

SECOND ORDER TOPOLOGICAL SENSITIVITY ANALYSIS

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ABSTRACT. The topological derivative provides the sensitivity of a given cost function with respect to the insertion of a hole at an arbitrary point of the domain. Classically, this derivative comes from the second term of the topological asymptotic expansion, dealing only with infinitesimal holes. However, for practical applications, we need to insert holes of finite size. Therefore, we consider one more term in the expansion which is defined as the second order topological derivative. In order to present these ideas, in this work we apply the Topological-Shape Sensitivity Method as a systematic approach to calculate first as well as second order topological derivative for the Poisson's equations, taking the total potential energy as cost function and the state equation as constraint. Furthermore, we also study the effects of different boundary conditions on the hole: Neumann and Dirichlet (both homogeneous). Finally, we present some numerical experiments showing the influence of the second order topological derivative in the topological asymptotic expansion, which has two main features: it allows us to deal with hole of finite size and provides a better descent direction in optimization process.

1. INTRODUCTION

The topological derivative provides the sensitivity of a given cost function with respect to the insertion of an infinitesimal hole at an arbitrary point of the domain [4, 5, 19, 23]. This derivative has been used as a descent direction to solve several problems, among others: topology optimization and inverse problems [1, 2, 7, 8, 9, 10, 16, 20, 22]. Classically, the topological derivative comes from the second term of the topological asymptotic expansion, dealing only with infinitesimal holes. However, for practical applications, we need to insert holes of finite size. Therefore, as a natural extension of the topological derivative concept, we can consider higher order terms in the expansion. In particular, we define the next one as the second order topological derivative. This term provides a more accurate estimation for the size of the holes and also it may be used to improve the optimality conditions given by the first order topological derivative (see, for instance, [4]). These features are essential in the context of topology optimization and inverse problems, for instance.

In order to present the basic idea, let us consider an open bounded domain $\Omega \subset \mathbb{R}^2$, with a smooth boundary $\partial\Omega$ and a cost function $\psi(\Omega)$. If the domain Ω is perturbed by introducing a small hole B_ε of radius ε at an arbitrary point $\hat{\mathbf{x}} \in \Omega$, we have a new domain $\Omega_\varepsilon = \Omega \setminus \overline{B}_\varepsilon$, whose boundary is denoted by $\partial\Omega_\varepsilon = \partial\Omega \cup \partial B_\varepsilon$. From these elements, the topological asymptotic expansion of the cost function may be expressed as

$$\psi(\Omega_\varepsilon) = \psi(\Omega) + f_1(\varepsilon)D_T\psi + f_2(\varepsilon)D_T^2\psi + \mathcal{R}(f_2(\varepsilon)), \quad (1.1)$$

where $f_1(\varepsilon)$ and $f_2(\varepsilon)$ are positive functions that decreases monotonically such that $f_1(\varepsilon) \rightarrow 0$, $f_2(\varepsilon) \rightarrow 0$ when $\varepsilon \rightarrow 0^+$ and

$$\lim_{\varepsilon \rightarrow 0} \frac{f_2(\varepsilon)}{f_1(\varepsilon)} = 0, \quad \lim_{\varepsilon \rightarrow 0} \frac{\mathcal{R}(f_2(\varepsilon))}{f_2(\varepsilon)} = 0. \quad (1.2)$$

Dividing eq. (1.1) by $f_1(\varepsilon)$ and after taking the limit $\varepsilon \rightarrow 0$ we obtain

$$D_T\psi = \lim_{\varepsilon \rightarrow 0} \frac{\psi(\Omega_\varepsilon) - \psi(\Omega)}{f_1(\varepsilon)}, \quad (1.3)$$

where term $D_T\psi$ is classically defined as the (first order) topological derivative of ψ . In addition, if we divide eq. (1.1) by $f_2(\varepsilon)$ and after taking the limit $\varepsilon \rightarrow 0$, we can recognize term $D_T^2\psi$ as

Key words and phrases. topological asymptotic expansion, (first order) topological derivative, second order topological derivative.

the second order topological derivative of ψ , which is given by

$$D_T^2\psi = \lim_{\varepsilon \rightarrow 0} \frac{\psi(\Omega_\varepsilon) - \psi(\Omega) - f_1(\varepsilon)D_T\psi}{f_2(\varepsilon)}. \quad (1.4)$$

In this work we apply the Topological-Shape Sensitivity Method developed in [19] as a systematic approach to calculate first as well as second order topological derivative for the Poisson's equations, taking the total potential energy as cost function and the state equation as constraint. Furthermore, we also study the effects of different boundary conditions on the hole: Neumann and Dirichlet (both homogeneous). Finally, we present some numerical experiments showing the influence of the second order topological derivative in the topological asymptotic expansion, which has two main features: it allows us to deal with hole of finite size and provides a better descent direction in optimization process.

2. TOPOLOGICAL-SHAPE SENSITIVITY METHOD

In [19] was proposed an alternative procedure to calculate the (first order) topological derivative called Topological-Shape Sensitivity Method. This approach makes use of the whole mathematical framework (and results) developed for shape sensitivity analysis (see, for instance, the pioneering work of Murat & Simon [18]). The main result obtained in [19] is given by the following Theorem:

Theorem 1. *Let $f_1(\varepsilon)$ be a function chosen in order to $0 < |D_T\psi| < \infty$, then the (first order) topological derivative given by eq. (1.3) can be written as*

$$D_T\psi = \lim_{\varepsilon \rightarrow 0} \frac{1}{f_1'(\varepsilon)} \frac{d}{d\varepsilon} \psi(\Omega_\varepsilon), \quad (2.1)$$

where the derivative of the cost function with respect to the parameter ε may be seen as its classical shape sensitivity analysis.

A remarkable fact concerning the Topological-Shape Sensitivity Method is that it can be easily extended to calculate higher order topological derivatives. In particular, following the same idea presented in theorem 1, it is straightforward to show that:

Theorem 2. *Let $f_2(\varepsilon)$ be a function chosen in order to $0 < |D_T^2\psi| < \infty$, then the second order topological derivative is given by*

$$D_T^2\psi = \lim_{\varepsilon \rightarrow 0} \frac{1}{f_2'(\varepsilon)} \left(\frac{d}{d\varepsilon} \psi(\Omega_\varepsilon) - f_1'(\varepsilon)D_T\psi \right). \quad (2.2)$$

In general the cost function $\psi(\Omega) := \mathcal{J}_\Omega(u)$ may depends explicitly and implicitly on the domain Ω . This last dependence comes from the solution of a variational problem associated to Ω : find $u \in \mathcal{U}(\Omega)$, such that

$$a(u, \eta) = l(\eta) \quad \forall \eta \in \mathcal{V}(\Omega), \quad (2.3)$$

where $\mathcal{U}(\Omega)$ and $\mathcal{V}(\Omega)$ respectively are the sets of admissible functions and admissible variations defined on Ω and $a(\cdot, \cdot) : \mathcal{U} \times \mathcal{V} \rightarrow \mathbb{R}$ is a bilinear form and $l(\cdot) : \mathcal{V} \rightarrow \mathbb{R}$ is a linear functional, which will be characterized later according to the problem under analysis. Likewise, the state equation written in the original configuration Ω (without hole) must also be satisfied in the perturbed configuration Ω_ε (with the introduction of a hole at point $\hat{\mathbf{x}} \in \Omega$). Therefore, we have the following variational problem associated to Ω_ε : find $u_\varepsilon \in \mathcal{U}_\varepsilon(\Omega_\varepsilon)$, such that

$$a_\varepsilon(u_\varepsilon, \eta) = l_\varepsilon(\eta) \quad \forall \eta \in \mathcal{V}_\varepsilon(\Omega_\varepsilon), \quad (2.4)$$

where $a_\varepsilon(\cdot, \cdot) : \mathcal{U}_\varepsilon \times \mathcal{V}_\varepsilon \rightarrow \mathbb{R}$, $l_\varepsilon(\cdot) : \mathcal{V}_\varepsilon \rightarrow \mathbb{R}$ and $\mathcal{U}_\varepsilon(\Omega_\varepsilon)$ and $\mathcal{V}_\varepsilon(\Omega_\varepsilon)$ respectively are the sets of admissible functions and admissible variations defined on Ω_ε , which will also be defined later according to the problem under analysis, the boundary condition on the hole and also the order of the topological derivative which is being calculated.

Formally, the shape derivative of the cost function $\psi(\Omega_\varepsilon) := \mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon)$ in relation to the parameter ε reads

$$\begin{cases} \text{Calculate :} & \frac{d}{d\varepsilon} \mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon) \\ \text{Subject to :} & a_\varepsilon(u_\varepsilon, \eta) = l_\varepsilon(\eta) \quad \forall \eta \in \mathcal{V}_\varepsilon(\Omega_\varepsilon) \end{cases}. \quad (2.5)$$

In general, this derivative can be expressed as

$$\frac{d}{d\varepsilon} \mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon) = \int_{\partial\Omega_\varepsilon} \boldsymbol{\Sigma}_\varepsilon \mathbf{n} \cdot \mathbf{v} dS, \quad (2.6)$$

where \mathbf{n} is the outward normal unit vector and $\boldsymbol{\Sigma}_\varepsilon$ can be interpreted as a generalization of the Eshelby energy-momentum tensor [6, 13, 24]. As a consequence, tensor $\boldsymbol{\Sigma}_\varepsilon$ plays a central role in the Topological-Shape Sensitivity Method and should be clearly identified according to the problem under consideration. In addition, the shape change velocity \mathbf{v} may be defined on the boundary $\partial\Omega_\varepsilon$ as [25, 3]

$$\begin{cases} \mathbf{v} = -\mathbf{n} & \text{on } \partial B_\varepsilon \\ \mathbf{v} = \mathbf{0} & \text{on } \partial\Omega \end{cases}. \quad (2.7)$$

Then, only the part of the boundary $\partial\Omega_\varepsilon$ associated to ∂B_ε is submitted to a perturbation (a uniform expansion of the ball B_ε in this case). Thus, the shape derivative of the cost function, given by eq. (2.6), results in an integral on the boundary ∂B_ε . Therefore, considering theorem 1, the (first order) topological derivative can be written as

$$D_T \psi = -\lim_{\varepsilon \rightarrow 0} \frac{1}{f'_1(\varepsilon)} \int_{\partial B_\varepsilon} \boldsymbol{\Sigma}_\varepsilon \mathbf{n} \cdot \mathbf{n} dS. \quad (2.8)$$

Analogously, from theorem 2, the second order topological derivative results in

$$D_T^2 \psi = -\lim_{\varepsilon \rightarrow 0} \frac{1}{f'_2(\varepsilon)} \left(\int_{\partial B_\varepsilon} \boldsymbol{\Sigma}_\varepsilon \mathbf{n} \cdot \mathbf{n} dS + f'_1(\varepsilon) D_T \psi \right). \quad (2.9)$$

In order to calculate the limit $\varepsilon \rightarrow 0$, we need to make an asymptotic analysis to estimate the behavior of the solution in the neighborhood of the hole.

3. TOPOLOGICAL DERIVATIVE FOR POISSON'S PROBLEM

In this section we will calculate the topological derivative for steady-state heat conduction considering homogeneous Neumann and Dirichlet boundary conditions on the hole and adopting the total potential energy as cost function.

The variational formulation of the problem associated to the original domain Ω can be stated as: find $u \in \mathcal{U}(\Omega)$, such that

$$\int_{\Omega} \nabla u \cdot \nabla \eta dV + \int_{\Gamma_N} q \eta dS = 0 \quad \forall \eta \in \mathcal{V}(\Omega), \quad (3.1)$$

where $\mathcal{U}(\Omega)$ and $\mathcal{V}(\Omega)$ are respectively defined, for n choosing in order to ensure a sufficient regularity of function u , as

$$\mathcal{U}(\Omega) := \{u \in H^n(\Omega) : u|_{\Gamma_D} = \varphi\}, \quad \mathcal{V}(\Omega) := \{\eta \in H^n(\Omega_\varepsilon) : \eta|_{\Gamma_D} = 0\}, \quad (3.2)$$

In addition, $\partial\Omega = \overline{\Gamma}_D \cup \overline{\Gamma}_N$ with $\Gamma_D \cap \Gamma_N = \emptyset$, when Γ_D and Γ_N are Dirichlet and Neumann boundaries, respectively. Thus φ is a Dirichlet data on Γ_D and q is a Neumann data on Γ_N , both assumed to be smooth enough.

Now, let us state the variational problem associated to the perturbed domain Ω_ε , that is: find $u_\varepsilon \in \mathcal{U}_\varepsilon(\Omega_\varepsilon)$, such that

$$\int_{\Omega_\varepsilon} \nabla u_\varepsilon \cdot \nabla \eta_\varepsilon dV + \int_{\Gamma_N} q \eta_\varepsilon dS = 0 \quad \forall \eta_\varepsilon \in \mathcal{V}_\varepsilon(\Omega_\varepsilon), \quad (3.3)$$

where $\mathcal{U}_\varepsilon(\Omega_\varepsilon)$ and $\mathcal{V}_\varepsilon(\Omega_\varepsilon)$ are given, respectively, by

$$\mathcal{U}_\varepsilon(\Omega_\varepsilon) := \{u_\varepsilon \in \mathcal{U}(\Omega_\varepsilon) : \alpha u_\varepsilon|_{\partial B_\varepsilon} = 0\}, \quad \mathcal{V}_\varepsilon(\Omega_\varepsilon) := \{\eta_\varepsilon \in \mathcal{V}(\Omega_\varepsilon) : \alpha \eta_\varepsilon|_{\partial B_\varepsilon} = 0\}, \quad (3.4)$$

with $\alpha \in \{0, 1\}$. This notation should be interpreted as follows: when $\alpha = 1$, $u_\varepsilon = 0$ and $\eta_\varepsilon = 0$ on ∂B_ε , and when $\alpha = 0$, u_ε and η_ε are free on ∂B_ε . Therefore, according to the values of α , we have Dirichlet or Neumann boundary condition on the hole.

As already mentioned, the total potential energy associated to the problem under analysis is adopted as cost function, that is

$$\psi(\Omega_\varepsilon) = \mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2} \int_{\Omega_\varepsilon} |\nabla u_\varepsilon|^2 dV + \int_{\Gamma_N} q u_\varepsilon dS. \quad (3.5)$$

Considering the Reynold's transport theorem and the concept of material derivative of spatial field (see for instance [12]) the Eshelby tensor Σ_ε is given by

$$\Sigma_\varepsilon = \frac{1}{2} |\nabla u_\varepsilon|^2 \mathbf{I} - (\nabla u_\varepsilon \otimes \nabla u_\varepsilon). \quad (3.6)$$

The gradient ∇u_ε defined on the boundary ∂B_ε can be decomposed into a normal and tangential components, that is

$$(\nabla u_\varepsilon \cdot \mathbf{n}) \mathbf{n} = \frac{\partial u_\varepsilon}{\partial n} \mathbf{n} \quad \text{and} \quad (\nabla u_\varepsilon \cdot \mathbf{t}) \mathbf{t} = \frac{\partial u_\varepsilon}{\partial t} \mathbf{t}, \quad (3.7)$$

where \mathbf{n} and \mathbf{t} are respectively the normal and tangential unit vectors, which define a curvilinear coordinate system on the boundary ∂B_ε . Therefore, substituting eq. (3.6) in eqs. (2.8, 2.9) and after a simple manipulation, we respectively obtain the following results:

$$D_T \psi = - \lim_{\varepsilon \rightarrow 0} \frac{1}{f'_1(\varepsilon)} \int_{\partial B_\varepsilon} \frac{1}{2} \left[\left(\frac{\partial u_\varepsilon}{\partial t} \right)^2 - \left(\frac{\partial u_\varepsilon}{\partial n} \right)^2 \right] dS, \quad (3.8)$$

and

$$D_T^2 \psi = - \lim_{\varepsilon \rightarrow 0} \frac{1}{f'_2(\varepsilon)} \left\{ \int_{\partial B_\varepsilon} \frac{1}{2} \left[\left(\frac{\partial u_\varepsilon}{\partial t} \right)^2 - \left(\frac{\partial u_\varepsilon}{\partial n} \right)^2 \right] dS + f'_1(\varepsilon) D_T \psi \right\}. \quad (3.9)$$

Finally, in order to calculate the final expression for $D_T \psi$ and $D_T^2 \psi$, we need to know the behavior of the solution u_ε in the neighborhood of the hole. Therefore, from an asymptotic analysis of u_ε , whose justification is given in Appendix A [11, 15, 17], we can choose functions $f_1(\varepsilon)$ and $f_2(\varepsilon)$ depending on each type of boundary condition on ∂B_ε , that allow us to calculate the limit $\varepsilon \rightarrow 0$ in eqs. (3.8, 3.9).

3.1. Neumann boundary condition on the hole. Taking $\alpha = 0$ in eq. (3.3), we have homogeneous Neumann boundary condition on the hole. Then, the following asymptotic expansion holds (see Appendix A)

$$u_\varepsilon(\mathbf{x}) = u(\mathbf{x}) + \frac{\varepsilon^2}{\|\mathbf{x} - \hat{\mathbf{x}}\|^2} \nabla u(\hat{\mathbf{x}}) \cdot (\mathbf{x} - \hat{\mathbf{x}}) + \frac{\varepsilon^4}{2\|\mathbf{x} - \hat{\mathbf{x}}\|^4} \nabla \nabla u(\hat{\mathbf{x}}) (\mathbf{x} - \hat{\mathbf{x}}) \cdot (\mathbf{x} - \hat{\mathbf{x}}) + \mathcal{O}(\varepsilon^2). \quad (3.10)$$

In addition, from eq. (3.8), we have

$$D_T \psi = - \lim_{\varepsilon \rightarrow 0} \frac{1}{f'_1(\varepsilon)} \int_{\partial B_\varepsilon} \frac{1}{2} \left(\frac{\partial u_\varepsilon}{\partial t} \right)^2 dS. \quad (3.11)$$

Thus, considering the expansion given by eq. (3.10) in eq. (3.11), we observe that $f_1(\varepsilon) = \pi \varepsilon^2$. Then, after computing the limit $\varepsilon \rightarrow 0$, we get the final expression for the **first order topological derivative**, which is given by

$$D_T \psi = - \nabla u(\hat{\mathbf{x}}) \cdot \nabla u(\hat{\mathbf{x}}) \quad \forall \hat{\mathbf{x}} \in \Omega, \quad \text{for } f_1(\varepsilon) = \pi \varepsilon^2. \quad (3.12)$$

Remark 3. The result given by eq. (3.12) can be continuously extended to the boundary with homogeneous Neumann condition [21], then

$$D_T \psi = - \nabla u(\hat{\mathbf{x}}) \cdot \nabla u(\hat{\mathbf{x}}) \quad \forall \hat{\mathbf{x}} \in \partial \Omega, \quad \text{for } f_1(\varepsilon) = \frac{1}{2} \pi \varepsilon^2. \quad (3.13)$$

Furthermore, according to eq. (3.9), we have

$$D_T^2 \psi = - \lim_{\varepsilon \rightarrow 0} \frac{1}{f'_2(\varepsilon)} \left[\int_{\partial B_\varepsilon} \frac{1}{2} \left(\frac{\partial u_\varepsilon}{\partial t} \right)^2 dS + f'_1(\varepsilon) D_T \psi \right]. \quad (3.14)$$

Taking into account eqs. (3.10, 3.12) in eq. (3.14) and choosing $f_2(\varepsilon) = \pi \varepsilon^4$, we can calculate limit $\varepsilon \rightarrow 0$ to obtain the final expression for the **second order topological derivative**, that is

$$D_T^2 \psi = - \frac{1}{4} \left(\nabla \nabla u(\hat{\mathbf{x}}) \cdot \nabla \nabla u(\hat{\mathbf{x}}) - \frac{1}{2} \text{tr}^2 \nabla \nabla u(\hat{\mathbf{x}}) \right) \quad \forall \hat{\mathbf{x}} \in \Omega, \quad \text{for } f_2(\varepsilon) = \pi \varepsilon^4, \quad (3.15)$$

and since $\Delta u = 0$ in Ω , we finally obtain

$$D_T^2 \psi = \frac{1}{2} \det \nabla \nabla u(\hat{\mathbf{x}}) \quad \forall \hat{\mathbf{x}} \in \Omega, \quad \text{for } f_2(\varepsilon) = \pi \varepsilon^4. \quad (3.16)$$

3.2. Dirichlet boundary condition on the hole. Taking $\alpha = 1$ in eq. (3.3), we have homogeneous Dirichlet boundary condition on the hole. Then, the following asymptotic expansion holds (see Appendix A)

$$u_\varepsilon(\mathbf{x}) = u(\mathbf{x}) - u(\widehat{\mathbf{x}}) \left(1 - \frac{\log(\|\mathbf{x} - \widehat{\mathbf{x}}\|/\varepsilon)}{\log(R/\varepsilon)} \right) + \frac{\varepsilon^2}{\|\mathbf{x} - \widehat{\mathbf{x}}\|^2} \nabla u(\widehat{\mathbf{x}}) \cdot (\mathbf{x} - \widehat{\mathbf{x}}) + \mathcal{O}(\varepsilon^2), \quad (3.17)$$

which is restricted to a ball B_R , where $R \gg \varepsilon$, with $B_\varepsilon \subset B_R \subset \Omega$.

According to eq. (3.8), we have

$$D_T \psi = \lim_{\varepsilon \rightarrow 0} \frac{1}{f'_1(\varepsilon)} \int_{\partial B_\varepsilon} \frac{1}{2} \left(\frac{\partial u_\varepsilon}{\partial n} \right)^2 dS. \quad (3.18)$$

Thus, considering the expansion given by eq. (3.17) in eq. (3.18), we observe that

$$f_1(\varepsilon) = -\frac{\pi}{\log \varepsilon}, \quad \text{and since } R \gg \varepsilon, \quad \log(R/\varepsilon) \simeq -\log \varepsilon. \quad (3.19)$$

Then, after computing the limit $\varepsilon \rightarrow 0$, we get the final expression for the **first order topological derivative**, which is given by

$$D_T \psi = u^2(\widehat{\mathbf{x}}) \quad \forall \widehat{\mathbf{x}} \in \Omega, \quad \text{for } f_1(\varepsilon) = -\frac{\pi}{\log \varepsilon}. \quad (3.20)$$

Remark 4. *The result given by eq. (3.20) cannot be continuously extended to the boundary. In fact, the first order topological derivative calculated on the boundary with homogeneous Dirichlet condition is given by [21]*

$$D_T \psi = \nabla u(\widehat{\mathbf{x}}) \cdot \nabla u(\widehat{\mathbf{x}}) \quad \forall \widehat{\mathbf{x}} \in \partial\Omega, \quad \text{for } f_1(\varepsilon) = \frac{1}{2} \pi \varepsilon^2. \quad (3.21)$$

In addition, from eq. (3.9), we have

$$D_T^2 \psi = \lim_{\varepsilon \rightarrow 0} \frac{1}{f'_2(\varepsilon)} \left[\int_{\partial B_\varepsilon} \frac{1}{2} \left(\frac{\partial u_\varepsilon}{\partial n} \right)^2 dS - f'_1(\varepsilon) D_T \psi \right]. \quad (3.22)$$

Taking into account eqs. (3.17, 3.20) in eq. (3.22) and choosing $f_2(\varepsilon) = \pi \varepsilon^2$, we can calculate limit $\varepsilon \rightarrow 0$ to obtain the final expression for the **second order topological derivative**, that is

$$D_T^2 \psi = \nabla u(\widehat{\mathbf{x}}) \cdot \nabla u(\widehat{\mathbf{x}}) \quad \forall \widehat{\mathbf{x}} \in \Omega, \quad \text{for } f_2(\varepsilon) = \pi \varepsilon^2. \quad (3.23)$$

4. NUMERICAL EXPERIMENTS

In this work the Topological-Shape Sensitivity Method has been used as a systematic procedure to calculate the first (Theorem 1) and the second (Theorem 2) order topological derivatives for the Poisson's problem, taking the total potential energy as cost function and the state equation as constraint. Furthermore, two boundary conditions on the hole, Neumann and Dirichlet (both homogeneous), were also considered. Therefore, the topological asymptotic expansions (eq. 1.1) are given respectively by:

- for homogeneous Neumann boundary condition on the hole (eqs. 3.12 and 3.16)

$$\psi(\Omega_\varepsilon) = \psi(\Omega) - \pi \varepsilon^2 \nabla u(\widehat{\mathbf{x}}) \cdot \nabla u(\widehat{\mathbf{x}}) + \frac{1}{2} \pi \varepsilon^4 \det \nabla \nabla u(\widehat{\mathbf{x}}) + \mathcal{R}(\varepsilon^4); \quad (4.1)$$

- for homogeneous Dirichlet boundary condition on the hole (eqs. 3.20 and 3.23)

$$\psi(\Omega_\varepsilon) = \psi(\Omega) - \frac{\pi}{\log \varepsilon} u^2(\widehat{\mathbf{x}}) + \pi \varepsilon^2 \nabla u(\widehat{\mathbf{x}}) \cdot \nabla u(\widehat{\mathbf{x}}) + \mathcal{R}(\varepsilon^2). \quad (4.2)$$

Our main objective with the numerical experiments presented in this section is to compare the above asymptotic expansions (4.1, 4.2) with the value of the cost functional computed in the perturbed domain Ω_ε , considering or not the term associated to the second order topological derivative. In doing so, it will be possible to obtain, for example, an insight concerning the influence of the second topological derivative on the estimation of the cost function associated to the perturbed domain with a hole of finite size.

To this end, we consider a domain $\Omega = (0, 1) \times (0, 1)$ and a perturbed one $\Omega_\varepsilon = \Omega \setminus \overline{B_\varepsilon}$, where B_ε has center at point $\mathbf{x}^* = (0.5, 0.5)$ and radius $\varepsilon \in \{0.01, 0.02, 0.04, 0.08\}$. The solutions u and u_ε ,

respectively associated to Ω and Ω_ε , are approximated using the standard three node triangular finite element. In particular and for all cases, the meshes were constructed maintaining the same number of elements $ne = 120$ along the boundary of the hole for whichever value of its radius ε . Since an automatic mesh generation was used, the following expected size h^e for the elements was adopted for all meshes

$$h^e \approx \frac{2\pi}{ne} \|\mathbf{x}^* - \mathbf{x}\| . \quad (4.3)$$

Moreover, we firstly compute the topological asymptotic expansion associated to the domain Ω at the point \mathbf{x}^* for the above values of ε . Then we effectively create the holes with center at the fixed point \mathbf{x}^* and compute the cost function $\psi(\Omega_\varepsilon)$ for each ε . Finally, we compare the obtained numerical results.

4.1. Example 1. In this example, we have a body submitted to a temperature $u = 0$ on Γ_{D_1} and Γ_{D_2} , and a heat flux $q_1 = 1$ on Γ_{N_1} and $q_1 = 2$ on Γ_{N_2} , as shown in Fig. (1, where $a = 0.2$). In addition, the remainder part of the boundary remains insulated.

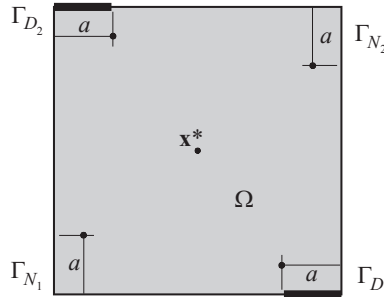


FIGURE 1. example 1.

4.1.1. Neumann boundary condition on the hole. Considering Neumann boundary condition on the hole, the topological asymptotic expansion obtained for the original domain Ω and for the perturbed one Ω_ε are shown in Fig. (2) and Fig. (3) respectively. We observe that $f_2(\varepsilon)D_T^2\psi$ does not produce significant changes in the results, at least from the qualitative point of view. However, this term furnishes an important correction factor for the expansion as clearly depicted in Fig. (4) showing, at the point \mathbf{x}^* , the behavior of the topological asymptotic expansion as a function of ε . Therefore, when finite holes are introduced, which is an important requirement in several applications, we can use, for example, this information to estimate:

- the size of the holes, according to the energy to be dissipated;
- the energy when creating holes of finite size.

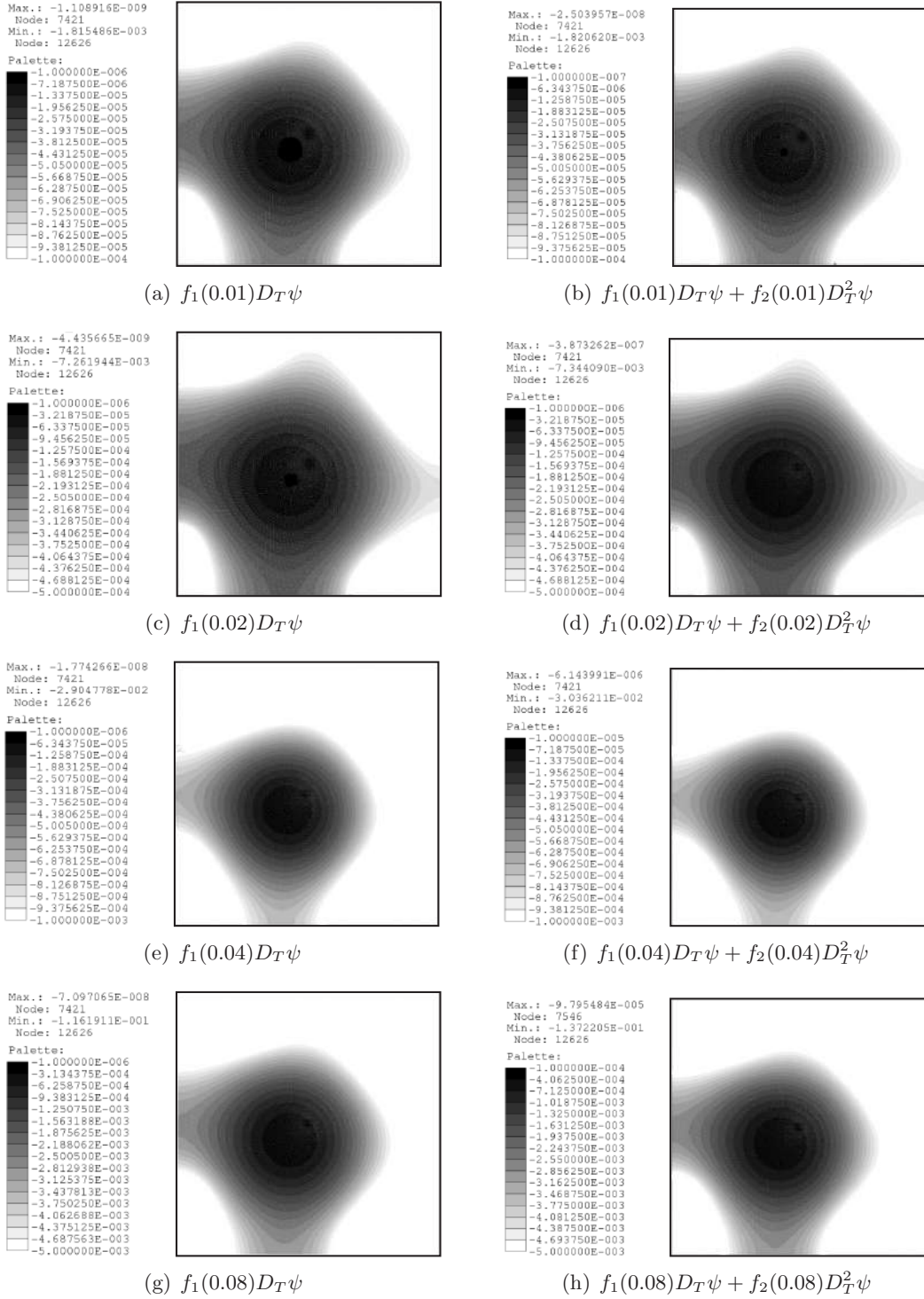
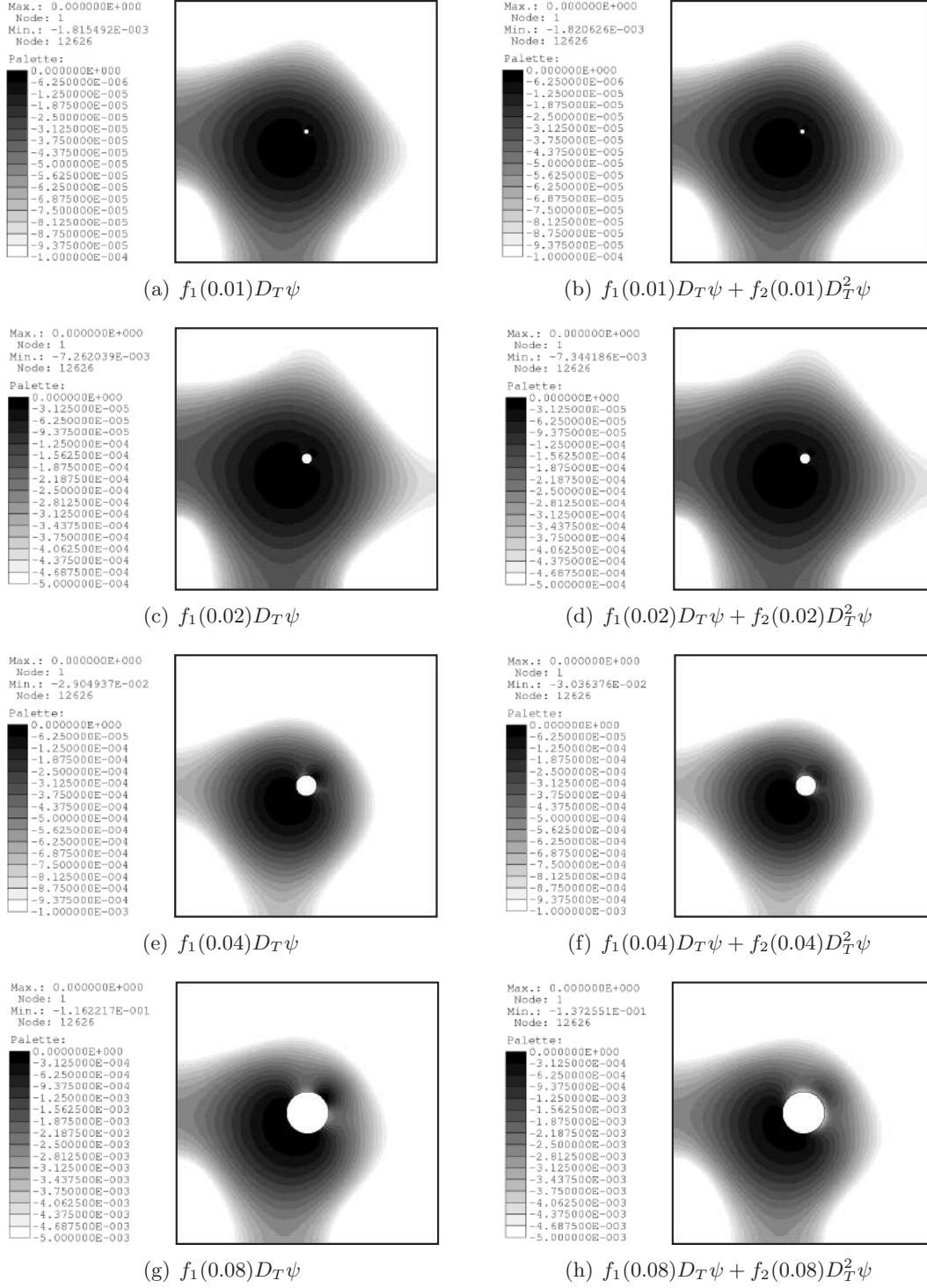


FIGURE 2. topological asymptotic expansion in the original domain Ω .

FIGURE 3. topological asymptotic expansion in the perturbed domain Ω_ϵ .

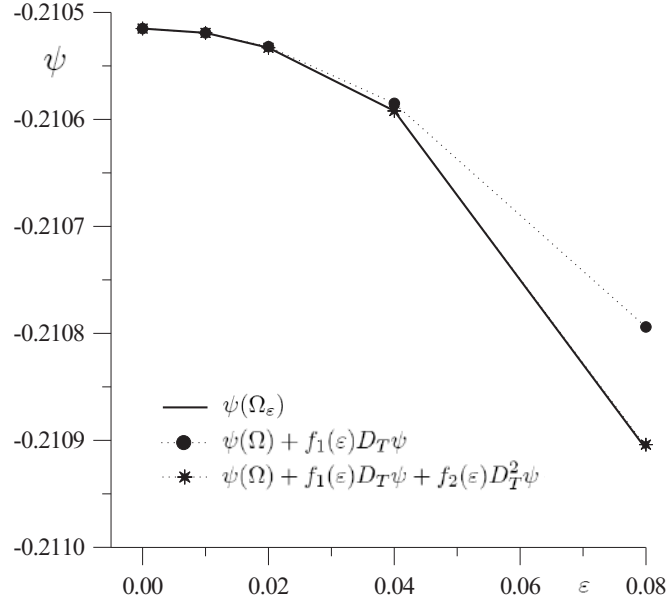


FIGURE 4. estimation of $\psi(\Omega_\varepsilon)$ considering first and second order terms of the topological asymptotic expansion.

Remark 5. Considering a larger variation of $\varepsilon \in \{0.08, 0.16, 0.24, 0.32\}$, we observe in Fig. (5) that the estimation becomes bad only for very large holes.

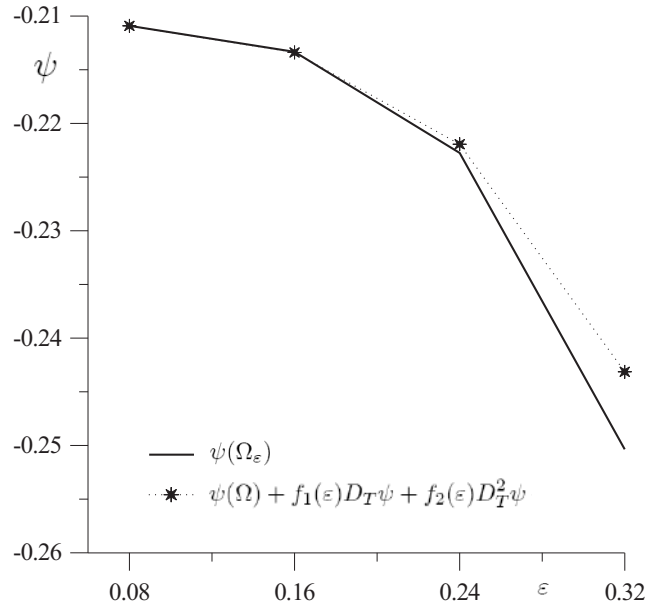
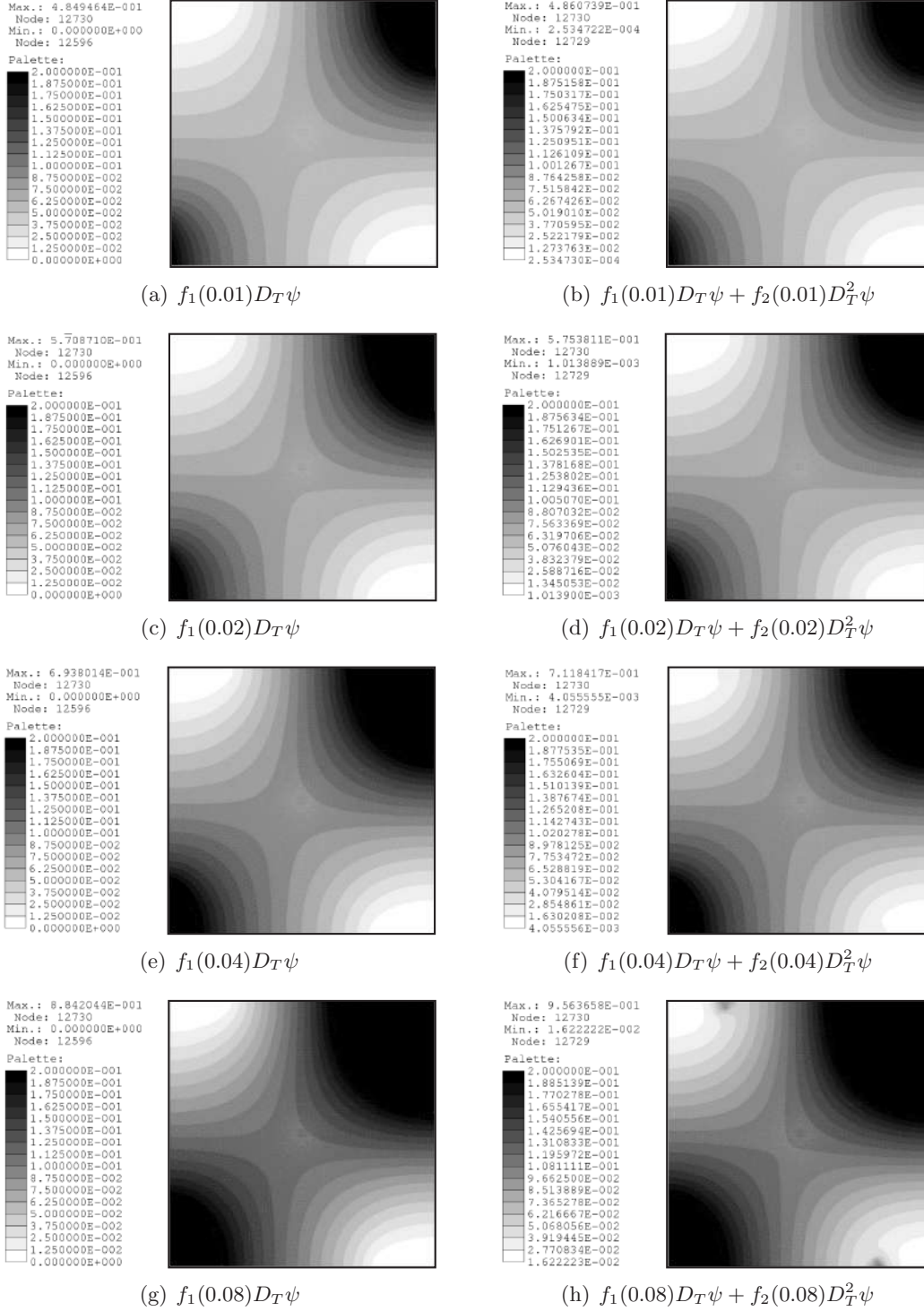


FIGURE 5. estimation of $\psi(\Omega_\varepsilon)$ considering the second order term of the topological asymptotic expansion for $\varepsilon \in \{0.08, 0.16, 0.24, 0.32\}$.

4.1.2. *Dirichlet boundary condition on the hole.* For Dirichlet boundary condition on the hole, the influence of the first and second order term in the topological asymptotic expansion are shown in Fig. (6) and Fig. (7) for original and perturbed domains respectively. From these figures, we observe that $f_2(\varepsilon)D_T^2\psi$ produces significant changes in the results only for the perturbed domain Ω_ε (this issue will be discussed again in the next example).

FIGURE 6. topological asymptotic expansion in the original domain Ω .

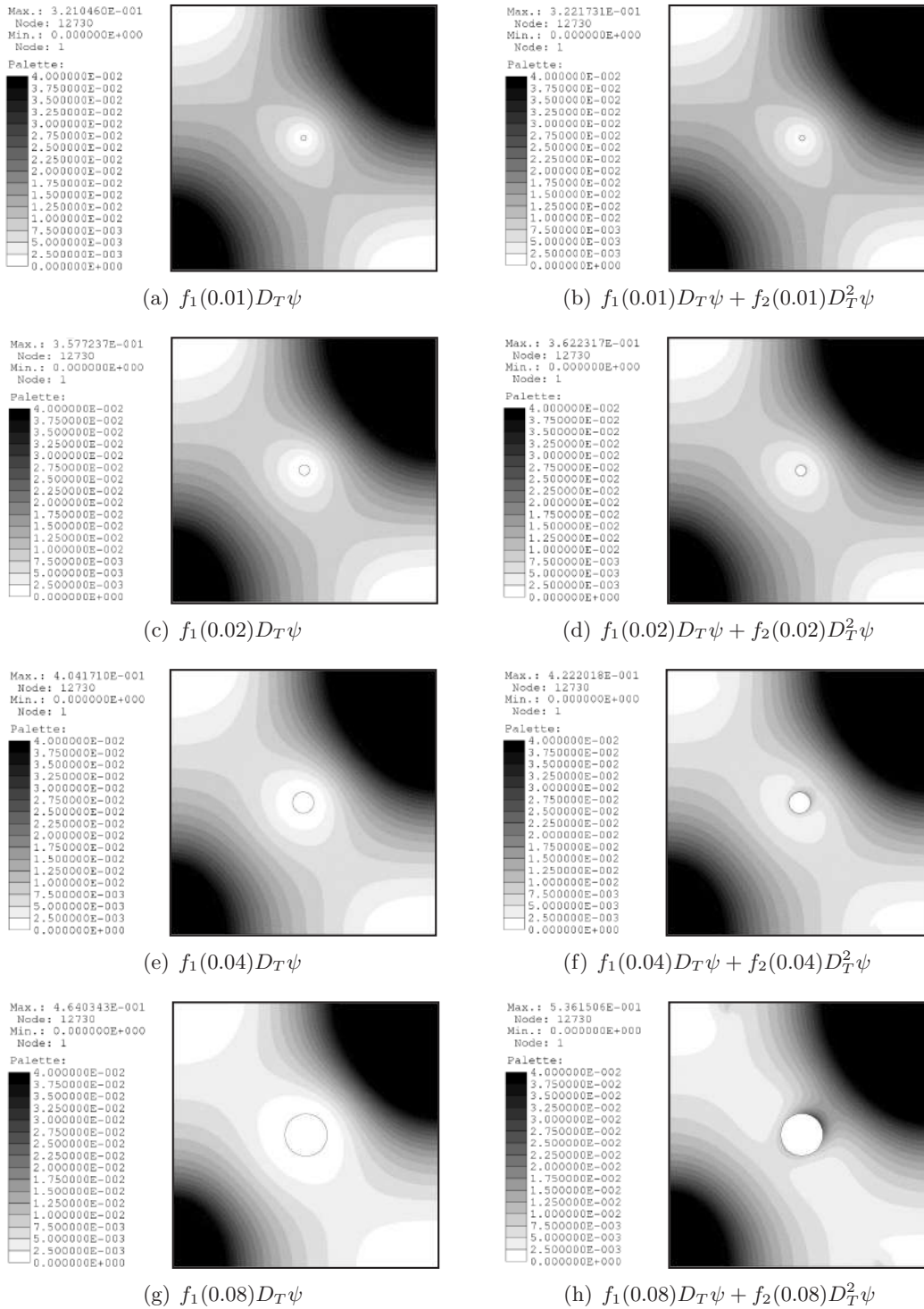
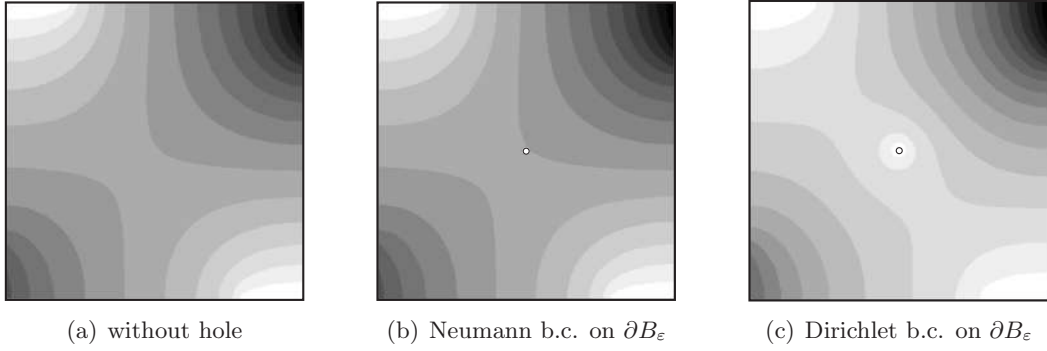
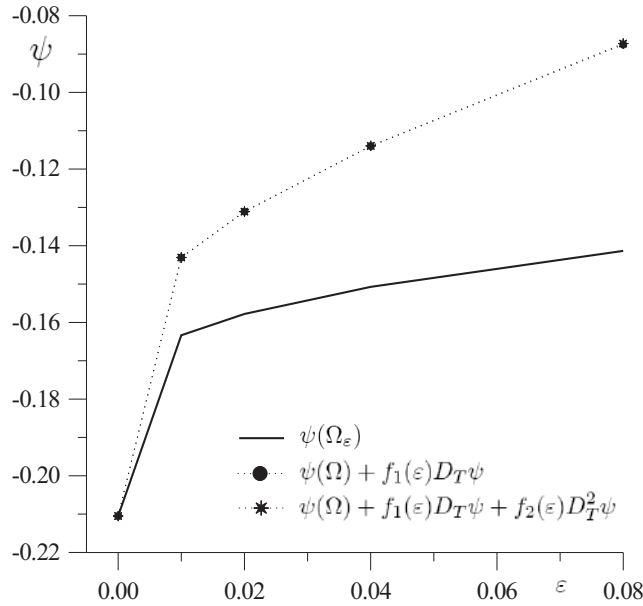


FIGURE 7. topological asymptotic expansion in the perturbed domain Ω_ε .

On the other hand, the behavior at \mathbf{x}^* of the topological asymptotic expansion as a function of ε is shown in Fig. (9). From this figure it follows that the asymptotic expansion gives a bad estimation for the cost function for values of ε greater than 0.01. However, Fig. (9) also suggests that the estimation, even though imprecise, furnishes a good decent direction in optimization problems.

Remark 6. From a comparison between Fig. (4) and Fig. (9) we observe that the estimation in the case of Neumann boundary condition on the hole is quite better than the one for Dirichlet boundary condition. This behavior was expected for this example because the perturbation in the solution is more severe for the last case than for the first one as can be seen in Fig. (8).

FIGURE 8. solutions u and u_ε for $\varepsilon = 0.01$.FIGURE 9. estimation of $\psi(\Omega_\varepsilon)$ considering first and second order terms of the topological asymptotic expansion.

4.2. Example 2. In this example, the problem considered can be seen in Fig. (10), where we have a body submitted to a temperature $u = 0$ on Γ_D and a heat flux given by a piecewise linear distribution on Γ_N , with $q_1 = 1$ and $q_2 = 2$. Further, homogeneous Dirichlet boundary condition on the holes will be considered. Due to the periodical symmetry of the problem, only a part, denoted by Ω , is considered.

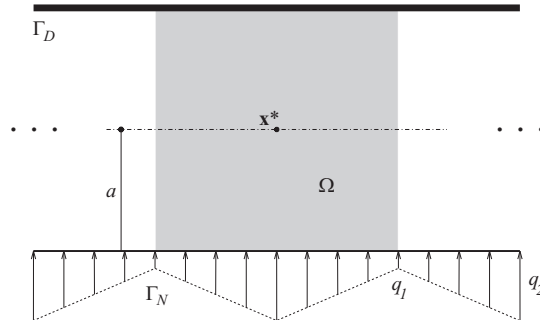


FIGURE 10. example 2.

In this case, the holes can be interpreted as cooling channels in a heat exchanger. Then, we will estimate the variation of the energy when the cooling channels (holes) are centered at the

point \mathbf{x}^* and, in a next step, at any point of the line defined by $a = 0.5$, which can be seen as a constraint in the problem.

The effects of the first and second order terms in the topological asymptotic expansion are shown in Fig. (11) and Fig. (12) for the original and perturbed domains respectively. From the last figure, we observe that, for $\varepsilon = 0.04$ and $\varepsilon = 0.08$, while $f_1(\varepsilon)D_T\psi$ suggests the creation of a new hole, the term $f_1(\varepsilon)D_T\psi + f_2(\varepsilon)D_T^2\psi$ suggests a growth of the cooling channel (see a detail for $\varepsilon = 0.04$ in Fig. (13)).

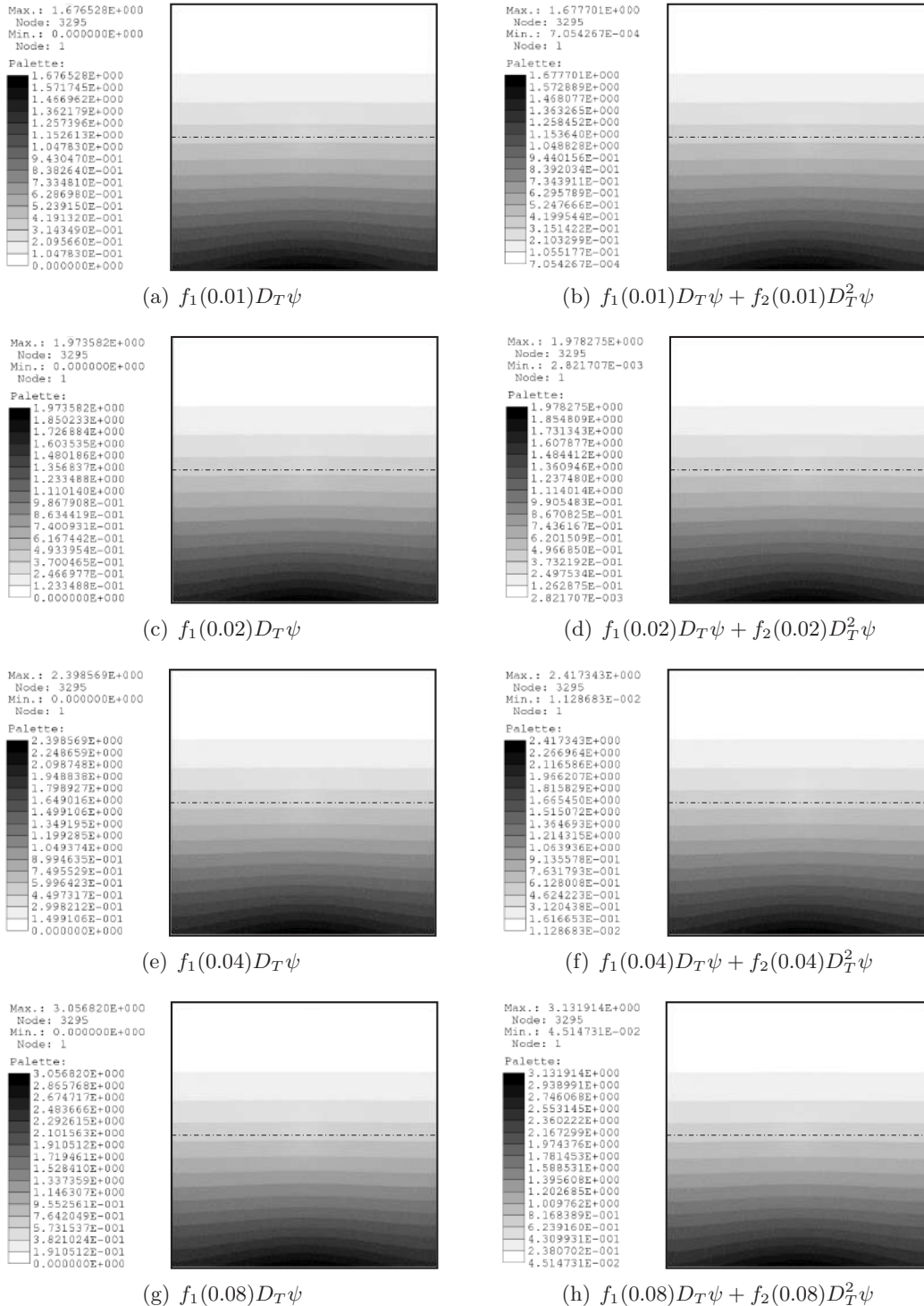
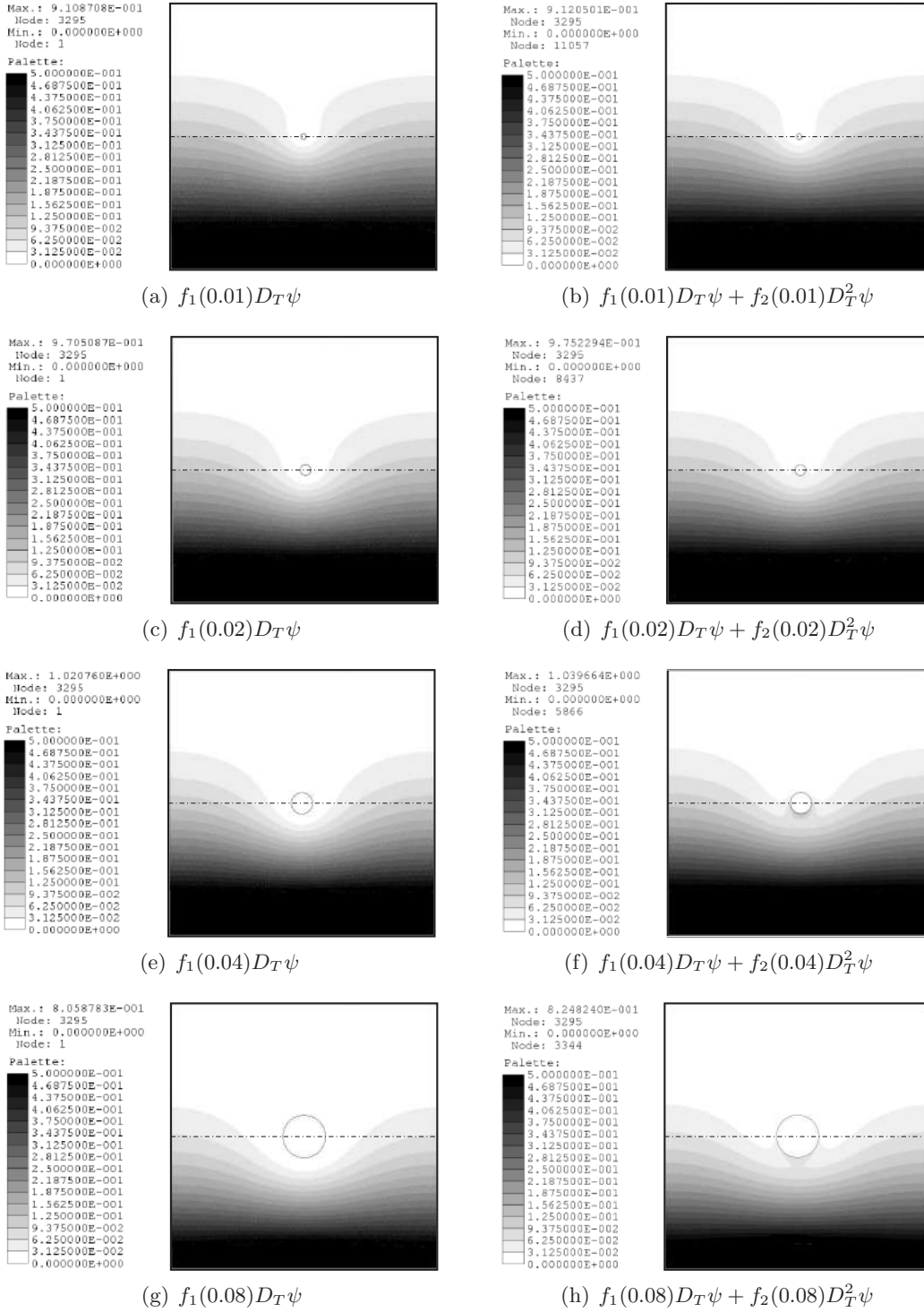


FIGURE 11. topological asymptotic expansion in the original domain Ω .

FIGURE 12. topological asymptotic expansion in the perturbed domain Ω_ϵ .

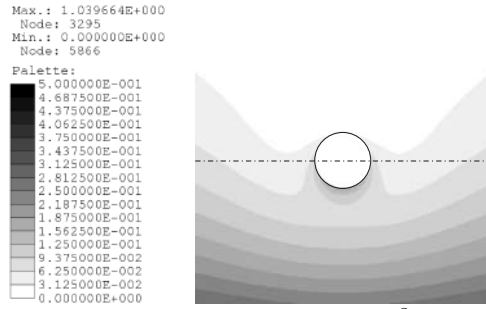


FIGURE 13. detail of term $f_1(0.04)D_T\psi + f_2(0.04)D_7^2\psi$ of the topological asymptotic expansion.

Nonetheless, it is important to mention that, formally the topological derivatives calculated in this work are defined only for interior points of the domain. Thus, according to Remark 4, we need to compute the topological derivative defined in interior ($\forall \hat{\mathbf{x}} \in \Omega$) and boundary ($\forall \hat{\mathbf{x}} \in \partial B_\varepsilon$) points. Taking into account the above consideration, the results obtained with only the first order topological derivative for $\varepsilon = 0.08$ are shown in Fig. (14), which was enough to suggest that the cooling channel should be expanded.

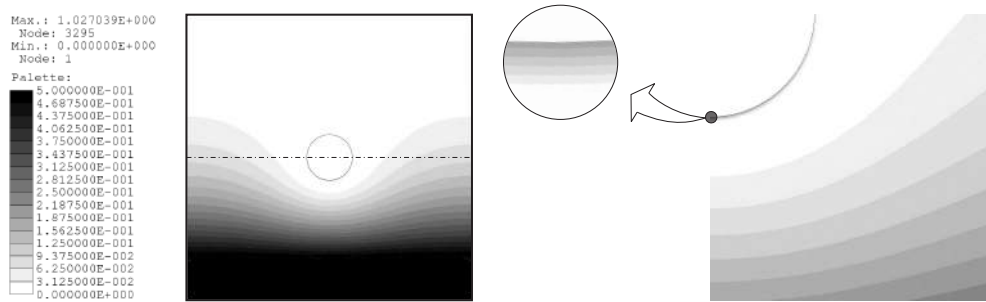


FIGURE 14. correct values for the term $f_1(\varepsilon)D_T\psi$ for $\hat{\mathbf{x}} \in \Omega$ and $\hat{\mathbf{x}} \in \partial B_\varepsilon$, for $\varepsilon = 0.08$.

5. CONCLUSIONS

In this work, we have considered one more term in the topological asymptotic expansion that can be recognized as the second order topological derivative. Then, we have applied the Topological-Shape Sensitivity Method as a systematic procedure to calculate the first and second order topological derivative. In particular, we have considered the Poisson's equation, taking into account homogeneous Neumann and Dirichlet boundary condition on the hole and the total potential energy as cost function. Finally, we have presented some numerical experiments showing the influence of the second order topological derivative in the topological asymptotic expansion. From these results, we have observed that the second order correction term plays an important role in the analysis, allowing a more accurate estimation for the size of the holes and also a better decent direction in optimization problems than the one given only by the first order correction term.

Acknowledgments. This research was partly supported by CNPq/FAPERJ-PRONEX (Brazil), under Grant E-26/171.199/2003 and CONICET (Argentina). Jairo Rocha de Faria was partially supported by Brazilian government fellowship from CAPES. The support from these Institutions is greatly appreciated.

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APPENDIX A. ASYMPTOTIC ANALYSIS

In this section we give a justification for the asymptotic expansions (eqs. 3.10 and 3.17) adopted to calculate the final expressions for the first and second order topological derivatives. The Euler-Lagrange equations associated to the variational problems given by eq. (3.1) and eq. (3.3) are respectively stated as

$$\begin{cases} \Delta u = 0 & \text{in } \Omega \\ u = \varphi & \text{on } \Gamma_D \\ -\frac{\partial u}{\partial n} = q & \text{on } \Gamma_N \end{cases}, \quad (\text{A.1})$$

and

$$\begin{cases} \Delta u_\varepsilon = 0 & \text{in } \Omega_\varepsilon \\ u_\varepsilon = \varphi & \text{on } \Gamma_D \\ -\frac{\partial u_\varepsilon}{\partial n} = q & \text{on } \Gamma_N \\ \alpha u_\varepsilon + (1 - \alpha) \frac{\partial u_\varepsilon}{\partial n} = 0 & \text{on } \partial B_\varepsilon \end{cases}. \quad (\text{A.2})$$

Our goal is to observe the asymptotic behavior of $u_\varepsilon(\mathbf{x})$ in confrontation with $u(\mathbf{x})$, which will be represented by power series of ε (or $\log \varepsilon$). These kind of solutions provide good approximations when $\varepsilon \rightarrow 0$.

Let us assume that u^D and u^N are solutions of Dirichlet and Neumann boundary-value problems, given respectively by

$$P_D : \begin{cases} \Delta u^D = 0 & \text{in } \Omega \\ u^D = \varphi & \text{on } \partial\Omega \end{cases} \quad \text{and} \quad P_N : \begin{cases} \Delta u^N = 0 & \text{in } \Omega \\ -\frac{\partial u^N}{\partial n} = q & \text{on } \partial\Omega \end{cases}, \quad (\text{A.3})$$

where q satisfies the compatibility condition. Then we can define the Steklov-Poincaré operator:

Definition 7. Let u^D be solution of the Dirichlet problem P_D , then the associated Steklov-Poincaré operator $\Lambda : H^{1/2}(\partial\Omega) \rightarrow H^{-1/2}(\partial\Omega)$ is defined as

$$\Lambda(\varphi) := \left. \frac{\partial u^D}{\partial n} \right|_{\partial\Omega}, \quad (\text{A.4})$$

that can be analogously defined for any part of $\partial\Omega$ with a Dirichlet data.

From these elements, we have that:

Proposition 8. Let u^D be solution of the Dirichlet problem (P_D) and $q = -\Lambda(\varphi)$, then $u^N = u^D$, where u^N is solution of the Neumann problem (P_N).

Proof. The proof of this result came immediately from the well-posedness of problems P_D and P_N \square

Therefore, we can transform the mixed problem given by eq. (A.2) in a Neumann problem using the Steklov-Poincaré operator. In addition, we have an estimation for a Neumann problem given by the following theorem:

Theorem 9. Let v_ε be solution of a Neumann boundary-value problem given by

$$\begin{cases} \Delta v_\varepsilon = 0 & \text{in } \Omega_\varepsilon \\ -\frac{\partial v_\varepsilon}{\partial n} = q_1 & \text{on } \partial B_\varepsilon \\ -\frac{\partial v_\varepsilon}{\partial n} = q_2 & \text{on } \partial\Omega \end{cases}, \quad (\text{A.5})$$

where q_1, q_2 are smooth functions satisfying the compatibility condition

$$\int_{\partial B_\varepsilon} q_2 dS = \int_{\partial\Omega} q_1 dS = 0. \quad (\text{A.6})$$

Then the estimative

$$|v_\varepsilon|_{H^1(\Omega_\varepsilon)} \leq C \left\{ \varepsilon \max_{\partial B_\varepsilon} |q_1| + \max_{\partial\Omega} |q_2| \right\} \quad (\text{A.7})$$

holds, where constant C is independent of ε and $|\cdot|_{H^1(\Omega_\varepsilon)}$ is used to denote a semi-norm (energy norm) in $H^1(\Omega_\varepsilon)$.

Proof. See [15] \square

Now we are able to obtain the estimates used in the topological derivative calculation for each kind of boundary condition on the holes.

A.1. Neumann boundary condition on the hole. Taking $\alpha = 0$ in eq. (A.2), we can propose an asymptotic expansion given by

$$u_\varepsilon(\mathbf{x}) = u(\mathbf{x}) + w_\varepsilon(\mathbf{x}/\varepsilon) + \tilde{u}_\varepsilon(\mathbf{x}). \quad (\text{A.8})$$

Let us expand $u(\mathbf{x})$ around $\hat{\mathbf{x}}$, then its normal derivative on ∂B_ε can be expressed as

$$\begin{aligned} \left. \frac{\partial u}{\partial n} \right|_{\partial B_\varepsilon} &= \nabla u(\hat{\mathbf{x}}) \cdot \mathbf{n} - \varepsilon D(\nabla u(\hat{\mathbf{x}}))(\mathbf{n})^2 + \varepsilon^2 D^2(\nabla u(\boldsymbol{\xi}))(\mathbf{n})^3 \\ &= \nabla u(\hat{\mathbf{x}}) \cdot \mathbf{n} - \varepsilon \nabla \nabla u(\hat{\mathbf{x}}) \mathbf{n} \cdot \mathbf{n} + \varepsilon^2 D^3 u(\boldsymbol{\xi})(\mathbf{n})^3, \end{aligned} \quad (\text{A.9})$$

where $\boldsymbol{\xi}$ is an intermediate point between $\hat{\mathbf{x}}$ and \mathbf{x} . Thus, function $w_\varepsilon(\mathbf{y})$, with $\mathbf{y} = \mathbf{x}/\varepsilon$, is solution of an exterior problem given by

$$\begin{cases} \Delta w_\varepsilon = 0 & \text{in } \mathbb{R}^2 \setminus \overline{B}_1 \\ w_\varepsilon \rightarrow 0 & \text{at } \infty \\ -\frac{\partial w_\varepsilon}{\partial n} = \varepsilon \nabla u(\hat{\mathbf{x}}) \cdot \mathbf{n} - \varepsilon^2 \nabla \nabla u(\hat{\mathbf{x}}) \mathbf{n} \cdot \mathbf{n} & \text{on } \partial B_1 \end{cases}, \quad (\text{A.10})$$

which can be solved by separation of variables, that is

$$w_\varepsilon(\mathbf{x}/\varepsilon) = \frac{\varepsilon^2}{\|\mathbf{x}-\widehat{\mathbf{x}}\|^2} \nabla u(\widehat{\mathbf{x}}) \cdot (\mathbf{x}-\widehat{\mathbf{x}}) + \frac{\varepsilon^4}{2\|\mathbf{x}-\widehat{\mathbf{x}}\|^4} \nabla \nabla u(\widehat{\mathbf{x}}) (\mathbf{x}-\widehat{\mathbf{x}}) \cdot (\mathbf{x}-\widehat{\mathbf{x}}). \quad (\text{A.11})$$

In addition, the discrepancy produced by w_ε on $\partial\Omega$ and by the remainder term of the expansion $\varepsilon^2 D^3 u(\boldsymbol{\xi})(\mathbf{n})^3$ on ∂B_ε shall be compensated by \tilde{u}_ε . Therefore, \tilde{u}_ε satisfies

$$\begin{cases} \Delta \tilde{u}_\varepsilon = 0 & \text{in } \Omega_\varepsilon \\ \tilde{u}_\varepsilon = -w_\varepsilon & \text{on } \Gamma_D \\ -\frac{\partial \tilde{u}_\varepsilon}{\partial \mathbf{n}} = \frac{\partial w_\varepsilon}{\partial \mathbf{n}} & \text{on } \Gamma_N \\ -\frac{\partial \tilde{u}_\varepsilon}{\partial \mathbf{n}} = \varepsilon^2 D^3 u(\boldsymbol{\xi})(\mathbf{n})^3 & \text{on } \partial B_\varepsilon \end{cases}. \quad (\text{A.12})$$

which is equivalent to the following one

$$\begin{cases} \Delta \tilde{u}_\varepsilon^N = 0 & \text{in } \Omega_\varepsilon \\ -\frac{\partial \tilde{u}_\varepsilon^N}{\partial \mathbf{n}} = \Lambda(w_\varepsilon) & \text{on } \Gamma_D \\ -\frac{\partial \tilde{u}_\varepsilon^N}{\partial \mathbf{n}} = \frac{\partial w_\varepsilon}{\partial \mathbf{n}} & \text{on } \Gamma_N \\ -\frac{\partial \tilde{u}_\varepsilon^N}{\partial \mathbf{n}} = \varepsilon^2 D^3 u(\boldsymbol{\xi})(\mathbf{n})^3 & \text{on } \partial B_\varepsilon \end{cases}, \quad (\text{A.13})$$

that is, considering Proposition 8, we observe that $\tilde{u}_\varepsilon^N = \tilde{u}_\varepsilon$. Finally, from Theorem 9, we obtain

$$|\tilde{u}_\varepsilon|_{H^1(\Omega_\varepsilon)} \leq C\varepsilon^2. \quad (\text{A.14})$$

where the constant C is independent of ε .

A.2. Dirichlet boundary condition on the hole. Considering $\alpha = 1$ in eq. (A.2), we observe that the technique used in the previous section fails in this case since the Dirichlet boundary value problem in $\mathbb{R}^2 \setminus \overline{B}_1$ does not necessarily has a solution that decays at infinity. In order to avoid this problem, we will consider a ball B_R , such that $R \gg \varepsilon$, and $B_\varepsilon \subset B_R \subset \Omega$. In addition, let us adopt again the asymptotic expansion written as

$$u_\varepsilon(\mathbf{x}) = u(\mathbf{x}) + v_\varepsilon(\mathbf{x}) + w_\varepsilon(\mathbf{x}/\varepsilon) + \tilde{u}_\varepsilon(\mathbf{x}), \quad (\text{A.15})$$

where function $v_\varepsilon(\mathbf{x})$ is given by [11]

$$v_\varepsilon(\mathbf{x}) = \begin{cases} -u(\widehat{\mathbf{x}}) \left(1 - \frac{\log(\|\mathbf{x}-\widehat{\mathbf{x}}\|/\varepsilon)}{\log(R/\varepsilon)}\right), & \forall \mathbf{x} \in B_R \setminus \overline{B}_\varepsilon \\ 0, & \forall \mathbf{x} \in \Omega \setminus \overline{B}_R \end{cases}. \quad (\text{A.16})$$

Now, considering the expansion of $u(\mathbf{x})|_{\partial B_\varepsilon}$ around $\widehat{\mathbf{x}}$ we have

$$u(\mathbf{x})|_{\partial B_\varepsilon} = u(\widehat{\mathbf{x}}) - \varepsilon D u(\widehat{\mathbf{x}}) \cdot \mathbf{n} + \varepsilon^2 D^2 u(\boldsymbol{\xi})(\mathbf{n})^2, \quad (\text{A.17})$$

where $\boldsymbol{\xi}$ is an intermediate point between $\widehat{\mathbf{x}}$ and \mathbf{x} . We can observe that $v_\varepsilon(\mathbf{x})|_{\partial B_\varepsilon} = -u(\widehat{\mathbf{x}})$. Therefore, is natural to define $w_\varepsilon(\mathbf{y})$, with $\mathbf{y} = \mathbf{x}/\varepsilon$, as solution of an exterior problem given by

$$\begin{cases} \Delta w_\varepsilon = 0 & \text{in } \mathbb{R}^2 \setminus \overline{B}_1 \\ w_\varepsilon \rightarrow 0 & \text{at } \infty \\ -\frac{\partial w_\varepsilon}{\partial \mathbf{n}} = \varepsilon \nabla u(\widehat{\mathbf{x}}) \cdot \mathbf{n} & \text{on } \partial B_1 \end{cases}, \quad (\text{A.18})$$

By separation of variables we have

$$w_\varepsilon(\mathbf{x}/\varepsilon) = \frac{\varepsilon^2}{\|\mathbf{x}-\widehat{\mathbf{x}}\|^2} \nabla u(\widehat{\mathbf{x}}) \cdot (\mathbf{x}-\widehat{\mathbf{x}}). \quad (\text{A.19})$$

Thus, the restriction of $u_\varepsilon(\mathbf{x})$ in the ball B_R can be expressed as

$$u_\varepsilon(\mathbf{x})|_{B_R} = u(\mathbf{x}) - u(\widehat{\mathbf{x}}) \left(1 - \frac{\log(\|\mathbf{x}-\widehat{\mathbf{x}}\|/\varepsilon)}{\log(R/\varepsilon)}\right) + \varepsilon^2 \nabla u(\widehat{\mathbf{x}}) \cdot \frac{(\mathbf{x}-\widehat{\mathbf{x}})}{\|\mathbf{x}-\widehat{\mathbf{x}}\|^2} + \tilde{u}_\varepsilon(\mathbf{x}), \quad (\text{A.20})$$

and $\tilde{u}_\varepsilon(\mathbf{x})$ is solution of the following boundary value problem:

$$\begin{cases} \Delta \tilde{u}_\varepsilon = 0 & \text{in } \Omega_\varepsilon \\ \tilde{u}_\varepsilon = -w_\varepsilon & \text{on } \Gamma_D \\ -\frac{\partial \tilde{u}_\varepsilon}{\partial \mathbf{n}} = \frac{\partial w_\varepsilon}{\partial \mathbf{n}} & \text{on } \Gamma_N \\ \tilde{u}_\varepsilon = -\varepsilon^2 D^2 u(\boldsymbol{\xi})(\mathbf{n})^2 & \text{on } \partial B_\varepsilon \end{cases}. \quad (\text{A.21})$$

In analogous way to the previous section, we can consider a new problem \tilde{u}_ε^N given by

$$\left\{ \begin{array}{ll} \Delta \tilde{u}_\varepsilon^N = 0 & \text{in } \Omega_\varepsilon \\ -\frac{\partial \tilde{u}_\varepsilon^N}{\partial n_N} = \Lambda(w_\varepsilon) & \text{on } \Gamma_D \\ -\frac{\partial \tilde{u}_\varepsilon^N}{\partial n} = \frac{\partial w_\varepsilon}{\partial n} & \text{on } \Gamma_N \\ -\frac{\partial \tilde{u}_\varepsilon^N}{\partial n} = \Lambda\left(\varepsilon^2 D^2 u(\boldsymbol{\xi})(\mathbf{n})^2\right) & \text{on } \partial B_\varepsilon \end{array} \right. . \quad (\text{A.22})$$

Then, taking into account Proposition 8, $\tilde{u}_\varepsilon^N = \tilde{u}_\varepsilon$. Finally, from Theorem 9, we obtain the required estimative given by,

$$|\tilde{u}_\varepsilon|_{H^1(\Omega_\varepsilon)} \leq C\varepsilon^2. \quad (\text{A.23})$$

where the constant C is independent of ε .

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