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Topological Derivatives of Shape Functionals. Part I: Theory in Singularly Perturbed Geometrical Domains

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Abstract

Mathematical analysis and numerical solutions of problems with unknown shapes or geometrical domains is a challenging and rich research field in the modern theory of the calculus of variations, partial differential equations, differential geometry as well as in numerical analysis. In this series of three review papers, we describe some aspects of numerical solution for problems with unknown shapes, which use tools of asymptotic analysis with respect to small defects or imperfections to obtain sensitivity of shape functionals. In classical numerical shape optimization, the boundary variation technique is used with a view to applying the gradient or Newton-type algorithms. Shape sensitivity analysis is performed by using the velocity method. In general, the continuous shape gradient and the symmetric part of the shape Hessian are discretized. Such an approach leads to local solutions, which satisfy the necessary optimality conditions in a class of domains defined in fact by the initial guess. A more general framework of shape sensitivity analysis is required when solving topology optimization problems. A possible approach is asymptotic analysis in singularly perturbed geometrical domains. In such a framework, approximations of solutions to boundary value problems (BVPs) in domains with small defects or imperfections are constructed, for instance by the method of matched asymptotic expansions. The approximate solutions are employed to evaluate shape functionals, and as a result topological derivatives of functionals are obtained. In particular, the topological derivative is defined as the first term (correction) 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, cavities, inclusions, defects, source terms and cracks. This new concept of variation has applications in many related fields, such as shape and topology optimization, inverse problems, image processing, multiscale material design and mechanical modeling involving damage and fracture evolution phenomena. In the first part of this review, the topological derivative concept is presented in detail within the framework of the domain decomposition technique. Such an approach is constructive, for example, for coupled models in multiphysics as well as for contact problems in elasticity. In the

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second and third parts, we describe the first- and second-order numerical methods of shape and topology optimization for elliptic BVPs, together with a portfolio of applications and numerical examples in all the above-mentioned areas.

1 Introduction

Shape and topology optimization is a broad field of modern research in pure (differential geometry) and applied mathematics, and in structural mechanics. In applied mathematics, it is a branch of the calculus of variations, partial differential equations and numerical methods. In structural mechanics, design and synthesis of metamaterials, fracture and damage modeling and structural optimization are areas of particular interest for shape and topology optimization techniques. Shape and topology optimization is also an efficient mathematical tool for numerical solution of inverse problems, involving defect identification for instance.

The problem of shape optimization is to minimize a shape functional over a family of admissible domains. The shape functional depends directly on geometrical domains and implicitly by means of solutions to the state equation defined in those domains. For example, in structural mechanics, the specific functional depends on solutions to elasticity BVPs defined in the domains of integration. From the mathematical point of view, the questions to address, as usual in the calculus of variations, are:

1. Existence of an optimal domain.
2. Necessary conditions for optimality, which can be obtained for differentiable shape functionals.
3. Convergence of numerical methods of solution of the shape optimization problem under study.

There is a vast literature on the subject; the representative sources are, for example, the monographs [1–5] on the theory and applications in mechanics of solids and fluids.

In general, we cannot expect the existence of a global solution to shape optimization problems, since shape functionals are nonconvex. Therefore, it makes sense to introduce generalized optimal solutions of shape optimization problems, for example, by means of the homogenization technique [6–8]. As a result, the optimization procedure leads to optimal microstructures and there appear subdomains of optimal domains filled with metamaterials. These methods are known in structural mechanics as the homogenization method [9] or the SIMP method [10].

In this review, we are interested in applications of asymptotic analysis tools and techniques to shape and topology optimization in singularly perturbed geometrical domains [11] (see also, e.g., [12–14]). Regarding the theoretical development of topological asymptotic analysis, see, for instance, [15–27]. An account of new developments in this

branch of shape optimization may be found in the book by Novotny and Sokołowski [28].

2 Classical Shape Optimization and Asymptotic Analysis Related to Topological Derivatives

Topological derivatives of shape functionals were introduced for elliptic BVPs quite recently. Instead of deformations of domains by diffeomorphism [1,3], asymptotic analysis in singularly perturbed geometrical domains is performed for the purposes of shape sensitivity analysis [11]. However, the approach based on deformations applies to all types of linear PDEs. In addition, the velocity method of shape sensitivity analysis is simpler compared to asymptotic analysis, but it has some drawbacks from the point of view of numerics. In general, there is a close relationship between the two approaches; the results obtained by the second approach can also be derived from the velocity method, under some local regularity assumptions on solutions of elliptic BVPs. In other words, the knowledge of shape gradients and shape Hessians leads to topological derivatives of, for example, energy functionals under additional regularity assumptions. Asymptotic analysis is performed in the original, unperturbed domains. It is worth mentioning that classical shape sensitivity analysis can be derived by using only asymptotic analysis tools. We present a general setting of asymptotic analysis in singularly perturbed geometrical domains in Appendices. In the main body of Part I, for simplicity, we restrict ourselves to the simple case of circular or ball-shaped voids.

As a result of asymptotic analysis, we obtain a function $\mathcal{T}(x)$, $x \in \Omega$, such that

$$J(\Omega_\varepsilon) = J(\Omega) + f(\varepsilon)\mathcal{T}(x) + o(f(\varepsilon))$$

for a given shape functional $\Omega \mapsto J(\Omega)$ and a given domain $\Omega \subset \mathbb{R}^d$, $d \geq 2$. Here, $\Omega_\varepsilon = \Omega \backslash \overline{\omega_\varepsilon}$, where $\overline{\omega_\varepsilon} \subset \Omega$ represents a singular domain perturbation of the size governed by a small parameter $\varepsilon \to 0$. Finally, $f(\varepsilon)$ is a positive function such that $f(\varepsilon) \to 0$ as $\varepsilon \to 0$. Therefore, the variation of the shape functional associated with the creation of a small singularity around $x \in \Omega$ is measured by the function $x \mapsto \mathcal{T}(x)$, which is called the topological derivative of the mapping $\Omega \mapsto J(\Omega)$.

In the first part of the review, we describe some qualitative results for the Laplacian and the elasticity system. In the second and third parts, we present, respectively, the first- and the second-order numerical methods of shape and topology optimization for elliptic BVPs, with many examples and numerical results. In order to fix ideas, let us give a very simple example.

Example 2.1 The notion of topological derivative extends the conventional definition of derivative to functionals depending on a *geometrical domain*, subjected to singular topology changes. The analogy between $\mathcal{T}(x)$ and the corresponding expressions for a conventional derivative should be noted. To illustrate the application of this concept, let us consider the very simple functional

$$J(\Omega) := |\Omega| = \int_\Omega 1, \tag{1}$$

with $\Omega \subset \mathbb{R}^2$ subject to the class of topological perturbations given by the nucleation of circular holes, namely $\omega_\varepsilon = B_\varepsilon(\widehat{x}) := \{\|x - \widehat{x}\| < \varepsilon\}$, for $\widehat{x} \in \Omega$. For two-dimensional domains Ω, the functional $J(\Omega)$ represents the area of the domain. The expansion with respect to ε in this case is trivial:

$$J(\Omega_\varepsilon) = |\Omega_\varepsilon| = \int_\Omega 1 - \int_{B_\varepsilon} 1 = J(\Omega) - \pi\varepsilon^2, \qquad (2)$$

and the topological derivative $\mathcal{T}(x)$ and the function $f(\varepsilon)$ are immediately found to be

$$\mathcal{T}(x) = -1, \quad f(\varepsilon) = \pi\varepsilon^2. \qquad (3)$$

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

A particular case of shape optimization is minimization of a functional over an admissible set of characteristic functions [3]. In Example 2.1, the integral is of this type,

$$J(\Omega) = \int_{\mathbb{R}^2} \chi_\Omega(x)\mathrm{d}x,$$

where χ_Ω is the characteristic function of Ω. We provide an example of a similar problem in the third part of the review.

The main idea of numerical methods based on topological derivatives is the construction of an auxiliary level set function, depending on the topological derivative in the actual domain (see, e.g., [29–32]). In this method, the shape gradient is simply replaced by the topological derivative. The line search procedure defined by simple rules in terms of the descent direction, given by the current value of the topological derivative, is used to modify the current shape. The shape is determined by the level set function. Therefore, within the topological derivative method, there is no need for the complicated Hamilton–Jacobi equation to control the shape evolution. During the optimization procedure, the shape evolution is governed by a simple updating algorithm based on the current topological derivative. In numerical examples, the procedure converges to a local solution of the topology-shape optimization problem. Therefore, this method belongs to the field of experimental mathematics. To our best knowledge, the convergence of the level set method is still to be shown, except for some particular cases. In contrast to the first-order method presented in the second part of this review, a novel method based on second-order topological derivatives is presented in the third part of the review. The two-term expansion of the functional is exploited, leading to a quadratic and strictly convex form with respect to the parameters under consideration. Therefore, a single optimization step gives the solution, without the need for an iterative algorithm. Second-order methods are discussed in the third part of the review, with details and examples.

In this paper, we are concerned with the ideas for elliptic problems and singular perturbations of the principal part of the elliptic operator. We refer the reader to [28]

for the case of penetrable inclusions and associated topological derivatives depending on the contrast parameter $0 < \gamma < \infty$, in particular for isotropic elasticity. There are also many problems where only lower order terms are perturbed, and in such cases asymptotic analysis substantially simplifies.

It is crucial for applications to know the exact form of topological derivatives. Sometimes, the expressions for topological derivatives depend on the unknown polarization tensor for the material, which is used to build geometrical domains.

3 Evaluation of Topological Derivatives

Evaluation of topological derivatives requires approximation of changes to solutions of elliptic BVPs with respect to small singular perturbations of geometrical domains. Such approximations are constructed, for example, in the monographs [33,34]; see also [35,36]. We refer the reader to [21] for the comparison of the known methods for evaluation of energy change due to the appearance of cavities in elastic solids. In Appendices, asymptotic analysis of scalar elliptic equations is discussed in a general setting.

We point out that in all methods listed below, for differentiable shape functionals, appropriate adjoint state equations can be introduced. Evaluation methods for topological derivatives depend on specific applications. The computational approaches of particular interest are:

1. The direct method of shape calculus combined with asymptotic expansions of solutions, proposed in the first paper on the topic [37]. In this method, the Taylor expansion of shape functionals, obtained in the framework of the velocity method [3], is used to pass to the limit with the small perturbation parameter, and as a result the topological derivative of the specific shape functional is obtained. The method is improved in [38] and finally uses the first shape derivatives only for a class of shape functionals. The method is difficult to apply for variational inequalities. See, for example, [39] for an application of standard asymptotic analysis to the Signorini problem, performed under the hypothesis of strict complementarity for unknown solutions. In the case of linear elliptic equations, the method can be combined with an adjoint equation approach [18,40].
2. The direct method of two-scale asymptotic analysis [11] performed for elliptic systems, and leading in particular to self-adjoint extensions of elliptic operators. In this method, appropriate adjoint state equations can be introduced at the end of the procedure, in order to simplify formulas for topological derivatives. In other words, first a two-scale asymptotic approximation of solutions with prescribed precision is constructed, and it is then used to construct an approximation of the functional. Finally, a convenient form of topological derivative is obtained, for the purposes of numerical methods. In [11], complete proofs of the results obtained for linearized elasticity boundary value problems are given.
3. The method using fundamental solutions in truncated domains and the standard two-scale expansion techniques of asymptotic analysis (see [41], for instance). In a sense, this method is substantially improved by the addition of the domain

decomposition technique with the Steklov–Poincaré operators; see the last point of this list. In addition, we refer to [15] for compound asymptotic analysis, combined with a modified adjoint sensitivity method.

4. The method using the technique of integral equations in electromagnetism, proposed, for instance, in [42] and [43]. We also refer to the recent book [44] for modeling influence of defects in elastic bodies, using well-established asymptotic formulas, with some applications to imaging.

5. The domain decomposition technique with asymptotic expansions of Steklov–Poincaré operators for small defects [27]. This framework is well adapted to the sensitivity analysis of coupled models in multiphysics, as well as of variational inequalities and contact problems in elasticity. The adjoint state equations are introduced in order to simplify the formulas for topological derivatives. The method has been used in many numerical examples: see, for example, [45,46].

The evaluation technique depends on the problem under consideration. If there is a state equation, the evaluation process usually includes asymptotic expansions of solutions with respect to a small parameter $\varepsilon \to 0$, which governs the size of singular geometrical perturbation. Asymptotic expansions of solutions to scalar equations for a model problem are given in Appendices. The case of the elasticity system is considered in [11].

We restrict ourselves to elliptic BVPs, namely the Laplace or Helmholtz equations, as well as to the BVPs of linear elasticity or for the Stokes system. The expansion depends on the spatial dimensions $d = 2, 3$, since we use the fundamental solutions to the associated elliptic equations. Most important for applications are elliptic equations in three spatial dimensions.

The differentiability of energy functionals is the first task of asymptotic analysis for the purposes of topological optimization. This property of functionals is used explicitly in numerical methods and implicitly when using the domain decomposition technique.

The general mathematical theory of solution's expansions, which applies to the elasticity system, can be found in [11]; see also [47] for the polarization tensors associated with the elasticity system. The results are given for arbitrary shapes of cavities or holes. However, closed formulas are available only for some specific shapes [47]. Usually, the results obtained for the contrast parameter $0 < \gamma < \infty$ lead to the limit cases for rigid inclusions and cavities [28].

Once the result of asymptotic analysis is known, there are some methods available which can be used to identify topological derivatives. We are particularly interested in numerical methods which are used in the framework of topological optimization. Therefore, topological derivatives should be given by robust expressions, which are approximated with the standard finite element techniques. The recommended way of identification is the application of the domain decomposition technique, in particular for topological derivatives of coupled models in multiphysics [27]. See also [41] for an early attempt at the truncated domain approach without Steklov–Poincaré operators.

In order to simplify asymptotic analysis, we are going to explain the application of Steklov–Poincaré operators to evaluation of topological derivatives for elliptic BVPs. Without the state equation, this evaluation is simpler and it becomes a purely geometrical problem; we refer to [48] for recent results in this direction. To be more specific,

we are going to explain in detail the asymptotic expansions for the elasticity system in Sects. 4.4.1 and 4.4.2. The Neumann problem on a hole of arbitrary shape is analyzed in Appendices.

To obtain the form of topological derivatives, appropriate asymptotic analysis of solutions to the associated partial differential equation should be performed. There are some monographs on the subject, for example, [33,34]. We also refer the reader to the related results obtained in collaboration with Nazarov [11,22,47,49–55]. See also [56] for further developments, using matched asymptotic expansions for the Laplacian. In general, the form of the topological derivative is given in terms of adjoint states and polarization tensors. This is an additional difficulty for numerical methods of topology optimization using topological derivatives, since the polarization tensor is known explicitly only for specific geometries of voids or cavities.

4 Asymptotic Expansions for the Domain Decomposition Technique

The domain decomposition technique seems to be the most important method of evaluation of topological derivatives for numerical methods of topology optimization. In particular, the topological derivatives for BVPs of coupled models in multiphysics can be obtained in the framework of this technique, combined with asymptotic expansions of Steklov–Poincaré operators. In control theory, at least for scalar elliptic problems, the Steklov–Poincaré operator becomes the Dirichlet-to-Neumann map. The domain decomposition method can be applied to linear elliptic problems, as well as to variational inequalities. Numerical applications of the method can be found in [45], for shape–topology optimization in piezo-elasticity, or in [46], for thermo-elasticity.

4.1 Asymptotic Expansions of Steklov–Poincaré Operators

Our goal is to apply the domain decomposition method to evaluate topological derivatives. The first step of such an evaluation for complex models is always the local analysis of singular perturbations of geometrical domains. Thus, for example, in linear elasticity in two or three spatial dimensions, with a traction-free hole or cavity, we consider a ring-shaped domain $C(R, \varepsilon)$ and obtain an asymptotic expansion of the Steklov–Poincaré operators associated with the elasticity problem, defined in its external boundary Γ_R, with respect to the small parameter $\varepsilon \to 0$. Let us consider a family of perturbations Ω_ε of the reference domain Ω by small holes or small cavities $\omega_\varepsilon(\widehat{x})$, with center $\widehat{x} \in \Omega$. The method consists in approximating singular domain perturbations by regular perturbations of the bilinear form $v \mapsto a(\Omega; v, v)$, in the variational formulation of the elliptic boundary value problem. The approximation means that the small domain ω_ε is replaced by the correction term to the bilinear form, given by the boundary bilinear form $v \mapsto \varepsilon^d b(\Gamma_R; v, v)$ concentrated on the curve or surface Γ_R. This bilinear form can be determined from asymptotic expansions of Steklov–Poincaré operators defined at the interface Γ_R, i.e., from the topological derivative of the energy functional in $\Omega_\varepsilon \setminus \overline{\Omega_R}$. In this section, we provide all the necessary details with some examples (Figs. 1, 2).

Fig. 1 Domain Ω_ε with small void ω_ε
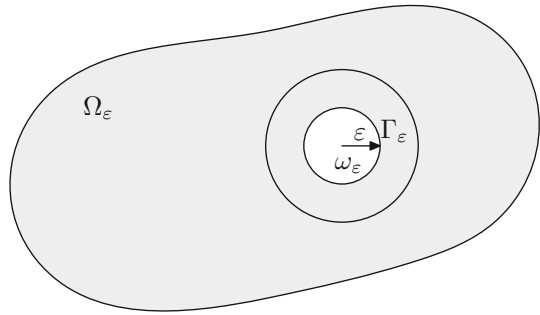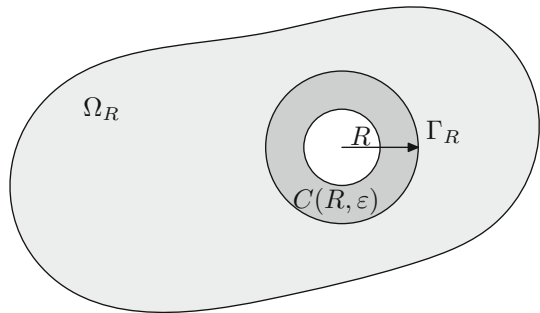

Fig. 2 Truncated domain Ω_R and the ring $C(R, \varepsilon)$

Remark 4.1 In a sense, our approach is similar, but not equivalent, to self-adjoint extensions of elliptic operators [57] as they are used in physics. See [11,22,52,54] for applications to asymptotic approximations, which lead to equivalent formulas for topological derivatives. In other words, we are able to define an approximate mathematical model in the original domain in such a way that the first-order asymptotic expansion of the energy functional is the same as for the original model in the perturbed domain. For self-adjoint extensions, the domain Ω_ε is replaced by the punctured domain $\Omega \setminus \{\widehat{x}\}$, while in our approach the truncated domain is $\Omega_R := \Omega \setminus \overline{B_R(\widehat{x})}$ for small $R > \varepsilon > 0$. This approximation is sufficient for most of the applications we have in mind. In any case, we need polarization tensors or matrices [47,49] in order to use topological derivatives in numerical methods applied to shape and topology optimization.

4.2 From Singular Domain Perturbations to Regular Perturbations of Bilinear Forms

In this section, we present the abstract scheme of asymptotic analysis for solutions of variational problems, posed in singularly perturbed geometrical domains. For simplicity, let us consider linear problems.

A weak solution of a linear elliptic problem with a symmetric, coercive and continuous bilinear form posed in $\Omega \subset \mathbb{R}^d$,

$$u := u_\Omega \in H \; : \; a(\Omega; u, \varphi) = L(\Omega; \varphi) \quad \forall \varphi \in H, \tag{4}$$

is given by a unique minimizer of the quadratic functional

$$I(\Omega; \varphi) := \frac{1}{2} a(\Omega; \varphi, \varphi) - L(\Omega; \varphi) = \frac{1}{2} a(\varphi, \varphi) - L(\varphi) \tag{5}$$

over the Sobolev space $H := H(\Omega)$ of functions defined in Ω. For simplicity, we write also

$$I(\varphi) := \frac{1}{2} a(\Omega; \varphi, \varphi) - L(\Omega; \varphi).$$

The energy shape functional is defined for Ω as

$$\Omega \mapsto \mathcal{E}(\Omega) := I(u) = \frac{1}{2} a(\Omega; u, u) - L(\Omega; u).$$

We consider the singular geometrical perturbation $\Omega_\varepsilon := \Omega \backslash \overline{B_\varepsilon(\widehat{x})}$ of the reference domain produced by a small circle or ball.

In order to evaluate the topological derivatives of the energy shape functional, as well as of some other shape functionals, we are going to use the domain decomposition technique. To this end, the reference domain is divided into two subdomains. The complement in Ω of the first subdomain $\Omega_R := \Omega \backslash \overline{B_R(\widehat{x})}$ is the ball $B_R(\widehat{x})$ which includes the singular geometrical perturbation of the reference domain. The energy functional in the perturbed domain is

$$\mathcal{E}(\Omega_\varepsilon) = \mathcal{E}(\Omega_R) + \mathcal{E}(C(R, \varepsilon)),$$

where $C(R, \varepsilon)$ is a ring,

$$C(R, \varepsilon) := B_R(\widehat{x}) \backslash \overline{B_\varepsilon(\widehat{x})}.$$

Now, we would like to introduce a bounded perturbation of the bilinear form

$$(\varphi, \varphi) \mapsto b_\varepsilon(\Gamma_R; \varphi, \varphi),$$

such that for $\varepsilon > 0$,

$$\mathcal{E}(C(R, \varepsilon)) = b_\varepsilon(\Gamma_R; u_\varepsilon, u_\varepsilon).$$

In fact, we can introduce such a form which is asymptotically exact for the first-order expansion of the solution u_ε, restricted to the truncated domain Ω_R, namely

$$u_\varepsilon^R = u^R + \varepsilon^d q^R + o(\varepsilon^d) \tag{6}$$

in $H(\Omega_R)$ for fixed $R > \varepsilon > 0$. Here, $f(\varepsilon) = \varepsilon^d$; thus, we assume implicitly that the homogeneous Neumann boundary conditions are prescribed on the cavity $B_\varepsilon(\widehat{x})$.

In this way, we could obtain the first-order topological derivatives for shape functionals defined in Ω_R, using the expansion of the energy functional in the ring $C(R, \varepsilon)$.

Let us fix $\widehat{x} \in \Omega$ and consider again the truncated domain $\Omega_R := \Omega \setminus \overline{B_R(\widehat{x})}$ and the perturbed domain $\Omega_\varepsilon := \Omega \setminus \overline{B_\varepsilon(\widehat{x})}$, where $R > \varepsilon > 0$ are two parameters such that $\varepsilon \to 0$ and $\overline{B_\varepsilon(\widehat{x})} \subset \Omega$. By definition (5), we associate with the domains the quadratic functionals

$$I_R(\varphi) := \frac{1}{2}a(\Omega_R; \varphi, \varphi) - L(\Omega_R; \varphi) = \frac{1}{2}a_R(\varphi, \varphi) - L_R(\varphi)$$

and

$$I_\varepsilon(\varphi) := \frac{1}{2}a_\varepsilon(\varphi, \varphi) - L_\varepsilon(\varphi), \tag{7}$$

obtained by restriction of the test functions $\varphi \in H(\Omega)$ to Ω_R (respectively, to Ω_ε). Our goal is to construct an approximation of the quadratic functional for which the minimizer u_ε^R is given by the restriction to Ω_R of the variational solution u_ε in the singularly perturbed domain. The variational solution in Ω is given by (4), and the variational problem in the perturbed domain Ω_ε is given by

$$u_\varepsilon \in H_\varepsilon \; : \; a_\varepsilon(u_\varepsilon, \varphi) = L_\varepsilon(\varphi) \quad \forall \varphi \in H_\varepsilon. \tag{8}$$

To this end, we introduce the nonlocal Steklov–Poincaré operator $\mathcal{A}_\varepsilon$ on the interior boundary Γ_R of Ω_R. The operator is defined by the nonhomogeneous Dirichlet boundary value problem over $C(R, \varepsilon)$. We determine the expansion of the Steklov–Poincaré operator

$$\mathcal{A}_\varepsilon = \mathcal{A} + \varepsilon^d \mathcal{B} + \mathcal{R}_\varepsilon$$

in the space of linear operators and introduce the bilinear form associated with the first term of the expansion,

$$b(h, h) := (\mathcal{B}(h), h)_{\Gamma_R}.$$

It can be shown that minimization of the first-order approximation of the quadratic functional (9), defined in the original domain, leads to the first-order expansion of the minimizers for the perturbed domain, which holds in the truncated domain Ω_R:

Theorem 4.1 *Let u_ε^R be the minimizer of the approximate quadratic functional*

$$I_\varepsilon^R(\varphi) = \frac{1}{2}a(\Omega; \varphi, \varphi) + \frac{1}{2}\varepsilon^d(\mathcal{B}(\varphi), \varphi)_{\Gamma_R} - L(\Omega_R; \varphi). \tag{9}$$

Then, the restriction of this minimizer to Ω_R (denoted by the same symbol u_ε^R) has in $H^1(\Omega_R)$ an expansion

$$u_\varepsilon^R = u^R + \varepsilon^d q^R + o(\varepsilon^d), \tag{10}$$

where $u^R = u_{|\Omega_R}$. This expansion coincides with the expansion of the solution to (8) in $H^1(\Omega_R)$.

Corollary 4.1 *In the case of variational equations resulting from the minimization of* (7), *we have the same result. Indeed, the first-order expansion of the minimizers* $\varepsilon \mapsto u_\varepsilon$, *restricted to the truncated domain* Ω_R, *i.e., for* $R > \varepsilon > 0$,

$$u_{\varepsilon|\Omega_R} = u_{|\Omega_R} + \varepsilon^d q^R + o(\varepsilon^d) \tag{11}$$

is preserved when using the minimization of (9), *since, for example, for the second-order elliptic boundary value problems,*

$$\|u_{\varepsilon|\Omega_R} - u_\varepsilon^R\|_{H^1(\Omega_R)} = o(\varepsilon^d).$$

Taking into account these estimates, the topological derivatives of shape functionals, defined by integrals in the truncated domain, can be obtained.

Corollary 4.2 *The topological derivative of the tracking-type functional,*

$$J(\Omega_\varepsilon) = \frac{1}{2} \int_{\Omega_R} (u_\varepsilon - z_d)^2 \mathrm{d}x, \tag{12}$$

is given by the expression

$$\mathcal{T}(\widehat{x}) = \int_{\Omega_R} (u^R(x) - z_d(x)) q^R(x) \mathrm{d}x = \int_{\Omega_R} (u(x) - z_d(x)) q(x) \mathrm{d}x, \tag{13}$$

where

$$q = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon^d} (u_\varepsilon - u) \quad in \ \ \Omega_R.$$

Remark 4.2 The topological derivative of the tracking-type functional (12) can be simplified for variational equations by using the adjoint state equation. Then, the full potential of the topological derivative is seen, since it becomes a function of the point $\widehat{x}$, obtained at the expense of solving only two sets of state-like systems. The corresponding formulas are given in Parts II [58] and Part III [59] of the paper. However, even if we cannot use adjoint equations, the domain decomposition method based on the asymptotic expansion of the Steklov–Poincaré operator has its advantages. They consist in replacing the influence of the small hole (inclusion) by the small, localized disturbance of the main bilinear form (see (9)), defined in the original domain. In this way, the method facilitates and speeds up numerical approximations, for example, using finite element methods.

4.3 Signorini Problem in Two Spatial Dimensions

Now we shall explain the domain decomposition technique used in approximation of quadratic energy functionals to evaluate topological derivatives for the Laplace operator [27]. We restrict ourselves to the homogeneous Neumann boundary conditions on holes in order to use $f(\varepsilon) \approx \varepsilon^2$.

Let us consider the Signorini problem in a domain $\Omega \subset \mathbb{R}^2$ with smooth boundary $\partial \Omega = \Gamma_0 \cup \Gamma_s$. The bilinear form

$$a(u, v) = a(\Omega; u, v) = \int_\Omega \nabla u \cdot \nabla v \mathrm{d}x$$

is coercive and continuous over the Sobolev space

$$H^1_{\Gamma_0}(\Omega) = \{v \in H^1(\Omega) \ : \ v = 0 \text{ on } \Gamma_0\},$$

and the linear form

$$L(v) = L(\Omega; v) = \int_\Omega f v \mathrm{d}x$$

is continuous on $L^2(\Omega)$. There is a unique solution to the variational inequality

$$u \in K \ : \ a(u, v - u) \geq L(v - u) \qquad \forall v \in K,$$

where K is the convex and closed cone

$$K = K(\Omega) = \{v \in H^1_{\Gamma_0}(\Omega) \ : \ v \geq 0 \text{ on } \Gamma_s\}.$$

Let us consider the variational inequality over the singularly perturbed domain $\Omega_\varepsilon = \Omega \backslash \overline{B}_\varepsilon$,

$$u_\varepsilon \in K_\varepsilon = K(\Omega_\varepsilon) \ : \ a_\varepsilon(u_\varepsilon, v - u_\varepsilon) \geq L_\varepsilon(v - u_\varepsilon) \qquad \forall v \in K_\varepsilon,$$

with the solution given by the unique minimizer of the quadratic functional

$$I_\varepsilon(v) = \frac{1}{2} a_\varepsilon(v, v) - L_\varepsilon(v) \tag{14}$$

over the convex set $K_\varepsilon := K(\Omega_\varepsilon)$. Let us assume that L_ε is supported in Ω_R.

We can show that there is an approximation of (14), denoted by

$$I^R_\varepsilon(v) = \frac{1}{2} a_\varepsilon(\Omega_R; v, v) - L_\varepsilon(\Omega_R; v),$$

such that the first-order expansion of the minimizers with respect to the small parameter $\varepsilon^2 \to 0$ is the same in $H^1(\Omega_R)$ as in the perturbed problem. Namely, we can introduce a continuous, symmetric and nonlocal bilinear form on the circle $\Gamma_R = \{\|x - \widehat{x}\| = R > \varepsilon > 0\}$,

$$H^{1/2}(\Gamma_R) \times H^{1/2}(\Gamma_R) \ni (v, v) \mapsto b(\Gamma_R; v, v) \in \mathbb{R},$$

such that

$$I_\varepsilon^R(v) = \frac{1}{2}a(\Omega; v, v) - L(\Omega; v) + \varepsilon^2 b(\Gamma_R; v, v).$$

Furthermore, if the solution to the perturbed variational inequality has an expansion in $H^1(\Omega_R)$,

$$u_\varepsilon = u + \varepsilon^2 q + o(\varepsilon^2),$$

then the minimizer u_ε^R of $v \mapsto I_\varepsilon^R(v)$ over the convex cone $K(\Omega)$ has in $H^1(\Omega_R)$ the same first-order expansion,

$$u_\varepsilon^R = u + \varepsilon^2 q + o(\varepsilon^2).$$

Corollary 4.3 *The topological derivative of the tracking-type functional for the variational inequality,*

$$J(\Omega_\varepsilon) = \frac{1}{2}\int_{\Omega_R}(u_\varepsilon - z_d)^2 dx, \tag{15}$$

is given by

$$\mathcal{T}(\widehat{x}) = \int_{\Omega_R}(u^R(x) - z_d(x))q^R(x)dx = \int_{\Omega_R}(u(x) - z_d(x))q(x)dx, \tag{16}$$

where

$$q = \lim_{\varepsilon \to 0}\frac{1}{\varepsilon^2}(u_\varepsilon - u) \ \ in \ \Omega_R.$$

For variational inequalities, we cannot introduce adjoint states.

Thus, we are able to replace the singular geometrical domain perturbation $B_\varepsilon(\widehat{x})$ by the regular perturbation $v \mapsto \varepsilon^2 b(\Gamma_R; v, v)$ of the bilinear form $v \mapsto a(\Omega; v, v)$ and preserve the first-order expansion of minimizers in the truncated domain. The bilinear form is constructed using the expansion of the Steklov–Poincaré operator, defined in Γ_R and given by the expansion of the energy functional in the ring $C(R, \varepsilon)$:

$$a(\Omega_\varepsilon; v, v) \cong a(\Omega; v, v) + \varepsilon^2 b(\Gamma_R; v, v),$$

where

$$b(\Gamma_R; v, v) = \left(\frac{1}{\pi R^3}\int_{\Gamma_R} v \cdot (x_1 - \widehat{x}_1)\, ds\right)^2 + \left(\frac{1}{\pi R^3}\int_{\Gamma_R} v \cdot (x_2 - \widehat{x}_2)\, ds\right)^2.$$

For the elasticity system, the relevant formulas are given in Sects. 4.4.1 and 4.4.2.

4.4 Domain Decomposition Method for Elasticity BVPs

The domain decomposition method has been used to evaluate topological derivatives for coupled BVPs [28,45,46]. In this section, we shall consider asymptotic corrections to the energy functional corresponding to the elasticity system in $\mathbb{R}^d$, where $d = 2, 3$. The change of energy is caused by creating a small ball-like void of variable radius ε in the interior of the domain Ω, with the homogeneous Neumann boundary condition on its surface. We assume that the void is centered at the origin $\mathcal{O}$. We take $\Omega_R = \Omega \setminus \overline{B_R}$, where $B_R := B(\mathcal{O}, R)$ is an open ball with fixed radius R. In this way, the void $B_\varepsilon := B(\mathcal{O}, \varepsilon)$ is surrounded by $B_R \subset \Omega$. We also denote the ring or spherical shell as $C(R, \varepsilon) = B_R \setminus \overline{B_\varepsilon}$, and its boundaries as $\Gamma_R = \partial B_R$ and $\Gamma_\varepsilon := \partial B_\varepsilon$.

Using these notations, we define our main tool, the Dirichlet-to-Neumann mapping for linear elasticity, which is called the Steklov–Poincaré operator:

$$\mathcal{A}_\varepsilon \: : \: H^{1/2}(\Gamma_R; \mathbb{R}^d) \to H^{-1/2}(\Gamma_R; \mathbb{R}^d)$$

by means of the boundary value problem

$$\begin{aligned} \mu \Delta w + (\lambda + \mu) \nabla(\operatorname{div} w) &= 0, \quad \text{in } C(R, \varepsilon), \\ w = v \ \text{ on } \ \Gamma_R, \quad \sigma(u)n &= 0 \ \text{ on } \ \Gamma_\varepsilon, \end{aligned} \tag{17}$$

so that

$$\mathcal{A}_\varepsilon(v) = \sigma(w)n \quad \text{on} \ \ \Gamma_R. \tag{18}$$

Here, μ, λ are the Lamé coefficients, and $\sigma(w)$ is the Cauchy stress tensor,

$$\sigma(w) = 2\mu(\nabla w)^s + \lambda \operatorname{div}(w) \, \mathrm{I}, \quad \text{with} \quad (\nabla w)^s = \frac{1}{2}(\nabla w + (\nabla w)^\top).$$

Let u^R be the restriction of u to Ω_R, and $\gamma^R(\varphi)$ the trace of φ on Γ_R, still denoted by φ for simplicity. We may then define the functional

$$I_\varepsilon^R(\varphi) := \frac{1}{2} \int_{\Omega_R} \sigma(\varphi) \cdot (\nabla \varphi)^s \, \mathrm{d}x - \int_{\Gamma_N} h \cdot \varphi \, \mathrm{d}s + \frac{1}{2} \int_{\Gamma_R} \mathcal{A}_\varepsilon(\varphi) \cdot \varphi \, \mathrm{d}s \tag{19}$$

and the solution u_ε^R as a minimizer for

$$I_\varepsilon^R(u_\varepsilon^R) := \inf_{\varphi \in K \subset H(\Omega_R)} I_\varepsilon^R(\varphi), \tag{20}$$

We have replaced the variable domain $\varepsilon \mapsto \Omega_\varepsilon$ by a fixed truncated domain Ω_R, at the price of introducing a variable boundary operator $\mathcal{A}_\varepsilon$. Thus, the goal is to find an asymptotic expansion

$$\mathcal{A}_\varepsilon = \mathcal{A} + \varepsilon^d \mathcal{B} + \mathcal{R}_\varepsilon, \tag{21}$$

where the remainder $\mathcal{R}_\varepsilon$ is of order $o(\varepsilon^d)$ in the operator norm in

$$\mathcal{L}(H^{1/2}(\Gamma_R; \mathbb{R}^2), H^{-1/2}(\Gamma_R; \mathbb{R}^2))$$

and the operator $\mathcal{B}$ is regular enough, namely it is bounded and linear:

$$\mathcal{B} \in \mathcal{L}(L^2(\Gamma_R; \mathbb{R}^2), L^2(\Gamma_R; \mathbb{R}^2)).$$

Under this assumption, the following propositions hold true.

Proposition 4.1 *Assume that* (21) *holds in the operator norm. Then,*

$$u_\varepsilon^R \to u^R \tag{22}$$

strongly in the $H^1(\Omega_R)$-norm.

Proposition 4.2 *The energy functional has a representation*

$$I_\varepsilon^R(u_\varepsilon^R) = I(u) + \varepsilon^d \langle \mathcal{B}(u), u \rangle_R + o(\varepsilon^d), \tag{23}$$

where $o(\varepsilon^d)/\varepsilon^d \to 0$ as $\varepsilon \to 0$ in the same energy norm.

Here, $I^R(u^R)$ denotes the functional I_ε^R on the original domain, i.e., $\varepsilon = 0$, with $\mathcal{A}_\varepsilon$ replaced by $\mathcal{A}$ applied to truncation of u.

Generally, the energy correction for the elasticity system has the form

$$\langle \mathcal{B}(u^R), u^R \rangle_R = -c_d e_u(\mathcal{O}),$$

where $c_d = \mathrm{vol}(B_1)$, with B_1 being the unit ball in $\mathbb{R}^d$. The energy-like density function $e_u(\mathcal{O})$ has the form

$$e_u(\mathcal{O}) = \frac{1}{2} \mathbb{P}\sigma(u^R) \cdot (\nabla u^R)^s(\mathcal{O}),$$

where for $d = 2$ and the plane stress,

$$\mathbb{P} = \frac{1}{1 - \nu}(4\mathbb{I} - \mathrm{I} \otimes \mathrm{I}),$$

and for $d = 3$,

$$\mathbb{P} = \frac{1 - \nu}{7 - 5\nu}\left(10\mathbb{I} - \frac{1 - 5\nu}{1 - 2\nu}\mathrm{I} \otimes \mathrm{I}\right).$$

Here, $\mathbb{I}$ is the fourth-order identity tensor, and I is the second-order identity tensor.

This approach is important for variational inequalities, since it allows us to derive formulas for topological derivatives which are similar to expressions obtained for the corresponding linear BVPs.

4.4.1 Explicit Form of the Operator $\mathcal{B}$ in Two Spatial Dimensions

Let us denote, for the plane stress case,

$$k = \frac{\lambda + \mu}{\lambda + 3\mu}.$$

It has been proved in [27] that the following exact formulas hold:

$$u_{1,1}(\mathcal{O}) + u_{2,2}(\mathcal{O}) = \frac{1}{\pi R^3} \int_{\Gamma_R} (u_1 x_1 + u_2 x_2) \, ds,$$

$$u_{1,1}(\mathcal{O}) - u_{2,2}(\mathcal{O}) = \frac{1}{\pi R^3} \int_{\Gamma_R} \left[(1 - 9k)(u_1 x_1 - u_2 x_2) + \frac{12k}{R^2} (u_1 x_1^3 - u_2 x_2^3) \right] ds,$$

$$u_{1,2}(\mathcal{O}) + u_{2,1}(\mathcal{O}) = \frac{1}{\pi R^3} \int_{\Gamma_R} \left[(1 + 9k)(u_1 x_2 + u_2 x_1) - \frac{12k}{R^2} (u_1 x_2^3 + u_2 x_1^3) \right] ds.$$

These expressions contain additional integrals of third powers of x_i. Therefore, strains evaluated at $\mathcal{O}$ may be expressed as linear combinations of integrals over the circle of the form

$$\int_{\Gamma_R} u_i x_j \, ds, \qquad \int_{\Gamma_R} u_i x_j^3 \, ds.$$

The same is true, due to Hooke's law, for the stresses $\sigma_{ij}(\mathcal{O})$. They may then be inserted into the expression for $\mathcal{B}$, yielding

$$\langle \mathcal{B}(u^R), u^R \rangle_R = -\frac{1}{2} c_2 \mathbb{P}\sigma(u) \cdot (\nabla u)^s.$$

These formulas are quite easy to compute numerically.

4.4.2 Explicit Form of the Operator $\mathcal{B}$ in Three Spatial Dimensions

It turns out that a similar situation holds in three spatial dimensions, but obtaining exact formulas is more difficult. Assuming given values of u on Γ_R, the solution of the elasticity system in B_R may be expressed, following partially the derivation from [60] (pp. 285 ff.), as

$$u = \sum_{n=0}^{\infty} [U_n + (R^2 - r^2) k_n(\nu) \nabla(\text{div } U_n)], \tag{24}$$

where $k_n(\nu) = 1/2[(3 - 2\nu)n - 2(1 - \nu)]$ and $r = \|x\|$, with ν denoting the Poisson ratio. In addition,

$$U_n = \frac{1}{R^n} [a_{n0} d_n(x) + \sum_{m=1}^{n} (a_{nm} c_n^m(x) + b_{nm} s_n^m(x))]. \tag{25}$$

The vectors

$$a_{n0} = (a_{n0}^1, a_{n0}^2, a_{n0}^3)^\top,$$
$$a_{nm} = (a_{nm}^1, a_{nm}^2, a_{nm}^3)^\top,$$
$$b_{nm} = (b_{nm}^1, b_{nm}^2, b_{nm}^3)^\top$$

are constants, and the set of functions

$$\{d_0; \; d_1, c_1^1, s_1^1; \; d_2, c_2^1, s_2^1, c_2^2, s_2^2; \; d_3, c_3^1, s_3^1, c_3^2, s_3^2, c_3^3, s_3^3; \; \ldots\}$$

constitutes a complete system of orthonormal harmonic polynomials on Γ_R, related to Laplace spherical functions. Specifically,

$$c_k^l(x) = \frac{\hat{P}_k^{l,c}(x)}{\|\hat{P}_k^{l,c}\|_R}, \quad s_k^l(x) = \frac{\hat{P}_k^{l,s}(x)}{\|\hat{P}_k^{l,s}\|_R}, \quad d_k = \frac{P_k(x)}{\|\hat{P}_k\|_R}.$$

For example,

$$c_3^2(\mathbf{x}) = \frac{1}{R^4}\sqrt{\frac{7}{240\pi}}(15x_1^2 x_3 - 15x_2^2 x_3).$$

If the value of u on Γ_R is assumed to be given, then, denoting

$$\langle \phi, \psi \rangle_R = \int_{\Gamma_R} \phi\psi \, ds,$$

we have for $n \geq 0$, $m = 1..n$, $i = 1, 2, 3$:

$$a_{n0}^i = R^n \langle u_i, d_n(x) \rangle_R,$$
$$a_{nm}^i = R^n \langle u_i, c_n^m(x) \rangle_R,$$
$$b_{nm}^i = R^n \langle u_i, s_n^m(x) \rangle_R. \tag{26}$$

Since we are looking for $u_{i,j}(\mathcal{O})$, only the part of u which is linear in x is relevant. It contains two terms:

$$\hat{u} = U_1 + R^2 k_3(v)\nabla(\operatorname{div} U_3). \tag{27}$$

For any $f(x)$, $\nabla \operatorname{div}(af) = H(f) \cdot a$, where a is a constant vector and $H(f)$ is the Hessian matrix of f. Therefore,

$$\hat{u} = \frac{1}{R}[a_{10}d_1(x) + a_{11}c_1^1(x) + b_{11}s_1^1(x))]$$

$$+ R^2 k_3(v)\frac{1}{R^3}\left[H(d_3)(x)a_{30} + \sum_{m=1}^{3}\left(H(c_3^m)(x)a_{3m} + H(s_3^m)(x)b_{3m}\right)\right]. \tag{28}$$

From the above, we may single out the coefficients of x_1, x_2, x_3 in u_1, u_2, u_3. For example,

$$
\begin{aligned}
u_{1,1}(\mathcal{O}) =& \frac{1}{R^3}\sqrt{\frac{3}{4\pi}}a_{11}^1 + \frac{1}{R^5}k_3(v)\Big[-3\sqrt{\frac{7}{4\pi}}a_{30}^3 9\sqrt{\frac{7}{24\pi}}a_{31}^1 \\
&-3\sqrt{\frac{7}{24\pi}}b_{31}^2 + 30\sqrt{\frac{7}{240\pi}}a_{32}^3 + 90\sqrt{\frac{7}{1440\pi}}a_{33}^1 + 90\sqrt{\frac{7}{1440\pi}}b_{33}^2\Big], \\
u_{1,2}(\mathcal{O}) =& \frac{1}{R^3}\sqrt{\frac{3}{4\pi}}(b_{11}^1 + a_{11}^2) + \frac{1}{R^5}k_3(v)\Big[-3\sqrt{\frac{7}{24\pi}}a_{31}^2 - \sqrt{\frac{7}{24\pi}}b_{31}^1 \\
&+ 15\sqrt{\frac{7}{60\pi}}b_{32}^3 - 90\sqrt{\frac{7}{1440\pi}}a_{33}^2 + 90\sqrt{\frac{7}{1440\pi}}b_{33}^1\Big].
\end{aligned}
$$

Observe that

$$
u_{1,1}(\mathcal{O}) + u_{2,2}(\mathcal{O}) + u_{3,3}(\mathcal{O}) = \frac{1}{R^3}\sqrt{\frac{3}{4\pi}}\big(R\langle u_1, c_1^1\rangle_R + R\langle u_2, s_1^1\rangle_R + R\langle u_3, d_1\rangle_R\big)
$$

and $c_1^1 = \frac{1}{R^2}\sqrt{\frac{3}{4\pi}}x_1$, $s_1^1 = \frac{1}{R^2}\sqrt{\frac{3}{4\pi}}x_2$, $d_1 = \frac{1}{R^2}\sqrt{\frac{3}{4\pi}}x_3$, which is in agreement with the fact that the trace of the strain tensor is a harmonic function.

As a result, the operator $\mathcal{B}$ may be defined by

$$
\langle \mathcal{B}u^R, u^R\rangle_R := -c_3\mathbb{P}\sigma(u) \cdot (\nabla u)^s(\mathcal{O}),
$$

where the right-hand side consists of integrals of u multiplied by first- and third-order polynomials in x_i over Γ_R resulting from (26). This is a very similar situation to the case of two spatial dimensions. Thus, the new expressions for strains make it possible to rewrite $\mathcal{B}$ in the form of the desired regularity. We refer the reader to [61–63] for supplementary material on elasticity models.

5 Perspectives and Open Problems

The topological derivative method in shape and topology optimization introduces the asymptotic analysis of elliptic BVPs, for example, into the field of structural optimization in elasticity. The method requires the local regularity of solutions to elliptic problems. Nowadays, classical shape optimization techniques are not restricted to elliptic problems, but can be applied to evolution problems, including linear parabolic and hyperbolic equations. Extension of the topological derivative method to evolution problems is one of the challenging issues in the field of shape optimization. In particular, for transport equations, the notion of topological derivative is still to be discovered. Let us mention that the transport equations are components of compressible Navier–Stokes equations. The modern theory of shape optimization for compressible Navier–Stokes equations can be found in the monograph [2]. Another domain which is promising for developments of shape optimization is nonlinear elasticity. Evolution of

geometrical domains is also used in growth modeling. Shape and topology optimization for nonlinear elasticity is still poorly understood. There is already some numerical evidence that topological derivatives are well adapted to the design of metamaterials in elasticity.

In order to state some open problems for applications of topological sensitivity analysis to numerical solution of shape optimization and inverse problems, we specify the mathematical framework, which combines analysis of weak solutions to elliptic BVPs with the domain decomposition method, as well as with asymptotic approximation of solutions in singularly perturbed geometrical domains.

1. *Applications of Γ-convergence to topological differentiability of shape functionals*. It is known that the shape derivatives of energy-type functionals can be obtained by the Γ-limit procedure; see the derivation of the elastic energy with respect to crack length [64,65] or [66–70] for related topics. It is not known whether the same Γ-convergence can be used for topological derivatives.

2. *Sensitivity analysis of evolution variational inequalities*. Shape optimization for stationary variational inequalities is studied in [3]. The results are based on Hadamard differentiability of the metric projection onto convex sets in Sobolev spaces [71–73]. The results are obtained by using potential theory in Dirichlet spaces [74], which leads to Hadamard differentiability of the metric projection. For stationary variational inequalities with local constraints on gradients or on stresses, shape and topological sensitivity analysis is an open problem. For example, for Hencky plasticity, there are no results, either in shape optimization or for topological derivatives. Extension of such results to evolution variational inequalities is a challenging problem, necessary for development of topological derivatives.

3. *Asymptotic analysis of evolution variational inequalities*. Asymptotic analysis of stationary variational inequalities was studied, for example, by Argatov and Sokolowski [39]. The concept of polyhedral subsets of Sobolev spaces can be used in order to derive topological derivatives for contact problems in solid mechanics. Open problems for stationary variational inequalities include some models of plates and shells and plasticity. This domain of research has stagnated for a long time. The mathematical result required concerns directional differentiability of the metric projection onto a convex set defined by local constraints on the stresses. Extending such results to asymptotic analysis of evolution variational inequalities is another challenging problem.

4. *Second-order necessary optimality conditions in topological optimization*. First-order necessary optimality conditions are known for linear state equations [26]. Using second-order topological derivatives to derive optimality conditions seems to be an open problem.

5. *Exact solutions in singularly perturbed geometrical domains for anisotropic elasticity, transient wave equations and nonlinear transport problems for evaluation of topological derivatives*. Exact solutions of elliptic BVPs in a ring are used to evaluate topological derivatives within the domain decomposition technique. Such results are of interest for the PDEs listed below.

    (a) *Elasticity with complex Kolosov potentials and Steklov–Poincaré formalism in domain decomposition*. Using complex potentials of Kolosov, one can obtain

exact solutions of the elasticity system in two spatial dimensions. These results lead to topological derivatives of arbitrary order. Extending such results to a full range of models in mechanics is an interesting line of research, which is still to be taken up.

(b) *Wave equations*. An important field of applications is electromagnetism and exact solutions, which are not standard from the mathematical point of view for asymptotic analysis. We refer the reader to [75–77] for related results in the static case. Open problems in the field of wave equations include all aspects of time-dependent problems, including asymptotic analysis in singularly perturbed geometrical domains. Wave equations with self-adjoint extensions of elliptic operators are used in [78].

(c) *Transport equations in singularly perturbed domains*. The domain decomposition method is also used for transport problems. Open problems in this field involve all aspects of asymptotic analysis. The compressible Navier–Stokes equations can also be considered from the point of view of singular domain perturbations, provided the related results for the transport equation component are established.

6 Conclusions

The proposed approach to evaluation of topological derivatives applies to some classes of variational inequalities and to multiphysics BVPs. From the mathematical point of view, the domain decomposition method of evaluation of topological derivatives uses asymptotic expansions of the energy functional in a small neighborhood of the singular domain perturbation, produced by a hole or a cavity. In our applications, the energy expansions are equivalent to expansions of nonlocal Steklov–Poincaré boundary operators. In the truncated domain, perturbations of boundary conditions with the expansion of Steklov–Poincaré boundary operators lead to regular perturbations of the bilinear form and allow us to avoid self-adjoint extensions of elliptic operators in punctured domains. Topological derivatives are known for linear elliptic BVPs. They remain almost unknown for some nonlinear problems, including nonlinear elasticity and plasticity. See [79] for some recent developments in this direction. Extension of this approach to shape optimization to evolution problems should also be considered for variational inequalities modeling compressible fluids.

Appendices

Formal asymptotic analysis for a scalar elliptic equation is presented. The same method is used for linear elasticity in [11].

A.1 Asymptotic Expansions of Solutions and Functionals

In previous sections, basic derivations are conducted for the simplest case of circular or ball-shaped voids, which nevertheless illustrate the most important features of the approach. In a similar way, ball-shaped penetrable inclusions with contrast $0 < \gamma < \infty$ can be obtained [28].

If more general shapes of voids (inclusions) are required, the asymptotic analysis approach applies as well, as is shown below. We refer the reader to [34] for the general theory and examples of asymptotic expansions.

For the convenience of the reader, a two-scale asymptotic analysis of a nonhomogeneous boundary value problem is performed, for a simple model problem. The small cavity $\omega_\varepsilon := \varepsilon\omega$ with center at the origin $\mathcal{O} \in \omega_\varepsilon \subset \omega$ can be considered without loss of generality. We denote by the same symbol $\omega_\varepsilon(\widehat{x}) := \widehat{x} + \omega_\varepsilon$ the cavity with center at $\widehat{x} \in \Omega$. Matched asymptotic expansions are used in two spatial dimensions for scalar problems with the Laplacian, where we consider singular perturbations of the principal part of the elliptic operator. In the case of a penetrable inclusion with contrast parameter $0 < \gamma < \infty$, the results are obtained in a similar way, since it is a regular perturbation of the main part of the elliptic operator.

A.2 Asymptotic Expansions of Steklov–Poincaré Operators

We consider a smooth domain $\Omega_\varepsilon := \Omega\backslash\overline{\omega_\varepsilon}$ for $\varepsilon \to 0$ and the nonhomogeneous Dirichlet problem with $h \in H^{1/2}(\Gamma)$,

$$
\begin{aligned}
\Delta w_\varepsilon &= 0 & &\text{in } \Omega_\varepsilon, \\
w_\varepsilon &= h & &\text{on } \Gamma, \\
\frac{\partial w_\varepsilon}{\partial n} &= 0 & &\text{on } \partial\omega_\varepsilon,
\end{aligned}
\tag{29}
$$

where $\Gamma = \partial\Omega$ is the boundary of Ω.

The energy associated with (29) is given by a symmetric bilinear form on the fractional Sobolev space $H^{1/2}(\Gamma)$,

$$
a_\varepsilon(h, h) = \int_{\Omega_\varepsilon} \|\nabla w_\varepsilon\|^2 \mathrm{d}x.
$$

We are interested in the asymptotic expansion of this quadratic functional for $\varepsilon \to 0$. To this end, the technique of matched asymptotic expansions [33,34] is used.

Using Green's formula, we derive equivalent forms of the energy (here, the boundary integrals stand for the duality pairing between $H^{1/2}(\Gamma)$ and its dual $H^{-1/2}(\Gamma)$):

$$
a_\varepsilon(h, h) = \int_\Gamma w_\varepsilon \frac{\partial w_\varepsilon}{\partial n} \mathrm{d}s = \int_\Gamma h \frac{\partial w_\varepsilon}{\partial n} \mathrm{d}s.
\tag{30}
$$

Now, we introduce two-scale asymptotic approximation of solutions. We use the method of matched asymptotic expansions and look for two types of expansions, the

outer expansion valid far from the cavity ω_ε,

$$w_\varepsilon(x) = w_0(x) + \varepsilon^2 w_1(x) + \varepsilon^3 w_2(x) + \cdots,$$

and the inner expansion, valid in a small neighborhood of ω_ε,

$$w_\varepsilon(x) = W_0(\xi) + \varepsilon W_1(\xi) + \varepsilon^2 W(\xi) + \cdots,$$

where the fast variable ξ is defined by

$$\xi := \frac{x}{\varepsilon}.$$

Following [33,34], we obtain

$$W_0(\xi) \equiv w_0(0),$$

and

$$W_1(\xi) = \sum_{j=1}^{2} \mathcal{Y}^j(\xi) \frac{\partial w_0}{\partial x_j}(0),$$

where $\mathcal{Y}^j$ is harmonic in $\mathbb{R}^2 \backslash \overline{\omega}$ and $\omega := \omega_1$. In addition, $\mathcal{Y}^j$ satisfies the homogeneous Neumann boundary conditions on $\partial \omega$ and enjoys the following behavior at infinity:

$$\mathcal{Y}^j(\xi) = \xi_j + \frac{1}{2\pi \|\xi\|^2} \sum_{k=1}^{2} m_{kj}^\omega \xi_k + O(\|\xi\|^{-2}), \quad \|\xi\| \to \infty.$$

Its regular part is denoted by

$$\mathcal{Y}_0^j(\xi) := \frac{1}{2\pi \|\xi\|^2} \sum_{k=1}^{2} m_{kj}^\omega \xi_k + O(\|\xi\|^{-2}),$$

and we denote its higher order term $O(\|\xi\|^{-2})$ by

$$\mathfrak{h}_0^j(\xi) := \mathcal{Y}_0^j(\xi) - \frac{1}{2\pi \|\xi\|^2} \sum_{k=1}^{2} m_{kj}^\omega \xi_k.$$

Taking into account this expansion, we get

$$w_1(x) = \sum_{j,k=1}^{2} \frac{\partial w_0}{\partial x_j}(0) m_{kj}^\omega \mathcal{G}^{(k)}(x).$$

We denote by $\mathcal{G}^{(k)}$ the singular solutions to the problem posed in the punctured domain,

$$
\begin{aligned}
\Delta_x \mathcal{G}^{(k)}(x) &= 0 && \text{in } \Omega \backslash \mathcal{O}, \\
\mathcal{G}^{(k)}(x) &= 0 && \text{on } \Gamma, \\
\mathcal{G}^{(k)}(x) &= \frac{x_k}{2\pi \|x\|^2} + O(1) && \|x\| \to 0.
\end{aligned}
\tag{31}
$$

We set

$$
\mathcal{G}^{(k)}(x) = \frac{x_k}{2\pi \|x\|^2} + \mathcal{G}_0^{(k)}(x),
$$

where $\mathcal{G}_0^{(k)}$ stands for the regular part. Therefore, far from the cavity ω_ε, we have

$$
w_\varepsilon(x) = w_0(x) + \varepsilon^2 \sum_{j,k=1}^2 \frac{\partial w_0}{\partial x_j}(0) m_{kj}^\omega \mathcal{G}^{(k)}(x) + O(\varepsilon^2).
$$

Substituting this representation into formula (30), we obtain the one-term expansion

$$
a_\varepsilon(h,h) = a(h,h) + \varepsilon^2 b(h,h) + O(\varepsilon^{3-\alpha}).
$$

Here, $\alpha \in \,]0, 1[$ and

$$
b(h,h) = \int_\Gamma h(x) \sum_{j,k=1}^2 \frac{\partial w_0}{\partial x_j}(0) m_{kj}^\omega \frac{\partial \mathcal{G}^{(k)}}{\partial n}(x)\,\mathrm{d}s.
$$

If we combine this with the integral equality on the sphere of radius $\delta > 0$,

$$
\int_{\mathbb{S}_\delta(\mathcal{O})} \left(x_j \frac{\partial}{\partial n} \frac{x_k}{2\pi \|x\|^2} - \frac{x_k}{2\pi \|x\|^2} \frac{\partial x_j}{\partial n} \right) \mathrm{d}s = \delta_{jk},
$$

we get

$$
b(h,h) = -m^\omega \nabla w_0(0) \cdot \nabla w_0(0).
$$

Since

$$
\int_\Gamma w_0(x) \partial_n \mathcal{G}^{(k)}(x)\,\mathrm{d}s = -\frac{\partial w_0}{\partial x_k}(0),
$$

it follows that

$$
b(h,h) = -\left(\int_\Gamma h(x) \partial_n \mathcal{G}^{(j)}(x)\,\mathrm{d}s \right) m_{jk}^\omega \left(\int_\Gamma h(x) \partial_n \mathcal{G}^{(k)}(x)\,\mathrm{d}s \right) \mathrm{d}s.
$$

Remark A.1 It can be shown that the following supremum taken with respect to the $H^{1/2}(\Gamma)$-norm is bounded with respect to $\varepsilon \to 0$:

$$\sup_{\|h\|\leq 1} \left| a_\varepsilon(h, h) - a(h, h) - \varepsilon^2 b(h, h) \right| \leq C_\alpha \varepsilon^{3-\alpha}.$$

Since the operators associated with the bilinear forms $(h, h) \mapsto a_\varepsilon(h, h)$ are positive and self-adjoint, the one-term expansion of Steklov–Poincaré operators is obtained for $\varepsilon \to 0$,

$$\mathcal{A}_\varepsilon = \mathcal{A} - \varepsilon^2 \mathcal{B} + O(\varepsilon^{3-\alpha}),$$

with the remainder bounded in the operator norm $H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$. The self-adjoint positive linear operators $\mathcal{A}_\varepsilon$ are uniquely determined by the symmetric and coercive bilinear forms $h \mapsto a_\varepsilon(h, h)$. The operator $\mathcal{B}$ is determined by $h \mapsto b(h, h)$.

A.3 Asymptotic Expansion of a Linear Form

Let us now consider the linear form

$$L_\varepsilon(h) = \int_{\Omega_\varepsilon} f(x) w_\varepsilon(x) \mathrm{d}x.$$

We use the method of matched asymptotic expansions and set

$$w_\varepsilon(w) = w_0(x) + \varepsilon \sum_{j=1}^{2} \frac{\partial w_0}{\partial x_j}(0) \mathcal{Y}_0^j(\xi) + \varepsilon^2 \sum_{j,k=1}^{2} \frac{\partial w_0}{\partial x_j}(0) m_{jk}^\omega \mathcal{G}_0^{(k)}(x) + \cdots,$$

hence

$$L_\varepsilon(h) = \int_{\Omega_\varepsilon} f(x) w_0(x) \mathrm{d}x + \varepsilon \int_{\Omega_\varepsilon} f(x) \sum_{j=1}^{2} \frac{\partial w_0}{\partial x_j}(0) \mathcal{Y}_0^j(\xi)$$

$$+ \varepsilon^2 \int_{\Omega_\varepsilon} f(x) \sum_{j,k=1}^{2} \frac{\partial w_0}{\partial x_j}(0) m_{jk}^\omega \mathcal{G}_0^{(k)}(x) \mathrm{d}x.$$

Taking into account that

$$\left| \mathcal{Y}_0^j(\xi) \right| \leq C_0 \frac{1}{\|\xi\|} = C_0 \frac{\varepsilon}{\|x\|} \quad \text{in} \quad \Omega_\varepsilon,$$

it follows that

$$
L_\varepsilon(h) = \int_\Omega f(x) w_0(x) \mathrm{d}x - \int_{\omega_\varepsilon} f(x) w_0(x) \mathrm{d}x
$$

$$
+ \varepsilon^2 \int_\Omega f(x) \sum_{j,k=1}^2 \frac{\partial w_0}{\partial x_j}(0) m_{jk}^\omega \mathcal{G}^{(k)}(x) \mathrm{d}x + \cdots
$$

In order to replace the integrals over Ω_ε by integrals over Ω, we use the estimates

$$
\varepsilon \int_{\omega_\varepsilon} f(x) \sum_{j,k=1}^2 \frac{\partial w_0}{\partial x_j}(0) m_{jk}^\omega \frac{\varepsilon x_k}{2\pi \|x\|^2} \mathrm{d}x \leq C_0 \varepsilon^2 \sup_{x \in \overline{\Omega}} |f(x)| \int_0^\varepsilon \frac{1}{r} r \mathrm{d}r
$$

and

$$
\int_{\omega_\varepsilon} f(x) \sum_{j,k=1}^2 \frac{\partial w_0}{\partial x_j}(0) m_{jk}^\omega \mathcal{G}_0^{(k)}(x) \leq C_0 \varepsilon^2.
$$

Finally,

$$
L_\varepsilon(h) = L_0(h) - \varepsilon^2 f(0) w_0(0) |\omega| + \varepsilon^2 \int_\Omega f(x) \sum_{j,k=1}^2 \frac{\partial w_0}{\partial x_j}(0) m_{jk}^\omega \mathcal{G}^{(k)}(x) \mathrm{d}x + \cdots
$$

A.4 Energy Functional of the Nonhomogeneous Dirichlet Problem in a Perturbed Domain

The energy functional

$$
\mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2} \int_{\Omega_\varepsilon} \|\nabla u_\varepsilon\|^2 \mathrm{d}x - \int_{\Omega_\varepsilon} f u_\varepsilon \mathrm{d}x = \frac{1}{2} \int_\Gamma u_\varepsilon \frac{\partial u_\varepsilon}{\partial n} \mathrm{d}s - \frac{1}{2} \int_{\Omega_\varepsilon} f u_\varepsilon \mathrm{d}x
$$

depends on solutions to the boundary value problem

$$
\begin{aligned}
-\Delta u_\varepsilon &= f && \text{in } \Omega_\varepsilon, \\
u_\varepsilon &= h_\varepsilon && \text{on } \Gamma, \\
\frac{\partial u_\varepsilon}{\partial n} &= 0 && \text{on } \partial\omega_\varepsilon.
\end{aligned}
\tag{32}
$$

with the associated Green formula

$$
\int_{\Omega_\varepsilon} \|\nabla u_\varepsilon\|^2 \mathrm{d}x = \int_\Gamma h_\varepsilon \frac{\partial u_\varepsilon}{\partial n} \mathrm{d}s + \int_{\Omega_\varepsilon} f u_\varepsilon \mathrm{d}x.
$$

For completeness of our analysis, we assume that the Dirichlet boundary datum also depends on the small parameter,

$$h_\varepsilon = h_0 + \varepsilon^2 h_1 + o(\varepsilon^2) \quad \text{in} \quad H^{1/2}(\Gamma),$$

and that there is a source term inside the perturbed domain Ω_ε.

The approximation of solutions takes the form

$$u_\varepsilon(x) = v_0(x) + \varepsilon^2 v_1(x) + \varepsilon \sum_{j=1}^{2} \frac{\partial v_0}{\partial x_j}(0) \mathcal{Y}_0^j(\xi) + \varepsilon^2 \sum_{j,k=1}^{2} \frac{\partial v_0}{\partial x_j}(0) m_{jk}^\omega \mathcal{G}_0^{(k)}(x) + \cdots$$

where

$$-\Delta v_0 = f \quad \text{in } \Omega, \qquad \text{and} \qquad -\Delta v_1 = 0 \quad \text{in } \Omega,$$
$$v_0 = h_0 \quad \text{on } \Gamma, \qquad\qquad\qquad v_1 = h_1 \quad \text{on } \Gamma.$$

The approximation of the normal derivatives is

$$\frac{\partial u_\varepsilon}{\partial n}(x) = \frac{\partial v_0}{\partial n}(x) + \varepsilon^2 \frac{\partial v_1}{\partial n}(x) + \varepsilon \sum_{j=1}^{2} \frac{\partial v_0}{\partial x_j}(0) \frac{\partial \mathcal{Y}_0^j}{\partial \nu}(\xi)$$

$$+ \varepsilon^2 \sum_{j,k=1}^{2} \frac{\partial v_0}{\partial x_j}(0) m_{jk}^\omega \frac{\partial \mathcal{G}_0^{(k)}}{\partial n}(x) + \cdots$$

where $\dfrac{\partial}{\partial n} = n \cdot \nabla_x$, $\dfrac{\partial}{\partial \nu} = n \cdot \nabla_\xi$ and $\xi = x/\varepsilon$. We recall that the higher order term of $\mathcal{Y}_0^j(\xi)$ satisfies

$$\left| \mathfrak{y}_0^j(\xi) \right| \leq C_0 \frac{1}{\|\xi\|^2} = C_0 \frac{\varepsilon^2}{\|x\|^2} \quad \text{for} \quad \xi = \frac{x}{\varepsilon} \in \mathbb{R}^2 \backslash \omega \quad \text{or for} \quad x \in \Omega_\varepsilon.$$

Thus, in the approximation of $u_\varepsilon(x)$, the terms of order $O(\varepsilon^3)$,

$$\varepsilon \sum_{j=1}^{2} \frac{\partial v_0}{\partial x_j}(0) \mathfrak{y}_0^j(\xi)$$

can be neglected. Therefore, from the formula

$$u_\varepsilon(x) = v_0(x) + \varepsilon^2 v_1(x) + \varepsilon \sum_{j=1}^{2} \frac{\partial v_0}{\partial x_j}(0) \mathfrak{y}_0^j(\xi) + \varepsilon^2 \sum_{j,k=1}^{2} \frac{\partial v_0}{\partial x_j}(0) m_{jk}^\omega \mathcal{G}^{(k)}(x) + \cdots$$

we deduce

$$\frac{\partial u_\varepsilon}{\partial n}(x) = \frac{\partial v_0}{\partial n}(x) + \varepsilon^2 \frac{\partial v_1}{\partial n}(x) + \varepsilon^2 \sum_{j,k=1}^{2} \frac{\partial v_0}{\partial x_j}(0) m_{jk}^\omega \frac{\partial \mathcal{G}^{(k)}}{\partial n}(x) + \cdots,$$

and it follows that

$$u_\varepsilon(x) \frac{\partial u_\varepsilon}{\partial n}(x) = v_0(x) \frac{\partial v_0}{\partial n}(x)$$

$$+ \varepsilon^2 \left(v_1(x) \frac{\partial v_0}{\partial n}(x) + v_0(x) \frac{\partial v_1}{\partial n}(x) \right.$$

$$\left. + v_0(x) \sum_{j,k=1}^{2} \frac{\partial v_0}{\partial x_j}(0) m_{jk}^\omega \mathcal{G}^{(k)}(x) \right) + \cdots$$

since the second-order term

$$\frac{\partial v_0}{\partial n}(x) \sum_{j,k=1}^{2} \frac{\partial v_0}{\partial x_j}(0) m_{jk}^\omega \mathcal{G}^{(k)}(x)$$

vanishes, by taking into account that $\mathcal{G}^{(k)}(x) = 0$ on the boundary Γ. We return to the shape functional,

$$\mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2} \int_\Gamma u_\varepsilon(x) \frac{\partial u_\varepsilon}{\partial n}(x) \mathrm{d}s - \frac{1}{2} \int_{\Omega_\varepsilon} f u_\varepsilon \mathrm{d}x,$$

and find approximations for the integrals

$$\frac{1}{2} \int_\Gamma u_\varepsilon(x) \frac{\partial u_\varepsilon}{\partial n}(x) \mathrm{d}s = \frac{1}{2} \int_\Gamma v_0(x) \frac{\partial v_0}{\partial n}(x) \mathrm{d}s$$

$$+ \frac{\varepsilon^2}{2} \int_\Gamma \left(v_1(x) \frac{\partial v_0}{\partial n}(x) + v_0(x) \frac{\partial v_1}{\partial n}(x) \right) \mathrm{d}s$$

$$+ \frac{\varepsilon^2}{2} \int_\Gamma v_0(x) \sum_{j,k=1}^{2} \frac{\partial v_0}{\partial x_j}(0) m_{jk}^\omega \frac{\partial \mathcal{G}^{(k)}}{\partial n}(x) \mathrm{d}s + \cdots$$

and

$$-\frac{1}{2} \int_{\Omega_\varepsilon} f u_\varepsilon \mathrm{d}x = -\frac{1}{2} \int_{\Omega_\varepsilon} f v_0 \mathrm{d}x - \frac{\varepsilon^2}{2} \int_{\Omega_\varepsilon} f v_1 \mathrm{d}x$$

$$-\frac{\varepsilon^2}{2} \int_{\Omega_\varepsilon} f \sum_{j,k=1}^{2} \frac{\partial v_0}{\partial x_j}(0) m_{jk}^\omega \mathcal{G}^{(k)}(x) + \cdots,$$

which can be written as

$$
-\frac{1}{2}\int_{\Omega_\varepsilon} f u_\varepsilon dx = -\frac{1}{2}\int_{\Omega} f v_0 dx + \frac{1}{2}\int_{\omega_\varepsilon} f v_0 dx - \frac{\varepsilon^2}{2}\int_{\Omega} f v_1 dx + \frac{\varepsilon^2}{2}\int_{\omega_\varepsilon} f v_1 dx
$$

$$
-\frac{\varepsilon^2}{2}\int_{\Omega} f \sum_{j,k=1}^{2} \frac{\partial v_0}{\partial x_j}(0) m_{jk}^\omega \mathcal{G}^{(k)}(x) dx
$$

$$
+\frac{\varepsilon^2}{2}\int_{\omega_\varepsilon} f \sum_{j,k=1}^{2} \frac{\partial v_0}{\partial x_j}(0) m_{jk}^\omega \mathcal{G}^{(k)}(x) dx + \cdots
$$

or as

$$
-\frac{1}{2}\int_{\Omega_\varepsilon} f u_\varepsilon dx = -\frac{1}{2}\int_{\Omega} f v_0 dx + \frac{\varepsilon^2}{2} f(0) v_0(0)|\omega| - \frac{\varepsilon^2}{2}\int_{\Omega} f v_1 dx
$$

$$
-\frac{\varepsilon^2}{2}\int_{\Omega} f \sum_{j,k=1}^{2} \frac{\partial v_0}{\partial x_j}(0) m_{jk}^\omega \mathcal{G}^{(k)}(x) dx + O(\varepsilon^3).
$$

Here, we take into account that the Taylor formula $\frac{1}{2}\int_{\omega_\varepsilon} f v_0 dx$ is replaced by $\frac{\varepsilon^2}{2} f(0) v_0(0)|\omega|$. In the same way, it follows that $\frac{\varepsilon^2}{2}\int_{\omega_\varepsilon} f v_1 dx$ is $O(\varepsilon^4)$; finally, the latter integral over ω_ε is $O\left(\int_0^\varepsilon \frac{1}{r} r\right)$. As a result,

$$
\mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon) = \frac{1}{2}\int_{\Gamma} v_0(x)\frac{\partial v_0}{\partial n}(x) ds - \frac{1}{2}\int_{\Omega} f v_0 dx
$$

$$
+\frac{\varepsilon^2}{2}\int_{\Gamma} \left(v_1(x)\frac{\partial v_0}{\partial n}(x) + v_0(x)\frac{\partial v_1}{\partial n}(x) \right) ds
$$

$$
+\frac{\varepsilon^2}{2}\int_{\Gamma} v_0(x) \sum_{j,k=1}^{2} \frac{\partial v_0}{\partial x_j}(0) m_{jk}^\omega \frac{\partial \mathcal{G}^{(k)}}{\partial n}(x) ds
$$

$$
-\frac{\varepsilon^2}{2}\int_{\Omega} f \sum_{j,k=1}^{2} \frac{\partial v_0}{\partial x_j}(0) m_{jk}^\omega \mathcal{G}^{(k)}(x) dx
$$

$$
+\frac{\varepsilon^2}{2} f(0) v_0(0)|\omega| - \frac{\varepsilon^2}{2}\int_{\Omega} f v_1 dx.
$$

We denote by $B_\delta(\mathcal{O})$ the ball at the origin of radius δ, with boundary $\mathbb{S}_\delta := \mathbb{S}_\delta(\mathcal{O})$. By the Green formula in the domain $\Omega_\delta = \Omega \setminus \overline{B_\delta(\mathcal{O})}$ with boundary $\partial \Omega_\delta = \Gamma \cup \mathbb{S}_\delta$, for $\delta \to 0$,

$$
\int_{\Omega_\delta} (v_0 \Delta \mathcal{G}^{(k)} - \mathcal{G}^{(k)} \Delta v_0) dx = \int_{\partial \Omega_\delta} \left(v_0 \frac{\partial \mathcal{G}^{(k)}}{\partial n} - \mathcal{G}^{(k)} \frac{\partial v_0}{\partial n} \right) ds.
$$

Since $\Delta v_0 = -f$, we find

$$\int_{\Omega_\delta} \mathcal{G}^{(k)} f \, \mathrm{d}x = \int_\Gamma v_0 \frac{\partial \mathcal{G}^{(k)}}{\partial n} \mathrm{d}s + \int_{\mathbb{S}_\delta} \left(v_0 \frac{\partial \mathcal{G}^{(k)}}{\partial n} - \mathcal{G}^{(k)} \frac{\partial v_0}{\partial n} \right) \mathrm{d}s.$$

Passage to the limit $\delta \to 0$ leads to

$$\int_{\Omega_\delta} \mathcal{G}^{(k)} f \, \mathrm{d}x - \int_\Gamma v_0 \frac{\partial \mathcal{G}^{(k)}}{\partial n} \mathrm{d}s = \frac{\partial v_0}{\partial x_k}(0)$$

Finally, we arrive at the expression

$$\begin{aligned}
\mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon) = {} & \mathcal{J}_\Omega(v_0) + \frac{\varepsilon^2}{2} f(0) v_0(0) |\omega| - \frac{\varepsilon^2}{2} \sum_{j,k=1}^2 \frac{\partial v_0}{\partial x_j}(0) m_{jk}^\omega \frac{\partial v_0}{\partial x_k}(0) \\
& + \frac{\varepsilon^2}{2} \int_\Gamma \left(v_1(x) \frac{\partial v_0}{\partial n}(x) + v_0(x) \frac{\partial v_1}{\partial n}(x) \right) \mathrm{d}s \\
& - \frac{\varepsilon^2}{2} \int_\Omega f(x) v_1(x) \mathrm{d}x + O(\varepsilon^3).
\end{aligned}$$

Remark A.2 The adjoint equations are commonly used in final formulas for topological derivatives. We refer the reader to[80] for related results. Some asymptotic expansions for the Laplace operator are given in [81,82].

Remark A.3 The case of the elasticity system in the same framework of asymptotic analysis is considered in [11], where the results obtained are given with complete proofs.

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