Johann Radon Institute for
Computational and Applied Mathematics
Austrian Academy of Sciences (ÖAW)

A bilevel shape optimization problem for the exterior Bernoulli free boundary value problem

H. Kasumba, K. Kunisch, A. Laurain

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A BILEVEL SHAPE OPTIMIZATION PROBLEM FOR THE EXTERIOR BERNOULLI FREE BOUNDARY VALUE PROBLEM

H. KASUMBA, K KUNISCH, AND A. LAURAIN

ABSTRACT. A bilevel shape optimization problem with the exterior Bernoulli free boundary problem as lower-level problem and the control of the free boundary as the upper-level problem is considered. Using the shape of the inner boundary as the control, we aim at reaching a specific shape for the free boundary. A rigorous sensitivity analysis of the bilevel shape optimization in the infinite-dimensional setting is performed. The numerical realization using two different cost functionals presented in this paper demonstrate the efficiency of the approach.

1. INTRODUCTION

Let $\omega \subset \mathscr{E}$ with ω a smooth and bounded domain in $\mathbb{R}^2$. Further $\mathscr{E}$ is a bounded domain in $\mathbb{R}^2$ which is supposed to contain all admissible shapes and is referred to as the *hold-all* domain. We define the set of admissible shapes as

$$\mathscr{O}_{ad} = \{\Omega \subset \mathbb{R}^2 \text{ a bounded domain}: \ \overline{\omega} \subset \Omega,\ \overline{\Omega} \subset \mathscr{E}\}.$$

For given $\mu \in \mathbb{R}, \mu < 0$, we consider the following free boundary problem:

$$(\mathscr{F}_\omega): \text{Find } \Omega \in \mathscr{O}_{ad} \text{ such that problem (1)} - \text{(4) has a solution,}$$

where

$$-\Delta u = 0 \quad \text{in} \quad \Omega \setminus \overline{\omega}, \tag{1}$$

$$u = 1 \quad \text{on} \quad \Sigma := \partial\omega, \tag{2}$$

$$u = 0 \quad \text{on} \quad \Gamma := \partial\Omega, \tag{3}$$

$$\partial_n u = \mu \quad \text{on} \quad \Gamma, \tag{4}$$

with u in $H^1_\Gamma(\Omega \setminus \overline{\omega})$, the standard Sobolev space of H^1-functions whose trace vanishes on Γ. This problem is known as the *exterior Bernoulli free boundary problem* due to $\overline{\omega} \subset \Omega$. Note that (1)-(4) is over-determined since two boundary conditions are specified on Γ, and in general does not have solutions. However for particular sets Ω, or equivalently free boundaries Γ, problem (1)-(4) may have a solution. Problem (1)-(4) originates, for instance, from the description of free boundaries for ideal fluids [DZ01, Pg. 138-140]. Other applications leading to similar formulations include electrochemistry and electromagnetics [FR97].

Typically, the shape of Γ is not known analytically except for some particular configurations of the inner boundary Σ. A number of authors have analyzed and solved problem

Key words and phrases. Bernoulli problem, Shape derivative, Free boundary problem.

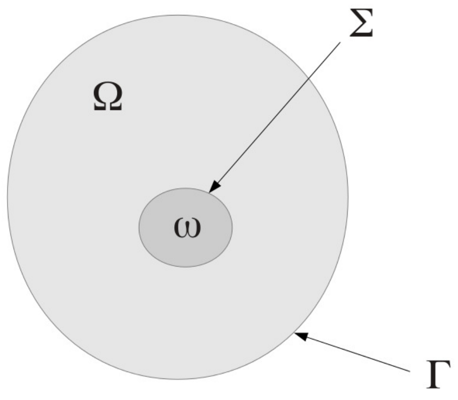

FIGURE 1. The exterior Bernoulli problem

$(\mathscr{F}_\omega)$ for a given fixed domain ω, see for instance [DZ01, Ch. 3], [FR97, IKP06, BCT05, BCT08, LP12] and references therein. We use the notation $(\mathscr{F}_\omega)$ to emphasize the dependence of the solution Γ on ω as we will use ω to control Γ in the problem considered in this paper.

The over-specification of conditions on Γ naturally suggests to formulate (1)-(4) as an optimization problem; this approach has been used in [IKP06] for instance. Subsequently, an interesting control problem arises when Σ is used to control the solution Γ of $(\mathscr{F}_\omega)$. This gives rise to a bilevel shape optimization problem, where the free boundary value problem constitutes the lower-level optimization problem, and the upper-level consists in minimization with respect to Σ. A similar bilevel problem has been treated for the Bernoulli problem in [THM08] in the discrete setting, where a sensitivity analysis was performed for the Bernoulli problem using an automatic differentiation technique. In the present work, we carry out a rigorous sensitivity analysis of the cost functionals with respect to the control ω (or equivalently Σ) in the infinite-dimensional setting using the tools of shape calculus [DZ01, SZ92]. For this purpose we introduce two cost functionals to drive the free set Ω as close as possible to a given desired set E.

In the literature on mathematical programs, multilevel optimization problems are programs which have a subset of their variables constrained to be an optimal solution of other programs. Such problems were first considered in [BM73]; see also [CMS05] for a review. In shape optimization only a few bilevel problems have been considered due to their inherent difficulty. In [SZ92, Section 4.3.2] shape controllability of the free boundary of an obstacle problem is studied. In [THM08, THM12] shape and topology optimization of Bernoulli free boundary problems are considered. Shape optimization problems in fluid dynamics governed by free surface flows are considered in [KK12] where a sensitivity analysis of the free surface problem with the Navier-Stokes equations as constraints is formally studied.

Turning to numerical realization of the bilevel optimization problem, a possible approach consists in discarding one of the two boundary conditions on the free boundary and to append it to the cost functional on the upper level by using a penalty or augmented Lagrangian approach. Using this strategy, solving for the state u becomes a classical linear boundary value problem with well-posed boundary data in the lower level problem. Unfortunately, as noted in [THM08], this approach leads to serious convergence problems. A further disadvantage that was noted in [THM08] is that, depending on the formulation, a locally optimal triplet (u,ω,Ω) might not represent a physical solution to the free boundary problem. For this reason, we adopt a segregation approach to solve the optimization problem, i.e., we find a solution to the free boundary problem $(\mathscr{F}_\omega)$ first and then proceed to the upper level represented by the minimization of the cost functional. In this iterative procedure, $(\mathscr{F}_\omega)$ has to be solved several times for varying interfaces Γ. Therefore, one needs an efficient and robust solver for this type of problem. Possible solution strategies include trial methods, linearization methods (continuous or discrete) [CS90], and shape optimization methods [HM03]. Here we use a regularized fixed point method, which is a trial method. The main advantage of this approach is that it solves $(\mathscr{F}_\omega)$ using some simple updating formula based only on the solution of a state system. Moreover this method locally converges super-linearly [FR97].

The remainder of this paper is organized as follows. Section 2 describes the setting of the free boundary and optimization problems. The sensitivity analysis of the bilevel problems is performed in Section 3. In Section 4, the numerical algorithm used to solve the optimization problems is given. Numerical examples that support the theoretical results are then presented.

2. Setting of the problem

In this section the mathematical notations, the algorithm for solving the free boundary problem, and the setting of the optimization problems are presented.

2.1. **Notations.**

Here we collect some notations and definitions that we need in our subsequent discussion. Throughout the paper we restrict ourselves to the two dimensional case.

Vectors: We use bold fonts for vectors $\mathbf{x} = (x_1, x_2)^T \in \mathbb{R}^2$ with norm $|\mathbf{x}|_{\mathbb{R}^2} = (\sum_{j=1}^2 x_j^2)^{1/2}$ and vector-valued functions are also indicated by bold letters.

Two notations for the inner product in $\mathbb{R}^2$ shall be used, namely (x,y) and $x \cdot y$, respectively. The latter shall be used in case of nested inner products. The unit outward normal and tangential vectors to a domain Ω shall be denoted by $\mathbf{n} = (n_1,n_2)$ and $\tau = (-n_2,n_1)$, respectively. For a given matrix A, we denote by A^t its transpose and by A^{-t} the transpose of its inverse.

Function spaces: When $\mathscr{S} \subset \mathbb{R}^2$ is open we denote by $\mathscr{C}_b^k(\mathscr{S})$ the spaces of k-times continuously differentiable scalar-valued functions u with $D^\beta u$ bounded whenever $0 \leq |\beta| \leq k$,where β is a multi-index, and equipped with the standard $\mathscr{C}^k$-norm. We write $\mathscr{C}_b^{k,\alpha}(\mathscr{S})$, $0 < \alpha \leq 1$ for the space of functions $u \in \mathscr{C}_b^k(\mathscr{S})$ such that $D^\beta u$ is Hölder continuous with exponent α whenever $|\beta| = k$. The space $\mathscr{C}_b^{k,\alpha}(\mathscr{S})$ equipped with the norm

$$\|u\|_{k,\alpha} := \sum_{|\beta|\le k} \sup_{\mathscr{S}}(D^\beta u) + \sum_{|\beta|=k} \sup_{x,y\in\mathscr{S},x\neq y} \frac{|D^\beta u(x) - D^\beta u(y)|}{|x-y|^\alpha}$$

is a Banach space. When $\mathscr{S}$ is a compact set we simply write $\mathscr{C}^{k,\alpha}(\mathscr{S})$. We denote by $W^{m,p}(\mathscr{S})$, $m \in \mathbb{N}$, $1 \le p \le \infty$ the standard L^p-Sobolev space of order m:

$$W^{m,p}(\mathscr{S}) := \left\{ u \in L^p(\mathscr{S}) \mid D^\beta u \in L^p(\mathscr{S}), \text{ for } 0 \le |\beta| \le m \right\},$$

where D^β is the weak (or distributional) partial derivative. Here $\mathscr{S}$ can be either $\mathbb{R}^2$, the flow domain Ω, its boundary $\partial\Omega$, or a subset of $\partial\Omega$. The norm $||\cdot||_{W^{m,p}(\mathscr{S})}$ associated with $W^{m,p}(\mathscr{S})$ is given by

$$||u||_{W^{m,p}(\mathscr{S})} = \left(\sum_{|\beta|\le m} \int_{\mathscr{S}} |D^\beta u|^p \, d\mathbf{x} \right)^{1/p}.$$

When $p = 2$ we write $H^m(\mathscr{S}) := W^{m,2}(\mathscr{S})$ for simplicity. We also denote

$$H^1_\Lambda(\mathscr{S}) := \left\{ u \in H^1(\mathscr{S}) \mid u = 0 \text{ on } \Lambda \right\},$$

where $\Lambda \subset \partial\mathscr{S}$ and $H^1_0(\mathscr{S})$ when $\Lambda = \partial\mathscr{S}$. When the function is vector-valued, we write $\mathscr{C}^{k,\alpha}_b(\mathscr{S},\mathbb{R}^2)$, $W^{m,p}_b(\mathscr{S},\mathbb{R}^2)$, etc ... for the function spaces.

Domains: The notation $|\Omega|$ denotes the Lebesgue measure of a set Ω and Ω^c its complementary. A domain Ω is said to be of class $\mathscr{C}^k$ or $\mathscr{C}^{k,\alpha}$ if its boundary is locally the graph of a $\mathscr{C}^k$ or $\mathscr{C}^{k,\alpha}$ function, respectively; see [DZ01, chapter 2, def. 3.1]. We write $\mathbb{1}_\Omega$ for the characteristic function of a set Ω, i.e.,

$$\mathbb{1}_\Omega(x) = \begin{cases} 1 & \text{if} \quad x \in E, \\ 0 & \text{if} \quad x \notin E. \end{cases} \tag{5}$$

For a a domain Ω of class $\mathscr{C}^2$ and a vector $\mathbf{v} \in \mathscr{C}^1(\mathbb{R}^2,\mathbb{R}^2)$, its tangential gradient $\nabla_\Gamma \mathbf{v}$ is defined as

$$\nabla_\Gamma \mathbf{v} := \nabla \mathbf{v}|_\Gamma - (\partial_n \mathbf{v})\mathbf{n}, \tag{6}$$

and its tangential divergence $\operatorname{div}_\Gamma(\mathbf{v})$ is defined as

$$\operatorname{div}_\Gamma(\mathbf{v}) := \operatorname{div}(\mathbf{v}) - D\mathbf{v}\,\mathbf{n}\cdot\mathbf{n}. \tag{7}$$

If $\mathbf{v}$ is only defined on Γ, then the tangential gradient and tangential divergence are defined similarly using an extension of $\mathbf{v}$ to $\mathbb{R}^2$ and they are independent of this extension. If the domain has enough regularity, the curvature $\mathscr{H}$ is given by $\mathscr{H} = \operatorname{div}_\Gamma \mathbf{n}$.

2.2. **Existence of solutions for the free boundary problem.** In this paper we work with bounded domains $\omega \in \mathscr{U}_{ad}$ where the admissible set of domains is

$$\mathscr{U}_{ad} := \{\omega \subset \mathbb{R}^2 \mid \omega_{min} \subset \omega \subset \omega_{max} \subset \mathscr{E},\ \omega \text{ is star-like with respect to all points in the ball } B_\delta(0) \text{ and } \omega \text{ is of class } \mathscr{C}^{2,\alpha}\}, \tag{8}$$

where $\omega_{min}, \omega_{max}$ are given non-empty domains in $\mathbb{R}^2$, ω_{min} contains the origin, $0 < \alpha < 1$ and the radius $\delta > 0$ is a given constant; see [THM08]. This choice of $\mathscr{U}_{ad}$ guarantees existence, uniqueness as well as stability (in the sense of [AM95, Theorem 3.9]) of the solution to $(\mathscr{F}_\omega)$ with respect to ω. Moreover, it is shown in [AM95] that if $\omega \in \mathscr{U}_{ad}$, then the boundary $\partial\Omega^*(\omega)$ is of class $\mathscr{C}^\infty$ and is star-like with respect to all points in $B_\delta(0)$. Here $\Omega^*(\omega)$ denotes the solution to $(\mathscr{F}_\omega)$.

2.3. **Fixed point approach for the free boundary problem.** The free boundary problem $(\mathscr{F}_\omega)$ can be formulated as a shape optimization problem [HIK+09, IKP06]. In this way, the numerical solution of $(\mathscr{F}_\omega)$ relies on the use of gradient information that depends on known state and adjoint systems. On the other hand, it would be helpful to have a method that solves $(\mathscr{F}_\omega)$ using some simple updating formula based only on the solution of some state system. The structure of such a scheme is as follows:

(1) Choose an initial approximation of the free boundary.
(2) Solve the boundary value problem (1)-(4) for u with one condition on Γ omitted.
(3) Update Γ using the discrepancy left by the remaining boundary condition.
(4) Iterate from step (2) until stationarity up to a specified accuracy is reached.

This scheme is simple to implement but it is not obvious how to construct the updating step in such a manner that the method converges and that the convergence is fast. In order to obtain an optimal updating step, Tilhonen [Til97] derived the first and second order derivatives for the cost $\mathscr{J}(\Omega)$ in the following shape optimization problem:

$$\begin{aligned} &\text{minimize} \quad \mathscr{J}(\Omega) := \frac{1}{2}\int_\Gamma u_\Omega^2\, ds \\ &\text{subject to} \quad \Omega \in \mathscr{O}_{ad}, u_\Omega \in H^1(\Omega \setminus \overline{\omega}) \end{aligned} \tag{9}$$

with

$$-\Delta u_\Omega = 0 \quad \text{in} \quad \Omega \setminus \overline{\omega}, \tag{10}$$

$$u_\Omega = 1 \quad \text{on} \quad \Sigma, \tag{11}$$

$$\alpha u_\Omega + \partial_n u_\Omega = \mu \quad \text{on} \quad \Gamma. \tag{12}$$

Here the coefficient α can be chosen freely without affecting the solution of the free boundary problem provided that the solution to (9) is such that $u_\Omega|_\Gamma = 0$. However, changes in α affect the conditioning of the Hessian of the cost functional $\mathscr{J}(\Omega)$. It has been shown in [Til97] that $\alpha = \mathscr{H}$, where $\mathscr{H} \geq 0$ is the mean curvature of Γ, is the optimal choice for an efficient resolution of the optimization problem (9). Furthermore, it has been shown using formal asymptotic expansions in [FR97], that the optimal updating step may be approximated by

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \frac{u(\mathbf{x}^{(k)})}{\mu}\mathbf{n}_\varepsilon(\mathbf{x}^{(k)}),$$

where $\mathbf{x}^{(k)} := (x_1^{(k)}, x_2^{(k)}) \in \Gamma^{(k)}$ is the k-th iterate and $\mathbf{n}_\varepsilon \in H^1(\Gamma)$ is the smoothed normal vector field on the free boundary Γ satisfying

$$\int_\Gamma \varepsilon \nabla_\Gamma \mathbf{n}_\varepsilon \nabla_\Gamma \varphi + \mathbf{n}_\varepsilon \varphi \, ds = \int_\Gamma \mathbf{n}\varphi \, ds, \text{ for all } \varphi \in H^1(\Gamma), \tag{13}$$

and ε is some fixed small parameter. The mean curvature $\mathscr{H}$ of Γ is defined as

$$\mathscr{H} := \mathrm{div}_\Gamma(\mathbf{n}_\varepsilon). \tag{14}$$

The algorithm to update the free boundary Γ at the k^{th} step now becomes

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Algorithm 1 Algorithm for solving $(\mathscr{F}_\omega)$

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1. Choose $\Gamma^{(0)}$ and compute $\mathscr{H}^{(0)}$. Set $k = 0$.
2. Solve the boundary value problem (10)-(12) in $\Omega^{(k)}$ with $\alpha = \mathscr{H}^{(k)}$.
3. Set $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \frac{u(\mathbf{x}^{(k)})}{\mu}\mathbf{n}_\varepsilon(\mathbf{x}^{(k)})$, where $\mathbf{x}^{(k)} = (x_1^{(k)}, x_2^{(k)}) \in \Gamma^{(k)}$.
4. If $u^{(k+1)}|_\Gamma$ is small enough, then stop. Otherwise set $k = k+1$ and go to 2.

Flucher and Rumpf [FR97] analyzed the convergence of Algorithm 1 in the continuous case. Their analysis shows that the convergence suffers from the smoothing procedure so that the convergence is less than quadratic but still super-linear. In two dimensions, one can obtain the convergence rate of order $3/2$.

2.4. **Bilevel shape optimization problems.** The solution of $(\mathscr{F}_\omega)$ is unique in view of the assumptions in section 2.2. Thus there exists a mapping

$$\Omega^* : \mathscr{U}_{ad} \ni \omega \mapsto \Omega^*(\omega) \in \mathscr{O}_{ad}, \tag{15}$$

such that $\Omega^*(\omega)$ is the solution of $(\mathscr{F}_\omega)$. We denote $\Gamma^*(\omega) := \partial\Omega^*(\omega)$.

We next turn to a shape optimization problem with respect to ω. Our control objective consists in determining ω such that $\Gamma^*(\omega)$ is as close as possible to the boundary ∂E of a target Lipschitz domain $E \in \mathscr{O}_{ad}$ such that $\omega \subset E$.

We study two functionals which allow us to achieve this goal. The first one is:

$$J_1(\Omega) := |\Omega \cap E^c| + |E \cap \Omega^c|. \tag{16}$$

The term $|\Omega \cap E^c| = 0$ forces Ω to be included in E while $|E \cap \Omega^c| = 0$ forces Ω to contain E. We may also write J_1 as

$$J_1(\Omega) = \int_{\Omega\cap E^c} 1 \, dx + \int_{E\cap\Omega^c} 1 \, dx. \tag{17}$$

Another approach consists in minimizing the functional

$$J_2(\Omega, \omega) = \frac{1}{2}\int_{\Omega\cap E^c} u^2 \, dx + \frac{1}{2}\int_{E\cap\omega^c} (u - u_l)^2 \, dx, \tag{18}$$

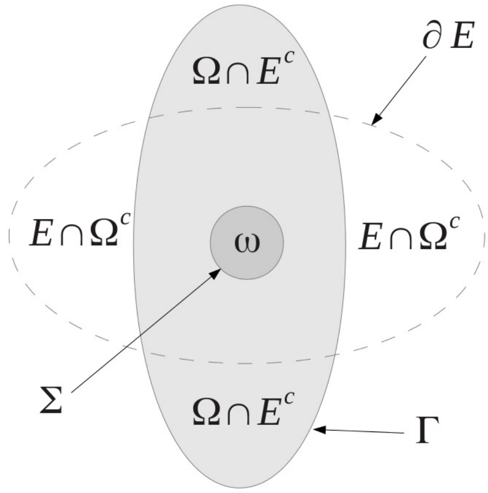


FIGURE 2. “Free” set Ω and target E

where $u \in H_0^1(\mathscr{E})$ is the extension by zero to $\mathscr{E}$ of the solution of (1)-(4). Such an extension exists as soon as $\Omega \subset \mathscr{E}$ is measurable and $u = 0$ on $\partial\Omega$; see [HP05]. The function u_l solves the linear problem

$$-\Delta u_l = 0 \quad \text{in } E \setminus \overline{\omega}, \tag{19}$$

$$u_l = 1 \quad \text{on } \Sigma, \tag{20}$$

$$u_l = 0 \quad \text{on } \partial E, \tag{21}$$

and is also extended by zero to a function in $H_0^1(\mathscr{E})$. The following proposition shows that minimizing J_1 and J_2 allows to drive Ω to E.

Proposition 1. *Let ω be a given open bounded set with $\omega \subset \Omega$. We have $J_1(\Omega) = 0$ and $J_2(\Omega, \omega) = 0$ if and only if $\Omega = E$ almost everywhere.*

Proof. We start with the case of J_1. If $\Omega = E$, then obviously $J_1(E) = 0$. On the other hand, if $J_1(\Omega) = 0$, then $|\Omega \cap E^c| = |E \cap \Omega^c| = 0$ and thus $\Omega = E$ almost everywhere.

Now we consider the case of J_2. Observe that if $\Omega = E$, then $\Omega \cap E^c = \emptyset$, $u = u_l$ a.e on $E \cap \omega^c$ and thus $J_2(\Omega, \omega) = 0$. Conversely we show that if $J_2(\Omega, \omega) = 0$, then $\Omega = E$ almost everywhere, which is equivalent to $|\Omega \cap E^c| + |\Omega^c \cap E| = 0$. We use a contradiction argument to support the latter assertion.

To this end, suppose that $|\Omega \cap E^c| + |\Omega^c \cap E| \neq 0$ and $J_2(\Omega, \omega) = 0$. Then we face two possibilities: (i) $|\Omega^c \cap E| > 0$ or (ii) $|\Omega^c \cap E| = 0$ and $|\Omega \cap E^c| > 0$. In case (i), since $J_2(\Omega, \omega) = 0$, we have $u - u_l = 0$ almost everywhere on $E \cap \omega^c$. Since $\Omega^c \cap E \subset \omega^c \cap E$ due to $\overline{\omega} \subset \Omega$ we have $u_l = u = 0$ on $\Omega^c \cap E$. By the maximum principle, since u_l is harmonic and its minimum is zero on ∂E, u_l must be equal to zero in all of $E \setminus \overline{\omega}$ which is a contradiction to $u_l = 1$ on Σ. Hence case (i) cannot happen.

We turn to case (ii). Since $J_2(\Omega,\omega)=0$ and $|\Omega\cap E^c|>0$ we have $u=0$ almost everywhere on $\Omega\cap E^c$. By the maximum principle and (1)-(4) we should have $u(x)=0$ for all $x\in\Omega\setminus\overline{\omega}$ which is a contradiction to $u(x)=1$ on Σ.

Hence we conclude that $\Omega=E$ almost everywhere whenever $J_2(\Omega,\omega)=0$. □

Writing $J_i(\Omega,\omega)=J_i(\Omega)$, $i=1,2$, we can now formulate the bilevel shape optimization problem as

$$(\mathscr{B}_i):\begin{cases}\text{minimize} & J_i(\Omega,\omega)\\ \text{subject to} & \omega\in\mathscr{U}_{ad}\text{ where }\Omega\text{ solves }(\mathscr{F}_\omega).\end{cases}$$

The problem of minimizing $J_i(\Omega,\omega)$ over $\omega\in\mathscr{U}_{ad}$ is called the *upper-level problem*, while the problem of solving $(\mathscr{F}_\omega)$ is called the *lower-level problem*. Similarly, Ω is the *lower-level variable* while ω is the *upper-level variable*. Defining the associated functionals

$$K_1(\omega):=J_1(\Omega^*(\omega)),\tag{22}$$

$$K_2(\omega):=J_2(\Omega^*(\omega),\omega),\tag{23}$$

we can rewrite the bilevel problem as

$$(\mathscr{B}_i):\begin{cases}\text{minimize} & K_i(\omega)\\ \text{subject to} & \omega\in\mathscr{U}_{ad}.\end{cases}$$

Remark 2.1. Note that the minimum of $K_1(\omega)$ and $K_2(\omega)$ need not exist and need not be 0 in general. In these cases we have $\Omega^*(\omega)\neq E$ even if ω minimizes $K_i(\omega)$. Indeed we have $K_i(\omega)=J_i(\Omega^*(\omega),\omega)$ but $\Omega^*(\mathscr{U}_{ad})\subsetneq\mathscr{O}_{ad}$ in general. So if $E\in\mathscr{O}_{ad}\setminus\Omega^*(\mathscr{U}_{ad})$, then we cannot find ω such that $K_i(\omega)=0$. It is easily seen that $\Omega^*(\mathscr{U}_{ad})\neq\mathscr{O}_{ad}$ in general since the domains $\Omega^*(\omega)$ have $\mathscr{C}^\infty$ regularity due to our choice of $\mathscr{U}_{ad}$ (see Section 2.2). However, if ω minimizes $K_i(\omega)$, then $\Omega^*(\omega)$ is the closest approximation of E (for $K_i(\omega)$) which solves the free boundary problem $(\mathscr{F}_\omega)$. We observe this phenomenon in Section 4.1.3 of the numerical results.

3. Sensitivity analysis

3.1. **Perturbation of identity.** In the study of the optimization problem $(\mathscr{B}_i)$, several issues arise including the sensitivity of $\Omega^*(\omega)$ with respect to ω. To deal with this issue concepts of shape differential calculus, described in detail in the monographs [DZ01, SZ92], are utilized. The inherent difficulty in dealing with shape functionals lies in the fact that sets of shapes are not vector spaces and the notion of differentiation cannot be used directly. Instead, one may consider perturbations of a reference shape by means of transformations in an appropriate function space which allows differentiation of the functional. These transformations can be constructed, for instance, by perturbation of the identity [DZ01] or by the flow of a velocity field [DZ01, SZ92]. We will use the perturbation of identity method in what follows. To this end let $\mathbf{V}\in\mathscr{C}_b^{k,\alpha}(\mathbb{R}^2,\mathbb{R}^2)$ with $k\geq 1$ and $0<\alpha<1$. We consider perturbations of identity $I+\mathbf{V}$ where $\mathbf{V}$ is in a neighborhood of 0 in $\mathscr{C}_b^{k,\alpha}(\mathbb{R}^2,\mathbb{R}^2)$ so that $I+\mathbf{V}$ is a bi-Lipschitz homeomorphism. In what follows we will denote by

$$\mathscr{S}_\mathbf{V} := (I+\mathbf{V})(\mathscr{S})$$

the transformation of a generic domain $\mathscr{S}$ by $I+\mathbf{V}$. Let $K(\omega)$ be a real-valued functional associated with $\omega \subset \mathbb{R}^2$. The functional $K(\omega)$ is Fréchet-differentiable at ω if there exists a linear and continuous functional $\nabla K(\omega)$ from $\mathscr{C}_b^{k,\alpha}(\mathbb{R}^2,\mathbb{R}^2)$ to $\mathbb{R}$ called *shape gradient* such that

$$K(\omega_\mathbf{V}) = K(\omega) + \nabla K(\omega)\cdot \mathbf{V} + r(\mathbf{V}),$$

where $|r(\mathbf{V})|/\|\mathbf{V}\|_{k,\alpha} \to 0$ as $\|\mathbf{V}\|_{k,\alpha} \to 0$.

We will also consider the particular case of directional derivative by introducing a family of transformations $T_t(\mathbf{V}) = I + t\mathbf{V}$, $t \in [0,\tau]$. The mapping T_t allows to define a family of transformed domains $\omega_t := T_t(\mathbf{V})(\omega)$ and boundaries $\Gamma_t := T_t(\mathbf{V})(\Gamma)$. Then we say that the functional $K(\omega)$ has an Eulerian derivative at ω in the direction $\mathbf{V}$ if the limit

$$dK(\omega;\mathbf{V}) = \lim_{t\to 0^+} \frac{K(\omega_t) - K(\omega)}{t}, \tag{24}$$

exists and is finite. The functional $K(\omega)$ is said to be shape differentiable at ω if the so-called *shape derivative* $dK(\omega;\mathbf{V})$ in direction $\mathbf{V}$ exists for all $\mathbf{V}$ and the *shape gradient*

$$\nabla K(\omega) : \mathbf{V} \mapsto dK(\omega;\mathbf{V}) \tag{25}$$

is linear and continuous from $\mathscr{C}_b^{k,\alpha}(\mathbb{R}^2,\mathbb{R}^2)$ to $\mathbb{R}$. We have that

$$\mathscr{C}_b^{k,\alpha}(\mathbb{R}^2,\mathbb{R}^2) \ni \mathbf{V} \mapsto dK(\omega;\mathbf{V}). \tag{26}$$

is a distribution on $\mathbb{R}^2$ with support on Σ, where Σ is the boundary of $\omega \subset \mathbb{R}^2$. In addition, if ω is of class $\mathscr{C}^{k+1,\alpha}$, then for all $\mathbf{V} \in \mathscr{C}_b^{k,\alpha}(\mathbb{R}^2,\mathbb{R}^2)$ such that $\mathbf{V}\cdot\mathbf{n} = 0$ on Σ, we have $dK(\omega;\mathbf{V}) = 0$. In other words, the shape derivative in direction $\mathbf{V}$ depends only on the normal component of the trace of $\mathbf{V}$ on Σ. This is the so-called Hadamard structure theorem in e.g., [DZ01, Ch. 8] or [HP05, Ch. 5]. If we assume that the data is smooth enough, then there exists an integrable function g such that the shape derivative can be expressed as

$$dK(\omega;\mathbf{V}) = \int_\Sigma g\mathbf{V}\cdot\mathbf{n}\, ds. \tag{27}$$

A similar definition can be used for the shape derivative of functionals taking their values in a Banach space. In particular, we would like to define the shape derivative of the solution of a partial differential equation such as (1)-(4). Let $u_\mathbf{V}$ denote the solution of a partial differential equation on the perturbed domain $\omega_\mathbf{V}$. Since $u_\mathbf{V}$ lives in a function space which depends on the moving domain $\omega_\mathbf{V}$, we cannot compute the shape derivative directly. Instead we take the derivative of $u_\mathbf{V}\circ(I+\mathbf{V})$ defined on ω. We call it *material derivative* and write $\dot{u}(\mathbf{V})$. Then one introduces the *shape derivative* by means of:

$$u'(\mathbf{V}) := \dot{u}(\mathbf{V}) - \nabla u\cdot\mathbf{V}.$$

3.2. **Sensitivity of u with respect to ω.** In order to compute (24), we proceed by first computing formally the derivative of the solution to (1)-(4) with respect to ω, using the classical results of shape calculus as in [SZ92]. To this end, let $T_t(\mathbf{V}) = I + t\mathbf{V}$ be the transformation associated with a vector field $\mathbf{V} \in \mathscr{C}_b^{k,\alpha}(\mathbb{R}^2, \mathbb{R}^2)$, and denote

$$\omega_t = T_t(\mathbf{V})(\omega), \quad t \geq 0. \tag{28}$$

Assume that there exists $\mathbf{W}^* \in \mathscr{C}_b^{k,\alpha}(\mathbb{R}^2, \mathbb{R}^2)$ such that $\Omega^*(\omega_t) = T_t(\mathbf{W}^*)(\Omega^*(\omega_0))$ for $t \in [0, \tau]$, $\tau > 0$, where $\Omega^*(\omega_t)$ is the solution to $(\mathscr{F}_{\omega_t})$ and $\omega_0 = \omega$. If such a $\mathbf{W}^*$ exists, then it depends on $\mathbf{V}$. In Theorem 3.1 we prove the existence of $\mathbf{W}^*$ as a function of $\mathbf{V}$. In this section we make explicit the dependence of $\mathbf{W}^*$ on $\mathbf{V}$. To obtain such a result, we study the sensitivity of the solution u to (1)-(4) with respect to ω. According to [SZ92], the shape derivative $u'(\mathbf{V}, \mathbf{W}^*)$ of u solution of (1)-(4) with respect to both transformations $T_t(\mathbf{V})$ and $T_t(\mathbf{W}^*)$ verifies

$$-\Delta u'(\mathbf{V}, \mathbf{W}^*) = 0 \quad \text{in} \quad \Omega^*(\omega) \setminus \overline{\omega}, \tag{29}$$

$$u'(\mathbf{V}, \mathbf{W}^*) = -\partial_n u \mathbf{V} \cdot \mathbf{n} \quad \text{on} \quad \Sigma, \tag{30}$$

$$u'(\mathbf{V}, \mathbf{W}^*) = -\partial_n u \mathbf{W}^* \cdot \mathbf{n} \quad \text{on} \quad \Gamma^*(\omega), \tag{31}$$

$$\partial_n u'(\mathbf{V}, \mathbf{W}^*) = \operatorname{div}_\Gamma(\nabla_\Gamma u \mathbf{W}^* \cdot \mathbf{n}) + \mu \mathscr{H} \mathbf{W}^* \cdot \mathbf{n} \quad \text{on} \quad \Gamma^*(\omega). \tag{32}$$

In view of (1)-(4) we have $\nabla_\Gamma u = 0$ and $\partial_n u = \mu$ on Γ, and we may simplify (29)-(32) as

$$-\Delta u'(\mathbf{V}, \mathbf{W}^*) = 0 \quad \text{in} \quad \Omega^*(\omega) \setminus \overline{\omega}, \tag{33}$$

$$u'(\mathbf{V}, \mathbf{W}^*) = -\partial_n u \mathbf{V} \cdot \mathbf{n} \quad \text{on} \quad \Sigma, \tag{34}$$

$$u'(\mathbf{V}, \mathbf{W}^*) = -\mu \mathbf{W}^* \cdot \mathbf{n} \quad \text{on} \quad \Gamma^*(\omega), \tag{35}$$

$$\partial_n u'(\mathbf{V}, \mathbf{W}^*) = \mu \mathscr{H} \mathbf{W}^* \cdot \mathbf{n} \quad \text{on} \quad \Gamma^*(\omega). \tag{36}$$

Since $\mathbf{W}^* = \mathbf{W}^*(\mathbf{V})$, we actually have $u'(\mathbf{V}, \mathbf{W}^*) = u'(\mathbf{V})$. Indeed, gathering the boundary conditions (35) and (36), we obtain the following partial differential equation with Robin boundary conditions on Γ for $u'(\mathbf{V})$

$$-\Delta u'(\mathbf{V}) = 0 \quad \text{in} \quad \Omega \setminus \overline{\omega}^*(\omega), \tag{37}$$

$$u'(\mathbf{V}) = -\partial_n u \mathbf{V} \cdot \mathbf{n} \quad \text{on} \quad \Sigma, \tag{38}$$

$$\partial_n u'(\mathbf{V}) + \mathscr{H} u'(\mathbf{V}) = 0 \quad \text{on} \quad \Gamma^*(\omega). \tag{39}$$

Assuming $\mathscr{H} \geq 0$, equation (37)-(39) has a unique solution $u'(\mathbf{V})$; see Lemma 3.1. Using boundary conditions (35), we formally obtain

$$\mathbf{W}^*(\mathbf{V}) = -\mu^{-1} u'(\mathbf{V}) \mathbf{n} \quad \text{on}\, \Gamma^*(\omega) \tag{40}$$

and the normal component of $\mathbf{W}^*(\mathbf{V})$ is uniquely defined on Γ. The tangential component of $\mathbf{W}^*$ can be chosen arbitrarily according to the Hadamard structure theorem [SZ92] mentioned in Section 3.1 and we take it equal to zero.

Before showing the existence of $\mathbf{W}^*(\mathbf{V})$ in Theorem 3.1, we need the following preliminary lemmae.

Lemma 3.1. *Let $m \geq 2$ be an integer and $0 < \alpha < 1$. If $\psi \in \mathscr{C}^{m-1,\alpha}(\Gamma)$, Ω is bounded of class $\mathscr{C}^{m+1,\alpha}$, ω is bounded of class $\mathscr{C}^{m,\alpha}$ and $\mathscr{H} \geq 0$ on Γ, then the linearized system*

$$\begin{aligned} -\Delta v &= 0 \quad \textit{in} \quad \Omega \setminus \overline{\omega}, \\ v &= 0 \quad \textit{on} \quad \Sigma, \\ \partial_n v + \mathscr{H} v &= \psi \quad \textit{on} \quad \Gamma. \end{aligned}$$

admits a unique solution $v \in \mathscr{C}_b^{m,\alpha}(\Omega \setminus \overline{\omega})$.

Proof. If Ω is of class $\mathscr{C}^{m+1,\alpha}$, then $\mathscr{H} = \mathrm{div}_\Gamma(\mathbf{n})$ is of class $\mathscr{C}^{m-1,\alpha}$. Applying standards regularity results for elliptic operators we obtain the result; see [Tro87, Lemma 3.19]. □

We introduce the functions $u_{1,\mathbf{V},\mathbf{W}}$ and $u_{2,\mathbf{V},\mathbf{W}}$, solutions of

$$-\Delta u_{1,\mathbf{V},\mathbf{W}} = 0 \quad \text{in} \quad \Omega_\mathbf{W} \setminus \overline{\omega_\mathbf{V}}, \tag{41}$$
$$u_{1,\mathbf{V},\mathbf{W}} = 1 \quad \text{on} \quad \Sigma_\mathbf{V}, \tag{42}$$
$$u_{1,\mathbf{V},\mathbf{W}} = 0 \quad \text{on} \quad \Gamma_\mathbf{W}, \tag{43}$$

and

$$-\Delta u_{2,\mathbf{V},\mathbf{W}} = 0 \quad \text{in} \quad \Omega_\mathbf{W} \setminus \overline{\omega_\mathbf{V}}, \tag{44}$$
$$u_{2,\mathbf{V},\mathbf{W}} = 1 \quad \text{on} \quad \Sigma_\mathbf{V}, \tag{45}$$
$$\partial_n u_{2,\mathbf{V},\mathbf{W}} = \mu \quad \text{on} \quad \Gamma_\mathbf{W}, \tag{46}$$

respectively.

Lemma 3.2. *Let $m \geq 2$, $0 < \alpha < 1$ and Ω, ω be bounded of class $\mathscr{C}^{m,\alpha}$. Then the functions*

$$(\mathbf{V}, \mathbf{W}) \in (\mathscr{C}_b^{m,\alpha}(\mathbb{R}^2, \mathbb{R}^2))^2 \to u_{1,\mathbf{V},\mathbf{W}} \circ (I + \mathbf{V} + \mathbf{W}) \in \mathscr{C}_b^{m,\alpha}(\Omega \setminus \overline{\omega})$$

and

$$(\mathbf{V}, \mathbf{W}) \in (\mathscr{C}_b^{m,\alpha}(\mathbb{R}^2, \mathbb{R}^2))^2 \to u_{2,\mathbf{V},\mathbf{W}} \circ (I + \mathbf{V} + \mathbf{W}) \in \mathscr{C}_b^{m,\alpha}(\Omega \setminus \overline{\omega})$$

are of class $\mathscr{C}^\infty$.

Proof. The proof follows the ideas of [HP05, Theorem 5.5.1] with some adaptations. We give here the proof in our context for the convenience of the reader. We only prove the case of $u_{2,\mathbf{V},\mathbf{W}}$, the case of $u_{1,\mathbf{V},\mathbf{W}}$ being a straightforward adaptation of it. We first set $z_{\mathbf{V},\mathbf{W}} := u_{2,\mathbf{V},\mathbf{W}} - 1$ so that z satisfies the following variational formulation

$$\int_{\Omega_\mathbf{W} \setminus \overline{\omega_\mathbf{V}}} \nabla z_{\mathbf{V},\mathbf{W}} \cdot \nabla \varphi = \mu \int_{\Gamma_\mathbf{W}} \varphi \qquad \text{for all } \varphi \in H^1_{\Sigma_\mathbf{V}}(\Omega_\mathbf{W} \setminus \overline{\omega_\mathbf{V}}). \tag{47}$$

Transporting back the problem on $\Omega \setminus \overline{\omega}$ by using the transformation $(I + \mathbf{V} + \mathbf{W})^{-1}$ we obtain

$$\int_{\Omega \setminus \overline{\omega}} A(\mathbf{V}, \mathbf{W}) \nabla Z_{\mathbf{V},\mathbf{W}} \cdot \nabla \varphi = \mu \int_\Gamma \varphi J_{\Gamma,\mathbf{W}} \qquad \text{for all } \varphi \in H^1_\Sigma(\Omega \setminus \overline{\omega}), \tag{48}$$

with

$$\begin{aligned}
Z_{\mathbf{V},\mathbf{W}} &:= z_{\mathbf{V},\mathbf{W}} \circ (I+\mathbf{V}+\mathbf{W}),\\
A(\mathbf{V},\mathbf{W}) &:= J_{\mathbf{V},\mathbf{W}}(I+D\mathbf{V}+D\mathbf{W})^{-1}(I+D\mathbf{V}^t+D\mathbf{W}^t)^{-1},\\
J_{\mathbf{V},\mathbf{W}} &:= \det(I+D\mathbf{V}+D\mathbf{W}),\\
J_{\Gamma,\mathbf{W}} &:= \det(I+D\mathbf{W})\|(I+D\mathbf{W})^{-t}\mathbf{n}\|,
\end{aligned}$$

where $J_{\mathbf{V},\mathbf{W}}$ is the Jacobian of transformation $I+\mathbf{V}+\mathbf{W}$ while $J_{\Gamma,\mathbf{W}}$ is the boundary Jacobian on Γ. We introduce the function

$$\begin{aligned}
G:(\mathscr{C}_b^{m,\alpha}(\mathbb{R}^2,\mathbb{R}^2))^2 \times \mathscr{C}_b^{m,\alpha}(\Omega\setminus\overline{\omega}) &\to [\mathscr{C}_b^{m-2,\alpha}(\Omega\setminus\overline{\omega})]_{(H^1_\Sigma(\Omega\setminus\overline{\omega}))'}\\
(\mathbf{V},\mathbf{W},z) &\mapsto \mathscr{A}_{\mathbf{V},\mathbf{W}}(z)-\mu\,\mathscr{J}_{\mathbf{W}},
\end{aligned}$$

where $[\mathscr{C}_b^{m-2,\alpha}(\Omega\setminus\overline{\omega})]_{(H^1_\Sigma(\Omega\setminus\overline{\omega}))'}$ denotes the subspace of $(H^1_\Sigma(\Omega\setminus\overline{\omega}))'$ composed of $\mathscr{C}_b^{m-2,\alpha}(\Omega\setminus\overline{\omega})$ functions and

$$\begin{aligned}
\mathscr{A}_{\mathbf{V},\mathbf{W}}(z) &: \varphi\in H^1_\Sigma(\Omega\setminus\overline{\omega}) \mapsto \int_{\Omega\setminus\overline{\omega}} A(\mathbf{V},\mathbf{W})\nabla z\cdot\nabla\varphi \in \mathbb{R},\\
\mathscr{J}_{\mathbf{W}} &: \varphi\in H^1_\Sigma(\Omega\setminus\overline{\omega}) \mapsto \int_\Gamma J_{\Gamma,\mathbf{W}}\varphi \in \mathbb{R}.
\end{aligned}$$

First of all the function

$$(\mathbf{V},\mathbf{W})\in(\mathscr{C}_b^{m,\alpha}(\mathbb{R}^2,\mathbb{R}^2))^2 \mapsto J_{\mathbf{V},\mathbf{W}} = \det(I+D\mathbf{V}+D\mathbf{W}) \in \mathscr{C}_b^{m-1,\alpha}(\mathbb{R}^2,\mathbb{R})$$

is of class $\mathscr{C}^\infty$ since $I+D\mathbf{V}+D\mathbf{W}$ is linear in $(\mathbf{V},\mathbf{W})$ and the determinant is polynomial and continuous for the $\mathscr{C}^{m,\alpha}$-norm. Writing $(I+D\mathbf{V}+D\mathbf{W})^{-1}=\sum_{q\ge 0}(-1)^q(D\mathbf{V}+D\mathbf{W})^q$, we can see that the function

$$(\mathbf{V},\mathbf{W})\in(\mathscr{C}_b^{m,\alpha}(\mathbb{R}^2,\mathbb{R}^2))^2 \mapsto (I+D\mathbf{V}+D\mathbf{W})^{-1} \in \mathscr{C}_b^{m-1,\alpha}(\mathbb{R}^2,\mathscr{M}_2)$$

is of class $\mathscr{C}^\infty$, where $\mathscr{M}_2$ is the set of 2×2-matrices. Thus $(\mathbf{V},\mathbf{W})\to A(\mathbf{V},\mathbf{W})$ is $\mathscr{C}^\infty$. Since the function

$$\begin{aligned}
\mathscr{C}_b^{m-1,\alpha}(\mathbb{R}^2,\mathscr{M}_2)\times H^1_\Sigma(\Omega\setminus\overline{\omega}) &\to (H^1_\Sigma(\Omega\setminus\overline{\omega}))'\\
(A,z) &\mapsto \left(\varphi\in H^1_\Sigma(\Omega\setminus\overline{\omega})\mapsto \int_{\Omega\setminus\overline{\omega}} A\nabla z\cdot\nabla\varphi\in\mathbb{R}\right)
\end{aligned}$$

is bilinear and continuous, this yields

$$\begin{aligned}
(\mathscr{C}_b^{m,\alpha}(\mathbb{R}^2,\mathbb{R}^2))^2 \times \mathscr{C}_b^{m,\alpha}(\Omega\setminus\overline{\omega}) &\to [\mathscr{C}_b^{m-2,\alpha}(\Omega\setminus\overline{\omega})]_{(H^1_\Sigma(\Omega\setminus\overline{\omega}))'}\\
(\mathbf{V},\mathbf{W},z) &\mapsto \mathscr{A}_{\mathbf{V},\mathbf{W}}(z)
\end{aligned}$$

is of class $\mathscr{C}^\infty$. For small $\mathbf{W}$ the function $\mathbf{W}\mapsto J_{\Gamma,\mathbf{W}}$ is $\mathscr{C}^\infty$ and since the trace operator is linear and continuous we obtain that

$$\mathbf{W}\in\mathscr{C}_b^{m,\alpha}(\mathbb{R}^2,\mathbb{R}^2)\mapsto \mathscr{J}_{\mathbf{W}} \in [\mathscr{C}_b^{m-2,\alpha}(\Omega\setminus\overline{\omega})]_{(H^1_\Sigma(\Omega\setminus\overline{\omega}))'}$$

is of class $\mathscr{C}^\infty$. Gathering the previous results we get that G is $\mathscr{C}^\infty$. We compute

$$D_zG(0,0,0)(\hat{z}) : \varphi \in H^1_\Sigma(\Omega\setminus\overline{\omega}) \mapsto \int_{\Omega\setminus\overline{\omega}} \nabla\hat{z}\cdot\nabla\varphi \in \mathbb{R}.$$

Since $\hat{z} \in \mathscr{C}_b^{m,\alpha}(\Omega\setminus\overline{\omega})$, $m \geq 2$, we actually have the strong form

$$D_zG(0,0,0)(\hat{z}) = -\Delta\hat{z} \in [\mathscr{C}_b^{m-2,\alpha}(\Omega\setminus\overline{\omega})]_{(H^1_\Sigma(\Omega\setminus\overline{\omega}))'}.$$

Since Ω and ω are of class $\mathscr{C}^{m,\alpha}$, $0<\alpha<1$, the theory of regularity of elliptic partial differential equations implies that

$$D_zG(0,0,0) : \mathscr{C}_b^{m,\alpha}(\Omega\setminus\overline{\omega}) \to [\mathscr{C}_b^{m-2,\alpha}(\Omega\setminus\overline{\omega})]_{(H^1_\Sigma(\Omega\setminus\overline{\omega}))'}$$

is an isomorphism. Therefore we can apply the implicit function theorem and there exists a function

$$(\mathbf{V},\mathbf{W}) \in (\mathscr{C}_b^{m,\alpha}(\mathbb{R}^2,\mathbb{R}^2))^2 \mapsto Z(\mathbf{V},\mathbf{W}) \in \mathscr{C}_b^{m,\alpha}(\Omega\setminus\overline{\omega})$$

of class $\mathscr{C}^\infty$ on a neighbourhood of $(0,0)$ such that $G(\mathbf{V},\mathbf{W},Z(\mathbf{V},\mathbf{W})) \equiv 0$. By uniqueness of the solution to (48) we get $Z(\mathbf{V},\mathbf{W}) = z_{\mathbf{V},\mathbf{W}} \circ (I+\mathbf{V}+\mathbf{W})$. Finally since $u_{2,\mathbf{V},\mathbf{W}} = z_{\mathbf{V},\mathbf{W}} + 1$, we have proved the claim. □

We now give a proof of the existence of $\mathbf{W}^*(\mathbf{V})$.

Theorem 3.1. *Assume there exists two bounded open sets Ω,ω of class $\mathscr{C}^{m+1,\alpha}$, $m\geq 2$, $0<\alpha<1$ such that the over-determined system (1)-(4) is satisfied in $\Omega\setminus\overline{\omega}$. Assume in addition that $\mathscr{H}\geq 0$ on $\Gamma=\partial\Omega$. Then there exists an open neighborhood $\mathscr{V}$ of 0 in $\mathscr{C}_b^{m,\alpha}(\mathbb{R}^2,\mathbb{R}^2)$ and a function*

$$\mathscr{V} \ni \mathbf{V} \mapsto \mathbf{W}^*(\mathbf{V}) \in \mathscr{C}_b^{m,\alpha}(\mathbb{R}^2,\mathbb{R}^2)$$

of class $\mathscr{C}^\infty$ such that (1)-(4) has a solution in $\Omega_{\mathbf{W}^*(\mathbf{V})}\setminus\overline{\omega_{\mathbf{V}}}$ for all $\mathbf{V}\in\mathscr{V}$ and $\mathbf{W}^*(0)\equiv 0$.

Proof. The main tool to prove this result is the implicit function theorem. First of all since Ω is of class $\mathscr{C}^{m+1,\alpha}$ we have $\mathscr{H} = \mathrm{div}_\Gamma(\mathbf{n}) \in \mathscr{C}^{m-1,\alpha}(\Gamma)$. Next, we introduce

$$\begin{aligned} F : \mathscr{C}^{m,\alpha}(\Sigma)\times\mathscr{C}^{m,\alpha}(\Gamma) &\to \mathscr{C}_b^{m,\alpha}(\Omega\setminus\overline{\omega}),\\ (v_n,w_n) &\mapsto (u_{1,\mathbf{V},\mathbf{W}} - u_{2,\mathbf{V},\mathbf{W}})\circ(I+\mathbf{V}+\mathbf{W})|_\Gamma, \end{aligned}$$

where $(\mathbf{V},\mathbf{W}) \in (\mathscr{C}_b^{m,\alpha}(\mathbb{R}^2,\mathbb{R}^2))^2$ are extensions along the normal of (v_n,w_n), i.e., $\mathbf{V}|_\Sigma := v_n\mathbf{n}_\Sigma$ and $\mathbf{W}|_\Gamma := w_n\mathbf{n}_\Gamma$. Since Ω,ω are of class $\mathscr{C}^{m+1,\alpha}$ we have $\mathbf{n}_\Gamma \in \mathscr{C}^{m,\alpha}(\Gamma)$ and $\mathbf{n}_\Sigma \in \mathscr{C}^{m,\alpha}(\Sigma)$ and we can find such extensions $\mathbf{V},\mathbf{W}$. With $(\mathbf{V},\mathbf{W}) \in (\mathscr{C}_b^{m,\alpha}(\mathbb{R}^2,\mathbb{R}^2))^2$ follows $u_{1,\mathbf{V},\mathbf{W}}$ and $u_{2,\mathbf{V},\mathbf{W}} \in \mathscr{C}_b^{m,\alpha}(\Omega_\mathbf{W}\setminus\overline{\omega_\mathbf{V}})$. Since we have assumed that there exists Ω and ω such that (1)-(4) has a solution, by uniqueness of the solution to (41)-(43) we get $u_{1,0,0} = u_{2,0,0}$ in $\Omega\setminus\overline{\omega}$ and therefore $F(0,0)=0$. From now on we write $u_1 = u_{1,0,0}$ and $u_2 = u_{2,0,0}$ for simplicity.

In order to apply the implicit function theorem and obtain $\mathbf{W}^*(\mathbf{V})$, we need to prove that F is continuously differentiable, and that its derivative is an isomorphism. According to Lemma 3.2 we have

$$(\mathbf{V},\mathbf{W}) \in (\mathscr{C}_b^{m,\alpha}(\mathbb{R}^2,\mathbb{R}^2))^2 \mapsto (u_{1,\mathbf{V},\mathbf{W}} - u_{2,\mathbf{V},\mathbf{W}})\circ(I+\mathbf{V}+\mathbf{W}) \in \mathscr{C}_b^{m,\alpha}(\Omega\setminus\overline{\omega})$$

is of class $\mathscr{C}^\infty$. Since the extensions $v_n \mapsto \mathbf{V}$ and $w_n \mapsto \mathbf{W}$ are linear and continuous, we also get

$$(v_n, w_n) \in \mathscr{C}^{m,\alpha}(\Sigma) \times \mathscr{C}^{m,\alpha}(\Gamma) \mapsto (u_{1,\mathbf{V},\mathbf{W}} - u_{2,\mathbf{V},\mathbf{W}}) \circ (I + \mathbf{V} + \mathbf{W}) \in \mathscr{C}_b^{m,\alpha}(\Omega \setminus \overline{\varpi})$$

is of class $\mathscr{C}^\infty$. The derivative of $u_{i,0,\mathbf{W}} \circ (I + \mathbf{W})$ with respect to $\mathbf{W}$ is the *material derivative* denoted $\dot{u}_i(\mathbf{W})$, i=1,2. Defining the so-called *shape derivative*:

$$u_i'(\mathbf{W}) := \dot{u}_i(\mathbf{W}) - \nabla u_i \cdot \mathbf{W},$$

we get

$$\begin{aligned} D_{w_n} F(0,0)(w_n) &= \dot{u}_1(\mathbf{W}) - \dot{u}_2(\mathbf{W}) = u_1'(\mathbf{W}) - u_2'(\mathbf{W}) + \nabla u_1 \cdot \mathbf{W} - \nabla u_2 \cdot \mathbf{W} \\ &= u_1'(\mathbf{W}) - u_2'(\mathbf{W}), \end{aligned}$$

since $u_1 = u_2$. According to standard shape calculus; see [SZ92] for instance, $u_1'(\mathbf{W})$ and $u_2'(\mathbf{W})$ satisfy the following equations

$$\begin{aligned} -\Delta u_1'(\mathbf{W}) &= 0 \quad \text{in} \quad \Omega \setminus \overline{\varpi}, \\ u_1'(\mathbf{W}) &= 0 \quad \text{on} \quad \Sigma, \\ u_1'(\mathbf{W}) &= -\partial_n u_1 w_n \quad \text{on} \quad \Gamma, \end{aligned}$$

and

$$\begin{aligned} -\Delta u_2'(\mathbf{W}) &= 0 \quad \text{in} \quad \Omega \setminus \overline{\varpi}, \\ u_2'(\mathbf{W}) &= 0 \quad \text{on} \quad \Sigma, \\ \partial_n u_2'(\mathbf{W}) &= \mathrm{div}_\Gamma(\nabla_\Gamma u_2 w_n) + \mu \mathscr{H} w_n \quad \text{on} \quad \Gamma. \end{aligned}$$

We prove first the injectivity of $D_{w_n} F(0,0)$. Assume that $D_{w_n} F(0,0)(w_n) = 0$. This implies $u_1'(\mathbf{W}) = u_2'(\mathbf{W})$. Taking into account that $u_1 = u_2 = 0$ and $\partial_n u_1 = \mu$ on Γ as well, we get that $w_n = -\mu^{-1} u_1'(\mathbf{W})$ on Γ and $u_2'(\mathbf{W})$ solves

$$\begin{aligned} -\Delta u_2'(\mathbf{W}) &= 0 \quad \text{in} \quad \Omega \setminus \overline{\varpi}, \\ u_2'(\mathbf{W}) &= 0 \quad \text{on} \quad \Sigma, \\ \partial_n u_2'(\mathbf{W}) + \mathscr{H} u_2'(\mathbf{W}) &= 0 \quad \text{on} \quad \Gamma. \end{aligned}$$

Since $\mathscr{H} \in \mathscr{C}^{m-1,\alpha}(\Gamma)$ and $\mathscr{H} \geq 0$ on Γ, this function has a unique solution $u_2'(\mathbf{W}) \equiv 0$ in view of Lemma 3.1. This implies that $w_n = 0$ and the injectivity is proved.

Next, we prove surjectivity. Let $\psi \in \mathscr{C}_b^{m,\alpha}(\Omega \setminus \overline{\varpi})$. We are looking for a solution of the equation

$$D_{w_n} F(0,0)(w_n) = u_1'(\mathbf{W}) - u_2'(\mathbf{W}) = \psi. \tag{49}$$

In view of the previous computation, $u_2'(\mathbf{W})$ solves

$$\begin{aligned} -\Delta u_2'(\mathbf{W}) &= 0 \quad \text{in} \quad \Omega \setminus \overline{\varpi}, \\ u_2'(\mathbf{W}) &= 0 \quad \text{on} \quad \Sigma, \\ \partial_n u_2'(\mathbf{W}) + \mathscr{H} u_2'(\mathbf{W}) &= -\mathscr{H} \psi \quad \text{on} \quad \Gamma. \end{aligned}$$

and $w_n = -\mu^{-1}(u_2'(\mathbf{W}) + \psi)$. Applying again Lemma 3.1 there exists a unique solution $u_2'(\mathbf{W}) \in \mathscr{C}_b^{m,\alpha}(\Omega \setminus \overline{\omega})$. Consequently we get

$$w_n = -\mu^{-1}(u_2'(\mathbf{W}) + \psi) \in \mathscr{C}^{m,\alpha}(\Gamma),$$

and this proves the surjectivity of $D_{w_n}F(0,0)$.

We have shown that $D_{w_n}F(0,0)$ is an isomorphism from $\mathscr{C}^{m,\alpha}(\Gamma)$ to $\mathscr{C}_b^{m,\alpha}(\Omega \setminus \overline{\omega})$. Therefore, we may apply the implicit function theorem to F, i.e., there exists a neighborhood $\mathscr{V}_\Gamma$ of 0 in $\mathscr{C}^{m,\alpha}(\Gamma)$ and a unique $\mathscr{C}^\infty$ function

$$\mathscr{C}^{m,\alpha}(\Sigma) \ni v_n \mapsto w_n^*(v_n) \in \mathscr{C}^{m,\alpha}(\Gamma)$$

such that $F(v_n, w_n^*(v_n)) \equiv 0$ for all $v_n \in \mathscr{V}_\Gamma$ with $w_n^*(0) = 0$.

The statement of the theorem is obtained by considering the trace

$$r : \begin{array}{rl} \mathscr{C}_b^{m,\alpha}(\mathbb{R}^2, \mathbb{R}^2) & \to \mathscr{C}^{m,\alpha}(\Sigma), \\ \mathbf{V} & \mapsto (\mathbf{V} \cdot \mathbf{n})|_\Gamma, \end{array}$$

and the linear extension along the normal $\mathbf{n}_\Gamma$

$$e : \begin{array}{rl} \mathscr{C}^{m,\alpha}(\Gamma) & \to \mathscr{C}_b^{m,\alpha}(\mathbb{R}^2, \mathbb{R}^2), \\ w_n & \mapsto \mathbf{W}. \end{array}$$

Note that the restriction r is well-defined due to $\mathbf{n}_\Sigma \in \mathscr{C}^{m,\alpha}(\Sigma, \mathbb{R}^2)$. Taking a neighborhood $\mathscr{V}$ of 0 in $\mathscr{C}_b^{m,\alpha}(\mathbb{R}^2, \mathbb{R}^2)$ such that $r(\mathscr{V}) \subset \mathscr{V}_\Gamma$ and applying the previous result with $v_n := r(\mathbf{V})$, we get a unique w_n^* in $\mathscr{C}^{m,\alpha}(\Gamma)$. Setting $\mathbf{W}^* := e(w_n^*)$ we obtain the main statement. Since the extension e is obviously not unique, $\mathbf{W}^*$ is not unique as well, even if w_n^* is. We can also note that $\mathbf{W}^*$ depends actually only on $v_n = (\mathbf{V} \cdot \mathbf{n})|_\Gamma$ and not on $\mathbf{V}$.

Finally, the trace r and extension e are linear and continuous, therefore the function

$$\mathscr{V} \ni \mathbf{V} \mapsto \mathbf{W}^*(\mathbf{V}) \in \mathscr{C}_b^{m,\alpha}(\mathbb{R}^2, \mathbb{R}^2)$$

is of class $\mathscr{C}^\infty$ by composition. □

From equation (33)-(35) for $u'(\mathbf{V})$, we may obtain a local monotonicity result.

Theorem 3.2. *Let Ω be convex, bounded and of class $\mathscr{C}^{2,\alpha}$. If $\mu < 0$ and $\mathbf{V}(x) \cdot \mathbf{n}(x) \leq 0$ for all $x \in \Sigma$, then $\mathbf{W}^*(x) \cdot \mathbf{n}(x) \geq 0$ for all $x \in \Gamma$.*

Proof. Since $u'(\mathbf{V})$ is harmonic, the maximum principle states that the minimum of $u'(\mathbf{V})$ is attained on $\Gamma \cup \Sigma$. The function u is also harmonic, therefore its maximum is attained on Σ, where $u = 1$ and $\partial_n u(x) \geq 0$ for all $x \in \Sigma$. Therefore, in view of the assumption $\mathbf{V}(x) \cdot \mathbf{n}(x) \leq 0$ on Σ, we have $u'(\mathbf{V}) \geq 0$ on Σ due to (38). Consequently, the minimum of $u'(\mathbf{V})$ is attained on Γ and not on Σ.

Due to (35) and since $\mu < 0$ by assumption, the claim $\mathbf{W}^*(x) \cdot \mathbf{n}(x) \geq 0$ for all $x \in \Gamma$ amounts to proving that $u'(\mathbf{V}) \geq 0$ on Γ. By contradiction, we assume that there exists a point $z \in \Gamma$ such that $u'(\mathbf{V})(z) < 0$. Since Ω is convex, we have $\mathscr{H}(z) \geq 0$ for all $z \in \Gamma$. Therefore, due to (39), we have

$$\partial_n u'(\mathbf{V})(z) = -\mathscr{H} u'(\mathbf{V})(z) \geq 0. \tag{50}$$

Since Ω is of class $\mathscr{C}^{2,\alpha}$, it satisfies the interior ball condition and we may apply Hopf's lemma (see [PW67] for details), so we must have $\partial_n u'(\mathbf{V})(z) < 0$ in contradiction with (50). Thus the initial assumption is wrong and $u'(\mathbf{V})(z) \geq 0$ on Γ. Therefore, since $u'(\mathbf{V})$ is harmonic, we have due to the maximum principle that $u'(\mathbf{V}) \geq 0$ in Ω, and in view of (40), that $\mathbf{W}^*(x) \cdot \mathbf{n}(x) \geq 0$ for all $x \in \Gamma$. □

Remark 3.1. *The convexity of Ω in Theorem 3.2 holds whenever ω is convex (See for instance* [HP05, Theorem 6.2.2]*)*

Remark 3.2. *Under the assumptions of Theorem 3.1, Theorem 3.2 leads to the monotonicity for the set inclusion of $\Omega^*(\omega)$ with respect to ω in a small neighbourhood of ω, i.e., if $\omega_1 \subset \omega_2$ are two convex sets and ω_2 is close to ω_1 in the sense that there exists a $\mathbf{V} \in \mathscr{V}$ such that $\omega_2 = (I+\mathbf{V})(\omega_1)$, then $\Omega^*(\omega_1) \subset \Omega^*(\omega_2)$. Indeed, we then have $\Omega^*(\omega_2) = (I+\mathbf{W}^*(\mathbf{V}))(\Omega^*(\omega_1))$. Since $\omega_1 \subset \omega_2$ we have $\mathbf{V}\cdot\mathbf{n} \leq 0$ on Σ and using Theorem 3.2 we get $\mathbf{W}^*(\mathbf{V})\cdot\mathbf{n} \geq 0$ and $\Omega^*(\omega_1) \subset \Omega^*(\omega_2)$ follows.*

In what follows, we will need the following standard lemma.

Lemma 3.3 ([HP05])**.** *Let ω be of class $\mathscr{C}^{m,\alpha}$, $\mathbf{V} \in \mathscr{C}_b^{m,\alpha}(\mathbb{R}^2,\mathbb{R}^2)$, $m \geq 2$ and $\omega_t = T_t(\mathbf{V})(\omega)$. Assume $t \in [0,\tau[\to f(t) \in L^1(\mathbb{R}^2)$ is differentiable at $t=0$ with derivative $f'(0)$ and $f(0) \in W^{1,1}(\mathbb{R}^2)$. Then*

$$\frac{d}{dt}\int_{\omega_t} f(t)(x)\,dx\,\Big|_{t=0} = \int_{\omega} f'(0)(x)\,dx + \int_{\partial\omega} f(0)(x)\,\mathbf{V}\cdot\mathbf{n}\,ds. \tag{51}$$

3.3. **Shape derivative of the cost functional K_1.** We express the shape derivative of K_1 as defined in (24) in the Hadamard-Zolesio structure form (27), under appropriate smoothness conditions on the boundary of Ω.

Theorem 3.3. *Let $\omega \subset \mathbb{R}^2$ be a bounded domain, with a boundary of class $\mathscr{C}^{2,\alpha}$, and let $\mathbf{V} \in \mathscr{C}_b^{2,\alpha}(\mathbb{R}^2,\mathbb{R}^2)$ be given. Assume $\mathscr{H} \geq 0$ on $\Gamma^*(\omega)$. Then the shape gradient $\nabla K_1(\omega)$ of the cost K_1 can be expressed as*

$$\nabla K_1(\omega) = [\nabla p \cdot \nabla u] \in \mathscr{C}^{1,\alpha}(\Sigma), \tag{52}$$

where all expressions are evaluated on Σ, and the adjoint state p satisfies

$$-\Delta p = 0 \quad in \quad \Omega^*(\omega)\setminus\overline{\omega}, \tag{53}$$

$$p = 0 \quad on \quad \Sigma, \tag{54}$$

$$\partial_n p + \mathscr{H} p = -\mu^{-1}\mathbb{1}_{E^c} + \mu^{-1}\mathbb{1}_E \quad on \quad \Gamma^*(\omega). \tag{55}$$

Proof. Using Lemma 3.3 we obtain the Eulerian derivative of $J_1(\Omega)$ at Ω in direction $\mathbf{W} \in \mathscr{C}_b^{2,\alpha}(\mathbb{R}^2,\mathbb{R}^2)$:

$$dJ_1(\Omega;\mathbf{W}) = \int_{\Gamma\cap E^c} \mathbf{W}\cdot\mathbf{n}\,ds + \int_{\Gamma\cap E} -\mathbf{W}\cdot\mathbf{n}\,ds. \tag{56}$$

Note that in (56), there is no contribution from the shape derivative along ∂E since E is fixed. The minus sign in the second integral comes from the orientation of the normal vector in $E \cap \Omega^c$. Since $K_1(\omega_{\mathbf{V}}) = J_1((I + \mathbf{W}^*(\mathbf{V}))(\Omega^*(\omega)))$ we may apply the chain rule thanks to Theorem 3.1 and (56). Using (40) we obtain

(57)
$$\begin{aligned} dK_1(\omega;\mathbf{V}) &= dJ_1(\Omega^*(\omega);\mathbf{W}^*(\mathbf{V})) \\ &= \int_{\Gamma^*\cap E^c} -\mu^{-1}u'\,ds + \int_{\Gamma^*\cap E} \mu^{-1}u'\,ds = \int_{\Gamma^*} (-\mu^{-1}\mathbb{1}_{E^c} + \mu^{-1}\mathbb{1}_E)u'\,ds. \end{aligned}$$

To simplify (57), we introduce the adjoint state p solution of (53)-(55), which is well-defined due to $\mathscr{H} \geq 0$ on $\Gamma^*(\omega)$. Using Green's formula in $\Omega \setminus \overline{\omega}$ and utilizing (53)-(55), we obtain

$$\begin{aligned} \int_{\Gamma^*} (-\mu^{-1}\mathbb{1}_{E^c} + \mu^{-1}\mathbb{1}_E)u'\,ds &= \int_{\Gamma^*} (\partial_n p + \mathscr{H} p)u'\,ds \\ &= \int_{\Omega^*\setminus\overline{\omega}} (\Delta p u' - p\Delta u')\,dx + \int_{\Gamma^*} p(\partial_n u' + \mathscr{H} u')\,ds \\ &\quad + \int_{\Sigma} (-u'\partial_n p + p\partial_n u')\,ds. \end{aligned} \tag{58}$$

Using (37)-(39) and (53)-(55), we get

$$\int_{\Gamma^*} (-\mu^{-1}\mathbb{1}_{E^c} + \mu^{-1}\mathbb{1}_E)u'\,ds = \int_{\Sigma} (\partial_n p \partial_n u)\mathbf{V}\cdot\mathbf{n}\,ds = \int_{\Sigma} \nabla p \cdot \nabla u\, \mathbf{V}\cdot\mathbf{n}\,ds.$$

Since ω is of class $\mathscr{C}^{2,\alpha}$ and $\Omega^* \setminus \omega$ is of class $\mathscr{C}^\infty$ due to assumption (8), we have $p|_\Sigma, u|_\Sigma \in \mathscr{C}^{2,\alpha}(\Sigma)$ due to standard regularity results and $\mathbf{n}_\Sigma \in \mathscr{C}^{1,\alpha}(\Sigma,\mathbb{R}^2)$. Therefore $\nabla K_1(\omega) = [\nabla p \cdot \nabla u] \in \mathscr{C}^{1,\alpha}(\Sigma)$ so we can integrate

$$dK_1(\omega;\mathbf{V}) = \int_{\Sigma} \nabla p \cdot \nabla u\, \mathbf{V}\cdot\mathbf{n}\,ds, \tag{59}$$

and $\mathbf{V} \mapsto dK_1(\omega;\mathbf{V})$ is linear and continuous. □

3.4. **Shape derivative of the cost functional K_2.** In a similar way we express the shape derivative of K_2 in the Hadamard-Zolesio structure form (27), under appropriate smoothness conditions on the boundary of Ω.

Theorem 3.4. *Let $\omega \subset \mathbb{R}^2$ be a bounded domain, with a boundary of class $\mathscr{C}^{2,\alpha}$, and let $\mathbf{V} \in \mathscr{C}_b^{2,\alpha}(\mathbb{R}^2,\mathbb{R}^2)$ be given. Assume $\mathscr{H} \geq 0$ on $\Gamma^*(\omega)$. Then the shape derivative of K_2 at ω in direction $\mathbf{V}$ is*

$$dK_2(\omega,\mathbf{V}) = \int_{\Sigma} [\nabla u \cdot \nabla p + \nabla p_l \cdot \nabla u_l]\mathbf{V}\cdot\mathbf{n}\,ds, \tag{60}$$

where all expressions are evaluated on Σ, and the adjoint states p_l and p satisfy

$$-\Delta p_l = -(u - u_l) \quad \text{in } E \setminus \overline{\omega}, \tag{61}$$

$$p_l = 0 \quad \text{on } \Sigma, \tag{62}$$

$$p_l = 0 \quad \text{on } \partial E, \tag{63}$$

and

$$-\Delta p = u\mathbb{1}_{\Omega^*(\omega)\cap E^c} + (u-u_l)\mathbb{1}_{E\cap\omega^c} \quad \text{in } \Omega^*(\omega)\setminus\overline{\omega}, \tag{64}$$

$$p = 0 \quad \text{on } \Sigma, \tag{65}$$

$$\partial_n p + \mathscr{H} p = 0 \quad \text{on } \Gamma^*(\omega), \tag{66}$$

respectively.

Proof. Using Lemma 3.3 and the chain rule we obtain the Eulerian derivative of $K_2(\omega)$ with respect to ω in direction $\mathbf{V}$:

$$\begin{aligned} dK_2(\omega;\mathbf{V}) &= dJ_2(\Omega^*(\omega),\omega;\mathbf{W}^*(\mathbf{V})) \\ &= \int_{\Omega^*\cap E^c} uu'\,dx + \int_{E\cap\omega^c}(u-u_l)(u'-u_l')\,dx \\ &\quad + \frac{1}{2}\int_{\Gamma^*\cap E^c} u^2\mathbf{W}^*(\mathbf{V})\cdot\mathbf{n}\,ds + \frac{1}{2}\int_\Sigma (u-u_l)^2\mathbf{V}\cdot\mathbf{n}\,ds, \end{aligned} \tag{67}$$

where u' is the solution of (37)-(39) and u_l' satisfies [SZ92]

$$-\Delta u_l' = 0 \quad \text{in} \quad E\setminus\overline{\omega}, \tag{68}$$

$$u_l' = -\partial_n u_l \mathbf{V}\cdot\mathbf{n} \quad \text{on} \quad \Sigma, \tag{69}$$

$$u_l' = 0 \quad \text{on} \quad \partial E. \tag{70}$$

In view of the boundary conditions for u and u_l we get

$$\begin{aligned} dK_2(\omega;\mathbf{V}) &= \int_{\Omega^*\cap E^c} uu'\,dx + \int_{E\cap\omega^c}(u-u_l)(u'-u_l')\,dx \\ &= \int_{\Omega^*\cap\omega^c}(u\mathbb{1}_{\Omega^*\cap E^c} + (u-u_l)\mathbb{1}_{E\cap\omega^c})u'\,dx + \int_{E\cap\omega^c} -(u-u_l)u_l'\,dx, \end{aligned} \tag{71}$$

using $u'\equiv 0$ on $(\Omega^*(\omega))^c$. Next, we simplify the second integral in (71) by introducing the adjoint state p_l, the solution to (61)-(63), and we obtain

$$\begin{aligned} \int_{E\cap\omega^c} -(u-u_l)u_l'\,dx &= \int_{E\cap\omega^c} -\Delta p_l u_l'\,dx \\ &= \int_{E\cap\omega^c} -p_l\Delta u_l'\,dx + \int_\Sigma(-\partial_n p_l u_l' + p_l\partial_n u_l')\,ds \\ &= \int_\Sigma \partial_n p_l \partial_n u_l \mathbf{V}\cdot\mathbf{n}\,ds = \int_\Sigma \nabla p_l\cdot\nabla u_l \mathbf{V}\cdot\mathbf{n}\,ds. \end{aligned}$$

Similarly, to simplify the first integral in (71), we introduce the adjoint state p solution of (64)-(66), which leads to

$$\begin{aligned}\int_{\Omega^*\cap\omega^c}(u\mathbb{1}_{\Omega^*\cap E^c}+(u-u_l)\mathbb{1}_{\Omega^*\cap\omega^c})u'\,dx &= \int_{\Omega^*\cap\omega^c}-\Delta p u'\,dx\\ &= \int_{\Omega^*\cap\omega^c}-p\Delta u'\,dx+\int_{\Gamma^*\cup\Sigma}(-\partial_n p u'+p\partial_n u')\,ds\\ &= \int_\Sigma \partial_n p\partial_n u\mathbf{V}\cdot\mathbf{n}\,ds+\int_{\Gamma^*}u'(-\partial_n p-\mathscr{H}p)\,ds\\ &= \int_\Sigma \partial_n p\partial_n u\mathbf{V}\cdot\mathbf{n}\,ds=\int_\Sigma \nabla u\cdot\nabla p\,\mathbf{V}\cdot\mathbf{n}\,ds,\end{aligned}$$

where we used (39). Since the mapping $dK_2(\omega;\mathbf{V})$ is linear and continuous, we have obtained (60). □

4. Numerical algorithm and examples

We solve the optimization problems using an iterative process, i.e., we find a solution to the lower-level problem $(\mathscr{F}_\omega)$ first and then proceed to the upper-level problem consisting of the minimization of K_1 and K_2. For the upper-level problem, we use the boundary variation technique [AP06]. One may use the negative shape gradients $\mathbf{V}_i=-\nabla K_i(\omega)\mathbf{n}$ on $\Sigma,\ i=1,2$ as a descent direction, which need to be extended to the entire domain for the numerical method. In Algorithm 2 we introduce an extension of $\mathbf{V}_i$ over the entire domain $\Omega^*\setminus\overline{\omega}$ such that

$$dK_i(\omega;\mathbf{V}_i)=\int_\Sigma \nabla K_i(\omega)\mathbf{V}_i\cdot\mathbf{n}\,ds=-\int_{\Omega^*\setminus\overline{\omega}}(|D\mathbf{V}_i|^2+|\mathbf{V}_i|^2)\,d\mathbf{x}<0.$$

Therefore it provides a descent direction for the cost functionals $K_i,\ i=1,2$.

Remark 4.1. The current form of Algorithm 2 does not satisfy the inequality constraints in $\mathscr{U}_{ad}$. To realize these constraints, a penalty approach is used. Furthermore, the extension $\mathbf{V}_i$ of $-\nabla K_i(\omega)\mathbf{n}$ on the basis of (72-74) is also regularizing. Namely, if ω is of class $\mathscr{C}^{2,\alpha}$ we have shown for instance in (52) that $\nabla K_1(\omega)\in\mathscr{C}^{1,\alpha}(\Sigma)$ and the extension $\mathbf{V}_i$ is in $\mathscr{C}_b^{2,\alpha}(\Omega^*(\omega)\setminus\overline{\omega})$ in view of (72-74). If the Neumann boundary condition in (73) is replaced by a Dirichlet condition, then the regularization is insufficient and undesired oscillations of the shapes may occur [KK11].

Remark 4.2. Note that the shape gradient in (60) for the reduced cost K_2 involves the functions u,p and u_l,p_l defined on domains $\Omega^*(\omega)\setminus\overline{\omega}$ and $E\setminus\overline{\omega}$, respectively. From the numerical implementation perspective, these domains and the associated grids must be updated separately and consequently, some modification of Algorithm 2 is necessary. Specifically, in addition to steps (72)-(77) in Algorithm 2, the domain $E\setminus\overline{\omega}$ is updated via

$$E\setminus\overline{\omega}^{(k+1)}=(I+t^{(k)}\hat{\mathbf{V}}^{(k)})(E\setminus\overline{\omega}^{(k)}),$$

Algorithm 2 Bilevel shape optimization problem

• Choose initial shape Ω_0, tol, N_{max};
while ($(err > tol)$ & $(k < N_{max})$) **do**
 • Solve $(\mathscr{F}_{\omega^{(k)}})$ using Algorithm 1.
 • Compute the mean curvature $\mathscr{H}^{(k)}$ of $\Gamma^{(k)}$ using (14).
 • Compute the adjoint system (53)-(55) for J_1 or (61)-(63) and (64)-(66) for J_2.
 • Evaluate the descent direction $\mathbf{V}_i^{(k)}$ for $i = 1, 2$ by using

$$-\Delta \mathbf{V}_i^{(k)} + \mathbf{V}_i^{(k)} = 0 \text{ in } \Omega^*(\omega^{(k)}) \setminus \overline{\omega}^{(k)}, \tag{72}$$

$$\partial_n \mathbf{V}_i^{(k)} = -\nabla K_i(\omega^{(k)})\mathbf{n} \text{ on } \Sigma^{(k)}, \tag{73}$$

$$\mathbf{V}_i^{(k)} = 0 \quad \text{on } \Gamma^{(k)}. \tag{74}$$

 • Compute $\mathbf{W}^*(\mathbf{V}_i^{(k)})$ using (40).
 • Set $\Omega^*(\omega^{(k+1)}) \setminus \overline{\omega}^{(k+1)} = (I + t^{(k)}\tilde{\mathbf{V}}^{(k)})(\Omega^*(\omega^{(k)}) \setminus \overline{\omega}^{(k)})$, where $\tilde{\mathbf{V}}^{(k)}$ solves

$$-\Delta \tilde{\mathbf{V}}^{(k)} + \tilde{\mathbf{V}}^{(k)} = 0 \text{ in } \Omega^*(\omega^{(k)}) \setminus \overline{\omega}^{(k)}, \tag{75}$$

$$\tilde{\mathbf{V}}^{(k)} = \mathbf{V}^{(k)} \text{ on } \Sigma^{(k)}, \tag{76}$$

$$\tilde{\mathbf{V}}^{(k)} = \mathbf{W}^*(\mathbf{V}^{(k)}) \quad \text{on } \Gamma^{(k)}, \tag{77}$$

 and $t^{(k)}$ is a positive scalar.
 • Set $err_k = \max(||\tilde{\mathbf{V}}^{(k)}||_{H^1(\Omega^* \setminus \overline{\omega})}, ||\tilde{\mathbf{V}}^{(k)}||_{\mathscr{C}(\overline{\omega})})$.
end while

where $\hat{\mathbf{V}}$ solves

$$-\Delta \hat{\mathbf{V}} + \hat{\mathbf{V}} = 0 \text{ in } E \setminus \overline{\omega}, \tag{78}$$

$$\partial_n \hat{\mathbf{V}} = -\nabla K_2(\omega)\mathbf{n} \text{ on } \Sigma, \tag{79}$$

$$\hat{\mathbf{V}} = 0 \quad \text{on } \partial E, \tag{80}$$

and $t^{(k)}$ is a positive scalar to be discussed in Section 4.1. For the computation of p and p_l, a data interpolation between $E \setminus \overline{\omega}$ and $\Omega \setminus \overline{\omega}$ is required.

4.1. **Numerical examples.** The state problem is discretized using standard triangular elements generated by the anisotropic mesh generator BAMG [Hec98]. The location of the free boundary corresponding to a given inner boundary is not known a priori. However, when considering the situation where both ω and Γ are concentric circles, then the location of the free boundary can be calculated analytically.

4.1.1. *Example 1.* We start with an example where the exact solution is known. Let $\omega = B_{r_1}(0)$ and $\Omega = B_C(0)$. It is straightforwardly seen that the function

$$u = \mu C \ln(r) + 1 + C \ln(r_1)$$

satisfies $\Delta u = 0$ in $\Omega \setminus \overline{\omega}$, $u = 1$ when $r = r_1$, and $\nabla u \cdot \mathbf{n} = \mu$ when $r = C$. Next, to solve the free boundary problem $(\mathscr{F}_\omega)$ we look for the value C^* giving $u = 0$ when $r = C^*$. For this, one needs to solve the equation

$$\mu C \ln(C) + 1 + C \ln(r_1) = 0,$$

for the value of C^*. In what follows, we shall take $\mu = -1$ and $r_1 = 1$, in which case, C^* is found to be $C^* \approx 1.76322$.

Therefore, by setting $E = B_{C^*}(0)$ where $\mu = -1$ in (4), we expect a circle of radius one to be the global minimizer of both J_1 and J_2, i.e.,

$$E = \Omega_T := \{(x,y) \in \mathbb{R}^2 \ : \ x^2 + y^2 = (C^*)^2\} \text{ and } \omega_T := \{(x,y) \in \mathbb{R}^2 \ : \ x^2 + y^2 = 1\}.$$

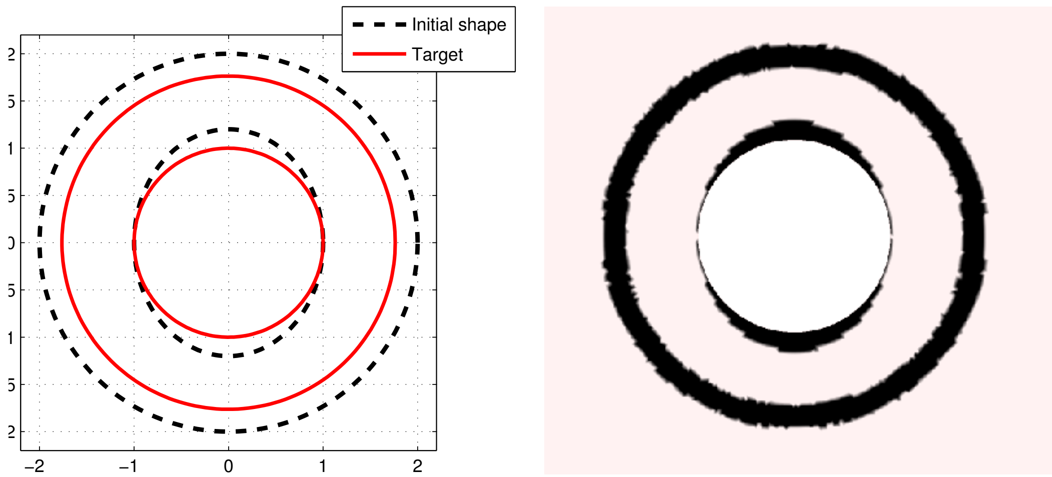
The optimization is performed using both cost functionals K_1 and K_2 starting from the same initial guess. The initial domains $\omega^{(0)}$ and $\Omega^{(0)}$ are given by

$$\omega^{(0)} := \left\{(x,y) \in \mathbb{R}^2 \ : \ \frac{x^2}{1} + \frac{y^2}{1.2^2} = 1\right\}, \quad \Omega^{(0)} := \{(x,y) \in \mathbb{R}^2 \ : \ x^2 + y^2 = 4\}, \tag{81}$$

respectively. The boundaries $\Gamma^{(0)}$, $\Sigma^{(0)}$ and ∂E, Σ_T of the initial and target shapes, respectively, are depicted in Figure 3(a). In order to compute the value of K_1, the hold-all $\mathscr{E} := [-4,4] \times [-4,4]$ embedding all admissible domains is utilized. The indicator function of the set $(\Omega \cap E^c) \cup (\Omega^c \cap E)$ is computed using

$$\mathbb{1}_{(\Omega \cap E^c) \cup (\Omega^c \cap E)}(x) = \mathbb{1}_\Omega(x) + \mathbb{1}_E(x) - \mathbb{1}_\Omega(x)\mathbb{1}_E(x).$$

This indicator function, corresponding to the initialization in (81), is depicted in Figure 3(b). For the initial value of the cost functional we get the numerical value $K_1(\omega^{(0)}) \approx$



(a) Initial and target shape *(b) Area to be minimized*

FIGURE 3. Initial shape $\Omega^{(0)}$ and target shape E

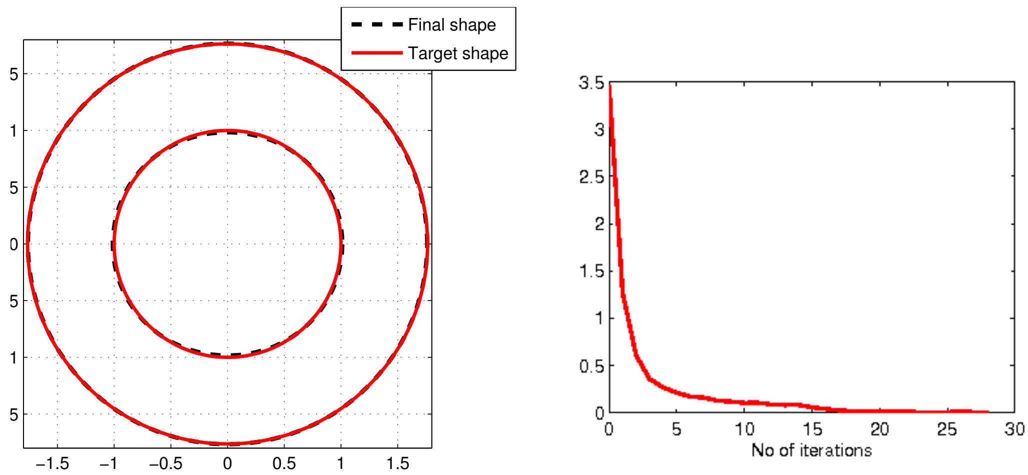
3.455. Our aim is to minimize the area of the dark region in Figure 3(b).

Remark 4.3. The motion of Σ is modeled explicitly using boundary nodes which are connected by line segments. These nodes are moved using the deformation field $\tilde{\mathbf{V}}$ computed in (72-77). During each optimization step, the step size $t^{(k)}$ is chosen on the basis of the Armijo-type line search and such that there are no reversed triangles within the mesh after the update. If reversed triangles occur or the mesh quality deteriorates, then a new mesh is generated, see, e.g., [AP06, THM08] for more details on mesh regeneration.

The parameters in $\mathscr{U}_{ad}$ are set to:

$$\omega_{min} := \{(x,y) \in \mathbb{R}^2 \mid x^2+y^2 \leq 0.61^2\}, \quad \omega_{max} := \{(x,y) \in \mathbb{R}^2 \mid x^2+y^2 \leq 1.75^2\}.$$

We set the value of tol to 1×10^{-3}. After 28 iterations and no mesh regeneration, we reach the target shape (see Figure 4(a)) with the final value $K_1(\omega^{final}) \approx 5.4 \times 10^{-3}$ for the cost. In Figure 4(b), we depict the convergence history of K_1. From this figure, we observe that



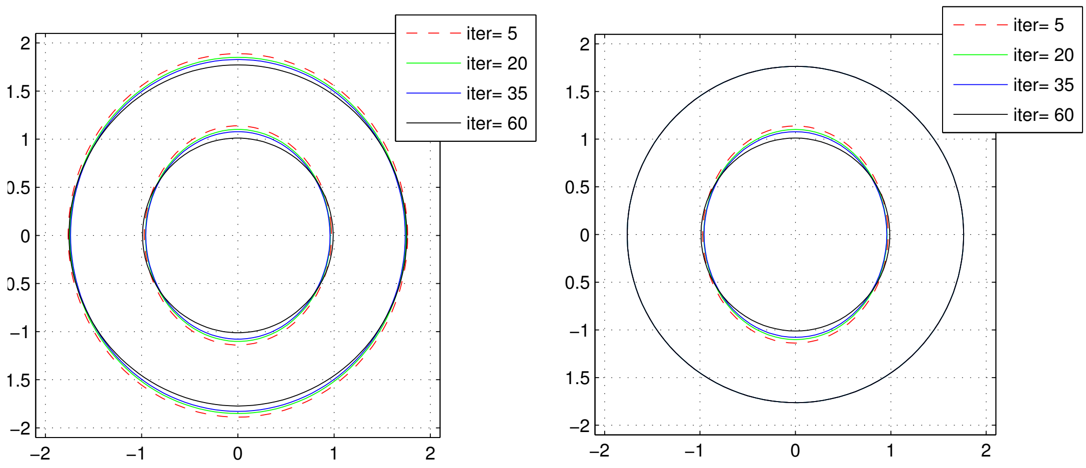
(a) Target and final shapes *(b) History of K_1*

FIGURE 4. Final shape $\Omega^{(final)}$ and target shape using K_1.

the cost is reduced during the optimization in a manner typical of gradient type methods, i.e., one observes a fast decrease in the beginning, and a slow convergence afterward. Moreover, since the target and final shapes of the boundaries practically coincide after optimization (see Figure 4(a)), the dark region is also minimized and tends to a set of measure zero.

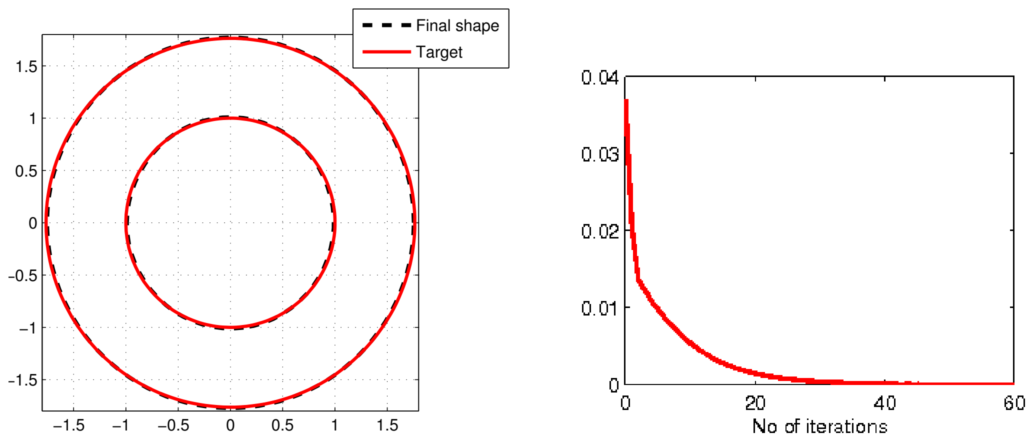
Next, we perform the optimization using K_2. The initial value of the cost is found to be $K_2(\omega^{(0)}) \approx 0.036987$. In Figure 5, we plot the variations of the domains $\Omega^*(\omega) \setminus \overline{\omega}$ and $E \setminus \overline{\omega}$ with the iteration count. It is observed that as the iteration count increases, the boundary Σ converges to the target (see Figure 5(b)). Similarly, the boundaries of $\Omega^*(\omega) \setminus \overline{\omega}$ converge to the target boundaries as well (see Figure 5(a)). The final boundaries are depicted in Figure 6(a). As expected, the final shape coincides with the target shape.

The convergence history of K_2 is depicted in Figure 6(b). After 60 iterations and no mesh regeneration, the value $K_2(\omega^{final}) \approx 2.527 \times 10^{-5}$ for the cost is obtained.



(a) *Domain $\Omega^*(\omega)\setminus\overline{\omega}$* (b) *Domain $E\setminus\overline{\omega}$*

FIGURE 5. Variations of domains $\Omega\setminus\overline{\omega}$ and $E\setminus\overline{\omega}$



(a) *Target and final shapes* (b) *History of K_2*

FIGURE 6. Initial and final shapes of the free boundary using K_2

Remark 4.4. *In the numerical experiments we observe that the domains obtained using K_1 tend to have an oscillatory behaviour near the optimal shape, which is not the case with K_2. Therefore, in the subsequent examples, we use only K_2 which provides a more stable convergence.*

4.1.2. *Example 2.* In this example our aim is to investigate the effect of increasing the value of μ on ω while the target boundary Γ_T remains fixed. We set the target boundary as $\Gamma_T := \{r(t)(\cos 2\pi t, \sin 2\pi t) \,|\, t \in [0,1]\}$, where

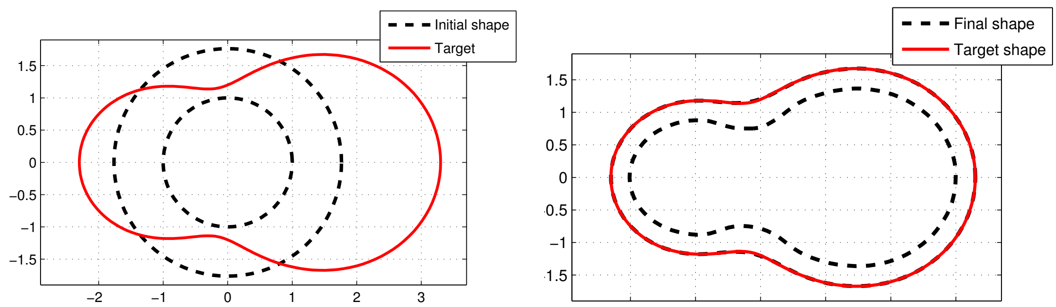
$$r(t) = 0.5\cos(2\pi t) + 0.8\cos(4\pi t) + 2.$$

It is known that for the exterior Bernoulli free boundary problems with fixed inner component of the boundary, the respective free boundaries for $\mu \to 0^-$ are asymptotic to a family of concentric circles with radii tending to infinity [FR97]. Therefore, one excepts the measure of the set $\Omega^*(\omega) \setminus \overline{\omega}$ to increase for $\mu \to 0^-$.

The initial design for Σ is a circle of radius one while that of Γ is a circle of radius C (see Figure 7(a)). We choose $\mu = -3$ and discretize the initial domains $\Omega^{(0)} \setminus \overline{\omega}^{(0)}$ and $E \setminus \overline{\omega}^{(0)}$ with triangular elements. The boundary nodes of the triangulations of $\Omega^{(k)} \setminus \overline{\omega}^{(k)}$ and $E \setminus \overline{\omega}^{(k)}$ are used as the control parameters for the optimization. The free boundary problem (1)-(4) is computed and the initial value of the cost is $K_2(\omega^{(0)}) \approx 0.1071$. The parameters in $\mathscr{U}_{ad}$ are set to:

$$\omega_{min} := \{(x,y) \in \mathbb{R}^2 \mid x^2 + y^2 \leq 0.75^2\} \quad \omega_{max} := \{(x,y) \in \mathbb{R}^2 \mid x^2 + y^2 \leq 3.15^2\}$$

.



(a) *Initial and target shape* (b) *Target and final shape*

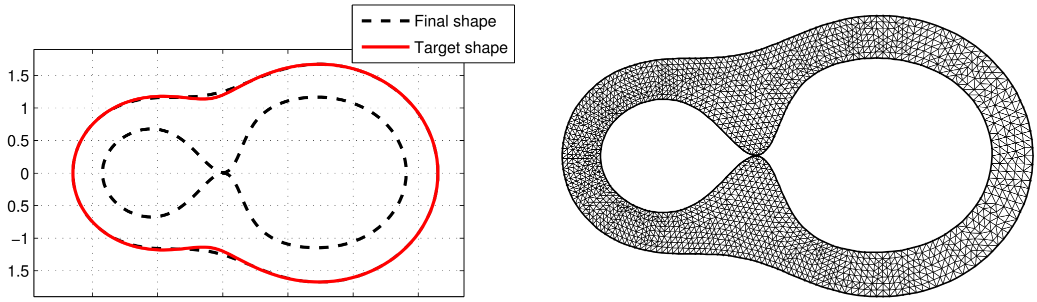
FIGURE 7. Target E, initial $\omega^{(0)}, \Omega^*(\omega^{(0)})$ and final shapes $\omega^{(final)}, \Omega^*(\omega^{(final)})$ using K_2 with $\mu = -3$.

The final value of the cost K_2 after 111 optimization iterations and 7 mesh regenerations is found to be 6×10^{-5}. The optimal domain is depicted in Figure 7(b). We observe that the final shape of $\Gamma^*(\omega)$ reaches almost perfectly the target boundary $\Gamma_T := \partial E$. We compute the measure $|\Omega^*(\omega^{final}) \setminus \overline{\omega}^{final}| \approx 4.36688$.

Next, we set $\mu = -1.8$ with an aim of checking whether the area of $\Omega^*(\omega) \setminus \overline{\omega}$ increases while $\Gamma^*(\omega)$ still coincides with the target Γ_T. We choose the same initialization as in Figure 7(a). The parameters in $\mathscr{U}_{ad}$ are now set to:

$$\omega_{min} := \{(x,y) \in \mathbb{R}^2 \mid x^2 + y^2 \leq 0.01^2\} \quad \omega_{max} := \{(x,y) \in \mathbb{R}^2 \mid x^2 + y^2 \leq 1.75^2\}.$$

The initial value is $K_2(\omega^{(0)}) \approx 0.128$. After 120 iterations one observes that the boundary Σ intersects itself at the origin (see Figure 8) and a meshing error occurs. At this point the optimization is stopped, the final value of $K_2(\omega^{final}) \approx 3.28 \times 10^{-4}$ is returned, and we compute $|\Omega^*(\omega^{final}) \setminus \overline{\omega}^{final}| \approx 7.51295$. The kind of parametrization used here does not allow topological changes to occur during the optimization process. Therefore, we arrive at a similar conclusion as in [THM08], i.e., that the inner boundary consists of more



(a) Target and final shapes *(b) Final mesh*

FIGURE 8. Target shape E and final shapes $\omega^{(final)}, \Omega^*(\omega^{(final)})$ using K_2 with $\mu = -1.8$

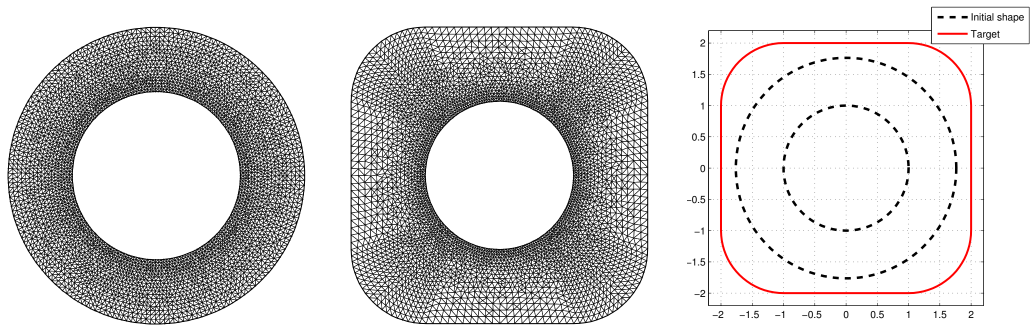
than one connected component. However, our numerical approach as well as the cost functionals K_1 and K_2 are completely different. Moreover, as expected, an increase in the value of μ for a fixed target, leads to an increase in the area of $\Omega^*(\omega) \setminus \overline{\omega}$, in agreement with the theory.

4.1.3. *Example 3.* In this example our aim is to check whether there exists a domain $\omega \in \mathscr{U}_{ad}$ such that $\Gamma^*(\omega)$ is as close as possible to a target Γ_T which is not of class $\mathscr{C}^\infty$. We minimize K_2 with the boundary ∂E of the target domain E represented by a square with rounded corners (see Figure 9). The square is of dimension $[-2,2] \times [-2,2]$. Each of the corners is rounded using a quarter of a circle of radius one and centers $(1,-1)$, $(1,1)$, $(-1,1)$, and $(-1,-1)$, numbered counter-clockwise starting from corner $(2,-2)$. This target boundary can also be described using the parametric equations

$$x(t) = 2|\cos(2\pi t)|^{\frac{1}{2}} \cdot \operatorname{sgn}(\cos(2\pi t)), \quad t \in (0,1), \tag{82}$$

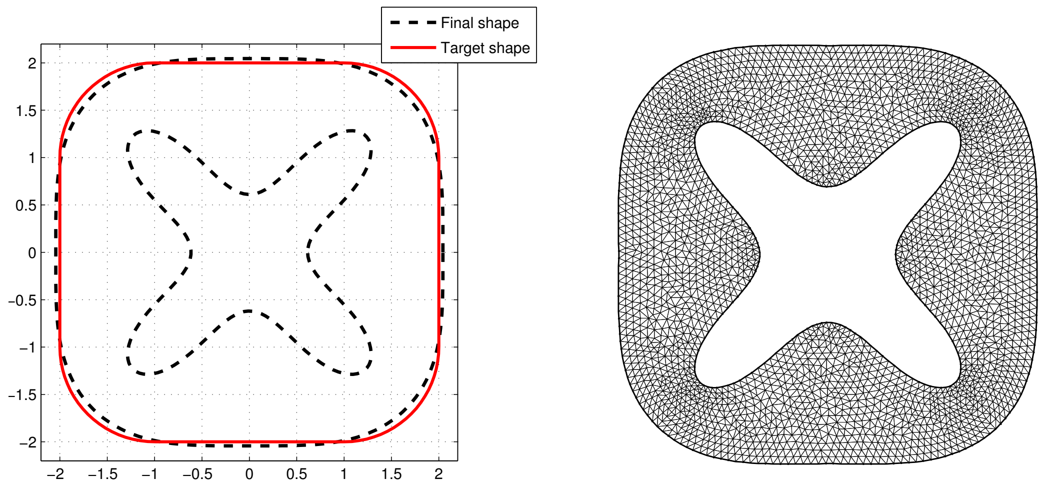
$$y(t) = 2|\sin(2\pi t)|^{\frac{1}{2}} \cdot \operatorname{sgn}(\sin(2\pi t)), \quad t \in (0,1). \tag{83}$$

With this parameterization, it is clear that the target is not of class $\mathscr{C}^\infty$. We set $\mu = -1$. The boundary Σ is initialized using a circle of radius one while Γ is initialized using a circle of radius C, both centered at the origin, cf. Figure 9. The parameters in $\mathscr{U}_{ad}$ are set as in the first example. The initial value of the cost is $K_2(\omega^{(0)}) \approx 0.0954102$. After 20 optimization steps and 5 remeshing, we obtain the final shape depicted in Figure 10(b). We compute the final value $K_2(\omega^{(final)}) \approx 1.1067 \times 10^{-3}$. In Figure 10(a), a comparison between the target outer boundary and the final outer boundary is made. We observe that the target is not reached exactly. In fact, some of the optimization variables attained the lower and upper bounds. Since the target is not of class $\mathscr{C}^\infty$, it cannot be reached using star-like boundaries Σ of class $\mathscr{C}^2$ [THM08, AM95]. The non-existence of $\omega \in \mathscr{U}_{ad}$ such that $\Gamma^*(\omega)$ is as close as possible to the target $\Gamma_T \notin \mathscr{C}^\infty$ usually manifests itself through oscillations of ω [THM08]. However, since we use a regularized velocity field (see Algorithm 2), these oscillations of the inner boundary do not occur in our case, cf. [THM08, Example 2].



(a) $\Omega^*(\omega^{(0)}) \setminus \overline{\omega}^{(0)}$ *(b) Target* $E \setminus \omega^{(0)}$ *(c) Initial and target shapes*

FIGURE 9. Initial domains and target E



(a) Target shape and Final shape *(b) Final mesh*

FIGURE 10. Initial and final shapes of the free boundary using K_2

5. CONCLUSIONS

In this paper, we have performed the mathematical analysis for the sensitivity of a Bernoulli free boundary problem with respect to a shape perturbation of the inner boundary using the concepts of shape calculus. A new segregation algorithm for solving this free boundary PDE constrained shape optimization problem has been proposed and implemented. The numerical results presented here indicate that the derived shape gradients produce similar results as those obtained by Haslinger et al [THM08] using an automatic differentiation technique. The results in this paper can be extended to other bilevel problems and control of the free boundary in shape optimization.

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(H. Kasumba) JOHANN RADON INSTITUTE FOR COMPUTATIONAL AND APPLIED MATHEMATICS, AUSTRIAN ACADEMY OF SCIENCES, ALTENBERGERSTRASSE 69, A-4040 LINZ, AUSTRIA

E-mail address: henry.kasumba@oeaw.at

(K. Kunisch) INSTITUTE FOR MATHEMATICS AND SCIENTIFIC COMPUTING, UNIVERSITY OF GRAZ, HEINRICHSTR. 36, A-8010 GRAZ, AUSTRIA

E-mail address: karl.kunisch@uni-graz.at

(A. Laurain) INSTITUT FÜR MATHEMATIK, TECHNICAL UNIVERSITY BERLIN, STRASSE DES 17. JUNI 136, 10623 BERLIN, GERMANY

E-mail address: laurain@math.tu-berlin.de