ON THE SECOND ORDER TOPOLOGICAL ASYMPTOTIC EXPANSION

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ABSTRACT. The topological derivative provides the sensitivity of a given shape functional with respect to an infinitesimal (non smooth) domain perturbation at an arbitrary point of the domain. Classically, this derivative comes from the second term of the topological asymptotic expansion, dealing only with infinitesimal perturbations. However, for practical applications, we need to insert perturbations 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 calculate first as well as second order topological derivatives for the total potential energy associated to the Laplace's equation, when the domain is perturbed with a hole. Furthermore, we also study the effects of different boundary conditions on the hole: Neumann and Dirichlet (both homogeneous). In the Neumann's case, the second order topological derivative depends explicitly on higher-order gradients of the state solution and also implicitly on the point where the hole is nucleated through the solution of an auxiliary problem. On the other hand, in the Dirichlet's case, the first order topological derivative depends explicitly on the state solution as well as implicitly through the solution of an auxiliary problem, and the second order topological derivative depends only explicitly on the solution associated to the original problem. Finally, we present two simple examples showing the influence of both terms in the second order topological asymptotic expansion for each case of boundary condition on the hole.

1. INTRODUCTION

The topological sensitivity analysis gives the topological asymptotic expansion of a shape functional with respect to an infinitesimal domain perturbation, like the insertion of holes, inclusions or source term [3, 12]. The second term of this expansion provides the topological derivative, which has been applied in several problems, such as topology optimization, image processing and inverse problems. Analogously to the classical Taylor's theorem, we can consider new terms in the topological asymptotic expansion of a smooth enough shape functional. As would be expected, we define the next one as the second order topological derivative. This procedure allows to deal with perturbation of finite size, which is an important requirement for practical applications.

In our previous work [5] we have extended the method proposed in [11] to calculate the second order topological asymptotic expansion for the Laplace's equation; considering the total potential energy as the shape functional, the state equation as the constraint and taking into account two different homogeneous boundary conditions on the hole: Neumann and Dirichlet. In particular, we will demonstrate that the second order topological derivative associated to the Neumann's case depends explicitly on higher-order gradients of the state solution and also implicitly on the point where the hole is nucleated through the solution of an auxiliary problem. Concerning the Dirichlet's case, the first order topological derivative depends explicitly on the state solution as well as implicitly through the solution of an auxiliary problem. However, in this last case, the second order topological derivative is given explicitly in terms of the state solution. Furthermore, for the sake of simplicity, in [5] we have disregarded all these implicit terms, leading to a discrepancy in the topological asymptotic expansion.

Therefore, in the present paper we calculate the complete second order topological asymptotic expansion for the two cases under consideration. Then, we present two simple examples with analytical solutions, where we discuss the effects of the *ad hoc* approximations adopted

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in [5] and also the influence of both explicit and implicit terms on the topological asymptotic expansion. More specifically, we show that these new implict terms play a crucial role in the analysis. Although very expansible to be computed in the whole domain, they cannot be simply disregarded in the case of bounded domains.

2. Topological-shape sensitivity method

Let us consider an open bounded domain $\Omega \subset \mathbb{R}^2$, with a smooth boundary $\partial\Omega$. Then, we drill a small hole $\mathcal{H}_\varepsilon$ of radius ε and center at point $\widehat{\mathbf{x}} \in \Omega$. Thus, we have a perforated domain $\Omega_\varepsilon = \Omega \backslash \overline{\mathcal{H}_\varepsilon}$, whose boundary is denoted by $\partial\Omega_\varepsilon = \partial\Omega \cup \partial\mathcal{H}_\varepsilon$. If we assume that a given shape functional ψ admits the following topological asymptotic expansion

$$\psi(\Omega_\varepsilon) = \psi(\Omega) + f_1(\varepsilon) D_T\psi + f_2(\varepsilon) D_T^2\psi + o(f_2(\varepsilon)) \ , \tag{2.1}$$

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

$$\lim_{\varepsilon\to 0} \frac{f_2(\varepsilon)}{f_1(\varepsilon)} = 0 \ , \qquad \lim_{\varepsilon\to 0} \frac{o(f_2(\varepsilon))}{f_2(\varepsilon)} = 0 \ , \tag{2.2}$$

then, $D_T\psi$ and $D_T^2\psi$ are the first and second order topological derivatives of ψ, respectively. In fact, from the approach presented in the work [11], the following results hold:

$$D_T\psi = \lim_{\varepsilon\to 0} \frac{1}{f_1'(\varepsilon)} \frac{d}{d\varepsilon} \psi(\Omega_\varepsilon) \ , \tag{2.3}$$

$$D_T^2\psi = \lim_{\varepsilon\to 0} \frac{1}{f_2'(\varepsilon)} \left(\frac{d}{d\varepsilon} \psi(\Omega_\varepsilon) - f_1'(\varepsilon) D_T\psi \right) \ . \tag{2.4}$$

The derivative of the shape function with respect to the parameter ε, that appears in eqs. (2.3,2.4), can be seen as its classical shape sensitivity analysis to the change in shape produced by a uniform expansion of the hole. In particular, for a circular hole, we can define a sufficiently regular shape change velocity field $\mathbf{v}$, such that on the boundary $\partial\Omega_\varepsilon$, $\mathbf{v}|_{\partial\mathcal{H}_\varepsilon} = -\mathbf{n}$ and $\mathbf{v}|_{\partial\Omega} = \mathbf{0}$, where $\mathbf{n}$ is the outward unit normal vector field to the hole $\mathcal{H}_\varepsilon$. Thus, it is possible to introduce an analogy to classical continuum mechanics [8] whereby the shape change velocity field $\mathbf{v}$ is identified with the classical velocity field of a deforming continuum and ε is identified as a time parameter (refer to [13] for analogies of this type in the context of shape sensitivity analysis). Then, the shape derivative of the cost functional results in an integral on the boundary $\partial\mathcal{H}_\varepsilon$, that is

$$\frac{d}{d\varepsilon}\psi(\Omega_\varepsilon) = -\int_{\partial\mathcal{H}_\varepsilon} \mathbf{\Sigma}_\varepsilon \mathbf{n} \cdot \mathbf{n} \ , \tag{2.5}$$

where tensor $\mathbf{\Sigma}_\varepsilon$ can be interpreted as a generalization of the Eshelby energy-momentum tensor [6, 9], which is derived by making use of Reynolds' transport theorem [8] and the concept of material derivative of a spatial field [13]. As a consequence, this tensor plays a central role in the topological-shape sensitivity method and should be clearly identified according to the problem under consideration.

3. Topological derivative for Laplace'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 the shape functional.

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

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

where $\mathcal{U}(\Omega)$ and $\mathcal{V}(\Omega)$ are respectively defined as

$$\mathcal{U}(\Omega) := \{u \in H^1(\Omega) : u|_{\Gamma_D} = \varphi\} \quad \text{and} \quad \mathcal{V}(\Omega) := \{\eta \in H^1(\Omega) : \eta|_{\Gamma_D} = 0\} . \tag{3.2}$$

In addition, $\partial\Omega = \overline{\Gamma_D \cup \Gamma_N}$ with $\Gamma_D \cap \Gamma_N = \varnothing$, 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

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

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

$$\mathcal{U}_\varepsilon(\Omega_\varepsilon) := \{u_\varepsilon \in \mathcal{U}(\Omega_\varepsilon) : \beta\, u_\varepsilon|_{\partial\mathcal{H}_\varepsilon} = 0\} \quad \text{and} \quad \mathcal{V}_\varepsilon(\Omega_\varepsilon) := \{\eta_\varepsilon \in \mathcal{V}(\Omega_\varepsilon) : \beta\, \eta_\varepsilon|_{\partial\mathcal{H}_\varepsilon} = 0\} \ , \tag{3.4}$$

with $\beta \in \{0,1\}$. This notation should be interpreted as follows: when $\beta = 1$, $u_\varepsilon = 0$ and $\eta_\varepsilon = 0$ on $\partial\mathcal{H}_\varepsilon$, and when $\beta = 0$, u_ε and η_ε are free on $\partial\mathcal{H}_\varepsilon$. Therefore, according to the values of β, we have Dirichlet or Neumann boundary condition on the hole, both homogeneous.

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

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

Considering the Reynold's transport theorem and the concept of material derivative of spatial field, the Eshelby tensor $\mathbf{\Sigma}_\varepsilon$ is given by [11]

$$\mathbf{\Sigma}_\varepsilon = \frac{1}{2}\|\nabla u_\varepsilon\|^2 \mathbf{I} - (\nabla u_\varepsilon \otimes \nabla u_\varepsilon) \, . \tag{3.6}$$

From an orthonormal curvilinear coordinate system $\mathbf{n}$ and $\mathbf{t}$ on the boundary $\partial\mathcal{H}_\varepsilon$, the gradient $\nabla u_\varepsilon|_{\partial\mathcal{H}_\varepsilon}$ can be decomposed into its normal and tangential components, that is

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

and we can apply the respective Neumann or Dirichlet boundary condition on the hole before perform the final topological derivatives calculation.

3.1. **Neumann boundary condition on the hole.** By taking $\beta = 0$ in eq. (3.4), we have homogeneous Neumann boundary condition on the hole. In the present case, we have the following expansion for u_ε (see Appendix)

$$\begin{aligned} u_\varepsilon(\mathbf{x}) &= u(\mathbf{x}) + \frac{\varepsilon^2}{\|\mathbf{x}-\widehat{\mathbf{x}}\|^2}\nabla u(\widehat{\mathbf{x}})\cdot(\mathbf{x}-\widehat{\mathbf{x}}) \\ &+ \frac{\varepsilon^4}{\|\mathbf{x}-\widehat{\mathbf{x}}\|^4}\mathbf{S}(\mathbf{x}-\widehat{\mathbf{x}})\cdot(\mathbf{x}-\widehat{\mathbf{x}}) + \frac{\varepsilon^6}{\|\mathbf{x}-\widehat{\mathbf{x}}\|^6}(\mathbf{T}(\mathbf{x}-\widehat{\mathbf{x}}))(\mathbf{x}-\widehat{\mathbf{x}})\cdot(\mathbf{x}-\widehat{\mathbf{x}}) \\ &+ \varepsilon^2\widetilde{u}(\mathbf{x}) + \frac{\varepsilon^4}{\|\mathbf{x}-\widehat{\mathbf{x}}\|^2}\nabla\widetilde{u}(\widehat{\mathbf{x}})\cdot(\mathbf{x}-\widehat{\mathbf{x}}) + v_\varepsilon(\mathbf{x}) \, , \end{aligned} \tag{3.8}$$

where the second-order tensor $\mathbf{S}$ and the third-order tensor $\mathbf{T}$ are respectively given by

$$\mathbf{S} = \frac{1}{2}\nabla\nabla u(\widehat{\mathbf{x}}) \quad \text{and} \quad \mathbf{T} = \frac{1}{6}\nabla\nabla\nabla u(\widehat{\mathbf{x}}) \ . \tag{3.9}$$

In addition, v_ε is such that $|v_\varepsilon|_{H^1(\Omega_\varepsilon)} \le C\varepsilon^3$, with C independent of ε, and function $\widetilde{u}$ is solution of the following variational problem: find $\widetilde{u} \in \mathcal{V}$, such that

$$\int_\Omega \nabla\widetilde{u}\cdot\nabla\eta + \int_{\Gamma_N}\frac{\partial g_N}{\partial n}\eta = 0 \quad \forall \eta \in \mathcal{W} \ , \tag{3.10}$$

where the admissible functions set $\mathcal{V}$ and the admissible variations space $\mathcal{W}$ are defined, respectively, as

$$\mathcal{V} = \{\widetilde{u} \in H^1(\Omega) : \widetilde{u}|_{\Gamma_D} = -g_N\} \quad \text{and} \quad \mathcal{W} = \{\eta \in H^1(\Omega) : \eta|_{\Gamma_D} = 0\} , \tag{3.11}$$

and function g_N is given by

$$g_N(\mathbf{x}) = \nabla u\,(\widehat{\mathbf{x}}) \cdot \frac{\mathbf{x} - \widehat{\mathbf{x}}}{\|\mathbf{x} - \widehat{\mathbf{x}}\|^2} . \tag{3.12}$$

In addition, according to the variational problem (3.3) we observe that $\partial u_\varepsilon/\partial n|_{\partial\mathcal{H}_\varepsilon} = 0$, for $\beta = 0$. Therefore, the shape derivative of the cost functional reads

$$\frac{d}{d\varepsilon}\psi(\Omega_\varepsilon) = -\frac{1}{2}\int_{\partial\mathcal{H}_\varepsilon} \left(\frac{\partial u_\varepsilon}{\partial t}\right)^2 . \tag{3.13}$$

Considering the expansion (3.8) in (3.13) and after analytically solving the integral on the boundary of the hole $\partial\mathcal{H}_\varepsilon$, we obtain, from eqs. (2.3,2.4) and taking into account that function u is harmonic, the following results

$$D_T\psi = -\|\nabla u\,(\widehat{\mathbf{x}})\|^2 , \tag{3.14}$$

$$D_T^2\psi = \frac{1}{2}\det\nabla\nabla u\,(\widehat{\mathbf{x}}) - \nabla u\,(\widehat{\mathbf{x}}) \cdot \nabla\widetilde{u}\,(\widehat{\mathbf{x}}) , \tag{3.15}$$

with $f_1(\varepsilon) = \pi\varepsilon^2$ and $f_2(\varepsilon) = \pi\varepsilon^4$. Finally, the topological asymptotic expansion of the energy shape functional reads

$$\psi(\Omega_\varepsilon) = \psi(\Omega) - \pi\varepsilon^2\,\|\nabla u(\widehat{\mathbf{x}})\|^2 + \frac{1}{2}\pi\varepsilon^4\,(\det\nabla\nabla u(\widehat{\mathbf{x}}) - 2\nabla u(\widehat{\mathbf{x}}) \cdot \nabla\widetilde{u}(\widehat{\mathbf{x}})) + o(\varepsilon^4) . \tag{3.16}$$

3.2. **Dirichlet boundary condition on the hole.** By taking $\beta = 1$ in eq. (3.4), we have homogeneous Dirichlet boundary condition on the hole. Let $\mathcal{G}\,(\mathbf{x})$ be solution of the following auxiliary variational problem: find $\mathcal{G} \in \mathcal{V}$, such that

$$\int_\Omega \nabla\mathcal{G} \cdot \nabla\eta + \int_{\Gamma_N} h_D\eta = 0 \quad \forall\eta \in \mathcal{W} , \tag{3.17}$$

where the admissible functions set $\mathcal{V}$ and the admissible variations space $\mathcal{W}$ are defined, respectively, as

$$\mathcal{V} = \{\mathcal{G} \in H^1(\Omega) : \mathcal{G}|_{\Gamma_D} = g_D\} \quad \text{and} \quad \mathcal{W} = \{\eta \in H^1(\Omega) : \eta|_{\Gamma_D} = 0\} , \tag{3.18}$$

and functions g_D and h_D are respectively given by

$$g_D(\mathbf{x}) = -\frac{1}{2\pi}\log\|\mathbf{x} - \widehat{\mathbf{x}}\| \quad \text{and} \quad h_D(\mathbf{x}) = \frac{1}{2\pi}\frac{\mathbf{x} - \widehat{\mathbf{x}}}{\|\mathbf{x} - \widehat{\mathbf{x}}\|^2} \cdot \mathbf{n} . \tag{3.19}$$

Then, we have the following expansion for u_ε (see Appendix A)

$$\begin{aligned} u_\varepsilon\,(\mathbf{x}) &= u\,(\mathbf{x}) - \alpha(\varepsilon)u\,(\widehat{\mathbf{x}})\left(\frac{1}{2\pi}\log\|\mathbf{x}-\widehat{\mathbf{x}}\| + \mathcal{G}\,(\mathbf{x})\right) \\ &- \frac{\varepsilon^2}{\|\mathbf{x}-\widehat{\mathbf{x}}\|^2}\left(\nabla u\,(\widehat{\mathbf{x}}) - \alpha(\varepsilon)u\,(\widehat{\mathbf{x}})\,\nabla\mathcal{G}\,(\widehat{\mathbf{x}})\right) \cdot (\mathbf{x} - \widehat{\mathbf{x}}) + \widetilde{u}_\varepsilon\,(\mathbf{x}) , \end{aligned} \tag{3.20}$$

where $\widetilde{u}_\varepsilon$ is such that $|\widetilde{u}_\varepsilon|_{H^1(\Omega_\varepsilon)} \leq C\varepsilon^2$, with C independent of ε, and $\alpha(\varepsilon)$ is given by (A.20). In addition, according to the variational problem (3.3) we observe that $\partial u_\varepsilon/\partial t|_{\partial\mathcal{H}_\varepsilon} = 0$, for $\beta = 1$. Therefore, the shape derivative of the cost functional reads

$$\frac{d}{d\varepsilon}\psi(\Omega_\varepsilon) = \frac{1}{2}\int_{\partial\mathcal{H}_\varepsilon} \left(\frac{\partial u_\varepsilon}{\partial n}\right)^2 . \tag{3.21}$$

Considering the expansion (3.20) in (3.21) and after analytically solving the integral on the boundary of the hole $\partial\mathcal{H}_\varepsilon$, we obtain, from eqs. (2.3,2.4), the following results

$$D_T\psi = u(\widehat{\mathbf{x}})^2 \ , \text{ with } f_1(\varepsilon) = -\frac{\pi}{\log\varepsilon + 2\pi\mathcal{G}(\widehat{\mathbf{x}})} \ , \tag{3.22}$$

$$D_T^2\psi = \|\nabla u(\widehat{\mathbf{x}})\|^2 \ , \text{ with } f_2(\varepsilon) = \pi\varepsilon^2 \ . \tag{3.23}$$

Finally, the topological asymptotic expansion of the energy shape functional reads

$$\psi(\Omega_\varepsilon) = \psi(\Omega) - \frac{\pi}{\log\varepsilon + 2\pi\mathcal{G}(\widehat{\mathbf{x}})} u(\widehat{\mathbf{x}})^2 + \pi\varepsilon^2 \|\nabla u(\widehat{\mathbf{x}})\|^2 + o(\varepsilon^2) \ . \tag{3.24}$$

It is important to mention that the *domain truncation technique* used in [5] introduces an artificial parameter R in the first order topological derivative, which cannot be explicitly calculated. Thus, the simplification $f_1(\varepsilon) \approx -\pi/\log\varepsilon$ has been widely adopted in the literature, leading to the following expansion (see, for instance, [7])

$$\psi(\Omega_\varepsilon) = \psi(\Omega) - \frac{\pi}{\log\varepsilon} u(\widehat{\mathbf{x}})^2 + o(\frac{-1}{\log\varepsilon}) \ . \tag{3.25}$$

The consequence of this approximation on the topological asymptotic expansion can be found in [5].

4. Examples

Now, we shall study, through some examples, the influence of the second order topological derivative in the complete topological asymptotic expansion. Therefore, we will compute the estimate for the shape functional taking into account only the first order topological derivative

$$\psi(\Omega_\varepsilon) \approx \psi(\Omega) + f_1(\varepsilon) D_T\psi \ . \tag{4.1}$$

Then we will compare it with the estimate considering both first and second order topological derivatives, that is

$$\psi(\Omega_\varepsilon) \approx \psi(\Omega) + f_1(\varepsilon) D_T\psi + f_2(\varepsilon) D_T^2\psi \ . \tag{4.2}$$

Thus, let us consider the Laplace problem defined in the domain $\Omega_\varepsilon = \Omega \backslash \overline{\mathcal{H}}_\varepsilon$, where, for $\varepsilon < \rho$, we have

$$\Omega = \left\{ \mathbf{x} \in \mathbb{R}^2 : \|\mathbf{x}\| < \rho, \ \rho \in \mathbb{R} \right\} \quad \text{and} \quad \mathcal{H}_\varepsilon = \left\{ \mathbf{x} \in \mathbb{R}^2 : \|\mathbf{x}\| < \varepsilon, \ \varepsilon \in \mathbb{R} \right\} \ . \tag{4.3}$$

4.1. **Example A: the Neumann's case.**

By taking $q = -(\cos\theta + \cos 2\theta)$, the problem formulation associated to the perturbed domain Ω_ε reads: find u_ε, such that

$$\left\{ \begin{array}{rcll} \Delta u_\varepsilon &=& 0 & \text{in } \Omega_\varepsilon \\ \frac{\partial u_\varepsilon}{\partial n} &=& \cos\theta + \cos 2\theta & \text{on } \partial\Omega \\ \frac{\partial u_\varepsilon}{\partial n} &=& 0 & \text{on } \partial\mathcal{H}_\varepsilon \end{array} \right. \ . \tag{4.4}$$

The analytical solution is given, up to an arbitrary additive constant, by

$$u_\varepsilon(r,\theta) = \frac{\rho^2}{r}\left(\frac{r^2+\varepsilon^2}{\rho^2-\varepsilon^2}\right)\cos\theta + \frac{\rho^3}{2r^2}\left(\frac{r^4+\varepsilon^4}{\rho^4-\varepsilon^4}\right)\cos 2\theta \ . \tag{4.5}$$

Thus, the shape functional is given by

$$\psi(\Omega_\varepsilon) = -\pi\frac{\rho^2}{2}\left(\frac{\rho^2+\varepsilon^2}{\rho^2-\varepsilon^2} + \frac{1}{2}\frac{\rho^4+\varepsilon^4}{\rho^4-\varepsilon^4}\right) \ , \tag{4.6}$$

which can by expanded in power of ε, such that

$$\psi(\Omega_\varepsilon) = -\frac{3}{4}\pi\rho^2 - \pi\varepsilon^2 - \pi\varepsilon^4\frac{3}{2\rho^2} + o\left(\varepsilon^4\right) \ . \tag{4.7}$$

Taking into account the influence associated to term $\widetilde{u}(\mathbf{x})$ in the topological asymptotic expansion, we have

$$\begin{aligned}\psi(\Omega_\varepsilon) &\approx \psi(\Omega) - \pi\varepsilon^2 \|\nabla u(\widehat{\mathbf{x}})\|^2 + \frac{1}{2}\pi\varepsilon^4 \left(\det \nabla\nabla u(\widehat{\mathbf{x}}) - 2\nabla u(\widehat{\mathbf{x}}) \cdot \nabla\widetilde{u}(\widehat{\mathbf{x}})\right) \\ &= -\frac{3}{4}\pi\rho^2 - \pi\varepsilon^2 - \pi\varepsilon^4 \left(\frac{1}{2\rho^2} + \frac{1}{\rho^2}\right) , \end{aligned} \tag{4.8}$$

that coincides with the above expansion in power of ε, where $\widetilde{u}(\mathbf{x})$ is solution of (3.10), that is

$$\widetilde{u}(r,\theta) = -\frac{1}{\rho^2} r\cos\theta \;\Rightarrow\; \nabla u(\widehat{\mathbf{x}}) \cdot \nabla\widetilde{u}(\widehat{\mathbf{x}}) = -\frac{1}{\rho^2} . \tag{4.9}$$

On the other hand, disregarding the influence of term associated to $\widetilde{u}(\mathbf{x})$, we obtain

$$\begin{aligned}\psi(\Omega_\varepsilon) &\approx \psi(\Omega) - \pi\varepsilon^2 \|\nabla u(\widehat{\mathbf{x}})\|^2 + \frac{1}{2}\pi\varepsilon^4 \det \nabla\nabla u(\widehat{\mathbf{x}}) \\ &= -\frac{3}{4}\pi\rho^2 - \pi\varepsilon^2 - \frac{1}{2\rho^2}\pi\varepsilon^4 . \end{aligned} \tag{4.10}$$

In particular, by taking $\rho = 1$, the first order topological asymptotic expansion is given by

$$\psi(\Omega_\varepsilon) \approx -\frac{3}{4}\pi - \pi\varepsilon^2 , \tag{4.11}$$

the second order topological asymptotic expansion, disregarding the influence of term associated to $\widetilde{u}(\mathbf{x})$, results in

$$\psi(\Omega_\varepsilon) \approx -\frac{3}{4}\pi - \pi\varepsilon^2 - \frac{1}{2}\pi\varepsilon^4 , \tag{4.12}$$

and, finally, taking into account the influence of term associated to $\widetilde{u}(\mathbf{x})$, we have

$$\psi(\Omega_\varepsilon) \approx -\frac{3\pi}{4} - \pi\varepsilon^2 - \frac{3}{2}\pi\varepsilon^4 . \tag{4.13}$$

These results are compared in the graphic of fig. 1, where we observe that the approximation associated only with higher-order gradients of solution u eq. (4.12) gives a better estimation for the shape functional than the first order topological asymptotic eq. (4.11). We also observe that the approximation taking into account the term associated to $\widetilde{u}$ eq. (4.13) plays an important role in the expansion for large values of ε.

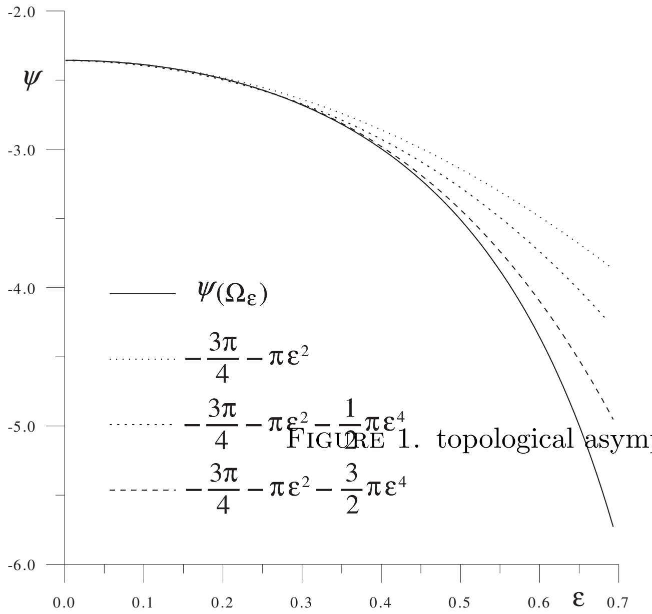

FIGURE 1. topological asymptotic expansions: the Neumann's case.

4.2. **Example B: the Dirichlet's case.** Now, let us consider $\varphi = \gamma + \cos\theta$. Then, the problem formulation associated to the perturbed domain Ω_ε reads: find u_ε, such that

$$\left\{\begin{array}{rcll} \Delta u_\varepsilon & = & 0 & \text{in} \quad \Omega_\varepsilon \\ u_\varepsilon & = & \gamma + \cos\theta & \text{on} \quad \partial\Omega \\ u_\varepsilon & = & 0 & \text{on} \quad \partial\mathcal{H}_\varepsilon \end{array}\right. , \tag{4.14}$$

whose analytical solution is given by

$$u_\varepsilon(r,\theta) = \gamma\frac{\log(r/\varepsilon)}{\log(\rho/\varepsilon)} + \frac{\rho}{r}\left(\frac{r^2-\varepsilon^2}{\rho^2-\varepsilon^2}\right)\cos\theta \ . \tag{4.15}$$

Thus, the shape functional results in

$$\psi\left(\Omega_\varepsilon\right) = \frac{\pi}{\log(\rho/\varepsilon)}\gamma^2 + \frac{\pi}{2}\frac{\rho^2+\varepsilon^2}{\rho^2-\varepsilon^2} \ . \tag{4.16}$$

which can by expanded in power of ε, such that

$$\psi\left(\Omega_\varepsilon\right) = \frac{\pi}{2} + \frac{\pi}{\log(\rho/\varepsilon)}\gamma^2 + \pi\varepsilon^2\frac{1}{\rho^2} + o\left(\varepsilon^2\right) \ . \tag{4.17}$$

Taking into account the final formulas for the first and second order topological derivatives, we have

$$D_T\psi = \gamma^2 \ , \ \text{with } f_1(\varepsilon) = \frac{\pi}{\log(\rho/\varepsilon)} \ , \tag{4.18}$$

$$D_T^2\psi = \frac{1}{\rho^2} \ , \ \text{with } f_2(\varepsilon) = \pi\varepsilon^2 \ . \tag{4.19}$$

that coincides with the above expansion in power of ε, where $\mathcal{G}(\mathbf{x})$ is solution of (3.17), that is

$$\left\{\begin{array}{rcll} \Delta\mathcal{G} & = & 0 & \text{in} \quad \Omega \\ \mathcal{G} & = & -\frac{1}{2\pi}\log\rho & \text{on} \quad \partial\Omega \end{array}\right. \quad \Rightarrow \ \mathcal{G}(\widehat{\mathbf{x}}) = -\frac{1}{2\pi}\log\rho \ . \tag{4.20}$$

Now, we shall study the influence of the second order topological derivative in the topological asymptotic expansion. Therefore, choosing $\rho = \gamma = 1$, we can compute the estimate for the shape functional taking into account only the first order topological derivative

$$\psi(\Omega_\varepsilon) \approx \frac{\pi}{2} - \frac{\pi}{\log\varepsilon} \ . \tag{4.21}$$

Then we will compare it with the estimate considering both first and second order topological derivatives, that is

$$\psi(\Omega_\varepsilon) \approx \frac{\pi}{2} - \frac{\pi}{\log\varepsilon} + \pi\varepsilon^2 \ . \tag{4.22}$$

These results are compared in the graphic of fig. 2, where we observe that the second order topological derivative is an important correction factor in the expansion for large values of ε.

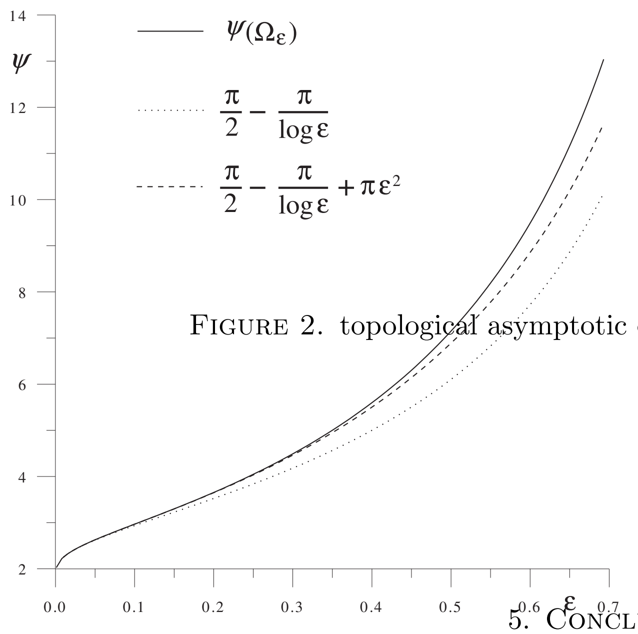

FIGURE 2. topological asymptotic expansions: the Dirichlet's case.

5. CONCLUSIONS

In this work, we have obtained a close formula for the topological asymptotic expansion considering first and second order approximations. In particular, we have applied the topological-shape sensitivity method to calculate first and second order topological derivatives for the total potential energy associated to the Laplace equation in two-dimensional domain, which was perturbed through the insertion of a small hole with homogeneous Neumann or Dirichlet boundary conditions.

From these results we observe that, in the Neumann's case, the second order topological derivative depends explicitly on higher-order gradients of the solution u associated to the non-perturbed problem and also implicitly through the function $\widetilde{u}$, solution of an auxiliary boundary value problem. On the other hand, in the Dirichlet's case, we have observed that the first order topological derivative depends explicitly on the solution u as well as implicitly on the solution $\mathcal{G}$ of an auxiliary problem. However, in this last case, the second order topological derivative depends only explicitly on the solution u. In addition, the incorporation of the terms associated to $\widetilde{u}$ (Neumann's case) and $\mathcal{G}$ (Dirichlet's case) in the calculation of the topological asymptotic expansion for all points $\widehat{\mathbf{x}} \in \Omega$ is impracticable from the computational point of view, since they depend on the point $\widehat{\mathbf{x}} \in \Omega$ where the hole is positioned, as can be seen in eqs. (3.10,3.17). Thus, it is natural to use the optimality condition given by the first order topological derivative ($D_T\psi$) to chose the points where the holes should be introduced. Once these points are fixed, then we can compute the complete topological asymptotic expansion until order two, considering both explicit and implicit terms, only for that points.

Then, we have presented two simple examples showing the influence of the second order approximation term in the topological asymptotic expansion. From these examples, we have observed that the estimate considering the second order topological derivative remains precise even for very large holes, allowing to deal with perturbations of finite size. This feature is very important in the development of topology optimization and reconstruction algorithms.

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Appendix A. Asymptotic Analysis

In this section we present the derivation of the asymptotic expansions (eqs. 3.8 and 3.20) adopted to calculate the final expressions for the first and second order topological derivatives. For a rigorous justification of the asymptotic expantions of the solution u_ε, the reader may refer to the work [1].

A.1. **Neumann boundary condition on the hole.** In order to obtain the derivation of the asymptotic formula given by eq. (3.8), let us propose the following expansion for u_ε

$$u_\varepsilon(\mathbf{x}) = u(\mathbf{x}) + w(\mathbf{x}/\varepsilon) + \widetilde{u}_\varepsilon(\mathbf{x}) \ , \tag{A.1}$$

where w is the solution of the following exterior problem: find w such that

$$\left\{ \begin{array}{rcll} \Delta w &=& 0 & \text{in} \quad \mathbb{R}^2 \backslash \overline{\mathcal{H}}_1 \\ w &\to& 0 & \text{at} \quad \infty \\ \frac{\partial w}{\partial n} &=& -(\varepsilon \nabla u(\widehat{\mathbf{x}}) - 2\varepsilon^2 \mathbf{S}\mathbf{n} + 3\varepsilon^3 (\mathbf{T}\mathbf{n})\mathbf{n}) \cdot \mathbf{n} & \text{on} \quad \partial \mathcal{H}_1 \end{array} \right. \tag{A.2}$$

with $\mathbf{S}$ and $\mathbf{T}$ given by eq. (3.9). The above boundary value problem has an explicit solution, namely

$$\begin{aligned} w\left(\mathbf{x}/\varepsilon\right) &= \frac{\varepsilon^2}{\|\mathbf{x}-\widehat{\mathbf{x}}\|^2}\nabla u(\widehat{\mathbf{x}})\cdot(\mathbf{x}-\widehat{\mathbf{x}}) \\ &+ \frac{\varepsilon^4}{\|\mathbf{x}-\widehat{\mathbf{x}}\|^4}\mathbf{S}(\mathbf{x}-\widehat{\mathbf{x}})\cdot(\mathbf{x}-\widehat{\mathbf{x}}) \\ &+ \frac{\varepsilon^6}{\|\mathbf{x}-\widehat{\mathbf{x}}\|^6}(\mathbf{T}(\mathbf{x}-\widehat{\mathbf{x}}))(\mathbf{x}-\widehat{\mathbf{x}})\cdot(\mathbf{x}-\widehat{\mathbf{x}}). \end{aligned} \tag{A.3}$$

In addition, the remaining term of expansion (A.1) solves: find $\widetilde{u}_\varepsilon$ such that

$$\left\{\begin{array}{rcll} \Delta\widetilde{u}_\varepsilon &=& 0 & \text{in} \quad \Omega_\varepsilon \\ \widetilde{u}_\varepsilon &=& -w\left(\mathbf{x}/\varepsilon\right) & \text{on} \quad \Gamma_D \\ \frac{\partial\widetilde{u}_\varepsilon}{\partial n} &=& -\frac{\partial}{\partial n}w\left(\mathbf{x}/\varepsilon\right) & \text{on} \quad \Gamma_N \\ \frac{\partial\widetilde{u}_\varepsilon}{\partial n} &=& \varepsilon^3 D^4 u(\boldsymbol{\xi}(\mathbf{x}))\,(\mathbf{n})^4 & \text{on} \quad \partial\mathcal{H}_\varepsilon \end{array}\right. \tag{A.4}$$

where $\boldsymbol{\xi}(\mathbf{x})$ is an intermediate point between $\mathbf{x}$ and $\widehat{\mathbf{x}}$. Likewise, we assume that $\widetilde{u}_\varepsilon$, solution of the boundary value problem (A.4), satisfies the expansion

$$\widetilde{u}_\varepsilon\left(\mathbf{x}\right) = \varepsilon^2\widetilde{u}\left(\mathbf{x}\right) + \widetilde{w}\left(\mathbf{x}/\varepsilon\right) + v_\varepsilon\left(\mathbf{x}\right)\ , \tag{A.5}$$

where $\widetilde{w}$ is the solution of the following exterior problem: find $\widetilde{w}$ such that

$$\left\{\begin{array}{rcll} \Delta\widetilde{w} &=& 0 & \text{in} \quad \mathbb{R}^2\backslash\overline{\mathcal{H}}_1 \\ \widetilde{w} &\to& 0 & \text{at} \quad \infty \\ \frac{\partial\widetilde{w}}{\partial n} &=& -\varepsilon^3\nabla\widetilde{u}\left(\widehat{\mathbf{x}}\right)\cdot\mathbf{n} & \text{on} \quad \partial\mathcal{H}_1 \end{array}\right. \tag{A.6}$$

which also has explicit solution, that is

$$\widetilde{w}\left(\mathbf{x}/\varepsilon\right) = \frac{\varepsilon^4}{\|\mathbf{x}-\widehat{\mathbf{x}}\|^2}\nabla\widetilde{u}\left(\widehat{\mathbf{x}}\right)\cdot(\mathbf{x}-\widehat{\mathbf{x}})\ . \tag{A.7}$$

By introducing the notation,

$$g\left(\mathbf{x}\right) = \frac{1}{\|\mathbf{x}-\widehat{\mathbf{x}}\|^2}\nabla u(\widehat{\mathbf{x}})\cdot(\mathbf{x}-\widehat{\mathbf{x}})\ , \tag{A.8}$$

$$h\left(\mathbf{x}\right) = \frac{1}{\|\mathbf{x}-\widehat{\mathbf{x}}\|^4}\mathbf{S}(\mathbf{x}-\widehat{\mathbf{x}})\cdot(\mathbf{x}-\widehat{\mathbf{x}})\ , \tag{A.9}$$

$$p\left(\mathbf{x}\right) = \frac{1}{\|\mathbf{x}-\widehat{\mathbf{x}}\|^6}(\mathbf{T}(\mathbf{x}-\widehat{\mathbf{x}}))(\mathbf{x}-\widehat{\mathbf{x}})\cdot(\mathbf{x}-\widehat{\mathbf{x}})\ , \tag{A.10}$$

we have

$$w\left(\mathbf{x}/\varepsilon\right) = \varepsilon^2 g\left(\mathbf{x}\right) + \varepsilon^4 h\left(\mathbf{x}\right) + \varepsilon^6 p\left(\mathbf{x}\right)\ . \tag{A.11}$$

Thus, function $\widetilde{u}$ satisfies a boundary value problem stated as: find $\widetilde{u}$ such that

$$\left\{\begin{array}{rcll} \Delta\widetilde{u} &=& 0 & \text{in} \quad \Omega \\ \widetilde{u} &=& -g\left(\mathbf{x}\right) & \text{on} \quad \Gamma_D \\ \frac{\partial\widetilde{u}}{\partial n} &=& -\frac{\partial}{\partial n}g\left(\mathbf{x}\right) & \text{on} \quad \Gamma_N \end{array}\right. \tag{A.12}$$

and the remaining term of expansion (A.5) solves: find v_ε such that

$$\left\{\begin{array}{rcll} \Delta v_\varepsilon &=& 0 & \text{in} \quad \Omega_\varepsilon \\ v_\varepsilon &=& -\widetilde{w}(\mathbf{x}/\varepsilon) - \varepsilon^4 h(\mathbf{x}) - \varepsilon^6 p(\mathbf{x}) & \text{on} \quad \Gamma_D \\ \frac{\partial v_\varepsilon}{\partial n} &=& -\frac{\partial}{\partial n}(\widetilde{w}(\mathbf{x}/\varepsilon) + \varepsilon^4 h(\mathbf{x}) + \varepsilon^6 p(\mathbf{x})) & \text{on} \quad \Gamma_N \\ \frac{\partial v_\varepsilon}{\partial n} &=& \varepsilon^3(D^4 u(\boldsymbol{\xi}(\mathbf{x}))(\mathbf{n})^4 - D^2\widetilde{u}(\boldsymbol{\zeta}(\mathbf{x}))(\mathbf{n})^2) & \text{on} \quad \partial\mathcal{H}_\varepsilon \end{array}\right. \tag{A.13}$$

where $\boldsymbol{\zeta}(\mathbf{x})$ is an intermediate point between $\mathbf{x}$ and $\widehat{\mathbf{x}}$. Finally, we have the following expansion for solution u_ε,

$$u_\varepsilon\left(\mathbf{x}\right) = u\left(\mathbf{x}\right) + w(\mathbf{x}/\varepsilon) + \varepsilon^2\widetilde{u}(\mathbf{x}) + \widetilde{w}(\mathbf{x}/\varepsilon) + v_\varepsilon(\mathbf{x})\,, \tag{A.14}$$

where v_ε satisfies the estimate $|v_\varepsilon|_{H^1(\Omega_\varepsilon)} \leq C\varepsilon^3$, with constant C independent of ε [2, 4, 10].

A.2. **Dirichlet boundary condition on the hole.** Following the original ideas introduced in [10], we present the derivation of the asymptotic formula given by (3.20). Initially, we consider that u_ε can be decomposed as

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

where the function v_ε is defined as

$$v_\varepsilon(\mathbf{x}) = \alpha(\varepsilon) u(\widehat{\mathbf{x}}) G(\mathbf{x}) \ , \tag{A.16}$$

and G is solution of the following boundary value problem: find G, such that

$$\left\{ \begin{array}{rcll} -\Delta G & = & \delta(\mathbf{x}-\widehat{\mathbf{x}}) & \text{in} \quad \Omega \\ G & = & 0 & \text{on} \quad \Gamma_D \\ \frac{\partial G}{\partial n} & = & 0 & \text{on} \quad \Gamma_N \end{array} \right. \tag{A.17}$$

which admits the following representation in the neighborhood of the point $\widehat{\mathbf{x}} \in \Omega$

$$G(\mathbf{x}) = -\left(\frac{1}{2\pi}\log\|\mathbf{x}-\widehat{\mathbf{x}}\| + \mathcal{G}(\mathbf{x})\right), \quad \text{with} \quad \|\mathbf{x}-\widehat{\mathbf{x}}\| \to 0 \ , \tag{A.18}$$

where $\mathcal{G}$ is harmonic in $\overline{\Omega}$ and must compensate the discrepancy on $\partial\Omega$ introduced by the above representation, that is, $\mathcal{G}$ is solution of the auxiliary boundary value problem: find $\mathcal{G}$, such that

$$\left\{ \begin{array}{rcll} \Delta \mathcal{G} & = & 0 & \text{in} \quad \Omega \\ \mathcal{G} & = & -\frac{1}{2\pi}\log\|\mathbf{x}-\widehat{\mathbf{x}}\| & \text{on} \quad \Gamma_D \\ \frac{\partial \mathcal{G}}{\partial n} & = & -\frac{1}{2\pi}\frac{\mathbf{x}-\widehat{\mathbf{x}}}{\|\mathbf{x}-\widehat{\mathbf{x}}\|^2}\cdot\mathbf{n} & \text{on} \quad \Gamma_N \end{array} \right. \tag{A.19}$$

The choice

$$\alpha(\varepsilon) = \left(\frac{1}{2\pi}\log\varepsilon + \mathcal{G}(\widehat{\mathbf{x}})\right)^{-1} , \tag{A.20}$$

guarantees the decay at infinity of the remaining terms. Furthermore, function w is solution of the exterior problem: find w, such that

$$\left\{ \begin{array}{rcll} \Delta w & = & 0 & \text{in} \quad \mathbb{R}^2 \backslash \overline{\mathcal{H}_1} \\ w & \to & 0 & \text{as} \quad \|\mathbf{y}\| \to \infty \\ w & = & \varepsilon\left(\nabla u(\widehat{\mathbf{x}}) - \alpha(\varepsilon) u(\widehat{\mathbf{x}}) \nabla\mathcal{G}(\widehat{\mathbf{x}})\right)\cdot\mathbf{n} & \text{on} \quad \partial\mathcal{H}_1 \end{array} \right. \tag{A.21}$$

which has a close solution, given by

$$w(\mathbf{x}/\varepsilon) = -\frac{\varepsilon^2}{\|\mathbf{x}-\widehat{\mathbf{x}}\|^2}\left(\nabla u(\widehat{\mathbf{x}}) - \alpha(\varepsilon) u(\widehat{\mathbf{x}}) \nabla\mathcal{G}(\widehat{\mathbf{x}})\right)\cdot(\mathbf{x}-\widehat{\mathbf{x}}) \ . \tag{A.22}$$

Finally, function $\widetilde{u}_\varepsilon$ is constructed in such a way that compensate the discrepancy introduced by the previous terms of the expansion for u_ε, thus it solves: find $\widetilde{u}_\varepsilon$, such that

$$\left\{ \begin{array}{rcll} \Delta \widetilde{u}_\varepsilon & = & 0 & \text{in} \quad \Omega_\varepsilon \\ \widetilde{u}_\varepsilon & = & -w(\mathbf{x}/\varepsilon) & \text{on} \quad \Gamma_D \\ \frac{\partial \widetilde{u}_\varepsilon}{\partial n} & = & -\frac{\partial}{\partial n} w(\mathbf{x}/\varepsilon) & \text{on} \quad \Gamma_N \\ \widetilde{u}_\varepsilon & = & -\varepsilon^2 (D^2 u(\boldsymbol{\xi}(\mathbf{x})) - \alpha(\varepsilon) u(\widehat{\mathbf{x}}) D^2\mathcal{G}(\boldsymbol{\zeta}(\mathbf{x})))(\mathbf{n})^2 & \text{on} \quad \partial\mathcal{H}_\varepsilon \end{array} \right. \tag{A.23}$$

where $\boldsymbol{\xi}(\mathbf{x})$ and $\boldsymbol{\zeta}(\mathbf{x})$ are intermediate points between $\mathbf{x}$ and $\widehat{\mathbf{x}}$. In fact, this remaining term admits the following estimate $|\widetilde{u}_\varepsilon|_{H^1(\Omega_\varepsilon)} \leq C\varepsilon^2$, with C independent of ε [2, 4, 10].

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