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TOPOLOGICAL DERIVATIVES FOR SEMILINEAR ELLIPTIC EQUATIONS

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The form of topological derivatives for an integral shape functional is derived for a class of semilinear elliptic equations. The convergence of finite element approximation for the topological derivatives is shown and the error estimates in the L^∞ norm are obtained. The results of numerical experiments which confirm the theoretical convergence rate are presented.

Keywords: shape optimization, topological derivative, levelset method, variational inequality, asymptotic analysis.

1. Introduction

1.1. Topological derivatives in shape optimization. Topological derivatives are introduced for linear problems in (Sokolowski and Zochowski, 1999) and for variational inequalities in (Sokolowski and Zochowski, 2005). The mathematical theory of asymptotic analysis is applied in (Nazarov and Sokolowski, 2003; 2006) for the derivation of topological derivatives in shape optimization of elliptic boundary values problems. Numerical solutions of shape optimization problems for variational inequalities obtained by the level set method combined with topological derivatives are presented in (Fulmanski *et al.*, 2007)

In the paper we present topological derivatives for semilinear elliptic boundary value problems. In the first part, asymptotic analysis of a class of boundary value problems for a second order semilinear differential equation is performed. In the second part, the convergence of our finite element approximation for the topological derivatives is proved, and the results of numerical experiments are presented as well.

Topological sensitivity analysis aims to provide an asymptotic expansion of a shape functional with respect to the size of a small hole created inside the domain. For a criterion $j(\Omega) = \mathcal{J}(u_\Omega;\Omega)$, where $\Omega \subset \mathbb{R}^N$ ($N = 2$ or 3) and u_Ω is a solution of a set of partial differential equations defined over Ω, this expansion can be generally written in the form

$$j(\Omega\setminus(\overline{\mathcal{O}+\omega_\varepsilon}))-j(\Omega) = f(\varepsilon)\mathcal{T}_\Omega(\mathcal{O},\omega)+o(f(\varepsilon)). \quad (1)$$

Here ε and $\mathcal{O}$ denote respectively the diameter and the center of the hole, ω is a fixed domain containing the origin $\mathcal{O}$ and $f(\varepsilon)$ is a positive function tending to zero with ε. The coefficient $\mathcal{T}_\Omega$ is commonly called *the topological derivative*.

1.2. Semilinear elliptic equation. Let Ω and ω be bounded domains in $\mathbb{R}^3$ with the smooth boundaries $\partial\Omega$ and $\partial\omega$ and the compact closures $\overline{\Omega}$ and $\overline{\omega}$, respectively. The origin $\mathcal{O}$ of the coordinate system is assumed to belong to the domains Ω and ω. The following sets are introduced:

$$\begin{aligned}\omega_\varepsilon &= \left\{x \in \mathbb{R}^3 : \xi := \varepsilon^{-1}x \in \omega\right\},\\ \Omega(\varepsilon) &:= \Omega \setminus \overline{\omega_\varepsilon},\end{aligned} \quad (2)$$

where $x = (x_1, x_2, x_3)$ are Cartesian coordinates in the domain Ω and $\varepsilon > 0$ is a small parameter. The upper bound $\varepsilon_0 > 0$ is chosen in such a way that for $\varepsilon \in (0, \varepsilon_0]$ the set $\overline{\omega_\varepsilon}$ belongs to the domain Ω. We can diminish the value of $\varepsilon_0 > 0$ in the sequel, if necessary. However, the notation for the bound ε_0 remains unchanged. The set ω_ε is called a hole, or an opening, in the domain $\Omega(\varepsilon)$.

In this paper, we consider a nonlinear elliptic problem in the singularly perturbed domain $\Omega(\varepsilon)$:

$$\begin{cases} -\Delta_x u^\varepsilon(x) = F(x, u^\varepsilon(x)), & x \in \Omega(\varepsilon), \\ u^\varepsilon(x) = 0, & x \in \partial\Omega(\varepsilon). \end{cases} \tag{3}$$

Here $F \in C^{0,\alpha}(\Omega \times \mathbb{R})$ and $f \in C^{0,\alpha}(\Omega)$ are given functions, independent of the parameter ε. Asymptotic analysis in the linear case is well known (see the monographs (Il'in, 1989; Mazja *et al.*, 1991)), e.g., for the Dirichlet boundary value problem for the Poisson equation:

$$\begin{cases} -\Delta_x u^\varepsilon(x) = f(x), & x \in \Omega(\varepsilon), \\ u^\varepsilon(x) = 0, & x \in \partial\Omega(\varepsilon). \end{cases} \tag{4}$$

According to the method of compound asymptotic expansions (Mazja *et al.*, 1991), in asymptotic analysis of (4) there appear two limit problems. The first one is obtained by formally taking $\varepsilon = 0$, e.g., by filling the hole $\overline{\omega_\varepsilon}$:

$$\begin{cases} -\Delta_x u(x) = f(x), & x \in \Omega, \\ u(x) = 0, & x \in \partial\Omega, \end{cases} \tag{5}$$

and the second one is the boundary value problem, which furnishes the leading boundary layers term:

$$\begin{cases} -\Delta_\xi w(\xi) = 0, & \xi \in \mathbb{R}^3 \setminus \overline{\omega}, \\ w(\xi) = -u(\mathcal{O}), & \xi \in \partial\omega, \end{cases} \tag{6}$$

where $u(\mathcal{O})$ is the value at the origin of the solution of (5).

As in (Mazja *et al.*, 1981) (see also Ch. 5.7 in (Mazja *et al.*, 1991)), for the nonlinear problem (3) we obtain also two limit problems. The first one is nonlinear,

$$\begin{cases} -\Delta_x v(x) = F(x, v(x)), & x \in \Omega, \\ v(x) = 0, & x \in \partial\Omega, \end{cases} \tag{7}$$

and the second one is the linear exterior problem (6) with $u(\mathcal{O}) := v(\mathcal{O})$ given by the solution to (7).

Our aim in this paper is the construction of asymptotic approximations for solutions to (3) in such a way that we will be able to obtain an expansion of a given shape functional

$$\mathcal{J}(u^\varepsilon; \Omega(\varepsilon)) = \int_{\Omega(\varepsilon)} J(x, u^\varepsilon(x))\, \mathrm{d}x, \tag{8}$$

of the first order with respect to ε, namely,

$$\mathcal{J}(u^\varepsilon; \Omega(\varepsilon)) = \mathcal{J}(v; \Omega) + \varepsilon \mathcal{T}_\Omega(\mathcal{O}) + o(\varepsilon), \tag{9}$$

(cf. (1)), where

$$\mathcal{J}(v; \Omega) = \int_{\Omega} J(x, v(x))\, \mathrm{d}x, \tag{10}$$

and $\mathcal{T}_\Omega$ is the topological derivative of the functional $\mathcal{J}$.

Apart from that, we need the linearized problem (7), which gives us the regular terms in the asymptotic approximation,

$$\begin{cases} -\Delta_x V(x) - F'_v(x, v(x))V(x) = \mathcal{F}(x), & x \in \Omega, \\ V(x) = g(x), & x \in \partial\Omega. \end{cases} \tag{11}$$

The solution V is but the so-called the adjoint state. The adjoint state is introduced in order to simplify the expression for the topological derivative.

Appropriate function spaces are employed to analyze the solvability of all boundary value problems introduced above. The weighted Hölder spaces $\Lambda^{l,\alpha}_\beta(\Omega)$ are defined (Mazja and Plamenevskii, 1978) as the closure of $C_c^\infty(\overline{\Omega} \setminus \mathcal{O})$ (smooth functions vanishing in the vicinity of $\mathcal{O}$) in the norm

$$\begin{aligned} &\|Z; \Lambda^{l,\alpha}_\beta(\Omega)\| \\ &= \sum_{k=0}^{l} \sup_{x\in\Omega} |x|^{\beta-l-\alpha+k} |\nabla^k_x Z(x)| \\ &+ \sup_{x,y\in\Omega, |x-y|<|x|/2} |x|^\beta |x-y|^{-\alpha} |\nabla^l_x Z(x) - \nabla^l_y Z(y)|. \end{aligned}$$

The standard norm in the Hölder space $C^{l,\alpha}(\Omega)$ is as follows:

$$\begin{aligned} &\|Z; C^{l,\alpha}(\Omega)\| \\ &= \sum_{k=0}^{l} \sup_{x\in\Omega} |\nabla^k_x Z(x)| \\ &+ \sup_{x,y\in\Omega, |x-y|<|x|/2} |x-y|^{-\alpha} |\nabla^l_x Z(x) - \nabla^l_y Z(y)|. \end{aligned}$$

Here $l \in \{0, 1, \dots\}$, $\alpha \in (0, 1)$ and $\beta \in \mathbb{R}$.

Now we introduce several assumptions which are required to define the topological derivatives:

(H1) The limit problem (7) has a solution $v \in C^{2,\alpha}(\Omega)$ and $F \in C^{0,1}(\overline{\Omega} \times \mathbb{R})$ with a certain $\alpha \in (0, 1)$.

(H2) The linear problem (11) with $\mathcal{F} \in C^{0,\alpha}(\Omega)$, $g \in C^{2,\alpha}(\partial\Omega)$ has a unique solution $V \in C^{2,\alpha}(\Omega)$,

$$\|V; C^{2,\alpha}(\Omega)\| \le c(\|\mathcal{F}; C^{0,\alpha}(\Omega)\| + \|g; C^{2,\alpha}(\partial\Omega)\|). \tag{12}$$

Here and in the sequel c stands for a positive constant that may change from place to place but never depends on ε.

(H3) $F'_v \in C^{0,\alpha}(\overline{\Omega} \times \mathbb{R})$.

If **(H3)** holds true and $F'_v(x, v(x)) \le 0$ for $x \in \Omega$, then **(H2)** is also satisfied.

The hypothesis **(H2)** means the existence and uniqueness of classical solutions to the linearized problem in Hölder spaces $C^{2,\alpha}(\Omega)$ with the a priori estimate (12). It turns out that the linear mapping for the problem (11), i.e.,

$$S : \{\mathcal{F}, g\} \longmapsto V, \tag{13}$$

is an isomorphism in the Hölder spaces $C^{0,\alpha}(\Omega) \times C^{2,\alpha}(\partial\Omega) \rightarrow C^{2,\alpha}(\Omega)$. By a general result in (Mazja and Plamenevskii, 1978), (see also (Nazarov and Plamenevsky, 1994)), the operator remains to be an isomorphism in weighted Hölder spaces under the proper choice of indices.

Theorem 1. *Under the assumptions **(H2)** and **(H3)**, the mapping (13) considered in the weighted Hölder spaces*

$$S : \Lambda_\beta^{0,\alpha}(\Omega) \times C^{2,\alpha}(\partial\Omega) \longmapsto \Lambda_\beta^{2,\alpha}(\Omega)$$

is an isomorphism if and only if $\beta - \alpha \in (2, 3)$.

The following result on asymptotics is due to (Kondratiev, 1967; Mazja and Plamenevskii, 1978) (see also (Mazja and Plamenevskii, 1973) and, e.g., (Nazarov and Plamenevsky, 1994)).

Theorem 2. *If the right hand side in (11)* $\mathcal{F} \in \Lambda_\gamma^{0,\alpha}(\Omega)$ *and* $\gamma - \alpha \in (1, 2)$, *then the solution* V *to (11) can be decomposed into* $V(x) = \widetilde{V}(x) + V(\mathcal{O})$ *and the following estimate holds:*

$$|V(\mathcal{O})| + \|\widetilde{V}; \Lambda_\gamma^{2,\alpha}(\Omega)\| \leq c(\|\mathcal{F}; \Lambda_\gamma^{0,\alpha}(\Omega)\| + \|g; C^{2,\alpha}(\partial\Omega)\|). \quad (14)$$

An assertion, similar to Theorem 1, is valid for the perforated domain $\Omega(\varepsilon)$ as well. The following result is due to (Mazja *et al.*, 1981) (see also (Mazja *et al.*, 1991; Nazarov and Plamenevsky, 1994))

Theorem 3. *Under the assumptions **(H2)** and **(H3)**, the linearized problem*

$$\begin{cases} -\Delta_x v^\varepsilon(x) - F'_v(x, v(x))v^\varepsilon(x) = \mathcal{F}^\varepsilon(x), & x \in \Omega(\varepsilon), \\ v^\varepsilon(x) = g^\varepsilon(x), & x \in \partial\Omega(\varepsilon) \end{cases} \quad (15)$$

is uniquely solvable and the solution operator

$$S_\varepsilon : \{\mathcal{F}^\varepsilon, g^\varepsilon\} \longmapsto v^\varepsilon \quad (16)$$

is bounded in the weighted Hölder spaces

$$S_\varepsilon : \Lambda_\beta^{0,\alpha}(\Omega(\varepsilon)) \times \Lambda_\beta^{2,\alpha}(\partial\Omega(\varepsilon)) \longmapsto \Lambda_\beta^{2,\alpha}(\Omega(\varepsilon)) .$$

Moreover, in the case when $\beta - \alpha \in (2, 3)$ *the estimate*

$$\|v^\varepsilon; \Lambda_\beta^{2,\alpha}(\Omega(\varepsilon))\| \leq c_\beta(\|\mathcal{F}^\varepsilon; \Lambda_\beta^{0,\alpha}(\Omega(\varepsilon))\| + \|g^\varepsilon; \Lambda_\beta^{2,\alpha}(\partial\Omega(\varepsilon))\|) \quad (17)$$

is valid, where the constant c_β *is independent of* $\varepsilon \in (0, \varepsilon_0]$.

Remark 1. Since $|x| \geq c\varepsilon > 0$ in $\Omega(\varepsilon)$, the weighted norm $\| \cdot ; \Lambda_\beta^{2,\alpha}(\Omega(\varepsilon))\|$ is equivalent to the usual norm $\| \cdot ; C^{2,\alpha}(\Omega(\varepsilon))\|$. However; the equivalence constants depend on ε. Thus $\Lambda_\beta^{2,\alpha}(\Omega(\varepsilon))$ and $C^{2,\alpha}(\Omega(\varepsilon))$ coincide algebraically and topologically but are normed in a different way. The norm of the operator S_ε is uniformly bounded for $\varepsilon \in (0, \varepsilon_0]$ for any β, although the constant c_β in (17) depends on ε provided $\beta \notin (2, 3)$, that is, the norm of the inverse operator is uniformly bounded in $\varepsilon \in (0, \varepsilon_1]$ only in the case of $\beta \in (2, 3)$.

For the nonlinear problem (3), we shall use the classical solutions to the boundary value problem (3), which means that for given $F \in C^{0,\alpha}(\overline{\Omega} \times \mathbb{R})$, $\alpha \in (0, 1)$, the solution lives in $C^{2,\alpha}(\overline{\Omega})$. We refer to (Ladyzhenskaya and Ural'tseva, 1968; Gilbarg and Trudinger, 2001) for a result on the existence and uniqueness of solutions to semilinear elliptic boundary value-problems. This means, in particular, that the problem (3) admits a unique solution $u^\varepsilon \in C^{2,\alpha}(\Omega(\varepsilon))$ for some $0 < \alpha < 1$ and for all $\varepsilon \in [0, \varepsilon_0)$.

2. Topological derivative for semilinear problems in 3D

We present here a complete analysis of the semilinear elliptic problem in three spatial dimensions. Such an analysis is interesting on its own, since in the existing literature there is no elementary derivation of the form of topological derivatives for nonlinear problems besides (Mazja *et al.*, 1981), (see also (Mazja *et al.*, 1991)), i.e., using asymptotic approximations of solutions to nonlinear PDEs. There are some results on topological derivatives of the shape functional for nonlinear problems, see, e.g., (Amstutz, 2006). However, such results are given in terms of one term exterior approximation of the solutions and without an asymtotically sharp estimate.

2.1. Formal asymptotic analysis.

Referring to (Mazja *et al.*, 1991), we set

$$u^\varepsilon(x) = v(x) + w(\varepsilon^{-1}x) + \varepsilon v'(x) + \cdots , \quad (18)$$

where v, v' and w are components of regular and boundary layer types, respectively. Thus,

$$\begin{aligned} -\Delta_x v(x) - \varepsilon^{-2}\Delta_\xi w(\xi) - \varepsilon\Delta_x v'(x) + \cdots \\ = F(x, v(x) + w(\varepsilon^{-1}x) + \varepsilon v'(x) + \cdots) \\ = F(x, v(x)) + (w(\varepsilon^{-1}x) \\ + \varepsilon v'(x))F'_v(x, v(x)) + \cdots . \end{aligned} \quad (19)$$

In view of (7), the first terms on the left and right-hand sides are cancelled and, moreover, w satisfies the problem (6) with $u(\mathcal{O}) = v(\mathcal{O})$,

$$\begin{cases} -\Delta_\xi w(\xi) = 0, & \xi \in \mathbb{R}^3 \setminus \overline{\omega}, \\ w(\xi) = -v(\mathcal{O}), & \xi \in \partial\omega, \end{cases} \quad (20)$$

while the boundary datum comes from the relation

$$v(x) + w(\varepsilon^{-1}x) + \varepsilon v'(x) = v(\mathcal{O}) + w(\varepsilon^{-1}x) + O(\varepsilon), \quad x \in \partial\omega_\varepsilon.$$

We have

$$w(\xi) = -v(\mathcal{O})P(\xi), \tag{21}$$

where P is the capacity potential (Landkof, 1966; Pólya and Szegö, 1951), e.g., a harmonic function in $\mathbb{R}^3 \setminus \overline{\omega}$ such that $P(\xi) = 1$ on $\partial\omega$ and

$$P(\xi) = |\xi|^{-1}\mathrm{cap}(\omega) + O(|\xi|^{-2}), \tag{22}$$

where $\mathrm{cap}(\omega)$ is the capacity of the set $\overline{\omega}$. Since

$$w(\varepsilon^{-1}x) = -|x|^{-1}\varepsilon v(\mathcal{O})\mathrm{cap}(\omega) + O(\varepsilon^2|x|^{-2}), \tag{23}$$

we collect coefficients on ε in (19) and obtain

$$\begin{cases} -\Delta_x v'(x) - v'(x)F'_v(x, v(x)) \\ \qquad = -a\Phi(x)F'_v(x, v(x)), \quad x \in \Omega, \\ \qquad v'(x) = a\Phi(x), \quad x \in \partial\Omega, \end{cases} \tag{24}$$

where $a = 4\pi v(\mathcal{O})\mathrm{cap}(w)$ and $\Phi(x) = (4\pi|x|)^{-1}$ is the fundamental solution of the Laplace equation in $\mathbb{R}^3$.

Since a direct calculation yields $F'(\cdot, v)\Phi \in \Lambda^{0,\alpha}_\gamma(\Omega)$ with any $\gamma > 1 + \alpha$, we obtain the solution $v' \in \Lambda^{2,\alpha}_\beta(\Omega)$ of the problem (24) such that $v' - v'(\mathcal{O}) \in \Lambda^{2,\alpha}_\gamma(\Omega)$ where $\beta - \alpha \in (2, 3)$ and $\gamma - \alpha \in (1, 2)$ can be taken arbitrarily in the prescribed intervals.

2.2. Justification of asymptotic.

We search for a solution of the problem (3) in the form

$$u^\varepsilon(x) = v(x) + w(\varepsilon^{-1}x) + \varepsilon v'(x) + \hat{u}^\varepsilon(x), \tag{25}$$

where $\hat{u}^\varepsilon$ is a small remainder, satisfying the problem

$$\begin{cases} -\Delta_x \hat{u}^\varepsilon(x) = \hat{\mathcal{F}}^\varepsilon(x; \hat{u}), & x \in \Omega(\varepsilon), \\ \hat{u}^\varepsilon(x) = \hat{g}^\varepsilon_\Omega(x), & x \in \partial\Omega, \\ \hat{u}^\varepsilon(x) = \hat{g}^\varepsilon_\omega(x), & x \in \partial\omega(\varepsilon). \end{cases} \tag{26}$$

Here

$$\begin{aligned} \hat{\mathcal{F}}^\varepsilon(x; \hat{u}) = {} & F(x, v(x) + w(\varepsilon^{-1}x) + \varepsilon v'(x) \\ & + \hat{u}^\varepsilon(x)) - F(x, v(x)) \\ & - \varepsilon(v'(x) - a\Phi(x))F'_v(x, v(x)), \end{aligned} \tag{27}$$

$$\hat{g}^\varepsilon_\Omega(x) = -w(\varepsilon^{-1}x) - a\varepsilon\Phi(x),$$
$$\hat{g}^\varepsilon_\omega(x) = -v(x) + v(\mathcal{O}) - \varepsilon v'(x).$$

We are going to employ the Banach contraction principle and, thus, we need to estimate the norms of (27).

Owing to (21), (22), the function $x \mapsto w(\varepsilon^{-1}x) + a\varepsilon\Phi(x)$ is smooth on the surface $\partial\Omega$, where $|x| \ge c > 0$, and

$$\begin{aligned} |w(\varepsilon^{-1}x) &+ a\varepsilon\Phi(x)| \\ &\le |v(\mathcal{O})||P(\xi) - \mathrm{cap}(\omega)|\xi|^{-1}| \\ &\le c\varepsilon^2|x|^{-2} \le c\varepsilon^2, \\ |\nabla^k_x w(\varepsilon^{-1}x) &+ a\varepsilon\nabla^k_x\Phi(x)| \\ &\le \varepsilon^{-k}|v(\mathcal{O})||\nabla^k_\xi P(\xi) - \mathrm{cap}(\omega)\nabla^k_\xi|\xi|^{-1}| \\ &\le c\varepsilon^{-k}|\xi|^{-2-k} = c\varepsilon^2|x|^{-2-k} \le c\varepsilon^2. \end{aligned} \tag{28}$$

Hence, by the above inequalities for the function $x \mapsto w(\varepsilon^{-1}x) + a\varepsilon\Phi(x)$, we obtain the following estimates of the norm of $\hat{g}^\varepsilon_\Omega$ in the weighted Hölder space :

$$\begin{aligned} \|\hat{g}^\varepsilon_\Omega; \Lambda^{2,\alpha}_\beta(\partial\Omega)\| &\le c\|\hat{g}^\varepsilon_\Omega; C^{2,\alpha}(\partial\Omega)\| \\ &\le c\|\hat{g}^\varepsilon_\Omega; C^3(\partial\Omega)\| \le c\varepsilon^2. \end{aligned} \tag{29}$$

Moreover, for $\beta - \beta' > 0$, we have

$$\begin{aligned} &\|\hat{g}^\varepsilon_\omega; \Lambda^{2,\alpha}_\beta(\partial\Omega)\| \\ &\le c(\sup_{x\in\partial\omega_\varepsilon}\sum_{k=0}^{2}|x|^{\beta-2-\alpha+k}(|\nabla^k_x(v(x) - v(\mathcal{O}))| \\ &\quad + \varepsilon|\nabla^k_x v'(x)|) + \sup_{x,y\in\partial\omega_\varepsilon}|x|^\beta|x-y|^{-\alpha}(|\nabla^2_x v(x) \\ &\quad - \nabla^2_y v(y)| + \varepsilon|\nabla^2_x v'(x) - \nabla^2_y v'(y)|)) \\ &\le c(\varepsilon^{\beta-1-\alpha}\|v; C^{2,\alpha}(\Omega)\| + \varepsilon^{1+\beta-\beta'}\|v'; \Lambda^{2,\alpha}_{\beta'}(\Omega)\|). \end{aligned} \tag{30}$$

Notice that $v' \in \Lambda^{2,\alpha}_{\beta'}(\partial\Omega)$ with arbitrary $\beta' \in (2 + \alpha, 3 + \alpha)$. We shall further select the indices β and β' in an appropriate way.

Write

$$\begin{aligned} \mathbf{F}(x, V(x)) = {} & F(x, v(x) + V(x)) \\ & - F(x, v(x)) - V(x)F'_v(x, v(x)), \end{aligned} \tag{31}$$

so that

$$\begin{aligned} &\hat{\mathcal{F}}^\varepsilon(x; \hat{u}^\varepsilon) \\ &= \mathbf{F}(x, w(\varepsilon^{-1}x) + \varepsilon v'(x) + \hat{u}^\varepsilon(x)) \\ &\quad + (w(\varepsilon^{-1}x) + \varepsilon a\Phi(x) + \hat{u}^\varepsilon(x))F'_v(x, v(x)). \end{aligned} \tag{32}$$

Since $(x \mapsto F'_v(x, v(x))) \in C^{0,\alpha}(\Omega)$, by **(H3)**, we take into account the representation (22) together with the inequality $\beta - \alpha > 2$ and, as a result, we obtain

$$\begin{aligned} &\|(w + \varepsilon a\Phi)F'_v; \Lambda^{0,\alpha}_\beta(\Omega(\varepsilon))\| \\ &\le c\left(\sup_{x\in\Omega(\varepsilon)}|x|^{\beta-\alpha}\left(\frac{|x|}{\varepsilon}\right)^{-2}\right. \\ &\quad + \left(\sup_{x,y\in\Omega(\varepsilon),|x-y|<|x|/2}|x|^\beta|x-y|^{-\alpha}\right. \\ &\quad \left.\left.\cdot\left|\frac{x}{\varepsilon} - \frac{y}{\varepsilon}\right|\left(\frac{|x|}{\varepsilon}\right)^{-3}\right)\right. \\ &\le c\varepsilon^2\sup_{x\in\Omega(\varepsilon)}(|x|^{\beta-\alpha}|x|^{-2} + |x|^{\beta+1-\alpha}|x|^{-3}) \\ &\le c\varepsilon^2. \end{aligned} \tag{33}$$

To estimate the first term on the right-hand side of (32), we need the following assumption on **F**:

(H4) With a certain $\kappa \in (0,1)$ and for $|V(x)| \le C$, $x \in \Omega$, the inequality $|\mathbf{F}(x,V(x))| \le c|V(x)|^{1+\kappa}$ and the following relations are valid:

$$\begin{aligned}&|\mathbf{F}(x,V_1(x)) - \mathbf{F}(y,V_2(y))|\\ &\quad\le c(|x-y|^\alpha(|V_1(x)|+|V_2(y)|)^{1+\kappa}\\ &\qquad + |V_1(x)-V_2(y)|(|V_1(x)|^\kappa + |V_2(y)|^\kappa)),\end{aligned}$$

$$\begin{aligned}&|\mathbf{F}(x,V_1(x)) - \mathbf{F}(x,V_2(x))\\ &\quad - (\mathbf{F}(y,V_1(y)) - \mathbf{F}(y,V_2(y)))|\\ &\le c(|V_1(x)-V_2(x)-(V_1(y)-V_2(y))|\mathbf{V}(x,y)^\kappa\\ &\quad + |x-y|^\alpha(|V_1(x)-V_2(x)|\\ &\quad + |V_1(y)-V_2(y)|)\mathbf{V}(x,y)^\kappa\\ &\quad + (|V_1(x)-V_2(x)|\\ &\quad + |V_1(y)-V_2(y)|)(|V_1(x)-V_2(y)|\\ &\quad + |V_1(y)-V_2(y)|)(1+\mathbf{V}(x,y))^{\kappa-1},\end{aligned} \tag{34}$$

where

$$\mathbf{V}(x,y) = |V_1(x)| + |V_2(x)| + |V_1(y)| + |V_2(y)|.$$

In other words, the mapping $\mathbf{F}$ satisfies the Hölder condition in both arguments and has a power-law growth in the second one. Moreover, the second order difference satisfies the estimate (34).

Lemma 1. (1) *Let $V \in \Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))$ and $\beta-\alpha \in (2,3), \alpha \in (0,1), \kappa \in (0,1)$. Then, for $x \in \Omega(\varepsilon)$ and $|x-y| < |x|/2$, the estimates*

$$\begin{aligned}|x|^{\beta-\alpha}|V(x)|^{1+\kappa} &\le c\|V;\Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))\|^{1+\kappa},\\ |x|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}|x-y|^{-\alpha}|V(x)-V(y)|^{1+\kappa}&\\ \le c\|V;\Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))\|^{1+\kappa}&\end{aligned}$$

are valid.
(2) Under the same restrictions on α,β,κ and x,y as above,

$$\begin{aligned}|x|^{\beta-\alpha}|w(\varepsilon^{-1}x)|^{1+\kappa} &\le c\varepsilon^{1+\kappa},\\ |x|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}|x-y|^{-\alpha}|w(\varepsilon^{-1}x)-w(\varepsilon^{-1}y)|^{1+\kappa}&\\ \le c\varepsilon.&\end{aligned}$$

Proof. First, we readily show the first assertion:

$$\begin{aligned}&|x|^{\beta-\alpha}|V(x)|^{1+\kappa}\\ &\quad\le |x|^{\beta-\alpha}|x|^{-(1+\kappa)(\beta-2-\alpha)}(|x|^{\beta-2-\alpha}|V(x)|)^{1+\kappa}\\ &\quad\le |x|^{2-\kappa(\beta-2-\alpha)}\|V;\Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))\|^{1+\kappa}\end{aligned}$$

The second inequality follows from the relation

$$2-\kappa(\beta-2-\alpha) \ge 2-1(3-2-\alpha) > 1 > 0.$$

Since

$$\frac{1}{2}|x| < |y| < \frac{3}{2}|x|,$$

in view of

$$|x-y| < \frac{x}{2}$$

and using the Newton-Leibnitz formula, we conclude that

$$\begin{aligned}&|x|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}|x-y|^{-\alpha}|V(x)-V(y)|^{1+\kappa}\\ &\quad\le c|x|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}|x-y|^{-\alpha}|x|^{-\beta+1+\alpha}|x-y|\\ &\qquad\cdot \sup_{x\in\Omega(\varepsilon)}(|x|^{\beta-1-\alpha}|\nabla_x V(x)|)\\ &\quad\le c|x|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}|x|^{1-\alpha}|x|^{-\beta+1+\alpha}\|V;\Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))\|\end{aligned}$$

while applying the inequalities

$$\begin{aligned}&\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}+1-\alpha-\beta+1+\alpha\\ &\quad = 2-(\beta-\alpha)\frac{\kappa}{1+\kappa} \ge \frac{2-(\beta-\alpha-2)\kappa}{1+\kappa} > 0.\end{aligned}$$

Based on the assumptions $\beta-\alpha > 2$ and $1+\kappa < 2$, we prove the second assertion. We have

$$\begin{aligned}|x|^{\beta-\alpha}|w(\varepsilon^{-1}x)|^{1+\kappa} &\le c|x|^{\beta-\alpha}(1+\frac{|x|}{\varepsilon})^{-1-\kappa}\\ &= c\varepsilon^{1+\kappa}\frac{|x|^{\beta-\alpha}}{(\varepsilon+|x|)^{1+\kappa}} \le c\varepsilon^{1+\kappa}.\end{aligned}$$

Owing to the estimate $|P(\xi)| \le c(1+|\xi|)^{-1}$ for the capacity potential and the boundary condition (21), it follows that

$$\begin{aligned}&|x|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}|x-y|^{-\alpha}|w(\varepsilon^{-1}x)-w(\varepsilon^{-1}y)|\\ &\quad\le c|x|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}|x-y|^{-\alpha}\Big|\frac{x}{\varepsilon}-\frac{y}{\varepsilon}\Big|\Big(1+\frac{|x|}{\varepsilon}\Big)^{-2}\\ &\qquad\cdot\sup_{\xi\in\mathbb{R}^3\setminus\omega}(1+|\xi|)^2|\nabla_\xi w(\xi)|)\\ &\quad\le c\varepsilon|x|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}|x|^{1-\alpha}(\varepsilon+|x|)^{-2}\\ &\quad\le c\varepsilon.\end{aligned}$$

Indeed, in the first inequality we have again applied the Newton-Leibnitz formula, and in the second one we have used the fact that $|\nabla_\xi P(\xi)| \le c(1+|\xi|)^{-2}$ and

$$\beta-\alpha-(\beta-\alpha)\frac{\kappa}{1+\kappa} = \frac{\beta-\alpha}{1+\kappa} \ge 1.$$

■

We now list the necessary estimates based on Lemma 1 and **(H5)**. We start with the boundedness of the first term in (32) multiplied by a weight. We obtain

$$\begin{aligned}&|x|^{\beta-\alpha}|\mathbf{F}(x,w(\varepsilon^{-1}x)+\varepsilon v'(x)+\hat{u}^\varepsilon(x))|\\ &\quad\le c|x|^{\beta-\alpha}(|w(\varepsilon^{-1}x)|^{1+\kappa}+\varepsilon^{1+\kappa}|v'(x)|^{1+\kappa}\\ &\qquad+|\hat{u}^\varepsilon(x))|^{1+\kappa})\\ &\quad\le c(\varepsilon^{1+\kappa}+\|\hat{u}^\varepsilon;\Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))\|^{1+\kappa}).\end{aligned} \tag{35}$$

Second, we verify the boundedness of the weighted difference, namely,

$$\begin{aligned}&|x|^\beta|x-y|^{-\alpha}|\mathbf{F}(x,\overbrace{w(\varepsilon^{-1}x)+\varepsilon v'(x)+\hat{u}^\varepsilon(x)}^{=V(x)})\\&\quad-\mathbf{F}(y,V(y))|\le c|x|^\beta(|V(x)|^{1+\kappa}+|x-y|^{-\alpha}|V(x)\\&\quad-V(y)|(|V(x)|^\kappa+|V(y)|^\kappa))\\&\le c\Big(\varepsilon^{1+\kappa}+\|\hat{u}^\varepsilon;\Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))\|^{1+\kappa}\\&\quad+(\varepsilon^\kappa+\|\hat{u}^\varepsilon;\Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))\|^\kappa)|x|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}|x-y|^{-\alpha}\\&\quad\cdot\Big\{\Big|w\Big(\frac{x}{\varepsilon}\Big)-w\Big(\frac{y}{\varepsilon}\Big)\Big|\\&\quad+\varepsilon|v'(x)-v'(y)|+|\hat{u}^\varepsilon(x)-\hat{u}^\varepsilon(y)|\Big\}\Big)\\&\le c(\varepsilon^{1+\kappa}+\|\hat{u}^\varepsilon;\Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))\|^{1+\kappa}).\end{aligned}\tag{36}$$

Now, we deduce the local Lipschitz continuity of the first part of the mapping (32):

$$\begin{aligned}&|x|^{\beta-\alpha}|\mathbf{F}(x,\overbrace{w(\varepsilon^{-1}x)+\varepsilon v'(x)+\hat{u}^\varepsilon_1(x)}^{=V_1(x)})\\&-\mathbf{F}(x,\overbrace{w(\varepsilon^{-1}x)+\varepsilon v'(x)+\hat{u}^\varepsilon_2(x)}^{=V_2(x)})|\\&\quad\le c|x|^{\beta-\alpha}|\hat{u}^\varepsilon_1(x)-\hat{u}^\varepsilon_2(x)|(|V_1(x)|^\kappa+|V_2(x)|^\kappa)\\&\quad\le c\|\hat{u}^\varepsilon_1-\hat{u}^\varepsilon_2;\Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))\|(\varepsilon^\kappa+\|\hat{u}^\varepsilon_1;\Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))\|^\kappa\\&\qquad+\|\hat{u}^\varepsilon_2;\Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))\|^\kappa).\end{aligned}\tag{37}$$

Finally, we prove the local Lipschitz continuity for the weighted second order differences of the mapping $\mathbf{F}$. For example, the first term on the right-hand side of (34) gets the bound

$$\begin{aligned}&c|x|^{\beta-(\beta-\alpha)\frac{\kappa}{1+\kappa}}|x-y|^{-\alpha}|(V_1(x)-V_2(x))\\&\quad-(V_1(y)-V_2(y))|(\varepsilon^\kappa+\|\hat{u}^\varepsilon_1;\Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))\|\\&\quad+\|\hat{u}^\varepsilon_2;\Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))\|)\\&\qquad\le c\|\hat{u}^\varepsilon_1-\hat{u}^\varepsilon_2;\Lambda^{2,\alpha}_\beta\\&\qquad\cdot(\Omega(\varepsilon))\|(\varepsilon^\kappa+\|\hat{u}^\varepsilon_1;\Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))\|^\kappa).\end{aligned}\tag{38}$$

The other two terms in (34) are estimated in the same way as in (35) and (36), respectively.

The above estimates allow us to apply the Banach fixed point theorem to verify the existence of the remainder $\hat{u}^\varepsilon$. To this end, we rewrite problem (26) in the form of an abstract equation in the Banach space $\mathfrak{R}=\Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))$, namely,

$$\hat{u}^\varepsilon=\mathfrak{G}\hat{u}^\varepsilon,\tag{39}$$

where

$$\mathfrak{G}\hat{u}^\varepsilon=\mathcal{S}_\epsilon(\hat{\mathcal{F}}^\varepsilon(.;\hat{u}^\varepsilon),\hat{g}^\varepsilon_\Omega,\hat{g}^\varepsilon_\omega)$$

and S_ε denotes the isomorphism (16). Let $\hat{u}^\varepsilon$ belong to the ball $\mathcal{B}\subset\mathfrak{R}$ of radius $\mathfrak{C}\varepsilon^{1+\kappa}$. We further need to verify two properties. First, the mapping $\mathfrak{C}$ maps the ball $\mathcal{B}$ into itself,

$$\mathcal{B}\ni\hat{u}^\varepsilon\Rightarrow\mathfrak{G}\hat{u}^\varepsilon\in\mathcal{B},\tag{40}$$

and second, the mapping becomes a strict contraction on the ball, i.e.,

$$\|\mathfrak{G}\mathfrak{v}-\mathfrak{G}\mathfrak{w};\mathfrak{R}\|\le k\|\mathfrak{v}-\mathfrak{w};\mathfrak{R}\|,\quad\mathfrak{v},\mathfrak{w}\in\mathfrak{R}\text{ with }k<1.\tag{41}$$

By (29), (30), (33) and (35), (36), we have

$$\begin{aligned}\|\mathfrak{G}\hat{u}^\varepsilon;\mathfrak{R}\|&\le c(\|\hat{\mathcal{F}}^\varepsilon;\Lambda^{0,\alpha}_\beta(\Omega(\varepsilon))\|+\|\hat{g}^\varepsilon_\Omega;\Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))\|\\&\quad+\|\hat{g}^\varepsilon_\omega;\Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))\|)\\&\le c(\varepsilon^{1+\kappa}+\|\hat{u}^\varepsilon;\mathfrak{R}\|^{1+\kappa}\\&\quad+\varepsilon^2+\varepsilon^{\beta-1-\alpha}+\varepsilon^{1+\beta-\beta'}).\end{aligned}\tag{42}$$

Let us fix β,α and β',κ such that

$$(1,2)\ni\beta-\alpha-1\ge1+\kappa,\tag{43}$$

$$\beta-\beta'\ge\kappa.\tag{44}$$

Recall that $\beta-\alpha$ and $\beta'-\alpha$ belong to the interval $(2,3)$. Thus, to satisfy (44), we must put $\beta-\alpha$ near 3 (satisfying (43) as well) and $\beta'-\alpha$ near 2. This allows us to create a gap of any length $\kappa\in(0,1)$.

If (43) and (44) hold true, we obtain

$$\|\mathfrak{G}\hat{u}^\varepsilon;\mathfrak{R}\|\le c(4\varepsilon^{1+\kappa}+\|\hat{u}^\varepsilon;\mathfrak{R}\|^{1+\kappa})\le\mathfrak{C}\varepsilon^{1+\kappa},$$

while the desired inequality $\mathfrak{C}\ge c(4+\mathfrak{C}^{1+\kappa}\varepsilon^{(1+\kappa)\kappa})$ is achieved by a proper choice of the constant $\mathfrak{C}$ (e.g., $\mathfrak{C}=5c$) and the bound for the parameter ε_0 in the condition $\varepsilon\in(0,\varepsilon_0]$.

By virtue of (37) and (38), the estimate

$$\|\mathfrak{G}\mathfrak{v}-\mathfrak{G}\mathfrak{w};\mathfrak{R}\|\le\underbrace{c(\varepsilon^\kappa+2\mathfrak{C}^\kappa\varepsilon^{(1+\kappa)\kappa})}_{k}\|v-w;\mathfrak{R}\|$$

is valid. The necessary relation $k<1$ can be achieved by diminishing, if necessary, the upper bound ε_0 for ε again.

Theorem 4. *Let the indices β,α and $\kappa\in(0,1)$ satisfy (43) and $\beta-2>\kappa$, while **(H2)** and **(H4)** hold true. Then there exist positive constants $\mathfrak{C}$ and ε_0 such that, for $\varepsilon\in(0,\varepsilon_0]$, the non-linear problem (26) has a unique small solution $\hat{u}^\varepsilon$, namely,*

$$\|\hat{u}^\varepsilon;\Lambda^{2,\alpha}_\beta(\Omega(\varepsilon))\|\le\mathfrak{C}\varepsilon^{1+\kappa}.\tag{45}$$

Consequently, the singularity perturbed problem (3) has at least one solution (25).

In the theorem we have proven the existence of a small remainder $\hat{u}^\varepsilon$ in (25), i.e., we have verified that the problem (3) has a unique solution in a small ball centred at the approximate asymptotic solution. If the uniqueness of the solution $\hat{u}^\varepsilon$ is known, for example, F in (3) gives rise to a monotone operator, the remainder is unique without any smallness assumption.

2.3. Formal asymptotic of the shape functional.

We have

$$\begin{aligned}
&\mathcal{J}(u^\varepsilon;\Omega(\varepsilon))\\
&\quad= \int_{\Omega(\varepsilon)} J(x,v(x))\,\mathrm{d}x\\
&\qquad+\int_{\Omega(\varepsilon)} (w(\varepsilon^{-1}x)+\varepsilon v'(x))J'_v(x,v(x))\,\mathrm{d}x+\cdots\\
&\quad=\int_\Omega J(x,v(x))\,\mathrm{d}x\\
&\qquad+\varepsilon\int_\Omega (v'(x)-a\Phi(x))J'_v(x,v(x))\,\mathrm{d}x+\cdots
\end{aligned} \tag{46}$$

We now introduce the following assumption:

(H5) $J\in C^{0,\alpha}(\Omega\times\mathbb{R})$, $J'_v\in C^{0,\alpha}(\Omega\times\mathbb{R})$.

Let $p\in C^{2,\alpha}(\Omega)$ be a solution of the problem

$$\begin{cases} -\Delta_x p(x)-F'_v(x,v(x))p(x) \\ \qquad\qquad = J'_v(x,v(x)), & x\in\Omega,\\ \qquad p(x)=0, & x\in\partial\Omega.\end{cases} \tag{47}$$

Integrating by parts in $\Omega\setminus\mathbb{B}_\delta=\{x\in\Omega: |x|>\delta\}$ yields

$$\begin{aligned}
&\int_\Omega (v'(x)-a\Phi(x))J'_v(x,v(x))\,\mathrm{d}x\\
&=-\lim_{\delta\to0}\int_{\Omega\setminus\mathbb{B}_\delta} (\Delta_x p(x)+F'_v(x,v(x))p(x))\\
&\quad\cdot(v'(x)-a\Phi(x))\,\mathrm{d}x\\
&=-\lim_{\delta\to0}\int_{\Omega\setminus\mathbb{B}_\delta} p(x)(\Delta_x+F'_v(x,v(x)))(v'(x)\\
&\quad-a\Phi(x))\,\mathrm{d}x-\lim_{\delta\to0}\int_{\partial\Omega}\partial_n p(x)(v'(x)-a\Phi(x))\,\mathrm{d}x\\
&\quad+\lim_{\delta\to0}\int_{\partial\mathbb{B}_\delta}(\partial_{|x|}p(x)(v'(x)-a\Phi(x))-p(x)\partial_{|x|}(v'(x)\\
&\quad-a\Phi(x)))\,\mathrm{d}x.
\end{aligned}$$

By (24), we have $v'(x)-a\Phi(x)=0$ for $x\in\Omega$ and

$$\begin{aligned}
(\Delta_x&+F'_v(x,v(x)))(v'(x)-a\Phi(x))\\
&=\Delta_x v'(x)\\
&\quad+v'(x)F'_v(x,v(x))-a\Phi(x)F'_v(x,v(x))\\
&=0.
\end{aligned}$$

On the other hand, $\partial_{|x|}p(x)(v'(x)-a\Phi(x))=O(\delta^{-1})$ and, hence,

$$\begin{aligned}
&\int_\Omega (v'(x)-a\Phi(x))J'_v(x,v(x))\,\mathrm{d}x\\
&\qquad-\lim_{\delta\to0}\int_{\partial\mathbb{B}_\delta}(\partial_{|x|}p(x)(v'(x)-a\Phi(x))\\
&\qquad-p(x)\partial_{|x|}(v'(x)-a\Phi(x)))\,\mathrm{d}x\\
&\qquad=-a\lim_{\delta\to0}\int_{\partial\mathbb{B}_\delta} p(0)(4\pi|x|^2)^{-1}\,\mathrm{d}s_x\\
&\qquad=-ap(0)=-4\pi v(\mathcal{O})p(0)\mathrm{cap}(\omega).
\end{aligned}$$

Thus,

$$\mathcal{J}(u^\varepsilon;\Omega(\varepsilon))=\mathcal{J}(v;\Omega)-\varepsilon4\pi v(\mathcal{O})p(0)\mathrm{cap}(\omega)+\cdots. \tag{48}$$

Similarly to the first inequality in **(H4)**, let the following assumption be valid:

(H6) With $\sigma\in(0,1)$,

$$\begin{aligned}|J(x,v(x)+V(x))-J(x,v(x))-V(x)J'_v(x,v(x))|\\ \le c|V(x)|^{1+\sigma}.\end{aligned}$$

Using this assumption leads to the relation

$$\begin{aligned}
&|\mathcal{J}(u^\varepsilon;\Omega(\varepsilon))-\mathcal{J}(v;\Omega(\varepsilon))\\
&\quad-\int_{\Omega(\varepsilon)}(w(\varepsilon^{-1}x)+\varepsilon v'(x)+\hat{u}^\varepsilon(x))J'_v(x,v(x))\,\mathrm{d}x|\\
&\le c\int_{\Omega(\varepsilon)}|w(\varepsilon^{-1}x)+\varepsilon v'(x)+\hat{u}^\varepsilon(x)|^{1+\sigma}\,\mathrm{d}x\\
&\le c\int_{\Omega(\varepsilon)}\Big(\Big|\frac{x}{\varepsilon}\Big|^{-1-\sigma}+|x|^{-(1+\sigma)(\beta-2-\alpha)}\\
&\quad\cdot(\varepsilon^{1+\sigma}\|v';\Lambda^{2,\alpha}_\beta(\Omega)\|^{1+\sigma}\\
&\quad+\|\hat{u}^\varepsilon(x);\Lambda^{2,\alpha}_\beta(\Omega)\|^{1+\sigma})\Big)\,\mathrm{d}x\\
&\le c\varepsilon^{1+\sigma}\Bigg(\int_\varepsilon^1 r^{-1-\sigma}r^2\,\mathrm{d}r\\
&\quad+\int_\varepsilon^1 r^{-(1+\sigma)(\beta-2-\alpha)}r^2\,\mathrm{d}r(\varepsilon^{1+\sigma}+\varepsilon^{(1+\kappa)(1+\sigma)})\Bigg)\\
&\le c\varepsilon^{1+\sigma}.
\end{aligned}$$

Here we have taken into account the fact that $1+\sigma \le 2$, $(1+\sigma)(\beta-2-\alpha) \le 2$, and both the integrals, extended on the interval $(0,1)$, do converge.

It suffices to mention the following inequalities:

$$|\mathcal{J}(u^\varepsilon;\Omega(\varepsilon)) - \mathcal{J}(v;\Omega)| \le c\,\mathrm{mes}_3(\omega_\varepsilon) \le c\varepsilon^3,$$

$$\int_{\Omega(\varepsilon)} |w(\varepsilon^{-1}x) + a\varepsilon\Phi(x)||J'_v(x,v(x))|\,\mathrm{d}x \le c\int_\varepsilon^1 \left(\frac{r}{\varepsilon}\right)^{-2} r\,\mathrm{d}r \le c\varepsilon^2,$$

$$\int_{\Omega(\varepsilon)} |\hat{u}^\varepsilon||J'_v(x,v(x))|\,\mathrm{d}x \le c\varepsilon^{1+\kappa}\int_{\Omega(\varepsilon)} |x|^{-(\beta-2-\alpha)}\,\mathrm{d}x \le c\varepsilon^{1+\kappa}.$$

This confirms the formal calculations performed above. Let us formulate the main result in three dimensions.

Theorem 5. *Under the assumptions listed above, we have*

$$|\mathcal{J}(u^\varepsilon;\Omega(\varepsilon)) - \mathcal{J}(v;\Omega) + \varepsilon 4\pi v(\mathcal{O})p(0)\mathrm{cap}(\omega)| \le c\varepsilon^{1+\min(\sigma,\kappa)}.$$

3. Topological derivative for a mixed semilinear elliptic problem in two spatial dimensions

The numerical analysis is performed in two spatial dimensions. Therefore, we introduce a mixed semilinear problem and analyze the asymptotic in such a case.

Since the proof uses the same arguments as in three spatial dimensions (note that we use the Hölder norms, which are insensitive to the space dimension), we provide only the formal analysis and impose the Neumann boundary conditions on the hole boundary $\partial\omega_\varepsilon$. Note that the Dirichlet condition on $\partial\omega_\varepsilon$ changes crucially the form of asymptotic expansions cf. (Il'in, 1989; Mazja *et al.*, 1981; Mazja *et al.*, 1991).

3.1. Formal asymptotic analysis.

Let Ω and ω be bounded domains in the plane $\mathbb{R}^2$. We consider the nonlinear mixed problem in the singularly perturbed domain $\Omega(\varepsilon)$, defined in (2):

$$\begin{cases} -\Delta_x u^\varepsilon(x) = F(x,u^\varepsilon(x)), & x\in\Omega(\varepsilon),\\ u^\varepsilon(x)=0, & x\in\partial\Omega,\\ \partial_n u^\varepsilon(x) = 0, & x\in\partial\omega_\varepsilon. \end{cases} \tag{49}$$

Referring to (Il'in, 1989) and especially to (Mazja *et al.*, 1981; Mazja *et al.*, 1991), we set

$$\begin{aligned} u^\varepsilon(x) =& v(x) + \varepsilon w_1(\varepsilon^{-1}x) + \varepsilon^2 w_2(\varepsilon^{-1}(x)\\ &+ \varepsilon^2 v'(x) + \cdots, \end{aligned} \tag{50}$$

where v, v' and w_1, w_2 are components of regular and boundary layer types, respectively. Precisely, v is a smooth solution of the problem (7) in the two dimensional entire domain Ω. The Taylor formula yields

$$v(x) = v(\mathcal{O}) + x^T\nabla_x v(\mathcal{O}) + \frac{1}{2}x^T\nabla_x^2 v(\mathcal{O})x + O(|x|^3).$$

The second term w_1 in the asymptotic ansatz (50) becomes a solution of the exterior problem

$$\begin{cases} -\Delta_\xi w_1(\xi) = 0, & \xi\in\mathbb{R}^2\setminus\overline{\omega},\\ \partial_{n(\xi)} w_1(\xi) = -\partial_{n(\xi)}\xi^T\nabla_x v(\mathcal{O}), & \xi\in\partial\omega. \end{cases} \tag{51}$$

Such a solution admits the asymptotic representation

$$w_1(\xi) = -\frac{1}{2\pi}\frac{\xi^T}{|\xi|^2}m(\omega)\nabla_x v(\mathcal{O}) + O(|\xi|^{-2}), \quad |\xi|\to\infty,$$

where m denotes the virtual mass matrix, see (Pólya and Szegö, 1951). Then the third term w_2 in (32) satisfies the problem

$$\begin{cases} -\Delta_\xi w_2(\xi) = 0, & \xi\in\mathbb{R}^2\setminus\overline{\omega},\\ \partial_{n(\xi)} w_2(\xi) = -\partial_{n(\xi)}\frac{1}{2}\xi^T\nabla_x v(\mathcal{O})\xi, & \xi\in\partial\omega. \end{cases} \tag{52}$$

For such a solution, we write down the classical asymptotic representation

$$w_2(\xi) = \frac{c}{2\pi}\ln\frac{1}{|\xi|} + O(\frac{1}{|\xi|}), \qquad |\xi|\to\infty,$$

where the constant c can be calculated as follows:

$$\int_{\partial\omega} \partial_{n(\xi)} w_2(\xi)\,\mathrm{d}s_\xi = -\int_{\partial\mathbb{B}_R} \frac{\partial}{\partial|\xi|}\frac{c}{2\pi}\ln\frac{1}{|\xi|}\,\mathrm{d}\xi = c. \tag{53}$$

By the Green formula, we compute the left boundary integral

$$\begin{aligned} -\int_{\partial\omega} \partial_{n(\xi)}\frac{1}{2}\xi^T\nabla_x^2 v(\mathcal{O})\xi\,\mathrm{d}s_\xi &= \int_\omega \Delta_\xi\frac{1}{2}\xi^T\nabla_x^2 v(\mathcal{O})\xi\,\mathrm{d}\xi \\ &= \mathrm{mes}_2\omega\Delta_x v(\mathcal{O})\\ &= -\mathrm{mes}_2\omega F(\mathcal{O};v(\mathcal{O})). \end{aligned} \tag{54}$$

Finally, the fourth term v' in (32) is to be found from the Dirichlet problem

$$\begin{cases} -\Delta_x v'(x) = (-\dfrac{1}{2\pi}\dfrac{x^T}{|x|^2}m(\omega)\nabla_x v(\mathcal{O}) \\ \qquad -\dfrac{1}{2\pi}\ln\dfrac{\varepsilon}{|x|}\mathrm{mes}_2\omega F(\mathcal{O};v(\mathcal{O})) \\ \qquad + v'(x))F'_v(x,v(x)), \quad x\in\Omega,\\ v'(x) = \dfrac{1}{2\pi}\dfrac{x^T}{|x|^2}m(\omega)\nabla_x v(\mathcal{O}) \\ \qquad + \dfrac{1}{2\pi}\ln\dfrac{\varepsilon}{|x|}\mathrm{mes}_2\omega F(\mathcal{O};v(\mathcal{O}), \quad x\in\partial\Omega. \end{cases} \tag{55}$$

3.2. Formal asymptotic of the shape functional. We introduce the following hypotheses:

(H7) $F \in C^{0,\alpha}(\overline{\Omega} \times \mathbb{R})$, $F'_v \in C^{0,\alpha}(\overline{\Omega} \times \mathbb{R})$ for some $\alpha \in (0,1)$ and $F'_v \le 0$.

(H8) $J \in C^{0,\alpha}(\overline{\Omega} \times \mathbb{R})$, $J'_v \in C^{0,\alpha}(\overline{\Omega} \times \mathbb{R})$

By the monotonicity of F, the Lax-Milgram lemma and the regularity of J, the problem

$$\begin{cases} -\Delta_x p(x) - F'_v(x, v(x))p(x) \\ \quad = J'_v(x, v(x)), & x \in \Omega, \\ p(x) = 0, & x \in \partial\Omega \end{cases} \tag{56}$$

admits a unique solution $p \in C^{2,\alpha}(\Omega)$.

We replace the solution u^ε by its asymptotic representation (32). As a result, we obtain the first asymptotic term of order ε^2 for the shape functional

$$\begin{aligned}
&\mathcal{J}(u^\varepsilon; \Omega(\varepsilon)) \\
&= \int_{\Omega(\varepsilon)} J(x, v(x))\,\mathrm{d}x + \int_{\Omega(\varepsilon)} (\varepsilon w_1(\varepsilon^{-1}x) \\
&\quad + \varepsilon^2 w_2(\varepsilon^{-1}x) + \varepsilon^2 v'(x))J'_v(x, v(x))\,\mathrm{d}x + \cdots \\
&= \mathcal{J}(v; \Omega(\varepsilon)) + \varepsilon^2 \int_{\Omega(\varepsilon)} \Big(-\frac{1}{2\pi}\frac{x^T}{|x|^2} m(\omega)\nabla_x v(\mathcal{O}) \\
&\quad - \frac{1}{2\pi} \ln\frac{\varepsilon}{|x|} \mathrm{mes}_2\omega F(\mathcal{O}; v(\mathcal{O})) \\
&\quad + v'(x)J'_v(x, v(x)\Big)\,\mathrm{d}x + \cdots \\
&= \mathcal{J}(v; \Omega) - \varepsilon^2 \mathrm{mes}_2\omega J(\mathcal{O}; v(\mathcal{O})) \\
&\quad + \varepsilon^2 \int_{\Omega} \Big(-\frac{1}{2\pi}\frac{x^T}{|x|^2} m(\omega)\nabla_x v(\mathcal{O}) \\
&\quad - \frac{1}{2\pi} \ln\frac{\varepsilon}{|x|} \mathrm{mes}_2\omega F(\mathcal{O}; v(\mathcal{O})) \\
&\quad + v'(x))\, J'_v(x, v(x))\,\mathrm{d}x + \cdots .
\end{aligned} \tag{57}$$

Now we replace the right-hand side of (56) according to the equation and twice integrate by parts in the domain $\Omega \setminus \mathbb{B}_\delta = \{x \in \Omega : |x| > \delta\}$. We have

$$\begin{aligned}
&\int_{\Omega} (-\frac{1}{2\pi}\frac{x^T}{|x|^2} m(\omega)\nabla_x v(\mathcal{O}) \\
&\quad - \frac{1}{2\pi} \ln\frac{\varepsilon}{|x|} \mathrm{mes}_2\omega F(\mathcal{O}; v(\mathcal{O})) + v'(x))J'_v(x, v(x))\,\mathrm{d}x \\
&= -\lim_{\delta\to 0} \int_{\Omega\setminus\mathbb{B}_\delta} (\Delta_x p(x) + F'_v(x, v(x))p(x)) \\
&\quad \cdot \Big(-\frac{1}{2\pi}\frac{x^T}{|x|^2} m(\omega)\nabla_x v(\mathcal{O}) \\
&\quad - \frac{1}{2\pi} \ln\frac{\varepsilon}{|x|} \mathrm{mes}_2\omega F(\mathcal{O}; v(\mathcal{O})) + v'(x)\Big)\,\mathrm{d}x \\
&= -\lim_{\delta\to 0} \int_{\Omega\setminus\mathbb{B}_\delta} p(x)(\Delta_x + F'_v(x, v(x))) \\
&\quad (-\frac{1}{2\pi}\frac{x^T}{|x|^2} m(\omega)\nabla_x v(\mathcal{O}) - \frac{1}{2\pi} \ln\frac{\varepsilon}{|x|} \mathrm{mes}_2\omega F(\mathcal{O}; v(\mathcal{O})) \\
&\quad + v'(x))\,\mathrm{d}x - \lim_{\delta\to 0} \int_{\partial\Omega} \partial_n p(x)(-\frac{1}{2\pi}\frac{x^T}{|x|^2} m(\omega)\nabla_x v(\mathcal{O}) \\
&\quad - \frac{1}{2\pi} \ln\frac{\varepsilon}{|x|} \mathrm{mes}_2\omega F(\mathcal{O}; v(\mathcal{O})) + v'(x))\,\mathrm{d}x \\
&\quad - \lim_{\delta\to 0} \int_{\partial\mathbb{B}_\delta} (\partial_{|x|} p(x)(-\frac{1}{2\pi}\frac{x^T}{|x|^2} m(\omega)\nabla_x v(\mathcal{O}) \\
&\quad - \frac{1}{2\pi} \ln\frac{\varepsilon}{|x|} \mathrm{mes}_2\omega F(\mathcal{O}; v(\mathcal{O})) + v'(x)) \\
&\quad - p(x)\partial_{|x|}(-\frac{1}{2\pi}\frac{x^T}{|x|^2} m(\omega)\nabla_x v(\mathcal{O}) \\
&\quad - \frac{1}{2\pi} \ln\frac{\varepsilon}{|x|} \mathrm{mes}_2\omega F(\mathcal{O}; v(\mathcal{O})) + v'(x))\,\mathrm{d}x.
\end{aligned}$$

On the other hand, the boundary condition (55) implies that

$$-\frac{1}{2\pi}\frac{x^T}{|x|^2} m(\omega)\nabla_x v(\mathcal{O}) - \frac{1}{2\pi} \ln\frac{\varepsilon}{|x|} \mathrm{mes}_2\omega F(\mathcal{O}; v(\mathcal{O})) + v'(x) = 0.$$

Furthermore, for the linearized operator $\Delta_x + F'_v$, the formula

$$\begin{aligned}
&(\Delta_x + F'_v(x, v(x))) + \Big(-\frac{1}{2\pi}\frac{x^T}{|x|^2} m(\omega)\nabla_x v(\mathcal{O}) \\
&\quad -\frac{1}{2\pi} \ln\frac{\varepsilon}{|x|} \mathrm{mes}_2\omega F(\mathcal{O}; v(\mathcal{O})) + v'(x)\Big) \\
&= \Delta_x v'(x) \\
&\quad + v'(x)F'_v(x, v(x)) \\
&\quad + \Big(-\frac{1}{2\pi}\frac{x^T}{|x|^2} m(\omega)\nabla_x v(\mathcal{O}) \\
&\quad -\frac{1}{2\pi} \ln\frac{\varepsilon}{|x|} \mathrm{mes}_2\omega F(\mathcal{O}; v(\mathcal{O}))\Big) F'_v(x, v(x)) = 0
\end{aligned}$$

is valid because the function

$$x \mapsto \Big(-\frac{1}{2\pi}\frac{x^T}{|x|^2} m(\omega)\nabla_x v(\mathcal{O}) -\frac{1}{2\pi} \ln\frac{\varepsilon}{|x|} \mathrm{mes}_2\omega F(\mathcal{O}; v(\mathcal{O})\Big)$$

is a harmonics. Hence, we obtain that

$$\begin{aligned}
&\int_{\Omega} \Big(-\frac{1}{2\pi}\frac{x^T}{|x|^2} m(\omega)\nabla_x v(\mathcal{O}) \\
&\quad - \frac{1}{2\pi} \ln\frac{\varepsilon}{|x|} \mathrm{mes}_2\omega F(\mathcal{O}); v(\mathcal{O})) \\
&\quad + v'(x))J'_v(x, v(x)\Big)\,\mathrm{d}x
\end{aligned}$$

$$
\begin{aligned}
&- \lim_{\delta\to 0}\int_{\partial\mathbb{B}_\delta}\Bigg(\partial_{|x|}p(x)\Big(-\frac{1}{2\pi}\frac{x^T}{|x|^2}m(\omega)\nabla_x v(\mathcal{O})\\
&-\frac{1}{2\pi}\ln\frac{\varepsilon}{|x|}\mathrm{mes}_2\omega F(\mathcal{O};v(\mathcal{O}))\Big)\\
&- p(x)\partial_{|x|}\Big(-\frac{1}{2\pi}\frac{x^T}{|x|^2}m(\omega)\nabla_x v(\mathcal{O})\\
&-\frac{1}{2\pi}\ln\frac{\varepsilon}{|x|}\mathrm{mes}_2\omega F(\mathcal{O};v(\mathcal{O}))\Big)\Bigg)\,\mathrm{d}x\\
&-\lim_{\delta\to 0}\sum_{i,j,k=1}^{2}\int_{\partial\mathbb{B}_\delta}\Bigg[\frac{x_i}{|x|}\frac{\partial p}{\partial x_i}(\mathcal{O})\Big(-\frac{1}{2\pi}\frac{x_k}{|x|^2}m_{kj}\frac{\partial v}{\partial x_j}(\mathcal{O})\Big)\\
&-(p(\mathcal{O})+x_i\frac{\partial p}{\partial x_i}(\mathcal{O}))\Big(-\frac{1}{2\pi}\frac{x_j}{|x|^3}m_{jk}\frac{\partial v}{\partial x_k}(\mathcal{O})\Big)\Bigg]\,\mathrm{d}x\\
&+\lim_{\delta\to 0}\int_{\partial\mathbb{B}_\delta}\Bigg[\sum_{i=1}^{2}(p(\mathcal{O})+x_i\frac{\partial p}{\partial x_i}(\mathcal{O}))\\
&\cdot\times\Big(\frac{1}{2\pi}\frac{1}{|x|}\mathrm{mes}_2\omega F(\mathcal{O};v(\mathcal{O}))\Big)\Bigg]\,\mathrm{d}x\\
&-\lim_{\delta\to 0}\int_{\partial\mathbb{B}_\delta}\Bigg[\sum_{i,j,k=1}^{2}\frac{x_i}{|x|}\frac{\partial p}{\partial x_i}(\mathcal{O})\Big(-\frac{1}{\pi}\frac{x_k}{|x|^2}m_{kj}\frac{\partial v}{\partial x_j}(\mathcal{O})\Big)\\
&-p(\mathcal{O})\Big(\frac{1}{2\pi}\frac{1}{|x|}\mathrm{mes}_2\omega F(\mathcal{O};v(\mathcal{O}))\Big)\Bigg]\,\mathrm{d}x\\
&\cdot\lim_{\delta\to 0}\int_{\partial\mathbb{B}_\delta}\Bigg[\sum_{i,j=1}^{2}\frac{x_i}{|x|}\frac{\partial p}{\partial x_i}(\mathcal{O})\Big(\frac{1}{\pi}\frac{x_i}{|x|^2}m_{ij}\frac{\partial v}{\partial x_j}(\mathcal{O})\Big)\\
&+p(\mathcal{O})\Big(\frac{1}{2\pi}\frac{1}{|x|}\mathrm{mes}_2\omega F(\mathcal{O};v(\mathcal{O}))\Big)\Bigg]\,\mathrm{d}x\\
={}& F(\mathcal{O};v(\mathcal{O}))\mathrm{mes}_2\omega p(\mathcal{O})\\
&+\nabla_x p(\mathcal{O})^T m(\omega)\nabla_x v(\mathcal{O}).
\end{aligned}
$$

Thus, recalling (57) we conclude the relation

$$
\begin{aligned}
&\mathcal{J}(u^\varepsilon;\Omega(\varepsilon))\\
&=\mathcal{J}(v;\Omega)+\varepsilon^2[-\mathrm{mes}_2\omega J(\mathcal{O};v(\mathcal{O}))\\
&\quad+F(\mathcal{O};v(\mathcal{O}))\mathrm{mes}_2\omega p(\mathcal{O})\\
&\quad+\nabla_x p(\mathcal{O})^T m(\omega)\nabla_x v(\mathcal{O})]+\cdots
\end{aligned}\tag{58}
$$

Theorem 6. *Under the assumptions **(H1)**, **(H7)** and **(H8)**, the asymptotic expansion* (58) *is valid with the remainder* $o(\varepsilon^2)$.

4. Finite element approximations of topological derivatives

Our aim in this section is to compute a numerical approximation of the topological derivative of the shape functional (8), with u^ε being the solution of the problem (49), and give L^∞-estimates of the error.

4.1. Family of finite elements. In $\overline{\Omega}$ we consider a family of triangulations $\{\mathscr{T}_h\}_{h>0}$. With each element $T\in\mathscr{T}_h$, we associate two parameters $\rho(T)$ and $\sigma(T)$, where $\rho(T)$ denotes the diameter of the set T, and $\sigma(T)$ is the diameter of the largest ball contained in T. We set $h=\max_{T\in\mathscr{T}_h}\rho(T)$. We make the following assumptions on the triangulations:

(H10) Regularity assumption: There exists $\sigma>0$ such that $\rho(T)/\sigma(T)\le\sigma$ for $T\in\mathscr{T}_h$ and $h>0$.

(H11) Inverse assumption: There exists $\rho>0$ such that $h/\rho(T)\le\rho$ for $T\in\mathscr{T}_h$ and $h>0$.

(H12) We denote by $\overline{\Omega}_h=\cup_{T\in\mathscr{T}_h}T$ the domain obtained by a triangulation, with Ω_h as its interior and $\partial\Omega_h$ its boundary. Then we assume that the vertices of $\mathscr{T}_h$ placed on the boundary $\partial\Omega_h$ also belong to $\partial\Omega$.

Consider the spaces

$$
\begin{aligned}
V_h=\big\{v_h\in C(\overline{\Omega}):v_h|_T\in P_1(T)\text{ for }T\in\mathscr{T}_h\\
\text{and }v_h=0\text{ in }\Omega\setminus\Omega_h\big\}
\end{aligned}
$$

and

$$
W_h=\big\{v_h\in C(\overline{\Omega}_h):v_h|_T\in P_1(T)\text{ for }T\in\mathscr{T}_h\big\},
$$

where $P_1(T)$ is the space of polynomials of degree 1 on T, V_h is a vector subspace of $H_0^1(\Omega)$ and W_h is a subspace of $H^1(\Omega)$.

We use the Lagrange interpolation operator

$$
\Pi_h: C(\overline{\Omega})\to W_h
$$

$\Pi_h z$ being the unique element in W_h such that $\Pi_h z(x_i)=z(x_i)$ for every node x_i of the triangulation. In the case of a function z vanishing on $\partial\Omega$, we extended $\Pi_h z$ to $\overline{\Omega}$ by zero and we denote this extension by $\Pi_h z$, too. In the last case, we have that $\Pi_h z\in V_h$.

4.2. Numerical solution of the semilinear problem. By virtue of the assumption $F\in C^{0,1}(\overline{\Omega}\times\mathbb{R})$ and by the mean value theorem, we deduce the following local Lipschitz condition: For all $M>0$ there exists $c_M>0$ such that

$$
\begin{aligned}
|F(x,v_1)-F(x,v_2)|\le c_M|v_1-v_2|,\quad x\in\Omega,\\
|v_1|,|v_2|\le M.
\end{aligned}\tag{59}
$$

Using classical arguments, we can deduce from the monotonicity of $F(x,\cdot)$ and (59) the existence of a unique solution to (7) in $H_0^1(\Omega)\cap C(\overline{\Omega})$. We refer to (Stampacchia, 1965) for the boundedness of the solution. From to the convexity of Ω, we can deduce that the solution is in $H^2(\Omega)$ (Ladyzhenskaya and Ural'tseva, 1968).

The weak formulation of the equation (7) is the following:

$$
a(v,z)=(F(x,v),z)_{L^2(\Omega)},\quad z\in H_0^1(\Omega),\tag{60}
$$

where

$$a(v,z) = \int_\Omega \nabla v(x)\nabla z(x)\,\mathrm{d}x.$$

The numerical approximation v_h of v is then the solution of the problem

$$\begin{cases} \text{Find } v_h \in V_h \text{ such that} \\ a(v_h, z_h) = (F(x, v_h), z_h)_{L^2(\Omega)}, \text{ for any } z_h \in V_h. \end{cases} \tag{61}$$

The proof of the existence of a solution of (61) is well known (Stampacchia, 1965). It is enough to apply, in a convenient way, Browder's fixed point theorem along with the monotonicity of $F(x,\cdot)$.

We rewrite problem (56) in the form

$$\begin{cases} -\Delta p(x) = F_0(x, p(x)), & x \in \Omega, \\ p(x) = 0, & x \in \partial\Omega, \end{cases} \tag{62}$$

where $F_0(x,p(x)) = F'_v(x,v(x))p(x) + J'(x,v(x))$. F_0 is linear with respect to the second variable, so that $F_0 \in C^{0,1}(\overline{\Omega}\times\mathbb{R})$.

Then the variational formulation of the linear problem (56) is the following:

$$a(p,z) = (F_0(x,p),z)_{L^2(\Omega)}, \quad z \in H_0^1(\Omega). \tag{63}$$

Thus, numerical approximation of p is the solution of the variational problem

$$\begin{cases} \text{Find } p_h \in V_h \text{ such that} \\ a(p_h, z_h) = (F_0(x, p_h), z_h)_{L^2(\Omega)} \text{ for any } z_h \in V_h. \end{cases} \tag{64}$$

Due to the hypotheses **(H1)** and **(H7)**, the linear problem (64) has a solution in space V_h.

In the next section we give L^∞-estimates for the finite element approximation of $v, \nabla v, p, \nabla p$ and the topological derivatives in the case of the semilinear elliptic problem.

4.3. Convergence of finite element approximation for the semilinear problem and the adjoint state problem.

We are going to use the recent results on the convergence of the finite element method in $W^{1,\infty}$ spaces. The topological derivative is a pointwise expression with the values of the solution and the adjoint state, as well as with the values of the gradient of these functions. In order to derive the error estimates in the L^∞ norm for the topological derivative, it is required to have in hand the error estimates in the $W^{1,\infty}$ norm for the solutions of the semilinear equation as well as the linear adjoint state equation. The results presented below lead to the error estimate for the topological derivative. We refer the reader to (Casas and Mateos, 2002; Demlov, 2007; Frehse and Rannacher, 1978), for the proofs of error estimates for linear and semilinear elliptic equations.

The following L^∞-estimate for approximation by finite elements of solutions to the problem (7) was proved in (Casas and Mateos, 2002).

Theorem 7. *Let v and v_h be solutions of the variational problems (60) and (61), respectively. Then there exists a constant $C>0$ independent of h such that*

$$\|v - v_h; L^\infty(\Omega_h)\| \le Ch\|v; H^2(\Omega)\|.$$

In addition, assuming that $\Omega_h \subset \Omega$, we have the following estimates, proved in (Demlov, 2007) (see also (Frehse and Rannacher, 1978)).

Theorem 8. *Let v and v_h be solutions of the variational problems (60) and (61), respectively. Then there exists a constant $C>0$ independent of h such that*

$$\|\nabla v - \nabla v_h; L^\infty(\Omega_h)\|_\infty \le Ch\|v; H^2(\Omega)\|.$$

On the other hand, we have the following L^∞ - estimates for the approximation of solutions to the linear problem (56).

Theorem 9. *Let $x_0 \in \Omega$, and let p and p_h be solutions of the variational problems (63) and (64), respectively. Then there exists a constant $C>0$ independent of h such that*

$$\|p - p_h; L^\infty(\Omega_h)\| + \|\nabla p - \nabla p_h; L^\infty(\Omega_h)\| \le Ch\|p; H^2(\Omega)\|.$$

4.4. L^∞- estimates for the approximation of the topological derivative.

We denote by $\mathcal{T}_{\Omega,h}$ numerical approximation by the finite element method of the topological derivative $\mathcal{T}_\Omega$. Then

$$\begin{aligned} \mathcal{T}_{\Omega,h}(\mathcal{O}) = &-\mathrm{mes}_2(\omega)J(\mathcal{O}, v_h(\mathcal{O})) \\ &+ \nabla_x p_h(\mathcal{O})^T m(\omega)\nabla_x v_h(\mathcal{O}) \\ &+ F(\mathcal{O}, v_h(\mathcal{O}))\mathrm{mes}_2(\omega)p_h(\mathcal{O}). \end{aligned} \tag{65}$$

We obtain

$$\begin{aligned} &|\mathcal{T}_\Omega(\mathcal{O}) - \mathcal{T}_{\Omega,h}(\mathcal{O})| \\ &\quad = |-\mathrm{mes}_2(\omega)[J(\mathcal{O},v(\mathcal{O})) - J(\mathcal{O},v_h(\mathcal{O}))] \\ &\qquad + [\nabla_x p(\mathcal{O})^T m(\omega)\nabla_x v(\mathcal{O}) \\ &\qquad - \nabla_x p_h(\mathcal{O})^T m(\omega)\nabla_x v_h(\mathcal{O})] \\ &\qquad + [F(\mathcal{O},v(\mathcal{O}))\mathrm{mes}_2(\omega)p(\mathcal{O}) \\ &\qquad - F(\mathcal{O},v_h(\mathcal{O}))\mathrm{mes}_2(\omega)p_h(\mathcal{O})]| \\ &\quad \le \mathrm{mes}_2(\omega)|J(\mathcal{O},v(\mathcal{O})) - J(\mathcal{O},v_h(\mathcal{O}))| \\ &\qquad + |\nabla_x p(\mathcal{O})^T m(\omega)\nabla_x v(\mathcal{O}) \\ &\qquad - \nabla_x p_h(\mathcal{O})^T m(\omega)\nabla_x v_h(\mathcal{O})| \\ &\qquad + \mathrm{mes}_2(\omega)|F(\mathcal{O},v(\mathcal{O}))p(\mathcal{O}) \\ &\qquad - F(\mathcal{O},v_h(\mathcal{O}))p_h(\mathcal{O})|. \end{aligned} \tag{66}$$

We have

$$|J(\mathcal{O},v(\mathcal{O})) - J(\mathcal{O},v_h(\mathcal{O}))| \le c\|v - v_h; L^\infty(\Omega_h)\|. \tag{67}$$

It follows that

$$\begin{aligned}
&|\mathcal{T}_\Omega(\mathcal{O}) - \mathcal{T}_{\Omega,h}(\mathcal{O})| \\
&\le c\|v - v_h; L^\infty(\Omega_h)\| \\
&\quad + |\nabla_x p(\mathcal{O})^T m(\omega) \nabla_x (v(\mathcal{O}) - v_h(\mathcal{O}))| \\
&\quad + |\nabla_x (p(\mathcal{O}) - p_h(\mathcal{O}))^T m(\omega) \nabla_x v_h(\mathcal{O})| \\
&\quad + \mathrm{mes}_2(\omega)|F(\mathcal{O}, v(\mathcal{O}))(p(\mathcal{O}) - p_h(\mathcal{O}))| \\
&\quad + \mathrm{mes}_2(\omega)|(F(\mathcal{O}, v(\mathcal{O})) - F(\mathcal{O}, v_h(\mathcal{O})))p_h(\mathcal{O})|.
\end{aligned} \tag{68}$$

Therefore,

$$\begin{aligned}
&|F(\mathcal{O}, v(\mathcal{O})) - F(\mathcal{O}, v_h(\mathcal{O}))| \\
&\qquad\qquad \le c\|v - v_h; L^\infty(\Omega_h)\|,
\end{aligned} \tag{69}$$

and we obtain

$$\begin{aligned}
&|\mathcal{T}_\Omega(\mathcal{O}) - \mathcal{T}_{\Omega,h}(\mathcal{O})| \\
&\quad \le c\|v - v_h; L^\infty(\Omega_h)\| \\
&\qquad + c\|\nabla_x (v(\mathcal{O}) - v_h(\mathcal{O})); L^\infty(\Omega_h)\| \\
&\qquad + c\|\nabla_x (p(\mathcal{O}) - p_h(\mathcal{O})); L^\infty(\Omega_h)\| \\
&\qquad + c\|p(\mathcal{O}) - p_h(\mathcal{O}); L^\infty(\Omega_h)\|.
\end{aligned} \tag{70}$$

Finally, by Theorems 8 and 9, we deduce the following result.

Theorem 10. *The following error estimate holds for the evaluation of the topological derivatives:*

$$\begin{aligned}
&|\mathcal{T}_\Omega(\mathcal{O}) - \mathcal{T}_{\Omega,h}(\mathcal{O})| \\
&\qquad \le Ch(\|v; H^2(\Omega)\| + \|p; H^2(\Omega)\|).
\end{aligned} \tag{71}$$

4.5. Numerical examples.

In this section, we present some numerical examples to show the behavior of topological derivative approximation with respect to the evolution of discretization step size. We derive errors and verify that the computed error satisfies the estimate from Theorem (10) in each case.

For each of the examples, we choose the domain Ω as a square $(0,1) \times (0,1)$ and the following energy functional:

$$\begin{aligned}
\mathcal{J}(v; \Omega) =& \frac{1}{2} \int_\Omega |\nabla v(x)|^2 \, \mathrm{d}x + \frac{1}{4} \int_\Omega v^4(x) \, \mathrm{d}x \\
&- \int_\Omega f(x) v(x) \, \mathrm{d}x
\end{aligned} \tag{72}$$

where v is the solution of the nonlinear problem

$$\begin{cases} -\Delta_x v(x) = -v(x)^3 + f(x), & x \in \Omega, \\ v(x) = 0, & x \in \partial\Omega. \end{cases} \tag{73}$$

We take different right-hand sides f in each of the examples. The size of discretization is determined by h, which decreases in each iteration. We compute the error in 20 iterations starting with $h = 0.2$ and reduce it by 0.01 in each step.

Example 1. In the first example the function f is given by

$$\begin{aligned}
f(x) =& f(x_1, x_2) = \left((x_1^2 + x_2^2) \sin \pi x_1 \sin \pi x_2\right)^3 \\
&+ 2\left(\pi^2(x_1^2 + x_2^2) - 2\right) \sin \pi x_1 \sin \pi x_2 \\
&- 4\pi \left(x_1 \cos \pi x_1 \sin \pi x_2 + \sin \pi x_1 \cos \pi x_2\right).
\end{aligned}$$

We calculate the exact solution of (73)

$$u(x_1, x_2) = \left(x_1^2 + x_2^2\right) \sin \pi x_1 \sin \pi x_2,$$

and the corresponding adjoint state

$$p(x_1, x_2) = -\frac{1}{2}\left(x_1^2 + x_2^2\right) \sin \pi x_1 \sin \pi x_2.$$

Exact and numerical approximations of the topological derivative are presented in Fig. 1. In Fig. 2 we plot the relative evolution of the error and the behavior of the error with respect to the discretization step size.

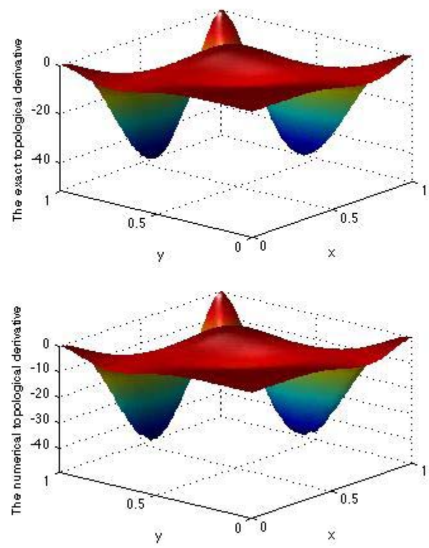

Fig. 1. Topological derivative: exact $\mathcal{T}_\Omega$ (left) and approximate $\mathcal{T}_{\Omega,h}$ (right).

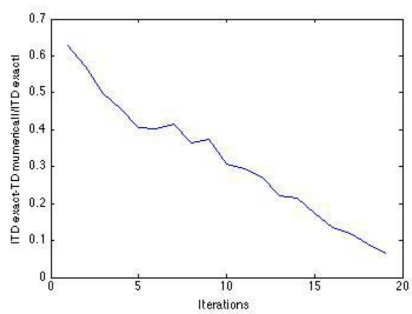

Fig. 2. Error : $|\mathcal{T}_\Omega - \mathcal{T}_{\Omega,h}|_\infty / |\mathcal{T}_\Omega|_\infty$.

Example 2. Let us choose

$$
\begin{aligned}
f(x) &= f(x_1, x_2) \\
&= (x_1(x_1-1)x_2(x_2-1))^3 \\
&\quad - 2\,(x_2(x_2-1) + x_1(x_1-1))\,.
\end{aligned}
$$

In this case,

$$u(x_1, x_2) = x_1(x_1-1)x_2(x_2-1)$$

and

$$p(x_1, x_2) = -\frac{1}{2}x_1(x_1-1)x_2(x_2-1).$$

The exact topological derivative and it numerical approximation are presented in Fig. 3 and in Fig. 4 we show the relative evolution of the error and the behavior of the error with respect to the discretization step size.

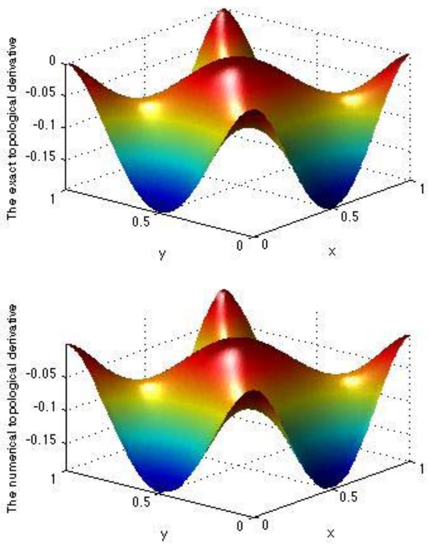

Fig. 3. Topological derivative: exact $\mathcal{T}_\Omega$ (left) and approximate $\mathcal{T}_{\Omega,h}$ (right).

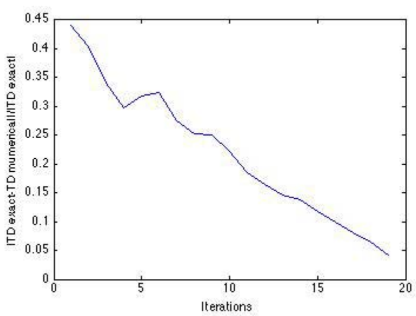

Fig. 4. Error : $|\mathcal{T}_\Omega - \mathcal{T}_{\Omega,h}|_\infty / |\mathcal{T}_\Omega|_\infty$.

Example 3. In the last example, we take

$$
\begin{aligned}
f(x_1, x_2) &= \left(100x_1^2x_2^2(x_1-1)^2(x_2-1)^2\right)^3 \\
&\quad - 200\left[x_1^2(x_1-1)^2(6x_2^2-6x_2+1)\right. \\
&\quad \left. + x_2^2(x_2-1)^2(6x_1^2-6x_1+1)\right].
\end{aligned}
$$

Then

$$u(x_1, x_2) = 100x_1^2x_2^2(x_1-1)^2(x_2-1)^2$$

and

$$p(x_1, x_2) = -50x_1^2x_2^2(x_1-1)^2(x_2-1)^2.$$

For this last example the exact topological derivative and it numerical approximation are presented in Fig. 5, and in Fig. 6 we show the relative evolution of the error and the behavior of the error with respect to the discretization step size.

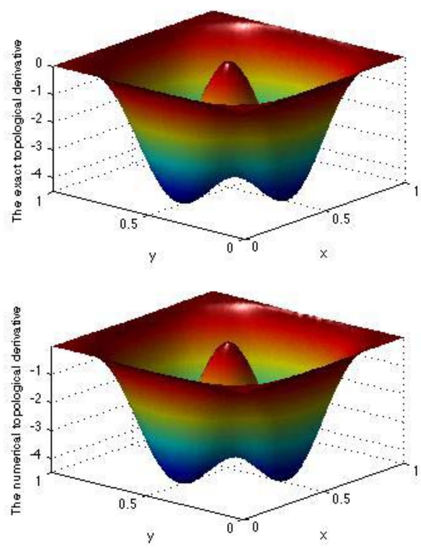

Fig. 5. Topological derivative: exact $\mathcal{T}_\Omega$ (left) and approximate $\mathcal{T}_{\Omega,h}$ (right).

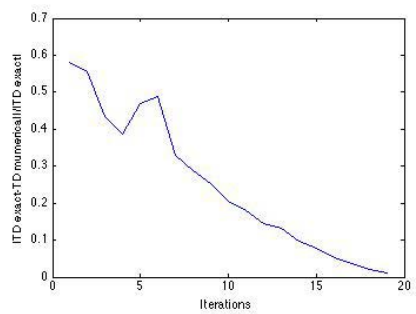

Fig. 6. Error : $|\mathcal{T}_\Omega - \mathcal{T}_{\Omega,h}|_\infty / |\mathcal{T}_\Omega|_\infty$.

5. Conclusions

In the paper the form of topological derivatives of the integral shape functional was obtained for semilinear elliptic boundary value problems in two and three spatial dimensions. The finite element method was used to compute an approximation of the topological derivatives. Convergence analysis of the finite element method was performed in two spatial dimensions. Since the application of topological derivatives in shape optimization requires pointwise values, we provided L^∞-estimates for finite element approximations. The results of computations confirmed the *a priori* estimate of the numerical approximation error. The presented results can be used for shape and topology optimization for semilinear elliptic boundary value problems.

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