TOPOLOGICAL DERIVATIVES OF SHAPE FUNCTIONALS. PART 1
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 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 admit the asymptotic analysis tools to perform the sensitivity of shape functionals with respect to small defects or imperfections. In classical numerical shape optimization the boundary variation technique is used for the purposes of the gradient or the Newton type algorithms. The shape sensitivity analysis is performed with 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 setting of shape sensitivity analysis is required for solution of topology optimization problems. A possible approach can be proposed in the framework of asymptotic analysis for singularly perturbed geometrical domains. In such a framework the approximations of solutions to boundary value problems (BVPs) in domains with small defects or imperfections are constructed e.g., by the methods of matched asymptotic expansions. The approximate solutions are employed in order to evaluate the shape functionals and as a result the topological derivatives of functionals are obtained, see e.g., [39]. 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 derivative has applications in many relevant fields such as shape and topology optimization, inverse problems, imaging processing, multiscale material design and mechanical modeling including damage and fracture evolution phenomena. In the first part of this review the topological derivative concept is presented in details within the framework of the domain decomposition technique.cSuch an approach is constructive e.g., for the coupled models in multiphysics as well as for contact problems in elasticity. In the second and third parts we respectively 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

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

The problem of shape optimization concerns minimization of a shape functional over a family of admissible domains. The shape functional depends directly on the geometrical domains Ω and implicitly by means of solutions $u = u(\Omega)$ to the state equation defined in Ω. For example, in structural mechanics the specific functional depends on solutions to the elasticity BVPs defined in the domains of integration

$$\Omega \mapsto \mathcal{J}_\Omega(u).$$

Key words and phrases. Topological derivatives, asymptotic analysis, singular perturbations, domain decomposition.

For practical applications we are interested in minimization of the shape functional over a family of admissible domains. From mathematical point of view there are questions to answer as usually in the calculus of variations:

(1) The existence of an optimal domain such that
$$\mathcal{J}_{\Omega^*}(u^*) \leq \mathcal{J}_{\Omega}(u).$$
(2) The necessary conditions for optimality which can be obtained for differentiable shape functionals.
(3) The convergence of numerical methods devised for solution of the shape optimization problem under considerations.

There is a vast literature on the subject, the representative sources are monographs [12, 51, 59] on the theory and applications in solids and fluids mechanics.

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 the generalized optimal solutions of shape optimization problems e.g. by means of the homogenization technique. As a result, the optimization procedure leads to optimal microstructures and there are subdomains of optimal domains filled with metamaterials. The methods are known in structural mechanics as the homogenization method, or the SIMP method, among others.

In this review we are interested in applications of asymptotic analysis tools and techniques in singularly perturbed geometrical domains [39] (see also e.g., [34, 36, 37]) to shape and topology optimization. Regarding the theoretical development of the topological asymptotic analysis, see for instance [4, 7, 8, 14, 16, 24, 30, 40, 47, 48, 52, 56, 57]. For an account of new developments in this branch of shape optimization we refer to the book by Novotny & Sokołowski [49].

2. Classical shape optimization and asymptotic analysis related to topological derivatives

Topological derivatives of shape functionals are introduced for elliptic BVPs quite recently. Instead of deformations of domains by diffeomorphism [12, 59], the asymptotic analysis in singularly perturbed geometrical domains is considered for the purposes of shape sensitivity analysis [39]. However, the first approach 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 numerical methods. In general, there is a close relationship between two types of approaches, the results obtained by the second approach can be also derived from the velocity method under some regularity assumptions for the elliptic BVPs. In another words, the knowledge of shape gradients and shape Hessians leads to the topological derivatives of e.g., the energy functionals under additional regularity assumptions. The asymptotic analysis is performed in the intact, unperturbed domains and locally requires the appropriate regularity of solutions. It is worth to say, that the classical shape sensitivity analysis can be performed by using the asymptotic analysis tools, only.

As a result of asymptotic analysis the function $\mathcal{T}(x)$ is identified for $x \in \Omega$, 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 $\Omega_\varepsilon = \Omega \setminus \overline{\omega_\varepsilon}$, where $\overline{\omega_\varepsilon} \subset \Omega$ represents the singular domain perturbation of size ε. Finally, $f(\varepsilon)$ is a positive function such that $f(\varepsilon) \to 0$ with $\varepsilon \to 0$. Therefore, the variation of the shape functional for 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 $\Omega \mapsto J(\Omega)$. In the first part of the review papers the qualitative results known for the Laplacian and the elasticity system are described. In the second and the third parts of review we respectively describe 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 these ideas, let us present a very simple example, namely:

Example 1. *The notion of topological derivative extends the conventional definition of derivative to functionals whose variable is 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*

$$J(\Omega) := |\Omega| = \int_\Omega 1, \tag{2.1}$$

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 can be obtained trivially in this case as

$$J(\Omega_\varepsilon) = |\Omega_\varepsilon| = \int_\Omega 1 - \int_{B_\varepsilon} 1 = J(\Omega) - \pi\varepsilon^2, \tag{2.2}$$

and the topological derivative $\mathcal{T}(x)$ and function $f(\varepsilon)$ promptly identified, respectively, as

$$\mathcal{T}(x) = -1, \quad f(\varepsilon) = \pi\varepsilon^2. \tag{2.3}$$

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

The particular case of shape optimization problems is minimization of a functional over an admissible set of characteristic functions [59]. In Example 1 the integral

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

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

The main idea of numerical methods based on the topological derivatives is the construction of an auxiliary level set function depending on the topological derivative in actual domain, see e.g., [5, 6, 20, 21]. In such a 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 actual topological derivative is used for modification of the actual shape. The shape is determined by the level set function. Therefore, within the topological derivative method there is no need for the complicated Hamilton-Jacoby equation to control the shape evolution. The shape evolution during the optimization procedure is governed by a simple updating algorithm based on the actual topological derivative. In numerical examples the proposed procedure converges to the local solution of the topology-shape optimization problem under considerations. Therefore, this method enters in the field of experimental mathematics. To our best knowledge the convergence of 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 the second order topological derivative concept is presented in the third part of the review. The two terms expansion of the functional is exploited, leading to a quadratic and strictly convex form with respect to the parameters under consideration. Thus, for the second order method, a trivial optimization step leads to a non-iterative algorithm, whose optimal solution is obtained in just one shot, we refer the reader to the third part of review for details and examples.

We speak on the ideas for elliptic problems and the singular perturbations of the principal part of the elliptic operator. There are also many problems when the lower order terms are only perturbed, and in such a case asymptotic analysis substantially simplifies.

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

3. Evaluation of topological derivatives

Evaluation of topological derivatives requires the approximation of solutions to elliptic BVPs with respect to small singular perturbations of geometrical domains. Such approximations are constructed e.g., in monographs [22, 32], see also [35, 38]. We refer the reader to [30] for the comparison of the known methods for evaluation of energy change due to the appearance of cavities in elastic solids. The methods of evaluation depend on the specific applications, we are particularly interested in numerical methods:

(1) The direct method of shape calculus combined with the asymptotic expansions of solutions proposed in the first paper on the topic [54]. In this method the Taylor expansion of shape functionals obtained in the framework of the speed method [59] is used to pass to the limit with the small perturbation parameter and obtain as a result the topological derivative of the specific shape functional. The method is improved in [55] and finally uses the first shape derivatives only. We present an example of the asymptotic expansions for the Laplacian in Appendix. The method is difficult to use for variational inequalities. See e.g., [10] for an application of the standard asymptotic analysis to the Signorini problem performed under the hypothesis of strict complementarity for unknown solutions.
(2) The direct method of two scale asymptotic analysis [39] performed for elliptic systems and leading in particular to the self-adjoint extensions of elliptic operators. In this method the appropriate adjoint state equations can be introduced at the end of the procedure of evaluation in order to simplify the formulas for the topological derivatives. In other words first, the two scale asymptotic approximation of solutions with prescribed precision is constructed, and it is used to derive the approximation of the functional. Finally, the convenient form of topological derivatives is given for the purposes of numerical methods. The complete proofs of obtained results are given in [39].
(3) The method using fundamental solutions in truncated domains and the standard two scale expansions techniques of asymptotic analysis, see e.g., [53]. 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. We also refer to [4] for the compound asymptotic analysis combined with a modified adjoint sensitivity method.
(4) The method using the technique of integral equations in electromagnetism proposed e.g., in [18] and [3], for instance. We refer to the recent book [2] for modeling the effect of defects in elasticity using well-established asymptotic formulas with some applications to imaging.
(5) The domain decomposition technique with the asymptotic expansions of Steklov-Poincaré operators for small defects [57]. 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 method has been used in many numerical examples, see e.g., [1, 17].

The evaluation technique depends on the shape functionals under considerations. If there is a state equation, the evaluation process usually includes the asymptotic expansions of solutions with respect to small parameter $\varepsilon \to 0$ which governs the size of singular geometrical perturbation. We restrict ourselves to the elliptic BVPs like the Laplace or Helmholtz equations as well as to the systems in linear elasticity or Stokes. The expansion depends on the spatial dimensions $d = 2, 3$, since we use the fundamental solutions to the associated elliptic equations. The most important for applications are the elliptic equations in three spatial dimensions. The general mathematical theory of solution's expansions which applies to the elasticity system can be found e.g., in [39], see also [46] for the polarization tensors associated with the elasticity system. The results are given for arbitrary shapes of cavities or holes however the closed formulas are available only for some shapes [46]. Once the result is known we have some methods which can be used for the identification of topological derivatives. We are particularly interested in numerical methods which are used in the framework of topological optimization. Therefore, the topological derivatives should be given by the robust expressions which are approximated by the standard finite element methods. The simplest way of evaluation, it seems, is the application of the domain decomposition technique, in order to determine the topological derivatives for nonlinear as well as for coupled models in multiphysics [57], see also [53] for an early attempt to the truncated domain approach without Steklov-Poincaré operators.

To be more specific we are going to explain in details the asymptotic expansions in two spatial dimensions in Appendix. The Neumann problem on the hole of arbitrary shape is analysed in Section 6. Such an analysis is required for the direct methods of asymptotic analysis. To simplify the derivation we are going also to explain the application of Steklov-Poincaré operators to the asymptotic analysis of the elliptic BVPs. Without the state equation the problem of evaluation is simpler, it becomes purely geometrical problem, we refer to [13] for recent results in this direction.

In order to obtain the form of topological derivatives, the appropriate asymptotic analysis of associated partial differential equation should be performed. There are some monographs on the subject, e.g., [22, 32]. We provide simple examples for singularly perturbed geometrical domains of scalar elliptic problems. The method of matched asymptotic expansions is applied. The obtained results in this domain are borrowed from the publications, which are due to the long and fruitful collaboration with the Russian mathematician Serguei A. Nazarov [11, 28, 39, 40, 41, 42, 43, 44, 45, 46]. In particular, the asymptotic analysis of elasticity BVPs for the purposes of topology optimization can be found e.g., in [39]. See also [9] for further developments within matched asymptotic expansions for the Laplacian. In general, the form of topological derivative is given in terms of the adjoint states and of the polarization tensors. This is an additional difficulty for numerical methods of topology optimization using the topological derivatives.

4. Asymptotic expansions for domain decomposition technique

The most important method of evaluation of topological derivatives for numerical methods of topology optimization is the domain decomposition technique. In particular, the topological derivatives for BVPs of coupled models in multiphysics are obtained in the framework of domain decomposition technique combined with the 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 considered for linear elliptic problems as well as for variational inequalities. Numerical applications of such a method can be found e.g., for shape-topology optimization in the piezo-elasticity [1] or in the thermo-elasticity [17].

4.1. **Asymptotic expansions of Steklov-Poincaré operators.** We want to apply the domain decomposition method for evaluation of topological derivatives. For complex models the first step od such evaluation is always the local analysis of singular perturbations of geometrical domains. Thus, e.g., in the linear elasticity in two or three spatial dimensions with the traction free hole or cavity we consider the ring $C(R, \varepsilon)$ like domain and obtain the asymptotic expansion of the Steklov-Poincaré operators associated to the elasticity problem, defined on its external boundary Γ_R, with respect to the small parameter $\varepsilon \to 0$. The second step of evaluation is the sensitivity analysis of regular perturbations of bilinear form in the truncated domain Ω_R.

We consider the family of perturbations Ω_ε of the reference domain Ω by small holes or a small cavities $\omega_\varepsilon(\widehat{x})$, with the centre $\widehat{x} \in \Omega$. The proposed method consists in the approximation of singular domain perturbations by the regular perturbation of the bilinear form $v \to a(\Omega; v, v)$ in variational formulation of elliptic boundary value problem under considerations. 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 $v \to \varepsilon^d b(\Gamma_R; v, v)$. The bilinear form $v \to b(\Gamma_R; v, v)$ can be determined from the asymptotic expansions of Steklov-Poincaré operators defined at the interface Γ_R i.e., from the topological derivative of the energy functional in the domain $\Omega_\varepsilon \setminus \overline{\Omega_R}$. We provide all necessary details in this section with some examples.

Remark 2. *In a sense our approach is similar but it is not equivalent, to the so-called self-adjoint extensions of the elliptic operators* [50] *as it is used in physics, see e.g.,* [39, 40, 42, 44] *for the applications to asymptotic approximations which lead to the equivalent formulae for topological derivatives. In another words, we are able to define another mathematical model in the intact domain in such a way that the first order asymptotic expansion of the energy functional is the same if compared to the original model. For the self-adjoint extensions the domain* Ω_ε *is replaced* *by the punctured domain $\Omega \setminus \{\widehat{x}\}$ while in our approach the resulting 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 the polarization tensors or matrices [11, 46] in order to use the topological derivatives in numerical methods e.g., of shape and topology optimization.

4.2. **Signorini problem in two spatial dimensions.** We explain the domain decomposition technique used in the approximation of the quadratic energy functionals for the purposes of evaluation of topological derivatives [57]. We restrict ourselves to the homogeneous Neumann boundary conditions on the holes to simplify the presentation.

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

$$a(u,v) = a(\Omega; u,v) = \int_\Omega \nabla u \cdot \nabla v dx$$

is coercive and continuous over the Sobolev space

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

and the linear form

$$L(v) = L(\Omega; v) = \int_\Omega f v dx$$

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

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

where the convex and closed set

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

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

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

with the solution given by the unique minimizer of quadratic functional

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

over the convex set $K_\varepsilon := K(\Omega_\varepsilon)$. We use the notation $(v,v) \to a_\varepsilon(v,v) = a(\Omega_\varepsilon; v,v)$ and $v \to L_\varepsilon(v) = L(\Omega_\varepsilon; v)$ in the singularly perturbed domain Ω_ε.

We can show that there is an approximation of the quadratic functional

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

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

$$H^{1/2}(\Gamma_R) \times H^{1/2}(\Gamma_R) \ni (v,v) \to b(\Gamma_R; v,v)$$

such that

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

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

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

then the minimizer u^R_ε of $v \to I^R_\varepsilon(v)$ over the convex cone $K(\Omega)$ admits in $H^1(\Omega_R)$ the same first order expansion

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

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

In this way the singular domain perturbation Ω_ε is replaced by a regular perturbation of the bilinear form, i.e., the bilinear form in Ω_ε is approximated by the bilinear form in the unperturbed domain Ω augmented by the correction term defined on the portion Γ_R of its boundary

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

To this end the topological derivatives of energy functional in singularly perturbed domain are used in order to evaluated the first order expansion of the Steklov-Poincaré operators.

4.3. **From singular domain perturbations to regular perturbations of bilinear forms.** Now, we are going to present the abstract scheme of asymptotic analysis for solutions of variational problems posed in singularly perturbed geometrical domains. For the sake of simplicity let us consider the linear problems.

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

$$u := u_\Omega \in H \ : \ a(u, \varphi) = L(\varphi) \qquad \forall \varphi \in H$$

is given by a unique minimizer of quadratic functional

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

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

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

The energy shape functional is defined for the domain Ω,

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

We consider the singular geometrical perturbation $\Omega_\varepsilon := \Omega \setminus \overline{B_\varepsilon(\widehat{x})}$ of the reference domain by a small circle or a 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 first subdomain Ω_R is a ball $B_R(\widehat{x})$ which includes the singular geometrical perturbation of the reference domain, say $B_\varepsilon(\widehat{x})$. The energy functional in perturbed domain

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

where $C(R, \varepsilon)$ is a ring. Now, we would like to introduce a bounded perturbation of bilinear form

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

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 in Ω_R of the solutions u_ε restricted to the truncated domain, namely it holds

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

in $H(\Omega_R)$ for $R > \varepsilon > 0$.

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 $C(R, \varepsilon)$.

Thus, we introduce two subdomains $\Omega_R := \Omega \setminus \overline{B_R(\widehat{x})}$ and $\Omega_\varepsilon := \Omega \setminus \overline{B_\varepsilon(\widehat{x})}$ of the reference domain. Here $\widehat{x} \in \Omega$ is a given point, $R > \varepsilon > 0$ are two parameters such that $\varepsilon \to 0$ and

$\overline{B_\varepsilon(\widehat{x})} \subset \Omega$. $\Omega_R \subset \Omega$ is the truncated domain, and Ω_ε is the singularly perturbed domain. Thus, we associate with the domains the quadratic functionals

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

and

$$I(\Omega_\varepsilon; \varphi) := \frac{1}{2} a(\Omega_\varepsilon; \varphi, \varphi) - L(\Omega_\varepsilon; \varphi) \tag{4.1}$$

obtained by restriction of the test functions $\varphi \in H(\Omega)$ to Ω_R (respectively to Ω_ε). For the sake of simplicity we denote

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

and

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

Our goal is to construct the quadratic functional which produces the restriction u_ε^R to Ω_R of the variational solution u_ε in the singularly perturbed domain. The variational solution in Ω is given by

$$u \in H \ : \ a(u, \varphi) = L(\varphi) \qquad \forall \varphi \in H$$

and the variational problem in perturbed domain is given by

$$u_\varepsilon \in H_\varepsilon \ : \ a_\varepsilon(u_\varepsilon, \varphi) = L_\varepsilon(\varphi) \qquad \forall \varphi \in H_\varepsilon$$

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 the ring

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

Thus, 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 latter expansion

$$b(h, h) := (\mathcal{B}(h), h)_{\Gamma_R} = \mathcal{T}(\widehat{x})(h, h)$$

It can be shown that minimization of the first order approximation of the quadratic functional (4.3) over the intact domain leads to the first order expansion of the minimizers for the perturbed domain, which holds however only restricted to the truncation domain (4.4), namely:

Theorem 3. *The first order expansion of the solution to the truncated problem posed in the intact domain reads*

$$u_\varepsilon^R = u^R + \varepsilon^d q^R + o(\varepsilon^d) \tag{4.2}$$

holds in $H^1(\Omega)$ for the variational problem obtained by the first order approximation of the quadratic functional

$$I_\varepsilon^R(\varphi) = \frac{1}{2} a(\Omega; \varphi, \varphi) + \frac{1}{2} \varepsilon^d (\mathcal{B}(\varphi), \varphi)_{\Gamma_R} - L(\Omega_R; \varphi). \tag{4.3}$$

Corollary 4. *In the case of variational equations for the minimization of* (4.1) *we have the same result. Indeed, the first order expansion of the minimizers $\varepsilon \to u_\varepsilon$ restricted to the truncated domain Ω_R, i.e., for $R > \varepsilon > 0$*

$$u_{\varepsilon|\Omega_R} = u_{|\Omega_R} + \varepsilon^d q^R + o(\varepsilon^d) \tag{4.4}$$

is preserved when using the minimization of (4.3) *since e.g., for the second order elliptic boundary value problems*

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

and $u^R = u_{|\Omega_R}$.

From this property we have the possibility to obtain the topological derivatives of shape functionals defined by integrals in the truncated domain only, which is a new result in the field of topological derivatives, it seems.

Corollary 5. *The topological derivative of the tracking type functional for variational inequalities*

$$J(\Omega_\varepsilon) = \frac{1}{2}\int_{\Omega_R} (u_\varepsilon - z_d)^2 dx \tag{4.5}$$

is simply given by the expression

$$\mathcal{T}(\widehat{x}) = \int_{\Omega_R} (u^R(x) - z_d(x))q^R(x)dx = \int_{\Omega_R} (u(x) - z_d(x))q(x)dx, \tag{4.6}$$

Remark 6. *The topological derivative of the tracking type functional* (4.5) *for variational equations can be simplified by using the adjoint state equation.*

4.4. **Regular perturbations of energy functional for the purposes of topological differentiability.** The domain decomposition method of evaluation of topological derivatives uses the asymptotic expansions of the energy functional is a small neighborhood of the singular domain perturbation created by a hole or a cavity. In our applications, the energy expansions are equivalent to the expansions of nonlocal Steklov-Poincaré boundary operators. In the truncated domain the perturbations of boundary conditions with the expansion of Steklov-Poincaré boundary operators lead to the regular perturbations of the bilinear form and allow us to avoid the self-adjoint extensions of elliptic operators in the punctured domains.

The energy functionals of elliptic BVPs are of great importance for shape and topology optimization. The topological derivatives of the energy shape functionals are given by expressions which contains the appropriate polarization tensors, see e.g., [49]. The domain decomposition method requires the asymptotic expansion of the Steklov-Poincaré operator on the interface Γ_R which is obtained from the asymptotic expansion of the energy in the ring $\Omega_\varepsilon \setminus \overline{\Omega_R}$.

Evaluation of topological derivatives of the energy in the ring $\Omega_\varepsilon \setminus \overline{\Omega_R}$ in two spatial dimensions is based on the explicit solutions to linear elliptic BVPs in function of small parameter. Thus, the perturbed domain Ω_ε is decomposed into two subdomains, a ring and its complement in Ω_ε. Exact solutions of BVP in the ring $C(R, \varepsilon) = \{0 < \varepsilon < \|x\| < R \subset \Omega\}$ give rise to the asymptotic expansion for the energy of the Steklov-Poincaré operator defined on $\Gamma_R = \{\|x\| = R\}$. The operator furnishes nonlocal boundary conditions on $\Gamma_R \subset \partial\Omega_R$ for the BVPs in the truncated domain Ω_R.

4.5. **Topological derivatives of energy functional for variational inequalities.** The variational inequalities which are considered in calculus of variations and lead to the free BVPs of elliptic type. The well known examples include the obstacle problems for Laplacian and bilaplacian, the frictionless contact problem in linearized elasticity as well as the contact problem with the Coulomb friction. Shape optimization for variational inequalities is performed in the framework of nonsmooth optimization [59]. The topological derivatives of shape functionals for the frictionless contact problems in elasticity are obtained in [57], see also [49]. The Hadamard differentiability of metric projection onto polyhedric convex sets [33] can be exploited for the purposes of shape sensitivity analysis of the unilateral problems. The case of polyhedric convex sets in the Sobolev spaces of Dirichlet type is well understood now from the point of view of shape and topology optimization [59, 49]. The domain decomposition technique is an efficient tool for evaluation of topological derivatives in such a case.

4.6. **Approximation of energy functionals combined with the domain decomposition method.** The standard topological derivative methodology developed by the authors in many papers requires knowledge of point-wise values of solutions to partial differential equations or variational equalities. However, the contact or unilateral problems are studied in the energy space setting, where point-wise values of weak solutions are not well defined. The authors proposed the new approach based on domain decomposition combined with the expansion of the

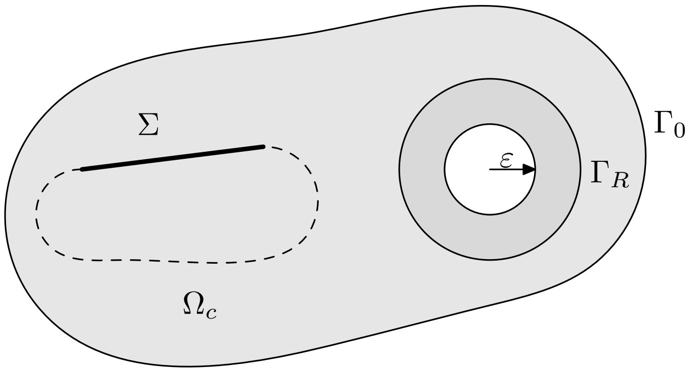

FIGURE 1. Domain Ω_ε with crack Σ.

Steklov-Poincaré operator with respect to small parameter which governs the size of imperfections to cope with such technical difficulties. As a result the regular perturbations of bilinear forms are determined in order to model the imperfections. The appropriate formulas were given for elasticity operator in 2D and 3D problems.

The proposed domain decomposition method is important for variational inequalities since the asymptotic analysis for variational inequalities is more involved compared to linear elliptic BVPs. The variational inequality under consideration results from the minimization problem of quadratic functional

$$v \mapsto I(v) = \frac{1}{2} a(v, v) - L(v) \tag{4.7}$$

over a convex, closed subset $K \subset H$ of the Hilbert space H called the energy space. The function space $H := H(\Omega)$ is a Sobolev space which contains the functions defined over a domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$.

The singular geometrical perturbation ω_ε (void) centred at $\widehat{x} \in \Omega$ of the domain Ω is denoted by Ω_ε, the size of perturbation is governed by a small parameter $\varepsilon \to 0$. The quadratic functional defined on $H := H(\Omega_\varepsilon)$ becomes

$$v \mapsto I_\varepsilon(v) = \frac{1}{2} a_\varepsilon(v, v) - L_\varepsilon(v) \tag{4.8}$$

with the minimizers $u_\varepsilon \in K := K(\Omega_\varepsilon)$. The expansion of associated energy functional

$$\varepsilon \mapsto \mathcal{E}(\Omega_\varepsilon) := I_\varepsilon(u_\varepsilon) = \frac{1}{2} a_\varepsilon(u_\varepsilon, u_\varepsilon) - L_\varepsilon(u_\varepsilon) \tag{4.9}$$

is considered at $\varepsilon = 0$. Namely, we are looking for its asymptotic expansion

$$\mathcal{E}(\Omega_\varepsilon) = \mathcal{E}(\Omega) + \varepsilon^d \mathcal{T}(\widehat{x}) + o(\varepsilon^d), \tag{4.10}$$

where $\widehat{x} \mapsto \mathcal{T}(\widehat{x})$ is the topological derivative.

It can be shown that there are regular perturbations of bilinear form defined on the energy space $H(\Omega)$,

$$v \mapsto b(v, v)$$

such that the perturbed quadratic functional defined on the unperturbed function space $H(\Omega)$

$$v \mapsto I^\varepsilon(v) = \frac{1}{2} \Big[a(v, v) + \varepsilon^d b(v, v) \Big] - L(v) \tag{4.11}$$

furnishes the first order expansion (4.10). In our applications to contact problems in linear elasticity it turns out that the bilinear form $v \mapsto b(v, v)$ is supported on $\Gamma_R := \{\|x - \widehat{x}\| = R\} \subset \Omega$ with $R > \varepsilon > 0$.

4.7. **Energy for elasticity BVPs.** 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 the 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 this void has its centre at the origin $\mathcal{O}$. In order to eliminate the variability of the domain, 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 denote also 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, namely the Dirichlet-to-Neumann mapping for linear elasticity which is called the Steklov-Poincaré operator

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

by means of the boundary value problem:

$$\begin{aligned} &\mu \Delta w + (\lambda + \mu) \nabla (\operatorname{div} w) = 0, \;\text{ in }\; C(R, \varepsilon), \\ &w = v \;\text{ on }\; \Gamma_R, \quad \sigma(u) n = 0 \;\text{ on }\; \Gamma_\varepsilon, \end{aligned} \tag{4.12}$$

so that

$$\mathcal{A}_\varepsilon(v) = \sigma(w) n \;\text{ on }\; \Gamma_R. \tag{4.13}$$

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

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

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

$$I_\varepsilon^R(\varphi_\varepsilon) = \frac{1}{2} \int_{\Omega_R} \sigma(\varphi_\varepsilon) \cdot (\nabla \varphi_\varepsilon)^s \, dx - \int_{\Gamma_N} h \cdot \varphi_\varepsilon \, ds + \frac{1}{2} \int_{\Gamma_R} \mathcal{A}_\varepsilon(\varphi_\varepsilon) \cdot \varphi_\varepsilon \, ds \tag{4.14}$$

and the solution u_ε^R as a minimal argument for

$$I_\varepsilon^R(u_\varepsilon^R) = \inf_{\varphi_\varepsilon \in K \subset V_\varepsilon} I_\varepsilon^R(\varphi_\varepsilon), \tag{4.15}$$

Here lies the essence of the domain decomposition concept: we have replaced the variable domain $\varepsilon \to \Omega_\varepsilon$ by a fixed truncated domain Ω_R, at the price of introducing variable boundary operator $\mathcal{A}_\varepsilon$. Thus, the goal is to find the asymptotic expansion

$$\mathcal{A}_\varepsilon = \mathcal{A} + \varepsilon^d \mathcal{B} + \mathcal{R}_\varepsilon, \tag{4.16}$$

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

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

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 7. *Assume that* (4.16) *holds in the operator norm. Then strong convergence takes place*

$$u_\varepsilon^R \to u^R \tag{4.17}$$

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

Proposition 8. *The energy functional has the representation*

$$I_\varepsilon^R(u_\varepsilon^R) = I^R(u^R) + \varepsilon^d \langle \mathcal{B}(u^R), u^R \rangle_R + o(\varepsilon^d) \;, \tag{4.18}$$

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

Here $I^R(u^R)$ denotes the functional I^R_ε on the intact 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 plane stress

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

and for $d = 3$

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

see [49, 56]. 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 the formulas for topological derivatives which are similar to the expressions obtained for the corresponding linear BVPs.

4.7.1. *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 [57] that the following exact formulae hold

$$\begin{aligned}
u_{1,1}(\mathcal{O}) + u_{2,2}(\mathcal{O}) &= \frac{1}{\pi R^3}\int_{\Gamma_R}(u_1x_1 + u_2x_2)\,ds,\\
u_{1,1}(\mathcal{O}) - u_{2,2}(\mathcal{O}) &= \frac{1}{\pi R^3}\int_{\Gamma_R}\Big[(1-9k)(u_1x_1 - u_2x_2) + \frac{12k}{R^2}(u_1x_1^3 - u_2x_2^3)\Big]\,ds,\\
u_{1,2}(\mathcal{O}) + u_{2,1}(\mathcal{O}) &= \frac{1}{\pi R^3}\int_{\Gamma_R}\Big[(1+9k)(u_1x_2 + u_2x_1) - \frac{12k}{R^2}(u_1x_2^3 + u_2x_1^3)\Big]\,ds.
\end{aligned}$$

These expressions are easy to compute numerically, but contain additional integrals of third powers of x_i. Therefore, strains evaluated at $\mathcal{O}$ may be expressed as linear combinations of integrals over circle which have 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 stresses $\sigma_{ij}(\mathcal{O})$. They may then be substituted into expression for the operator $\mathcal{B}$, 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.

4.7.2. *Explicit form of the operator $\mathcal{B}$ in three spatial dimensions.* It turns out that similar situation holds in three spatial dimensions, but obtaining the formulas is more difficult. Assuming given values of u on Γ_R, the solution of elasticity system in B_R may be expressed, following partially the derivation from [31] (pages 285 and later), as

$$u = \sum_{n=0}^{\infty}[U_n + (R^2 - r^2)k_n(\nu)\nabla(\operatorname{div} U_n)]. \tag{4.19}$$

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

$$U_n = \frac{1}{R^n}[a_{n0}d_n(x) + \sum_{m=1}^{n}(a_{nm}c_n^m(x) + b_{nm}s_n^m(x))]. \tag{4.20}$$

The vectors

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

are constant 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 the 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,

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

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

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

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

$$\begin{aligned} a_{n0}^i &= R^n\langle u_i, d_n(x)\rangle_R, \\ a_{nm}^i &= R^n\langle u_i, c_n^m(x)\rangle_R, \\ b_{nm}^i &= R^n\langle u_i, s_n^m(x)\rangle_R. \end{aligned} \tag{4.21}$$

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:

$$\hat{u} = U_1 + R^2k_3(\nu)\nabla(\operatorname{div} U_3). \tag{4.22}$$

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

$$\begin{aligned} \hat{u} &= \frac{1}{R}[a_{10}d_1(x) + a_{11}c_1^1(x) + b_{11}s_1^1(x))] \\ &\quad + R^2k_3(\nu)\frac{1}{R^3}\Big[H(d_3)(x)a_{30} + \sum_{m=1}^{3}\big(H(c_3^m)(x)a_{3m} + H(s_3^m)(x)b_{3m}\big)\Big] \end{aligned} \tag{4.23}$$

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

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

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 $c_1^1 = \frac{1}{R^2}\sqrt{\frac{3}{4\pi}}x_1$, $s_1^1 = \frac{1}{R^2}\sqrt{\frac{3}{4\pi}}x_2$, $d_1 = \frac{1}{R^2}\sqrt{\frac{3}{4\pi}}x_3$.

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

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

but the right-hand side consists of integrals of u multiplied by first and third order polynomials in x_i over Γ_R resulting from (4.21). This is a very similar situation as in two spatial dimensions. Thus, the new expressions for strains make possible to rewrite $\mathcal{B}$ in the form possessing the desired regularity.

5. Perspectives and Open Problems

The topological derivative method in shape and topology optimization introduces the asymptotic analysis of elliptic BVPs e.g., into the field of structural optimization in elasticity. The method requires the local regularity of solutions to elliptic problems. Nowadays, the classical shape optimization techniques are not restricted to elliptic problems, but can be applied to evolution problems including linear parabolic and hyperbolic equations. The extension of topological derivative method to evolution problems is one of challenging issues in the field of shape optimization. In particular, for the 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 [51]. Another domain which is promising for the developments of shape optimization is the nonlinear elasticity. The evolution of geometrical domains is used within the growth modeling. The shape and topology optimization for nonlinear elasticity is still poorly known issue. The topological derivatives can be also used for optimization of microstructures for the metamaterials design. This could be a modern application of topological derivatives for producing the new optimal microstructures for the metamaterials design. There is already some numerical evidence that this approach is well adapted to the design of metamaterials in elasticity.

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

(1) *Differentiability of energy functionals.* It is known that the shape derivatives of energy type functionals can be obtained by the Gamma-limit procedure, see e.g., the derivation of the elastic energy with respect to the crack length [26, 27], see also [23, 25, 29] for the related topics.
(2) *Sensitivity analysis of variational inequalities.* Shape optimization for variational inequalities is studied in [59]. The obtained results are based on the Hadamard differentiability of metric projection onto convex sets in Sobolev spaces [19, 33, 58]. The known results are obtained by using the potential theory in Dirichlet spaces [15] which leads to the Hadamard differentiablity of metric projection.
(3) *Asymptotic analysis of variational inequalities.* The asymptotic analysis of variational inequalities was studied e.g., by Argatov and Sokolowski [10]. The concept of polyhedral subsets of the Sobolev spaces can be used in order to derive the topological derivatives for contact problems in solid mechanics. The case of linearized elasticity can be considered. The open problems are some models of plates and the shells and the Hencky plasticity. This domain of research is in stagnation for a long time already. The mathematical result which is required concerns the directional differentiability of the metric projection onto the convex set defined by the local constraints on the stresses.

(4) *The necessary optimality conditions.* The first order necessary optimality conditions are known in the case of linear state equations [56]. Using the second order topological derivatives for the purposes of derivation of optimality conditions seems to be an open problem.
(5) *Exact solutions of elasticity with complex Kolosov potentials and Steklov-Poincaré formalism in domain decomposition.* Using complex potentials of Kolosov the exact solutions of elasticity system in two spatial dimensions are obtained. These results leads to topological derivatives of arbitrary order. The extension of such results to full range of models in mechanics is an interesting issue of research which is to be completed in the literature.
(6) *Exact solutions of wave equations.* The important field of application concerns electromagnetism, which are not standard from the mathematical point of view for the asymptotic analysis. The open problems are the field of wave equations in all aspects including the mathematical asymptotic analysis in singularly perturbed geometrical domains.
(7) *Exact solutions of transport equations.* The domain decomposition method is known for the transport problems. The open problems are the field of transport equations in all aspects including the mathematical asymptotic analysis in singularly perturbed geometrical domains. Finally, the compressible Navier-Stokes equations can be considered from the point of view of singular domain perturbations.
(8) *Open problems for variational inequalities.* Beside the energy functionals and the case of variational inequalities with polyhedric convex sets in ordered Sobolev spaces the shape and topology optimization is not developed. Namely, for other type variational inequalities with local constraints on gradients or on stresses the shape and topological sensitivity analysis is in general an open problem. The case of the Hencky plasticity is an example with no results, to our best knowledge, neither on shape optimization nor on topological derivatives.

6. Appendix

6.1. **Asymptotic expansions of solutions and functionals.** For the convenience of the reader the two scale asymptotic analysis of nonhomogeneous boundary value problem is performed for a simple model problem. The small cavity $\omega_\varepsilon := \varepsilon\omega$ with the centre at the origin $\mathcal{O} \in \omega_\varepsilon \subset \omega$ can be considered without loss of generality. In general we denote by the same symbol $\omega_\varepsilon(\widehat{x}) := \widehat{x}+\omega_\varepsilon$ the cavity with the centre at $\widehat{x} \in \Omega$. The matched asymptotic expansions are used in two spatial dimensions for scalar problems with the Laplacian.

6.2. **Asymptotic expansions of Steklov-Poincaré operators.** We denote the smooth domain $\Omega_\varepsilon := \Omega \setminus \overline{\omega_\varepsilon}$ for $\varepsilon \to 0$ and let us consider the nonhomogeneous Dirichlet problem with $h \in H^{1/2}(\Gamma)$,

$$\left\{ \begin{array}{rcll} \Delta w_\varepsilon &=& 0 & \text{in} \quad \Omega_\varepsilon \,, \\ w_\varepsilon &=& h & \text{on} \quad \Gamma \,, \\ \dfrac{\partial w_\varepsilon}{\partial n} &=& 0 & \text{on} \quad \partial\omega_\varepsilon \,, \end{array} \right. \tag{6.1}$$

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

The energy associated with (6.1) is given by the symmetric bilinear form on fractional Sobolev space $H^{1/2}(\Gamma)$

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

We are interested in the asymptotic expansion of the quadratic functional for $\varepsilon \to 0$. To this end the technique of matched asymptotic expansions [22, 32] is used.

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

$$a_\varepsilon(h,h) = \int_\Gamma w_\varepsilon \frac{\partial w_\varepsilon}{\partial n} ds = \int_\Gamma h \frac{\partial w_\varepsilon}{\partial n} ds \tag{6.2}$$

Now, we introduce the 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

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

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

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

where the fast variable ξ is defined by

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

Following [22, 32] 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 $\mathbb{R}^2 \setminus \overline{\omega}$ 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

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

Its regular part is denoted by

$$\mathcal{Y}^j_0(\xi) := \frac{1}{2\pi\|\xi\|^2} \sum_{k=1}^{2} m^\omega_{kj} \xi_k + O(\|\xi\|^{-2}),$$

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

$$\mathfrak{y}^j_0(\xi) := \mathcal{Y}^j_0(\xi) - \frac{1}{2\pi\|\xi\|^2} \sum_{k=1}^{2} m^\omega_{kj} \xi_k,$$

Taking into account this expansion, we get

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

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

$$\begin{cases} \Delta_x \mathcal{G}^{(k)}(x) = 0 & \text{in} \quad \Omega \setminus \mathcal{O}, \\ \mathcal{G}^{(k)}(x) = 0 & \text{on} \quad \Gamma, \\ \mathcal{G}^{(k)}(x) = \dfrac{x_k}{2\pi\|x\|^2} + O(1) & \|x\| \to 0. \end{cases} \tag{6.3}$$

We put

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

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

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

Substituting this representation into formula (6.2) we obtain 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

$$b(h,h) = \int_\Gamma h(x) \sum_{j,k=1}^{2} \frac{\partial w_0}{\partial x_j}(0) m^\omega_{kj} \frac{\partial \mathcal{G}^{(k)}}{\partial n}(x) ds$$

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

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

we get

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

Since

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

it follows that

$$b(h,h) = -\left(\int_\Gamma h(x) \partial_n \mathcal{G}^{(j)}(x) ds \right) m^\omega_{jk} \left(\int_\Gamma h(x) \partial_n \mathcal{G}^{(k)}(x) ds \right) ds.$$

Remark 9. *It can be shown that the following supremum taken with respect to $H^{1/2}(\Gamma)$-norm is bounded with respect to $\varepsilon \to 0$,*

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

Since the operators associated to 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 $H^{1/2}(\Gamma) \mapsto H^{-1/2}(\Gamma)$. 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 $h \mapsto b(h,h)$.

6.3. **Asymptotic expansion of linear form.** Let us now consider the linear form

$$L_\varepsilon(h) = \int_{\Omega_\varepsilon} f(x) w_\varepsilon(x) dx$$

We use the method of matched asymptotic expansions and set

$$w_\varepsilon(w) = w_0(x) + \varepsilon \sum_{j=1}^{2} \frac{\partial w_0}{\partial x_j}(0) \mathcal{Y}^j_0(\xi) + \varepsilon^2 \sum_{j,k=1}^{2} \frac{\partial w_0}{\partial x_j}(0) m^\omega_{jk} \mathcal{G}^{(k)}_0(x) + \dots$$

hence

$$L_\varepsilon(h) = \int_{\Omega_\varepsilon} f(x) w_0(x) dx + \varepsilon \int_{\Omega_\varepsilon} f(x) \sum_{j=1}^{2} \frac{\partial w_0}{\partial x_j}(0) \mathcal{Y}^j_0(\xi) + \varepsilon^2 \int_{\Omega_\varepsilon} f(x) \sum_{j,k=1}^{2} \frac{\partial w_0}{\partial x_j}(0) m^\omega_{jk} \mathcal{G}^{(k)}_0(x) dx$$

Taking into account that

$$\left| \mathcal{Y}^j_0(\xi) \right| \le C_0 \frac{1}{\|\xi\|} = C_0 \frac{\varepsilon}{\|x\|} \quad \text{in} \quad \Omega_\varepsilon$$

it follows that

$$L_\varepsilon(h) = \int_\Omega f(x) w_0(x) dx - \int_{\omega_\varepsilon} f(x) w_0(x) dx + \varepsilon^2 \int_\Omega f(x) \sum_{j,k=1}^{2} \frac{\partial w_0}{\partial x_j}(0) m^\omega_{jk} \mathcal{G}^{(k)}(x) dx + \dots$$

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

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

and

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

Finally,

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

6.4. **Energy functional of nonhomogeneous Dirichlet problem in peturbed domain.** The energy functional

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

depends on solutions to the boundary value problem

$$\left\{ \begin{array}{rcll} -\Delta u_\varepsilon &=& f & \text{in } \Omega_\varepsilon \,, \\ u_\varepsilon &=& h_\varepsilon & \text{on } \Gamma \,, \\ \dfrac{\partial u_\varepsilon}{\partial n} &=& 0 & \text{on } \partial\omega_\varepsilon \,. \end{array} \right. \tag{6.4}$$

with the associated Green's formula

$$\int_{\Omega_\varepsilon} \|\nabla u_\varepsilon\|^2 dx = \int_\Gamma h_\varepsilon \frac{\partial u_\varepsilon}{\partial n} ds + \int_{\Omega_\varepsilon} f u_\varepsilon dx$$

Here, 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 of the perturbated domain Ω_ε.

The approximation of solutions takes the form

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

where

$$\left\{ \begin{array}{rcll} -\Delta v_0 &=& f & \text{in } \Omega \,, \\ v_0 &=& h_0 & \text{on } \Gamma \,, \end{array} \right. \quad \text{and} \quad \left\{ \begin{array}{rcll} -\Delta v_1 &=& 0 & \text{in } \Omega \,, \\ v_1 &=& h_1 & \text{on } \Gamma \,. \end{array} \right.$$

The approximation of the normal derivatives

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

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

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

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

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

we deduce

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

and it follows that

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

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

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

and find the approximations for the integrals,

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

and

$$-\frac{1}{2}\int_{\Omega_\varepsilon} f u_\varepsilon dx = -\frac{1}{2}\int_{\Omega_\varepsilon} f v_0 dx - \frac{\varepsilon^2}{2}\int_{\Omega_\varepsilon} f v_1 dx - \frac{\varepsilon^2}{2}\int_{\Omega_\varepsilon} f \sum_{j,k=1}^{2} \frac{\partial v_0}{\partial x_j}(0) m_{jk}^\omega \mathcal{G}^{(k)}(x) + \dots,$$

which can be written as

$$-\frac{1}{2}\int_{\Omega_\varepsilon} f u_\varepsilon dx = -\frac{1}{2}\int_{\Omega} f v_0 dx + \frac{1}{2}\int_{\omega_\varepsilon} f v_0 dx - \frac{\varepsilon^2}{2}\int_{\Omega} f v_1 dx + \frac{\varepsilon^2}{2}\int_{\omega_\varepsilon} f v_1 dx - \frac{\varepsilon^2}{2}\int_{\Omega} f \sum_{j,k=1}^{2} \frac{\partial v_0}{\partial x_j}(0) m_{jk}^\omega \mathcal{G}^{(k)}(x)dx + \frac{\varepsilon^2}{2}\int_{\omega_\varepsilon} f \sum_{j,k=1}^{2} \frac{\partial v_0}{\partial x_j}(0) m_{jk}^\omega \mathcal{G}^{(k)}(x)dx + \dots$$

or as follows

$$-\frac{1}{2}\int_{\Omega_\varepsilon} f u_\varepsilon dx = -\frac{1}{2}\int_{\Omega} f v_0 dx + \frac{\varepsilon^2}{2} f(0) v_0(0)|\omega| - \frac{\varepsilon^2}{2}\int_{\Omega} f v_1 dx - \frac{\varepsilon^2}{2}\int_{\Omega} f \sum_{j,k=1}^{2} \frac{\partial v_0}{\partial x_j}(0) m_{jk}^\omega \mathcal{G}^{(k)}(x)dx + O(\varepsilon^3)$$

Where we take into account that using the Taylor formula $\frac{1}{2}\int_{\omega_\varepsilon} fv_0dx$ is replaced by $\frac{\varepsilon^2}{2}f(0)v_0(0)|\omega|$, in the same way it follows that $\frac{\varepsilon^2}{2}\int_{\omega_\varepsilon} fv_1dx$ is $O(\varepsilon^4)$; finally, the latter integral over ω_ε is of the type $O\left(\int_0^\varepsilon \frac{1}{r}r\right)$. As a result

$$\begin{aligned}\mathcal{J}_{\Omega_\varepsilon}(u_\varepsilon) &= \frac{1}{2}\int_\Gamma v_0(x)\frac{\partial v_0}{\partial n}(x)ds - \frac{1}{2}\int_\Omega fv_0dx \\ &+ \frac{\varepsilon^2}{2}\int_\Gamma\left(v_1(x)\frac{\partial v_0}{\partial n}(x) + v_0(x)\frac{\partial v_1}{\partial n}(x)\right)ds + \frac{\varepsilon^2}{2}\int_\Gamma v_0(x)\sum_{j,k=1}^{2}\frac{\partial v_0}{\partial x_j}(0)m_{jk}^\omega\frac{\partial \mathcal{G}^{(k)}}{\partial n}(x)ds \\ &- \frac{\varepsilon^2}{2}\int_\Omega f\sum_{j,k=1}^{2}\frac{\partial v_0}{\partial x_j}(0)m_{jk}^\omega\mathcal{G}^{(k)}(x)dx + \frac{\varepsilon^2}{2}f(0)v_0(0)|\omega| - \frac{\varepsilon^2}{2}\int_\Omega fv_1dx.\end{aligned}$$

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

$$\int_{\Omega_\delta}\mathcal{G}^{(k)}fdx = \int_\Gamma v_0\frac{\partial\mathcal{G}^{(k)}}{\partial n}ds + \int_{\mathbb{S}_\delta}\left(v_0\frac{\partial\mathcal{G}^{(k)}}{\partial n} - \mathcal{G}^{(k)}\frac{\partial v_0}{\partial n}\right)ds.$$

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

$$\int_{\Omega_\delta}\mathcal{G}^{(k)}fdx - \int_\Gamma v_0\frac{\partial\mathcal{G}^{(k)}}{\partial n}ds = \frac{\partial v_0}{\partial x_k}(0)$$

Finally, we arrive at the expression

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

Acknowledgements

This research was partly supported by CNPq (Brazilian Research Council), CAPES (Brazilian Higher Education Staff Training Agency) and FAPERJ (Research Foundation of the State of Rio de Janeiro). These supports are gratefully acknowledged.

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