Chapter 1
Introduction

The topological derivative is defined as the first term of the asymptotic expansion of a given shape functional with respect to a small parameter that measures the size of singular domain perturbations, such as holes, inclusions, source-terms, and cracks [75]. This relatively new concept has applications in many different fields such as shape and topology optimization, inverse problems, imaging processing, multi-scale material design, and mechanical modeling including damage and fracture evolution phenomena. For an account on the theoretical development and applications of the topological derivative method, see the series of review papers [79–81] and references therein.

The topological derivative method has been specifically designed to deal with topology optimization. It has been introduced by Sokołowski and Żochowski in 1999 through the fundamental paper [88] to fill a gap in the existing literature at that time. Actually, the idea was to give a precise (mathematical) answer to the following important question: What happens when a hole is nucleated? The answer to this question is not trivial at all, since singularities may appear once a hole is nucleated. Therefore, in order to deal with this problem, asymptotic analysis in singularly perturbed geometrical domains is needed. In this book, the topological derivative method is presented through some selected examples in a simple and pedagogical manner by using a direct approach based on calculus of variations combined with *matched* [54] and *compound* [67] asymptotic analysis of solution to boundary value problems. In addition, the topological derivative is used in numerical method of shape optimization including applications in the context of compliance structural topology optimization and topology design of compliant mechanisms. Finally, some exercises are proposed at the end of each chapter for the readers' convenience.

This chapter is organized as follows. In Sect. 1.1 the topological derivative concept is introduced and five simple examples are presented in order to fix the ideas. In Sect. 1.2 the adjoint sensitivity method is presented through the Lagrangian formalism and an example in the context of control theory with PDE constraint

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is fully developed. Finally, the content of the book is described in detail through Sect. 1.3.

1.1 The Topological Derivative Concept

Let us consider an open and bounded domain $\Omega \subset \mathbb{R}^d$, with $d \geq 2$, which is subject to a non-smooth perturbation confined in a small region $\omega_\varepsilon(\widehat{x}) = \widehat{x} + \varepsilon\omega$ of size ε, such that $\overline{\omega_\varepsilon} \subset \Omega$, where $\widehat{x}$ is an arbitrary point of Ω and ω represents a fixed domain in $\mathbb{R}^d$. See sketch in Fig. 1.1. We introduce a *characteristic function* $x \mapsto \chi(x)$, $x \in \mathbb{R}^d$, associated with the unperturbed domain, namely $\chi := \mathbb{1}_\Omega$, such that

$$|\Omega| = \int_{\mathbb{R}^d} \chi, \tag{1.1}$$

where $|\Omega|$ is the *Lebesgue measure* of Ω. Then, we define a characteristic function associated with the topologically perturbed domain of the form $x \mapsto \chi_\varepsilon(\widehat{x}; x)$, $x \in \mathbb{R}^d$. In the case of a perforation, for example, $\chi_\varepsilon(\widehat{x}) := \mathbb{1}_\Omega - \mathbb{1}_{\omega_\varepsilon(\widehat{x})}$ and the perturbed domain is obtained as $\Omega_\varepsilon = \Omega \setminus \overline{\omega_\varepsilon}$. Finally, we assume that a given shape functional $\psi(\chi_\varepsilon(\widehat{x}))$, associated with the topologically perturbed domain, admits a *topological asymptotic expansion* of the form

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) + f(\varepsilon)\mathscr{T}(\widehat{x}) + \mathscr{R}(\varepsilon), \tag{1.2}$$

where $\psi(\chi)$ is the shape functional associated with the reference (unperturbed) domain, $f(\varepsilon)$ is a positive *first order correction function*, which decreases monotonically such that $f(\varepsilon) \to 0$ with $\varepsilon \to 0$, and $\mathscr{R}(\varepsilon)$ is the *remainder term*, that is, $\mathscr{R}(\varepsilon)/f(\varepsilon) \to 0$ with $\varepsilon \to 0$. The function $\widehat{x} \mapsto \mathscr{T}(\widehat{x})$ is recognized as the *topological derivative* of ψ at $\widehat{x}$. Therefore, the product $f(\varepsilon)\mathscr{T}(\widehat{x})$ represents a first order correction over $\psi(\chi)$ to approximate $\psi(\chi_\varepsilon(\widehat{x}))$. In addition, after rearranging (1.2), we have

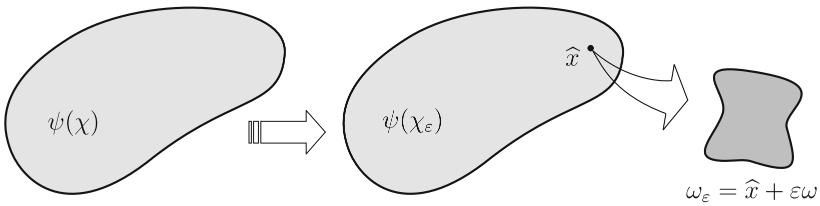

Fig. 1.1 The topological derivative concept

$$\frac{\psi(\chi_\varepsilon(\widehat{x})) - \psi(\chi)}{f(\varepsilon)} = \mathscr{T}(\widehat{x}) + \frac{\mathscr{R}(\varepsilon)}{f(\varepsilon)}. \tag{1.3}$$

The limit passage $\varepsilon \to 0$ in the above expression leads to the general definition for the *topological derivative*, namely

$$\mathscr{T}(\widehat{x}) := \lim_{\varepsilon \to 0} \frac{\psi(\chi_\varepsilon(\widehat{x})) - \psi(\chi)}{f(\varepsilon)}. \tag{1.4}$$

Assuming that the functional $\psi(\chi_\varepsilon(\widehat{x}))$ admits the topological asymptotic expansion (1.2), the applicability of this expansion depends on the procedure of evaluation of the unknown function $\widehat{x} \mapsto \mathscr{T}(\widehat{x})$. In particular, we are looking for an appropriate form for the topological derivative which can be used in numerical method of shape/topology optimization, for instance. Therefore, we need some properties of the shape functional and its asymptotic expansion in order to apply a simple method for evaluation of the topological derivative, which are:

1. The shape functional $\varepsilon \mapsto j(\varepsilon) := \psi(\chi_\varepsilon(\widehat{x}))$ is continuous with respect to a *topological perturbation* at 0^+, i.e., $\lim_{\varepsilon \to 0^+} f(\varepsilon) = 0$.
2. The limit passage $\lim_{\varepsilon \to 0^+} \mathscr{R}(\varepsilon)/f(\varepsilon) = 0$ holds true.

Note that since we are dealing with singular domain perturbations, in general the limit in (1.4) cannot be trivially evaluated. It is the case of topological perturbations consisting of nucleation of holes, for instance, where the shape functionals $\psi(\chi)$ and $\psi(\chi_\varepsilon(\widehat{x}))$ are associated with topologically different domains (see Remark 1.2 below). Therefore, we need to develop $\psi(\chi_\varepsilon(\widehat{x}))$ asymptotically with respect to the small parameter ε and collect the leading terms of the resulting expansion. How to construct a topological asymptotic expansion of the form (1.4) is, in fact, the main concern of this monograph.

Remark 1.1 The notion of topological derivative extends the conventional definition of derivative [34, 35], allowing to deal with functionals depending on a *geometrical domain* subjected to singular topology changes. According to (1.4), the analogy between the topological *derivative* and the corresponding expressions for a conventional derivative is to be noted.

Remark 1.2 We say *topological* derivative because we are dealing with topological changes in a geometrical domain given by, e.g., nucleation of holes. In fact, the *Euler-Poincaré characteristic* of any oriented surface Ω is given by the quantity

$$C(\Omega) = V - E + F, \tag{1.5}$$

where V, E, and F are respectively the numbers of vertices, edges, and faces of a given polyhedron produced by an arbitrary triangularization of Ω. In particular, if two distinct surfaces Ω_1 and Ω_2 have the same Euler-Poincaré characteristic, namely $C(\Omega_1) = C(\Omega_2)$, then they are topologically equivalents. Let us now suppose that we remove one single triangle from Ω_2, then Ω_1 and Ω_2 have the

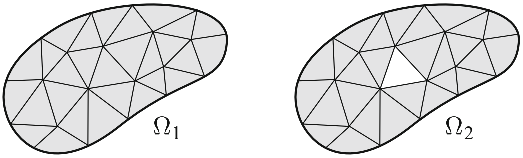

Fig. 1.2 An example of the Euler-Poincaré characteristic

same numbers of vertices and edges, but Ω_2 has one face less than Ω_1, so that $C(\Omega_2) = C(\Omega_1) - 1$. See sketch in Fig. 1.2. Therefore, according to the Euler-Poincaré characteristic, after creating a hole in Ω_2 by removing a triangle, its topology actually changes.

In order to fix these ideas let us present five (very) simple examples. The first one concerns the topological derivative of the volume of a given geometrical domain. The second and third examples deal with singular and regular domain perturbations, respectively. The fourth example shows that the topological derivative obeys the basic rules of differential calculus. Finally, the last example deals with the topological derivative of the energy shape functional associated with a second order ordinary differential equation into one spatial dimension.

Example 1.1 Let us consider a very simple functional given by the area of the domain $\Omega \subset \mathbb{R}^2$, that is

$$\psi(\chi) := |\Omega| = \int_\Omega 1, \tag{1.6}$$

with Ω subject to the class of topological perturbations produced by the nucleation of circular holes, namely $\omega_\varepsilon = B_\varepsilon(\widehat{x}) := \{x \in \Omega : \|x - \widehat{x}\| < \varepsilon\}$, for $\widehat{x} \in \Omega$. The expansion with respect to ε can be trivially obtained as follows:

$$\psi(\chi_\varepsilon(\widehat{x})) = |\Omega_\varepsilon(\widehat{x})| = \int_\Omega 1 - \int_{B_\varepsilon} 1 = \psi(\chi) - \pi\varepsilon^2. \tag{1.7}$$

Therefore, function $f(\varepsilon)$ and the topological derivative $\mathscr{T}(\widehat{x})$ are immediately identified as

$$f(\varepsilon) = \pi\varepsilon^2 \quad \text{and} \quad \mathscr{T}(\widehat{x}) = -1 \quad \forall\, \widehat{x} \in \Omega. \tag{1.8}$$

In this particular case $\mathscr{T}(\widehat{x})$ is independent of $\widehat{x}$, and the rightmost term of the topological asymptotic expansion is equal to zero.

Example 1.2 We consider a shape functional of the form

$$\psi(\chi_\varepsilon(\widehat{x})) := \int_{\Omega_\varepsilon(\widehat{x})} g(x), \tag{1.9}$$

where $\chi_\varepsilon(\widehat{x}) = \mathbb{1}_\Omega - \mathbb{1}_{B_\varepsilon(\widehat{x})}$ and $\Omega_\varepsilon(\widehat{x}) = \Omega \setminus \overline{B_\varepsilon(\widehat{x})}$, with $B_\varepsilon(\widehat{x})$ used to denote a ball of radius ε and center at $\widehat{x} \in \Omega$. The function $g : \mathbb{R}^2 \mapsto \mathbb{R}$ is assumed to be

Lipschitz continuous in $B_\varepsilon(\widehat{x})$, i.e., $|g(x) - g(\widehat{x})| \leq C\|x - \widehat{x}\| \ \forall x \in B_\varepsilon(\widehat{x})$, where $C \geq 0$ is the Lipschitz constant. In the context of problems governed by partial differential equations, this property comes out from the interior *elliptic regularity* of solutions. Note that this is the case regarding singular domain perturbation (see Remark 1.2). Since $|B_\varepsilon| \to 0$ with $\varepsilon \to 0$, we have

$$\psi(\chi) := \int_\Omega g(x). \tag{1.10}$$

We are looking for an asymptotic expansion of the form (1.2), namely

$$\begin{aligned}
\psi(\chi_\varepsilon(\widehat{x})) &= \int_{\Omega_\varepsilon} g(x) + \int_{B_\varepsilon} g(x) - \int_{B_\varepsilon} g(x) \\
&= \int_\Omega g(x) - \int_{B_\varepsilon} g(x) + \int_{B_\varepsilon} g(\widehat{x}) - \int_{B_\varepsilon} g(\widehat{x}) \\
&= \psi(\chi) - \pi\varepsilon^2 g(\widehat{x}) + \mathscr{E}(\varepsilon).
\end{aligned} \tag{1.11}$$

The remainder $\mathscr{E}(\varepsilon)$ is defined as

$$\mathscr{E}(\varepsilon) = -\int_{B_\varepsilon} (g(x) - g(\widehat{x})), \tag{1.12}$$

which can be bounded as follows:

$$|\mathscr{E}(\varepsilon)| = \left| \int_{B_\varepsilon} (g(x) - g(\widehat{x})) \right| \leq \int_{B_\varepsilon} |g(x) - g(\widehat{x})| \leq C_1 \int_{B_\varepsilon} \|x - \widehat{x}\|, \tag{1.13}$$

since function g is assumed to be locally Lipschitz continuous. From a polar coordinate system (r, θ) centered at the point $\widehat{x} \in \Omega$, there is

$$\int_{B_\varepsilon} \|x - \widehat{x}\| = \int_0^{2\pi} \left(\int_0^\varepsilon (r)\, r dr \right) d\theta = \frac{2\pi}{3}\varepsilon^3, \tag{1.14}$$

where we have used the fact that $\|x - \widehat{x}\| = r$. Finally, by combining the last two results, the following estimate for the remainder $\mathscr{E}(\varepsilon)$ holds true:

$$|\mathscr{E}(\varepsilon)| \leq C_2 \varepsilon^3, \tag{1.15}$$

with constant C_2 independent of the small parameter ε. Therefore, the term $-g(\widehat{x})$ is identified as the topological derivative of the shape functional ψ evaluated at the point $\widehat{x} \in \Omega$, namely

$$\mathscr{T}(\widehat{x}) = -g(\widehat{x}) \quad \forall\, \widehat{x} \in \Omega. \tag{1.16}$$

In addition, function $f(\varepsilon) = \pi\varepsilon^2$. Finally, the remainder $\mathscr{E}(\varepsilon)$ is of order $O(\varepsilon^3)$.

Example 1.3 Now, let us consider a shape functional defined as follows:

$$\psi(\chi_\varepsilon(\widehat{x})) := \int_\Omega g_\varepsilon(x), \tag{1.17}$$

where $\chi_\varepsilon(\widehat{x}) = \mathbb{1}_\Omega - (1-\gamma)\mathbb{1}_{B_\varepsilon(\widehat{x})}$. The function $g_\varepsilon = \chi_\varepsilon g$ is defined as

$$g_\varepsilon(x) := \begin{cases} g(x) \text{ if } x \in \Omega \setminus \overline{B_\varepsilon(\widehat{x})}, \\ \gamma g(x) \text{ if } x \in B_\varepsilon(\widehat{x}), \end{cases} \tag{1.18}$$

where $\gamma \in \mathbb{R}$ is the contrast and $B_\varepsilon(\widehat{x})$ is a ball of radius ε and center at $\widehat{x} \in \Omega$. In addition, function $g : \mathbb{R}^2 \mapsto \mathbb{R}$ is assumed to be Lipschitz continuous in B_ε (see Example 1.2). Observe that this case corresponds to regular domain perturbation where the shape functional depends on characteristic function of small sets. Since $|B_\varepsilon| \to 0$ with $\varepsilon \to 0$, there is

$$\psi(\chi) := \int_\Omega g(x). \tag{1.19}$$

We are looking for an asymptotic expansion of the form (1.2), that is

$$\begin{aligned} \psi(\chi_\varepsilon(\widehat{x})) &= \int_{\Omega\setminus\overline{B_\varepsilon}} g(x) + \int_{B_\varepsilon} \gamma g(x) \\ &= \int_{\Omega\setminus\overline{B_\varepsilon}} g(x) + \int_{B_\varepsilon} \gamma g(x) \pm \int_{B_\varepsilon} g(x) \\ &= \int_\Omega g(x) - (1-\gamma)\int_{B_\varepsilon} g(x) \pm (1-\gamma)\int_{B_\varepsilon} g(\widehat{x}) \\ &= \psi(\chi) - \pi\varepsilon^2(1-\gamma)g(\widehat{x}) + o(\varepsilon^2), \end{aligned} \tag{1.20}$$

where we have used the notation $0 = \pm(\cdot) = (\cdot) - (\cdot)$. From the above expansion, we can identify the term $-(1-\gamma)g(\widehat{x})$ as the topological derivative of the shape functional ψ evaluated at the point $\widehat{x} \in \Omega$, namely

$$\mathcal{T}(\widehat{x}) = -(1-\gamma)g(\widehat{x}) \quad \forall\, \widehat{x} \in \Omega, \tag{1.21}$$

with $f(\varepsilon) = \pi\varepsilon^2$. Note that the limit passage $\gamma \to 0$ leads to $\mathcal{T}(\widehat{x}) = -g(\widehat{x})$. It means that the former example can be seen as the singular limit of this one.

Example 1.4 We consider two functions g_1 and g_2 assumed to be Lipschitz continuous in B_ε. Let us return to the case regarding singularly perturbed geometrical domains of the form $\Omega_\varepsilon(\widehat{x}) = \Omega \setminus \overline{B_\varepsilon(\widehat{x})}$. According to Example 1.2, we have

$$\psi_i(\chi) := \int_\Omega g_i(x) \quad \Rightarrow \quad \mathcal{T}_i(\widehat{x}) = -g_i(\widehat{x}), \quad \text{for} \quad i = 1, 2. \tag{1.22}$$

Then, the topological derivative of the product between $\psi_1(\chi)$ and $\psi_2(\chi)$, namely

$$\psi(\chi) := \psi_1(\chi)\psi_2(\chi), \tag{1.23}$$

is given by

$$\begin{aligned} \mathscr{T}(\widehat{x}) &= \mathscr{T}_1(\widehat{x})\psi_2(\chi) + \mathscr{T}_2(\widehat{x})\psi_1(\chi) \\ &= -g_1(\widehat{x}) \int_\Omega g_2(x) - g_2(\widehat{x}) \int_\Omega g_1(x). \end{aligned} \tag{1.24}$$

Finally, the topological derivative of the quotient between $\psi_1(\chi)$ and $\psi_2(\chi)$, that is

$$\psi(\chi) := \frac{\psi_1(\chi)}{\psi_2(\chi)}, \tag{1.25}$$

can be written as

$$\begin{aligned} \mathscr{T}(\widehat{x}) &= \frac{\mathscr{T}_1(\widehat{x})\psi_2(\chi) - \mathscr{T}_2(\widehat{x})\psi_1(\chi)}{\psi_2(\chi)^2} \\ &= \frac{g_2(\widehat{x}) \displaystyle\int_\Omega g_1(x) - g_1(\widehat{x}) \int_\Omega g_2(x)}{\psi_2(\chi)^2}. \end{aligned} \tag{1.26}$$

Example 1.5 In this last example we consider that the problem is governed by a second order ordinary differential equation. The associated energy shape functional is defined as

$$\psi(\chi_\varepsilon(\widehat{x})) := \int_0^1 \gamma_\varepsilon |u_\varepsilon'|^2. \tag{1.27}$$

Note that in this case $\Omega = (0, 1)$, $\chi_\varepsilon(\widehat{x}) = \mathbb{1}_\Omega - (1-\gamma)\mathbb{1}_{\omega_\varepsilon(\widehat{x})}$, with $\omega_\varepsilon(\widehat{x}) = (0, \varepsilon)$, and $\gamma_\varepsilon := \chi_\varepsilon$. It means that $\gamma_\varepsilon(x) = \gamma$ for $0 < x \leq \varepsilon$ and $\gamma_\varepsilon(x) = 1$ for $\varepsilon < x < 1$, where $\gamma \in \mathbb{R}^+$, i.e., $0 < \gamma < \infty$, is the contrast on the material property. In addition, u_ε is the solution of the following boundary value problem

$$(\gamma_\varepsilon(x)u_\varepsilon'(x))' = 0, \qquad 0 < x < 1, \tag{1.28}$$

endowed with boundary conditions of the form

$$u_\varepsilon(0) = 0 \qquad \text{and} \qquad u_\varepsilon'(1) = 1, \tag{1.29}$$

and transmission conditions arising naturally from the variational formulation of problem (1.28), that is

$$u_\varepsilon(\varepsilon^+) = u_\varepsilon(\varepsilon^-) \qquad \text{and} \qquad u_\varepsilon'(\varepsilon^+) = \gamma u_\varepsilon'(\varepsilon^-). \tag{1.30}$$

The above boundary value problem admits an explicit solution of the form

$$\begin{cases} u_\varepsilon(x) = \frac{x}{\gamma}, & 0 < x \leq \varepsilon, \\ u_\varepsilon(x) = x + \varepsilon\frac{1-\gamma}{\gamma}, & \varepsilon < x < 1. \end{cases} \tag{1.31}$$

Since $|B_\varepsilon| \to 0$ with $\varepsilon \to 0$, there is

$$\psi(\chi) := \int_0^1 |u'|^2, \tag{1.32}$$

where u is the solution to the above boundary value problem for $\varepsilon = 0$, that is

$$u(x) = x. \tag{1.33}$$

We are looking for an asymptotic expansion of the form (1.2), namely

$$\psi(\chi_\varepsilon(\widehat{x})) = \int_0^\varepsilon \gamma|u'_\varepsilon|^2 + \int_\varepsilon^1 |u'_\varepsilon|^2 = 1 + \varepsilon\frac{1-\gamma}{\gamma} = \psi(\chi) + \varepsilon\frac{1-\gamma}{\gamma}. \tag{1.34}$$

Therefore, the associated topological derivative is given by

$$\mathcal{T}(\widehat{x}) = \frac{1-\gamma}{\gamma} \quad \forall\, \widehat{x} \in (0, 1), \tag{1.35}$$

with $f(\varepsilon) = \varepsilon$. Note that in the limit case $\gamma \to \infty$, $\mathcal{T}(\widehat{x}) = -1\ \forall \widehat{x} \in (0, 1)$. On the other hand, for $\gamma \to 0$ the topological derivative is not defined. This is in fact an intrinsic property of one-dimensional problems, which in general do not admit singular domain perturbations [18].

1.2 Evaluation of the Topological Derivative

Before concluding this chapter, let us present a last example concerning the simplest case of topological perturbation with PDEs constraints. It is given by a perturbation on the right-hand side of a boundary value problem, which can be seen as a simple variant of the case associated with singularly perturbed geometrical domains. We start by introducing the adjoint sensitivity method. Then we state an auxiliary result which will be used here, in this section, and later in the book. Finally, we present a simple example in the context of optimal control problem.

1.2.1 Adjoint Sensitivity Method

Let us introduce the *adjoint sensitivity method* through the *augmented Lagrangian formalism*. We consider the following minimization problem:

$$\underset{\Omega \in X}{\text{Minimize}} \; \mathscr{J}(u), \tag{1.36}$$

where X represents the set of admissible geometrical domains and $\mathscr{J} : \mathscr{U} \mapsto \mathbb{R}$ is the shape functional to be minimized with respect to the design variable domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$. In addition, function u is the solution of the abstract variational problem of the form

$$u \in \mathscr{U} \;:\; a(u, \eta) = \ell(\eta) \quad \forall \eta \in \mathscr{V}, \tag{1.37}$$

where $\mathscr{U} \in U$ is the set of admissible functions and $\mathscr{V} \in V$ is the space of admissible variations, with U and V used to denote linear Hilbert subspaces, respectively. Finally, $a : U \times V \mapsto \mathbb{R}$ is a bilinear form and $\ell : V \mapsto \mathbb{R}$ is a linear functional. From these elements, we can introduce the associated augmented Lagrangian, which consists in imposing the constraint of the minimization problem (1.36), given by the state equation (1.37), through Lagrangian multiplier, namely

$$\mathscr{L}(u, v) = \mathscr{J}(u) + a(u, v) - \ell(v) \quad \forall (u, v) \in \mathscr{U} \times \mathscr{V}. \tag{1.38}$$

Let us evaluate the *Fréchet derivative* of the Lagrangian function $\mathscr{L}(u, v)$ with respect to $v \in \mathscr{V}$ in the direction $\eta \in \mathscr{V}$, thus

$$\langle D_v \mathscr{L}(u, v), \eta \rangle = a(u, \eta) - \ell(\eta). \tag{1.39}$$

After applying the first order optimality condition in the above result we obtain

$$u \in \mathscr{U} \;:\; a(u, \eta) = \ell(\eta) \quad \forall \eta \in \mathscr{V}, \tag{1.40}$$

which is actually the state equation (1.37). On the other hand, the *Fréchet derivative* of the Lagrangian function $\mathscr{L}(u, v)$ with respect to $u \in \mathscr{U}$ in the direction $\varphi \in \mathscr{V}$ can be written as

$$\langle D_u \mathscr{L}(u, v), \varphi \rangle = \langle D_u \mathscr{J}(u), \varphi \rangle + a(\varphi, v). \tag{1.41}$$

Let us apply again the first order optimality condition, leading to the associated *adjoint equation*, namely

$$v \in \mathscr{V} \;:\; a(\varphi, v) = -\langle D_u \mathscr{J}(u), \varphi \rangle \quad \forall \varphi \in \mathscr{V}. \tag{1.42}$$

Note that, from (1.42), the adjoint state v always lives in the space $\mathscr{V}$ and appears on the second argument of the bilinear form. Finally, from the above discussion, the adjoint variable v can also be interpreted as the Lagrangian multiplier used to impose the state equation (1.37) as a constraint in the optimization problem (1.36).

1.2.2 Auxiliary Result

Now, let us state an auxiliary result which will be used in the next section in particular and in the whole book in general.

Lemma 1.1 *Let Ω be an open and bounded domain in $\mathbb{R}^2$ and let B_ε be a ball of radius ε, such that $\overline{B_\varepsilon} \subset \Omega$. Then, for a function $\varphi \in H^1(\Omega)$, the following estimate holds true*

$$\|\varphi\|_{L^2(B_\varepsilon)} \leq C\varepsilon^\delta \|\varphi\|_{H^1(\Omega)}, \tag{1.43}$$

with $0 < \delta < 1$ and the constant C independent of the small parameter ε.

Proof From the *Hölder inequality*, we have

$$\begin{aligned}
\|\varphi\|_{L^2(B_\varepsilon)} &\leq \left[\left(\int_{B_\varepsilon} (|\varphi|^2)^p \right)^{\frac{1}{p}} \left(\int_{B_\varepsilon} 1^q \right)^{\frac{1}{q}} \right]^{\frac{1}{2}} \\
&= \pi^{1/2q} \varepsilon^{1/q} \left(\int_{B_\varepsilon} |\varphi|^{2p} \right)^{\frac{1}{2p}} \\
&= \pi^{1/2q} \varepsilon^{1/q} \|\varphi\|_{L^{2p}(B_\varepsilon)} \\
&\leq C\varepsilon^{1/q} \|\varphi\|_{L^{2p}(\Omega)},
\end{aligned} \tag{1.44}$$

for all $p, q \in (1, +\infty)$ satisfying $1/p + 1/q = 1$. By choosing $q > 1$ and p accordingly, the *Sobolev embedding theorem* [33, Ch. IV, §8, Sec. 1.2, p. 139] implies $H^1(\Omega) \subset L^{2p}(\Omega)$ with a continuous embedding. Therefore, we have

$$\|\varphi\|_{L^2(B_\varepsilon)} \leq C\varepsilon^{1/q} \|\varphi\|_{H^1(\Omega)}, \tag{1.45}$$

which leads to the result by setting $\delta = 1/q$. □

1.2.3 A Simple Example

Let us consider the tracking type *shape functional*, which is useful in many practical applications including optimal control problem and imaging processing, namely

$$\psi(\chi) := \mathscr{J}(u) = \frac{1}{2}\int_\Omega |u - z_d|^2, \tag{1.46}$$

where $\Omega \subset \mathbb{R}^2$ and z_d is the target function, assumed to be smooth. The scalar field u is the solution of the following variation problem:

$$u \in H_0^1(\Omega) : \int_\Omega \nabla u \cdot \nabla \eta = \int_\Omega b\eta \quad \forall \eta \in H_0^1(\Omega), \tag{1.47}$$

where the source-term b is assumed to be locally Lipschitz continuous (see Example 1.2). According to Sect. 1.2.1, the associated augmented Lagrangian functional is given by

$$\mathscr{L}(u, v) = \frac{1}{2}\int_\Omega |u - z_d|^2 + \int_\Omega \nabla u \cdot \nabla v - \int_\Omega bv, \tag{1.48}$$

and the *adjoint equation* reads

$$\begin{aligned} v \in H_0^1(\Omega) : \int_\Omega \nabla \eta \cdot \nabla v &= -\langle D_u \mathscr{J}(u), \eta \rangle \\ &= -\int_\Omega (u - z_d)\eta \quad \forall \eta \in H_0^1(\Omega). \end{aligned} \tag{1.49}$$

Note that by symmetry of the above bilinear form, in this particular case the left-hand sides of (1.47) and (1.49) are precisely the same but for the appropriate test functions only. The only difference is their right-hand sides. This property simplifies enormously the numerics.

Now, we introduce a topological perturbation on the source term of the form $b_\varepsilon = \chi_\varepsilon b$, with $\chi_\varepsilon(\widehat{x}) = \mathbb{1}_\Omega - (1-\gamma)\mathbb{1}_{B_\varepsilon(\widehat{x})}$. Therefore, the perturbed source term b_ε can be written as

$$b_\varepsilon(x) := \begin{cases} b(x) \text{ if } x \in \Omega \setminus B_\varepsilon(\widehat{x}), \\ \gamma b(x) \text{ if } x \in B_\varepsilon(\widehat{x}), \end{cases} \tag{1.50}$$

with $\gamma \in \mathbb{R}$ used to denote the contrast in the source term. From these elements, the shape functional associated with the perturbed problem is defined as

$$\psi(\chi_\varepsilon) := \mathscr{J}_\varepsilon(u_\varepsilon) = \frac{1}{2}\int_\Omega |u_\varepsilon - z_d|^2. \tag{1.51}$$

The scalar function u_ε is the solution of the following variation problem

$$u_\varepsilon \in H_0^1(\Omega) : \int_\Omega \nabla u_\varepsilon \cdot \nabla \eta = \int_\Omega b_\varepsilon \eta \quad \forall \eta \in H_0^1(\Omega). \tag{1.52}$$

From the definition of the source term given by (1.50), we have $b_\varepsilon = b$ in $\Omega \setminus \overline{B_\varepsilon}$ and $b_\varepsilon = \gamma b$ in B_ε. Therefore, the state equation (1.52) can be rewritten as

$$\begin{aligned} u_\varepsilon \in H_0^1(\Omega) : \int_\Omega \nabla u_\varepsilon \cdot \nabla \eta &= \int_{\Omega\setminus\overline{B_\varepsilon}} b\eta + \gamma \int_{B_\varepsilon} b\eta \pm \int_{B_\varepsilon} b\eta \\ &= \int_\Omega b\eta - (1-\gamma) \int_{B_\varepsilon} b\eta \quad \forall \eta \in H_0^1(\Omega). \end{aligned} \tag{1.53}$$

Now, let us subtract (1.47) from (1.53) to obtain

$$\int_\Omega \nabla(u_\varepsilon - u) \cdot \nabla \eta = -(1-\gamma) \int_{B_\varepsilon} b\eta \quad \forall \eta \in H_0^1(\Omega). \tag{1.54}$$

Thus, the existence of the topological derivative of the problem we are dealing with is ensured by the following result:

Lemma 1.2 *Let u and u_ε be the solutions of* (1.47) *and* (1.52)*, respectively. Then the following estimate holds true*

$$\|u_\varepsilon - u\|_{H^1(\Omega)} \leq C\varepsilon^{1+\delta}, \tag{1.55}$$

with constant C independent of the small parameter ε and $0 < \delta < 1$.

Proof By taking $\eta = u_\varepsilon - u$ as test function in (1.54), we obtain the following equality:

$$\int_\Omega \|\nabla(u_\varepsilon - u)\|^2 = -(1-\gamma) \int_{B_\varepsilon} b(u_\varepsilon - u). \tag{1.56}$$

From the *Cauchy-Schwarz inequality*, we have

$$\begin{aligned} \int_\Omega \|\nabla(u_\varepsilon - u)\|^2 &\leq C_1 \|b\|_{L^2(B_\varepsilon)} \|u_\varepsilon - u\|_{L^2(B_\varepsilon)} \\ &\leq C_2 \varepsilon^{1+\delta} \|u_\varepsilon - u\|_{H^1(\Omega)}, \end{aligned}$$

where we have used Lemma 1.1 and the continuity of function b at the point $\widehat{x} \in \Omega$. Finally, from the *coercivity* of the bilinear form on the left-hand side of the above inequality, namely

$$c\|u_\varepsilon - u\|_{H^1(\Omega)}^2 \leq \int_\Omega \|\nabla(u_\varepsilon - u)\|^2, \tag{1.57}$$

we conclude that

$$c\|u_\varepsilon - u\|_{H^1(\Omega)} \leq C_2 \varepsilon^{1+\delta}, \tag{1.58}$$

which leads to the result with $C = C_2/c$ and $0 < \delta < 1$. □

The variation of the shape functional can be obtained by subtracting (1.46) from (1.51), that is

$$\mathscr{J}_\varepsilon(u_\varepsilon) - \mathscr{J}(u) = \int_\Omega (u - z_d)(u_\varepsilon - u) + \mathscr{E}_1(\varepsilon), \tag{1.59}$$

with the remainder $\mathscr{E}_1(\varepsilon)$ bounded as

$$\begin{aligned} \mathscr{E}_1(\varepsilon) &= \frac{1}{2}\int_\Omega |u_\varepsilon - u|^2, \\ |\mathscr{E}_1(\varepsilon)| &\leq C\|u_\varepsilon - u\|^2_{L^2(\Omega)} \\ &\leq C\|u_\varepsilon - u\|^2_{H^1(\Omega)} = o(\varepsilon^2), \end{aligned} \tag{1.60}$$

where we have used Lemma 1.2. Now, let us set $\eta = u_\varepsilon - u$ as test function in the adjoint Eq. (1.49) and $\eta = v$ as test function in (1.54) to obtain

$$\int_\Omega \nabla v \cdot \nabla(u_\varepsilon - u) = -\int_\Omega (u - z_d)(u_\varepsilon - u), \tag{1.61}$$

$$\int_\Omega \nabla v \cdot \nabla(u_\varepsilon - u) = -(1-\gamma)\int_{B_\varepsilon} bv. \tag{1.62}$$

From the above results we conclude that

$$\int_\Omega (u - z_d)(u_\varepsilon - u) = (1-\gamma)\int_{B_\varepsilon} bv. \tag{1.63}$$

Therefore, the variation (1.59) can be rewritten as an integral concentrated in the ball B_ε, namely

$$\begin{aligned} \mathscr{J}_\varepsilon(u_\varepsilon) - \mathscr{J}(u) &= (1-\gamma)\int_{B_\varepsilon} bv + \mathscr{E}_1(\varepsilon) \\ &= (1-\gamma)\pi\varepsilon^2 b(\widehat{x})v(\widehat{x}) + \mathscr{E}_1(\varepsilon) + \mathscr{E}_2(\varepsilon). \end{aligned} \tag{1.64}$$

The remainder $\mathscr{E}_2(\varepsilon)$ can be bounded as follows:

$$\mathscr{E}_2(\varepsilon) = (1-\gamma)\int_{B_\varepsilon} (bv - b(\widehat{x})v(\widehat{x})),$$

$$|\mathscr{E}_2(\varepsilon)| \leq C_1 \int_{B_\varepsilon} \|x - \widehat{x}\| \leq C_2 \varepsilon^3 = o(\varepsilon^2), \tag{1.65}$$

where we have used the interior elliptic regularity of function u. See Example 1.2. Finally, the topological asymptotic expansion of the shape functional is given by

$$\mathscr{J}_\varepsilon(u_\varepsilon) = \mathscr{J}(u) + \pi\varepsilon^2(1-\gamma)b(\widehat{x})v(\widehat{x}) + o(\varepsilon^2). \tag{1.66}$$

From the above expansion, we can identify function $f(\varepsilon) = \pi\varepsilon^2$ and the final formula for the topological derivative, namely

$$\mathscr{T}(\widehat{x}) = (1-\gamma)b(\widehat{x})v(\widehat{x}) \quad \forall\, \widehat{x} \in \Omega, \tag{1.67}$$

where u and v are the solutions of the direct (1.47) and adjoint (1.49) problems, respectively, both defined in the original (unperturbed) domain Ω.

Remark 1.3 This kind of topological perturbation, that is, on the right-hand side of the governing boundary value problem, can be treated by using simple arguments from the analysis. Actually, we have just used the fact that the boundary value problems are well posed. Therefore, in this context, it is possible to consider certain classes of nonlinear problems. However, this book is dedicated to the case of topological perturbations on the main part of the differential operator, such as the ones produced by the nucleation of holes. The mathematical analysis of this class of topological perturbations is much more involved, which is deeply discussed in Chap. 4 and also in [75], for instance.

1.3 Organization of the Book

In this chapter the topological derivative concept has been introduced, together with some selected examples. Note that the small parameter governing the asymptotic analysis represents the size of the topological domain perturbation, allowing for the nucleation of small inclusions or voids in a numerical procedure of optimization regarding shape/topology changes on the material properties distribution or in the geometrical domain itself, respectively. Therefore, this new concept in shape optimization has applications in many different fields such as topology optimization, inverse problems, imaging processing, multi-scale material design, and mechanical modeling including damage and fracture evolution phenomena. The central idea of this work is to introduce the topological derivative method from both theoretical and practical point of views, so that it is oriented to the readers interested in the mathematical aspects of the topological asymptotic analysis as well as in the applications of the topological derivative method in computational mechanics. In particular, this book is presented as follows:

- The topological asymptotic analysis of the energy shape functional associated with the Poisson's equation, with respect to singular domain perturbations, is formally developed through Chap. 2. In particular, we consider singular perturbations produced by the nucleation of small circular holes endowed with homogeneous Neumann, Dirichlet, or Robin boundary conditions.
- Chapter 3 deals with the topological derivative of the so-called compliance shape functional associated with a modified Helmholtz problem, with respect to the nucleation of a small circular inclusion with different material property from the background. By taking into account the boundary value problem we are dealing with, three different cases are considered: (1) perturbation on its right-hand side, (2) perturbation on the lower order term, and (3) perturbation on the higher order term. The existence of the associated topological derivatives is ensured by using simple arguments from the analysis. Then, we derive their explicit forms which are useful for numerical methods in shape/topology optimization. Finally, a priori estimates for the remainders left in the topological asymptotic expansions are rigorously obtained, which are used to justify the obtained results.
- The domain decomposition technique combined with the Steklov–Poincaré pseudo-differential boundary operator is presented in Chap. 4. The main idea is introduced in the context of coupled elliptic boundary value problems. Then, the same framework is used for deriving the topological asymptotic expansion of a tracking-type shape functional with respect to singular domain perturbations produced by the nucleation of small circular holes endowed with homogeneous Neumann boundary condition. The resulting asymptotic method allows for obtaining sharp a priori estimates for the remainders, so that it can be seen as a rigorous mathematical justification for the derivations presented in the former chapters.
- In Chap. 5 a topology optimization algorithm based on the topological derivative concept combined with a level-set domain representation method is presented. The model problem is governed by the elasticity system into two spatial dimensions. The topological asymptotic expansion of a tracking-type shape functional, associated with the nucleation of a small circular inclusion endowed with different material property from the background, is rigorously derived. Finally, the obtained theoretical result is used as a steepest-descent direction in the optimization process, which is applied in the context of compliance structural topology optimization and topology design of compliant mechanisms.
- Some useful basic results of tensor calculus are included in Appendix A for the readers' convenience. In particular, inner, vector, and tensor products are defined. In addition, gradient, divergence, and curl formulae, together with some integral theorems, are presented. Finally, some useful decompositions in curvilinear, polar, and spherical coordinate systems are provided.

1.4 Exercises

1. Repeat Example 1.2 by considering $g : \mathbb{R}^3 \mapsto \mathbb{R}$.
2. Let us consider one more term in the topological asymptotic expansion of the form

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) + f(\varepsilon)\mathscr{T}(\widehat{x}) + f_2(\varepsilon)\mathscr{T}^2(\widehat{x}) + o(f_2(\varepsilon)),$$

where $f_2(\varepsilon)$ is such that

$$\lim_{\varepsilon\to 0}\frac{f_2(\varepsilon)}{f(\varepsilon)} = 0.$$

Then, quantities $\mathscr{T}(\widehat{x})$ and $\mathscr{T}^2(\widehat{x})$ represent the first and *second order topological derivatives* of ψ, respectively. Assume that function $g(x)$ in Example 1.3 is of class $C^2(\Omega)$, with its second order gradient Lipschitz continuous in B_ε, namely $\exists\, C \geq 0 : \|\nabla\nabla g(x) - \nabla\nabla g(\widehat{x})\| \leq C\|x - \widehat{x}\|\ \forall x \in B_\varepsilon$, where $B_\varepsilon(\widehat{x})$ is used to denote a ball of radius ε and center at $\widehat{x} \in \Omega \subset \mathbb{R}^2$. Show that the topological asymptotic expansion of the functional $\psi(\chi_\varepsilon(\widehat{x}))$ is given by

$$\psi(\chi_\varepsilon(\widehat{x})) = \psi(\chi) - (1-\gamma)\pi\varepsilon^2 g(\widehat{x}) - \frac{1-\gamma}{8}\pi\varepsilon^4 \Delta g(\widehat{x}) + o(\varepsilon^4).$$

3. From the definition for the topological asymptotic expansion given by (1.2), show the results presented in Example 1.4.
4. Repeat Example 1.5 by considering the following conditions:

$$-u''(x) = 1 \quad \text{for} \quad 0 < x < 1 \quad \text{and} \quad u(0) = u'(1) = 0.$$

5. By taking into account the example presented in Sect. 1.2.3:

   (a) Replace the shape functional (1.46) by the total potential energy associated with the variational problem (1.47), namely

   $$\psi(\chi) := \mathscr{J}(u) = \frac{1}{2}\int_\Omega \|\nabla u\|^2 - \int_\Omega bu.$$

   Then compute its topological derivative by repeating the same derivations as presented in Sect. 1.2.3.

   (b) Take the total potential energy defined in a disk B_1 of unit radius and center at the origin. By setting $b = 1$ as source term, consider as topological perturbation the particular case given by (1.50), namely $b_\varepsilon(x) = 1$ if $x \in B_1 \setminus \overline{B_\varepsilon}$ and $b_\varepsilon(x) = \gamma$ if $x \in B_\varepsilon$, where B_ε is a disk of radius ε and center at the origin. From these elements, develop the topologically perturbed counter part of the total potential energy given by $\psi(\chi_\varepsilon)$ in power of ε around the origin. Finally, compare the obtained result with the one previously derived.