and 25322 elements, as can be see in Fig.4(b).

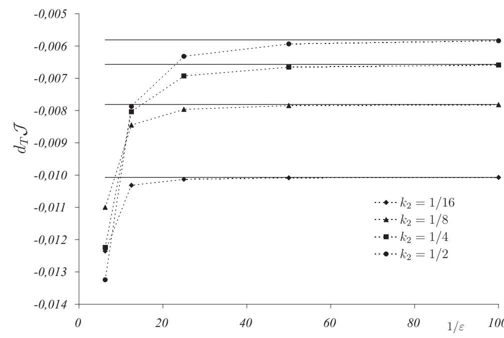


(a) Domain. (b) Finite element mesh.

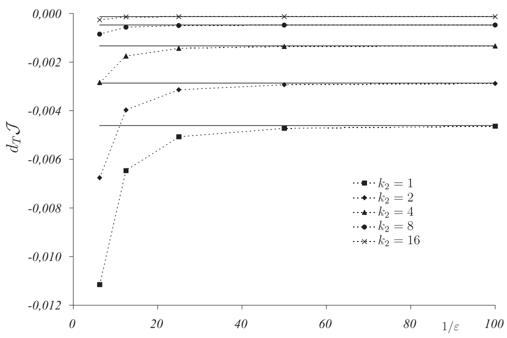
FIGURE 4. Numerical verification. Domain and finite elements mesh.

For this numerical verification two cases for the parameter γ are studied: *(i)* $\gamma = 1/2$; and *(ii)* $\gamma = 2$. The results of the analyses are plotted in Fig.5 and Fig.6, respectively, which shows the analytical topological derivative and the numerical approximations for each value of ε for values of parameters k_1 and k_2 between 1/16 and 16.

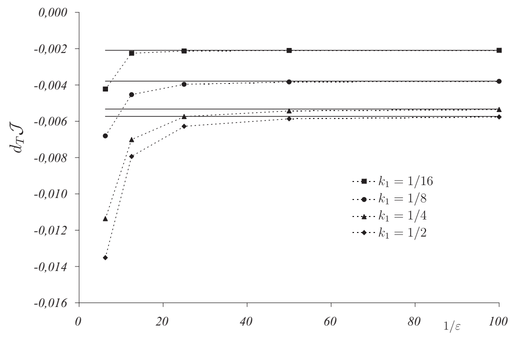
The convergence of the numerical topological derivatives to their corresponding analytical values with decreasing ε is obvious in all cases and confirm the correctness of formula (3.17).



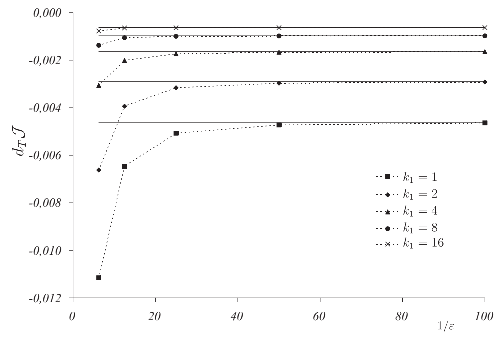
(a) $k_1 = 1$ and $k_2 < 1$.



(b) $k_1 = 1$ and $k_2 \geq 1$.

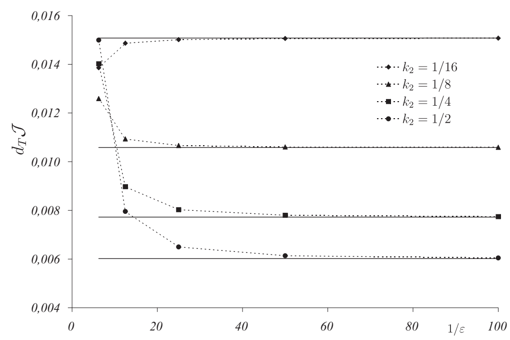


(c) $k_2 = 1$ and $k_1 < 1$.

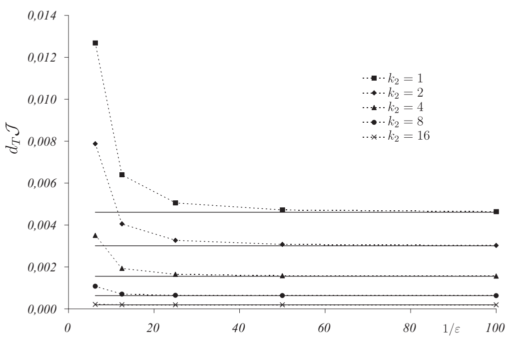


(d) $k_2 = 1$ and $k_1 \geq 1$.

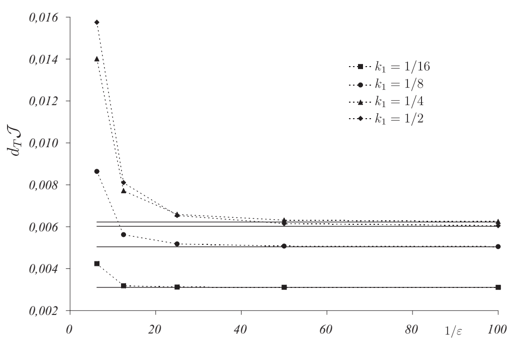
FIGURE 5. Numerical verification. Convergence of numerical topological derivative to analytical value for $\gamma = 1/2$.



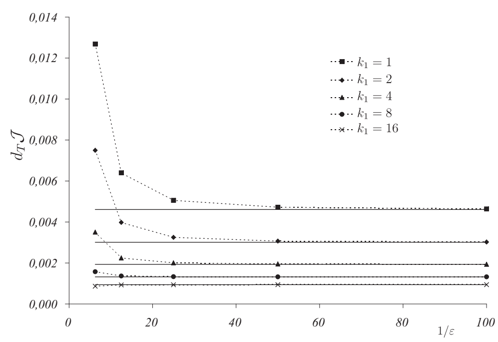
(a) $k_1 = 1$ and $k_2 < 1$.



(b) $k_1 = 1$ and $k_2 \geq 1$.



(c) $k_2 = 1$ and $k_1 < 1$.



(d) $k_2 = 1$ and $k_1 \geq 1$.

FIGURE 6. Numerical verification. Convergence of numerical topological derivative to analytical value for $\gamma = 2$.

4. Numerical examples

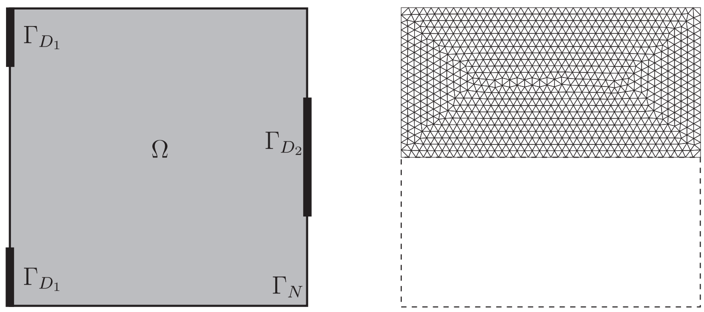
In this section we present two examples considering different values of the orthotropic thermal conductivities parameters k_1 and k_2, namely:

- **Case A:** $k_1 = k_2 = 2$ (isotropic behavior),
- **Case B:** $k_1 = 3$ and $k_2 = 1$,
- **Case C:** $k_1 = 1$ and $k_2 = 3$.

The first one concerns two numerical experiments showing the behavior of the topological sensitivity field taking into account the limit cases $\gamma \to 0$ and $\gamma \to \infty$. In the second example, the topological derivative is used in the optimal design of heat conductors. In all examples we consider a set $\mathcal{D} = (0, 10) \times (0, 10)$ such that the domain $\Omega \subseteq \mathcal{D}$, whose boundary is given by $\partial\Omega = \Gamma_D \cup \Gamma_N$ with $\Gamma_N \cap \Gamma_D = \varnothing$.

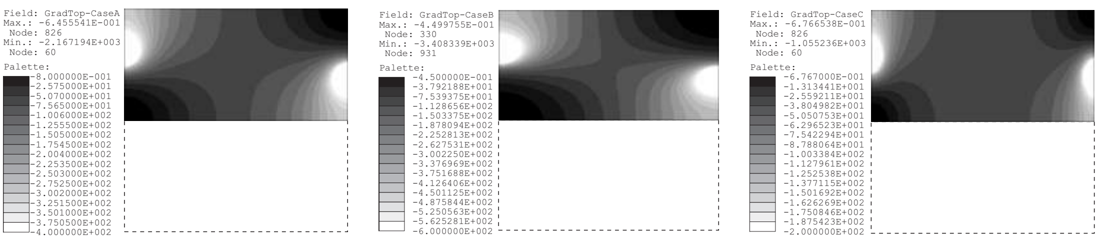
4.1. **Example 1.** For this example we consider a domain Ω without heat source ($b = 0$) and the Dirichlet boundary Γ_D is such that: $\Gamma_D = \Gamma_{D_1} \cup \Gamma_{D_2}$ with $meas(\Gamma_{D_1}) = meas(\Gamma_{D_2}) = 4$. We study the behavior of the limits cases given by (3.18) and (3.19).

Experiment 1. In this first experiment $\Omega = \mathcal{D}$ and the boundary condition are given by: on Γ_N we have that $\bar{q} = 0$ and on Γ_{D_1} and Γ_{D_2} are prescribed the temperatures $\bar{u}_1 = 0$ and $\bar{u}_2 = 100$, respectively. Due to the symmetry of the problem, only half of the domain is discretized. For discretization we use an uniform mesh with 1822 tree-noded (linear) triangular elements with a total of 972 nodes. The domain Ω and the finite element mesh are shown in Figs.7(a) and 7(b), respectively. The topological derivative field obtained for the ideal thermal insulator case ($\gamma \to 0$) is shown in Fig.8 and, for the ideal thermal conductor case ($\gamma \to \infty$) in Fig.9.



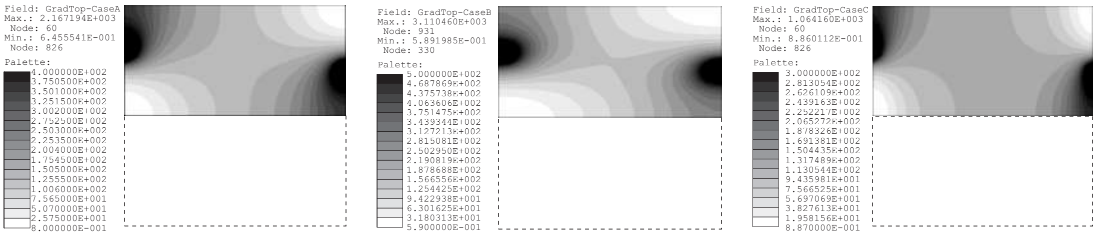
(a) Domain. (b) Mesh.

Figure 7. Example 1, Experiment 1. Domain and finite elements mesh.



(a) Case A. (b) Case B. (c) Case C.

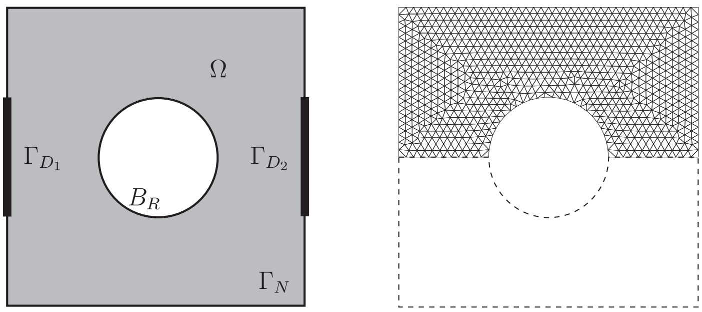
Figure 8. Example 1, Experiment 1. Topological derivative value for $\gamma \to 0$.



(a) Case A. (b) Case B. (c) Case C.

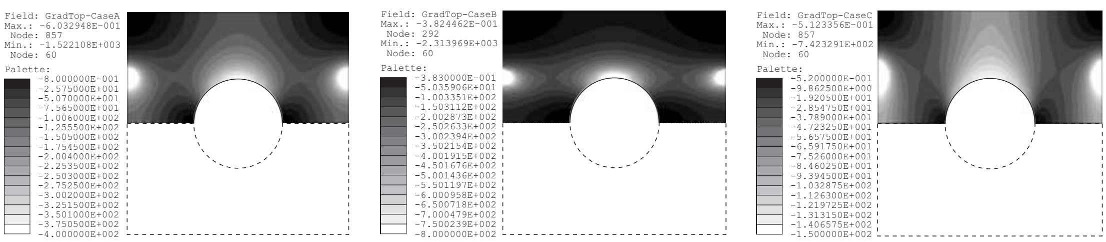
FIGURE 9. Example 1, Experiment 1. Topological derivative value for $\gamma \to \infty$.

Experiment 2. In Fig.10(a) we show the disposition of boundaries Γ_{D_1}, Γ_{D_2}, Γ_N and the domain $\Omega = \mathcal{D}\backslash\overline{B_R}$, where B_R denote a ball with radius $R = 2.0$ and centered at point $\mathbf{x} = (5.0, 5.0)$. In this case, the boundary conditions are the same that for the previous experiment. Due to the symmetry of the problem, only half of the domain is discretized. For discretization we use an uniform mesh with 1583 tree-noded (linear) triangular elements with a total of 857 nodes. In Fig. 10(b) is shown the finite element mesh used in this experiment. In Fig.11 is shown the topological derivative field for the ideal thermal insulator case ($\gamma \to 0$) and in Fig.12 for the ideal thermal conductor case ($\gamma \to \infty$) .



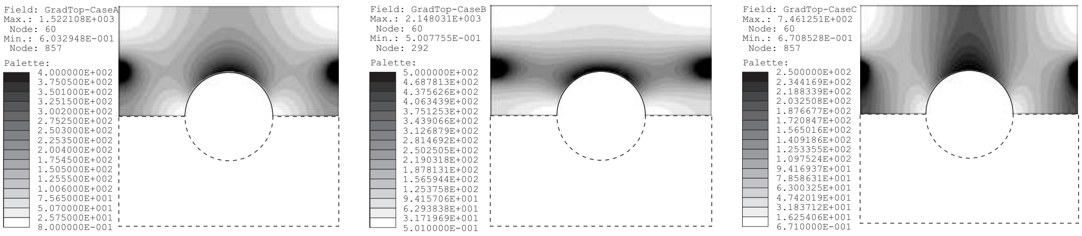
(a) Domain. (b) Mesh.

FIGURE 10. Example 1, Experiment 2. Domain and finite elements mesh.



(a) Case A. (b) Case B. (c) Case C.

FIGURE 11. Example 1, Experiment 2. Topological derivative value for $\gamma \to 0$.



(a) Case A. (b) Case B. (c) Case C.

FIGURE 12. Example 1, Experiment 2. Topological derivative value for $\gamma \to \infty$.

These experiments, although academic, shows that the topological derivative can be used to determine where the holes (or inclusion) must be positioned (points $\widehat{\mathbf{x}}$ in which $D_T(\widehat{\mathbf{x}})$ assumes the value closer to zero) in order to minimize (or maximize) the shape functional, in this case, the total potential energy associated to the steady-state orthotropic heat diffusion problem. In particular, in both examples the region in which the topological derivative assume the value closer to zero is almost the same for the three cases. But in Case C this region is bigger than in the others two cases, due to, in part, to the fact that the direction of the heat flux corresponds with the direction of higher coefficient of the thermal conductivity tensor.

4.2. **Example 2.** In this second example we use the topological derivative field (3.17) to perform the optimal design of heat conductors. To this ends we use the topology optimization algorithm developed in [17]. In Fig.13 is presented the design domain $\Omega = \mathcal{D}$, whose boundary remain isolated except for a region Γ_D of size $meas(\Gamma_D) = 2$, positioned in the middle of the left side in which the temperature is prescribed as $\bar{u} = 0$. We also consider an uniform heat generation $b = 1$ over all the domain Ω ($\delta = 1$). For this example, we have two materials: a good conductor characterized by the thermal conductivities previously mentioned (Case A, B or C) and a bad conductor (or insulator) characterized by the parameter $\gamma = 0.001$. Finally, the volume constraint is chosen to be 40% of good conductor material. Due to the symmetry of the problem, only half of the domain is discretized. For discretization we use an uniform mesh with 46212 tree-noded (linear) triangular elements with a total of 23407 nodes.

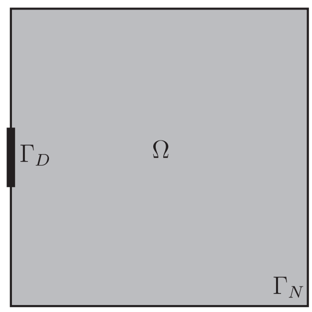
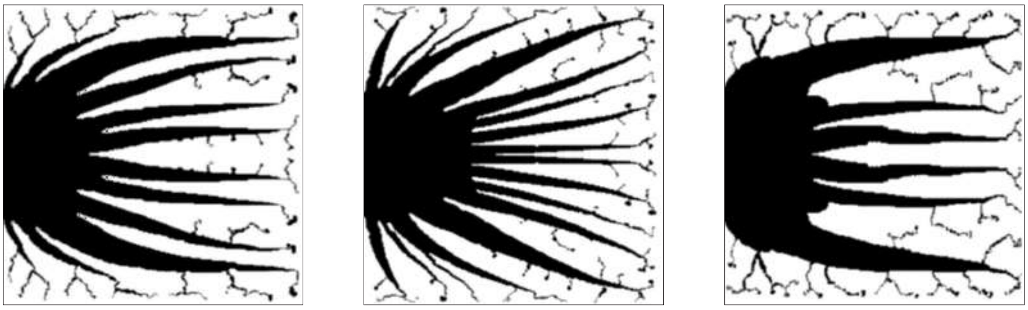


FIGURE 13. Example 2. Model.

In this final example, we show how the topological derivative field can be used in the topological design of heat conductors. As expected, the obtained result, Fig.14, show how the good conductor drains energy from all parts of the domain. Similar results, for the isotropic case, can be found in the literature, see [8] for instance.



(a) Case A. (b) Case B. (c) Case C.

FIGURE 14. Example 2. Obtained topologies.

The value of the shape functional $\psi(\Omega_\varepsilon)$ throughout the optimization procedure previously referred is presented in Fig.15. In Fig.14 we shown the obtained topologies for the three studied cases for the different values of the thermal conductivities. In the figures, the black material represents the good thermal conductor.

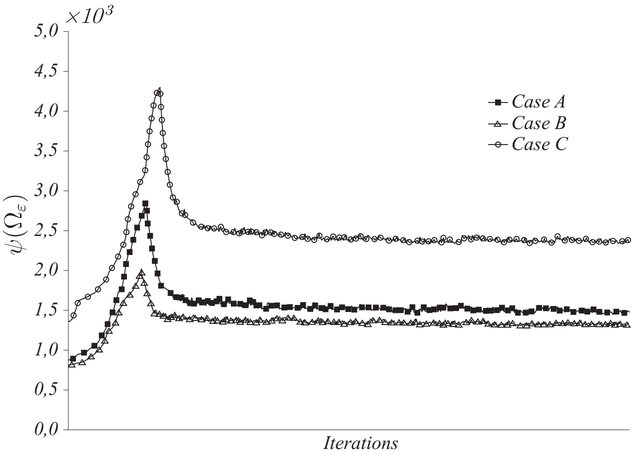


FIGURE 15. Example 2. Total potential energy.

5. Final remarks

An analytical expression for the topological derivative associated to the total potential energy in steady-state orthotropic heat diffusion problem, when a circular inclusion of the same nature as the bulk material is introduced at an arbitrary point of the domain, has been proposed in this paper. The final formula was obtained using a simple changing of variable and the first order Pólya-Szegö polarization tensor. Thus, besides to extend the result presented in [31], we have shown that the approach here adopted ([29]) can be in fact applied to arbitrary shaped holes or inclusions (an elliptical inclusion in this case), contrary to the comment by [5]. In order to verify the proposed analytical expression, we have developed a numerical validation showing the convergence of the numerical topological derivative to their corresponding analytical value. The obtained result was used to devise two numerical examples. The first one shows the behavior of the topological derivative field for different values of the orthotropic thermal conductivity. For the second numerical example, the topological derivative formula is used in the design of heat conductors. Finally, we remark that this information can be potentially used, as shown in the numerical examples, in a number of applications of practical interest such as, for instance: image restoration algorithm, optimization of mechanical or electronic pieces, design of an orthotropic material to achieve a specified thermal behavior.

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