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Shape optimization methods for the Inverse Obstacle Problem with generalized impedance boundary conditions

Fabien Caubet*, Marc Dambrine†, Djalil Kateb*

January 24, 2013

Abstract

We aim to reconstruct an inclusion ω immersed in a perfect fluid flowing in a larger bounded domain Ω via boundary measurements on $\partial\Omega$. The obstacle ω is assumed to have a thin layer and is then modeled using generalized boundary conditions (precisely Ventcel boundary conditions). We first obtain an identifiability result (*i.e.* the uniqueness of the solution of the inverse problem) for annular configurations through explicit computations. Then, this inverse problem of reconstructing ω is studied thanks to the tools of shape optimization by minimizing a least squares type cost functional. We prove the existence of the shape derivatives with respect to the domain ω and characterize the gradient of this cost functional in order to make a numerical resolution. We also characterize the shape Hessian and prove that this inverse obstacle problem is unstable in the following sense: the functional is degenerated for highly oscillating perturbations. Finally, we present some numerical simulations in order to confirm and extend our theoretical results.

Keywords: geometric inverse problem, shape calculus, generalized impedance boundary conditions, Ventcel boundary conditions, identifiability result

AMS Classification: 49Q10, 49Q12, 34A55, 35Q93

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1 Introduction

A method to solve the inverse problem of reconstructing an object living in a larger domain is the shape optimization methods and particularly the geometric shape optimization. This kind of studies was realized for the impedance electric tomography by Afraites *et al.* in [2] or for the Stokes and Navier-Stokes equations by Badra *et al.* in [6] or Caubet *et al.* in [14, 13, 12] using technics of shape differentiation with respect to the domain. These technics are exposed for example in the books of Henrot *et al.* and Sokołowski *et al.* [21, 27]. In the previous references [2, 6, 14, 13], the authors proved that the studied inverse problems, treated as a shape optimization problems, are severely ill-posed (*i.e.* unstable), for both Dirichlet and Neumann boundary conditions on the object. Thus, they have to use some regularization methods to solve them numerically.

Here, we focus on the case of generalized impedance boundary conditions (of order two) on the obstacle, precisely Ventcel boundary conditions which deal with a Laplace-Beltrami operator. This kind of non classical boundary conditions appear in the modeling of thin layer or of corrosion effects. The study of this type of boundary conditions is an emerging research theme and the analysis of the Ventcel boundary conditions was recently made by Bonnaillie-Noël *et al.* in [7]. We can here mentioned the work of Haddar *et al.* in [18] where they propose a new construction of generalized impedance boundary conditions and develop a complete mathematical analysis for the approximate problem. The construction of generalized impedance boundary conditions is also treated for example by Antoine *et al.* in [4], by Pognard in [26] or by Haddar *et al.* in [19]. One topic is then to identify the coefficients corresponding to these conditions as treated by Bourgeois *et al.* in [9, 8]. Another is to identify the shape while the coefficients are known. We consider this question here: our aim is to adapt the classical shape optimization methods used to solve inverse problems to the case of immersed obstacles modeled by Ventcel boundary conditions. In the recent work [11], Cakoni *et al.* address the question of recovering simultaneously the unknown boundary and the unknown coefficients by an integral equation approach.

A method to solve this inverse problem of determining the shape of an immersed obstacle is then to make a boundary measurement on the exterior boundary. A first study of this problem is given by Cakoni *et al.* in [10] using a boundary integral equation method in the spirit of the method proposed by Kress *et al.* in [22]. In particular, in [10], the authors give an example of non identifiability result. Even if we do not obtain a general identifiability result (as the one stated for Robin boundary conditions by Bacchelli in [5]), we here prove it for annular configurations with the same center using two well chosen measurements. Then, following previous works on electric impedance topography (see [17, 2, 3]) or on the same topic in the Stokes and Navier-Stokes cases (see [6, 14, 13]), our strategy is to minimize a least squares functional.

We prove the existence of shape derivatives for this type of boundary value problem pursuing the studies initiated by Dambrine *et al.* in [15]. We compute the shape gradient and characterize the shape Hessian. We then prove, using a local regularity argument, that the Riesz operator corresponding to this shape Hessian is compact and it follows that the functional is degenerated for highly oscillating perturbations. Finally, we make some numerical simulations in order to confirm and complete our theoretical study. These numerical experiments point out that, contrary to the case of classical boundary conditions treated in [2, 14], we can achieve acceptable reconstruction without regularization methods. Indeed, the presence of the Laplace-Beltrami operator in the generalized impedance boundary conditions of order two seems to somehow regularize the problem.

This paper is organized as follows. We first introduce the precise problem under consideration and useful results. Then, we prove an identifiability result in the case of an annulus in dimension two. In Section 4, we prove the existence of shape derivatives (of order one and two) when Ventcel boundary conditions are imposed. The differentiation with respect to the domain of the problem and of the cost functional are detailed in Section 5. This section ends with the proof of the instability of the inverse problem. Finally, we make some numerical experiments which underline the fact that we do not need some regularization method to obtain efficient results. In order to be complete, we recall some results concerning the Ventcel boundary conditions in Appendix A and some reminders of useful shape differential calculus in Appendix B.

2 The problem setting

2.1 General notations and reminders

Let us introduce the notations that we adopt in this paper. We denote by L^p , $W^{m,p}$ and H^s the usual Lebesgue and Sobolev spaces. For $k \in \mathbb{N}$ and an open set $\Omega \subset \mathbb{R}^d$ ($d \geq 2$), we denote by $C_c^k(\Omega)$ the space of functions with continuous k first derivatives compactly supported in Ω and by $\|\cdot\|_{k,\infty}$ its natural norm. We note in bold the vectorial functions and spaces: \mathbf{L}^p , $\mathbf{W}^{m,p}$, \mathbf{H}^s , etc. Moreover, \mathbf{n} represents the external unit normal to $\partial\Omega$, and for a smooth enough function u , we note respectively $\partial_n u$ and $\partial_{nn}^2 u$ the normal derivative and the second normal derivative of u . We also denote by $\mathcal{M}_{d,d}$ the space of the matrix of size $d \times d$. The tangential differential operators will be noted by the subscript τ . We recall some definitions and useful results in Appendix B. For more details on tangential differential operators, we refer for example to Section 5.4.3 in [21]. In particular, we recall the following integration by parts result which will be used many times in this paper.

Theorem 2.1. *Let Ω be a bounded open set of \mathbb{R}^d ($d \geq 2$) with a C^2 boundary. Let*

$f \in W^{1,1}(\partial\Omega)$ and $\mathbf{W} \in \mathbf{W}^{1,1}(\partial\Omega)$. Then,

$$\int_{\partial\Omega} \mathbf{W} \cdot \nabla_{\tau} f = \int_{\partial\Omega} -f \operatorname{div}_{\tau} \mathbf{W} + Hf \mathbf{W} \cdot \mathbf{n},$$

where H is the mean curvature of $\partial\Omega$.

2.2 The studied problem

Let Ω be a smooth (at least C^3) bounded open set of \mathbb{R}^d , where $d \geq 2$ is an integer representing the dimension. Let $\delta > 0$ be a fixed (small) real number. We define

$$\mathcal{O}_{\delta} := \left\{ \omega \subset\subset \Omega \text{ be a smooth (at least } C^3) \text{ open set such that } d(x, \partial\Omega) > \delta \ \forall x \in \omega \right. \\ \left. \text{and such that } \Omega \setminus \bar{\omega} \text{ is connected} \right\}. \quad (2.1)$$

Let $g \in H^{3/2}(\partial\Omega)$ be an admissible boundary measurement and let $f \in H^{5/2}(\partial\Omega)$ such that $f \neq 0$. We then consider, for $\omega \in \mathcal{O}_{\delta}$, the following overdetermined boundary values problem:

$$\begin{cases} -\Delta u = 0 & \text{in } \Omega \setminus \bar{\omega} \\ u = f & \text{on } \partial\Omega \\ \partial_{\mathbf{n}} u + \alpha u + \beta \Delta_{\tau} u = 0 & \text{on } \partial\omega \\ \partial_{\mathbf{n}} u = g & \text{on } \partial\Omega, \end{cases} \quad (2.2)$$

where $\alpha > 0$ and $\beta < 0$ are fixed real number.

We assume here that there exists $\omega^* \in \mathcal{O}_{\delta}$ such that (2.2) has a solution. This means that the measurement g is perfect, that is to say without error. Thus, we consider the following geometric inverse problem:

$$\text{find } \omega \in \mathcal{O}_{\delta} \text{ and } u \text{ which satisfy the overdetermined system (2.2)}. \quad (2.3)$$

To solve this inverse problem, we consider, for $\omega \in \mathcal{O}_{\delta}$, the least squares functional

$$J(\omega) := \frac{1}{2} \int_{\partial\Omega} |\partial_{\mathbf{n}} u(\omega) - g|^2, \quad (2.4)$$

where $u(\omega) \in H^1(\Omega \setminus \bar{\omega})$ solves

$$\begin{cases} -\Delta u = 0 & \text{in } \Omega \setminus \bar{\omega} \\ u = f & \text{on } \partial\Omega \\ \partial_{\mathbf{n}} u + \alpha u + \beta \Delta_{\tau} u = 0 & \text{on } \partial\omega, \end{cases} \quad (2.5)$$

measuring in the misfit to data in the L^2 sense. Notice that, according to Theorem A.2, the boundary value problem (2.5) admits a unique solution $u \in H^3(\Omega \setminus \bar{\omega})$.

Then, we try to minimize the least squares criterion J :

$$\omega^* \in \operatorname{argmin}_{\omega \in \mathcal{O}_{\delta}} J(\omega). \quad (2.6)$$

Indeed, if ω^* solves the inverse problem (2.3), then $J(\omega^*) = 0$ and (2.6) holds. Conversely, if ω^* solves the optimization problem (2.6) with $J(\omega^*) = 0$, then it is a solution of (2.3).

Remark 2.2. *Using the local regularity of the solutions in a neighborhood of $\partial\omega$, notice that we can only assume that $\partial\Omega$ is Lipschitz and that $f \in H^{1/2}(\partial\Omega)$ and $g \in H^{-1/2}(\partial\Omega)$ (see for example [6, 13, 14]). However, in order to simplify the proof and the notations, we assume the announced regularity.*

Moreover, we could assume that the measurement g is made only on a part $O \subset \partial\Omega$ and not on the whole exterior boundary as made for example in [6, 13].

The needed functional tools. Let us introduce the following notation for $k \in \mathbb{N}$:

$$\mathbf{H}_{\partial\Omega}^k(\Omega \setminus \bar{\omega}) := \left\{ u \in \mathbf{H}^k(\Omega \setminus \bar{\omega}), u = 0 \text{ on } \partial\Omega \right\}.$$

Let us define Ω_δ an open set with a C^∞ boundary such that

$$\{x \in \Omega; d(x, \partial\Omega) > \delta/2\} \subset \Omega_\delta \subset \{x \in \Omega; d(x, \partial\Omega) > \delta/3\}.$$

Then, in order to make a shape sensitivity analysis (of order two), we define

$$\mathbf{U} := \left\{ \boldsymbol{\theta} \in \mathbf{W}^{3,\infty}(\mathbb{R}^d); \text{supp}(\boldsymbol{\theta}) \subset \overline{\Omega_\delta} \right\} \quad \text{and} \quad \mathbf{U} := \left\{ \boldsymbol{\theta} \in \mathbf{U}; \|\boldsymbol{\theta}\|_{3,\infty} < \min\left(\frac{\delta}{3}, 1\right) \right\} \quad (2.7)$$

as the space of admissible deformations. These spaces permit to perturb only the object ω and not the fixed domain Ω . Notice that if $\boldsymbol{\theta} \in \mathbf{U}$, then $(\mathbf{I} + \boldsymbol{\theta})$ is a diffeomorphism. For such a $\boldsymbol{\theta} \in \mathbf{U}$ and $\omega \in \mathcal{O}_\delta$, we check that $\Omega = (\mathbf{I} + \boldsymbol{\theta})(\Omega)$ and we define the perturbed domain

$$\omega_\theta := (\mathbf{I} + \boldsymbol{\theta})(\omega)$$

which is so that $\omega_\theta \in \mathcal{O}_\delta$.

Let $T > 0$, that we will have to fix small. We use the shape calculus introduced by Murat and Simon in [25]. Thus, we consider the function

$$\phi : t \in [0, T] \mapsto \mathbf{I} + t\mathbf{V} \in \mathbf{W}^{3,\infty}(\mathbb{R}^d), \quad (2.8)$$

where $\mathbf{V} \in \mathbf{U}$. Note that for small t , $\phi(t)$ is a diffeomorphism of \mathbb{R}^d and that $\phi'(0) = \mathbf{V}$ vanishes on $\partial\Omega$ and even on the tubular neighborhood $\Omega \setminus \overline{\Omega_\delta}$ of $\partial\Omega$. For $t \in [0, T]$, we define

$$\omega_t := \phi(t)(\omega)$$

where ϕ is defined by (2.8). For the rest of the paper, we use a subscript " t " to indicate that the quantity is defined on the time t dependent domain. For instance, \mathbf{n}_t is the external unit normal of $\Omega \setminus \bar{\omega}_t$.

Finally, we introduce the following notation: for $\mathbf{V} \in \mathbf{U}$,

$$V_{\mathbf{n}} := \mathbf{V} \cdot \mathbf{n}.$$

3 On the identifiability result on rings

In this section, we will analyze the question of identifiability of the shape ω . The question is the following: *does a measurement (or several measurements) determine uniquely the domain ω ?* This kind of result was recently proved by Bacchelli in [5] for Robin boundary conditions. In the case of generalized impedance boundary condition, the literature is reduced to the discussion by Cakoni *et al.* in [11].

In order to try to answer to this question concerning the non classical Ventcel boundary conditions, let us focus on particular geometries in the bi-dimensional case. More precisely, we consider an annulus with two concentric circles: the inner circle $\Gamma_i := \partial\omega = \rho S^1$ has a radius ρ and we denote by R the radius of the outer circle $\Gamma := \partial\Omega = RS^1$ (where S^1 denotes the unit sphere). Hence,

$$\Omega \setminus \bar{\omega} := \{x \in \mathbb{R}^2, \rho < |x| < R\} = B_R \setminus \overline{B_\rho}.$$

Let u the solution of the following problem

$$\begin{cases} \Delta u = 0 & \text{in } \Omega \setminus \overline{\omega} = B_R \setminus \overline{B_\rho} \\ u = f & \text{on } \Gamma = \partial\Omega = RS^1 \\ \partial_n u + \alpha u + \beta \Delta_\tau u = 0 & \text{on } \Gamma_i = \partial\omega = \rho S^1. \end{cases} \quad (3.1)$$

We deal with the inverse problem of reconstructing the inner circle (*i.e.* find the radius ρ) from boundary measurements on the outer circle $\partial\Omega$. We give a result for identifying uniquely the obstacle from two pairs of Cauchy data $(f_1, \partial_n u_1 = g_1|_\Gamma)$ and $(f_2, \partial_n u_2 = g_2|_\Gamma)$, where u_1 and u_2 are the respective solutions of Problem (3.1) with the Dirichlet data f_1 and f_2 . Precisely, we show the following result:

Theorem 3.1. *Given $\alpha > 0$ and $\beta < 0$, one can determine uniquely Γ_i (*i.e.* the radius ρ) with two pairs of measurements (f_1, g_1) and (f_2, g_2) , provided f_1 and f_2 are suitably chosen.*

The idea of the proof is the following. We consider two inputs of the form $f_1 = R^{n_1} \cos(n_1\theta)$ and $f_2 = R^{n_2} \cos(n_2\theta)$. We assume that two inner radii ρ and $\tilde{\rho}$ generate the same Cauchy data for both inputs. We obtain a system of equations in $t := \rho/\tilde{\rho}$ with respect to n_1 and n_2 of the kind

$$h_{n_i}^1(t) = h_{n_i}^2(t) \quad \forall i = 1, 2,$$

where the $h_{n_i}^i$ are real valued functions of the real variable. We will show that for n_1 and n_2 suitably chosen, the unique solution of the previous system is $t = 1$ meaning $\rho = \tilde{\rho}$.

Proof. In the sequel, the couple (r, θ) represents the polar coordinates. Moreover, $a_n(f)$ and $b_n(f)$ (respectively $a_n(g)$ and $b_n(g)$) represent the respective Fourier coefficients of f and g . We subdivide the proof in two parts.

First step: preliminary computations. Assume that (f, g) is a Cauchy pair for Problem (3.1) set in the annulus $B_R \setminus \overline{B_\rho}$. Its solution is of the following form

$$u(r, \theta) = a_{-1} \ln r + a_0 + \sum_{n=1}^{\infty} (a_n r^n + a_{-n} r^{-n}) \cos(n\theta) + \sum_{n=1}^{\infty} (b_n r^n + b_{-n} r^{-n}) \sin(n\theta)$$

where, for $n \geq 1$,

$$\begin{cases} a_n R^n + a_{-n} R^{-n} & = a_n(f) \\ a_n R^n - a_{-n} R^{-n} & = \frac{R}{n} a_n(g) \\ a_n \rho^n \left(\frac{-\beta n^2}{\rho^2} - \frac{n}{\rho} + \alpha \right) + a_{-n} \rho^{-n} \left(\frac{-\beta n^2}{\rho^2} + \frac{n}{\rho} + \alpha \right) & = 0 \end{cases}$$

(and with the same system replacing a_n by b_n). Since the matrix of the linear system is of rank two, we get the relation

$$2a_n(f)X_n(\rho) = \left(\frac{R^{2n}}{\rho^{2n}} Y_n(\rho) - X_n(\rho) \right) \left(\frac{R}{n} a_n(g) - a_n(f) \right)$$

where we set

$$X_n(\rho) := \frac{-\beta n^2}{\rho^2} - \frac{n}{\rho} + \alpha \quad \text{and} \quad Y_n(\rho) := \frac{-\beta n^2}{\rho^2} + \frac{n}{\rho} + \alpha.$$

Hence,

$$\frac{2a_n(f)}{\frac{R}{n}a_n(g) - a_n(f)} = \frac{\frac{R^{2n}}{\rho^{2n}}Y_n(\rho) - X_n(\rho)}{X_n(\rho)}.$$

Notice that the left hand side does not depend on the inner radius ρ .

Second step: derivation of an equation using two measurements. Assume now that $(f = R^n \cos(n\theta), g)$ is a Cauchy pair for the boundary value problem (3.1) in the annuli $B_R \setminus \overline{B_\rho}$ and $B_R \setminus \overline{B_{\tilde{\rho}}}$ (where $0 < \tilde{\rho} < R$). The previous remark provides the relation

$$\frac{\frac{R^{2n}}{\rho^{2n}}Y_n(\rho) - X_n(\rho)}{X_n(\rho)} = \frac{\frac{R^{2n}}{\tilde{\rho}^{2n}}Y_n(\tilde{\rho}) - X_n(\tilde{\rho})}{X_n(\tilde{\rho})}.$$

Hence

$$\frac{\tilde{\rho}^{2n}}{\rho^{2n}}Y_n(\rho)X_n(\tilde{\rho}) = Y_n(\tilde{\rho})X_n(\rho).$$

Setting $t := \frac{\tilde{\rho}}{\rho}$, we then get

$$t^{2n} \frac{-\beta n^2 - n t \rho + \alpha t^2 \rho^2}{-\beta n^2 - n \rho + \alpha \rho^2} = \frac{-\beta n^2 + n t \rho + \alpha t^2 \rho^2}{-\beta n^2 + n \rho + \alpha \rho^2}.$$

Denoting $b_n := \frac{n\rho + \beta n^2 - \alpha \rho^2}{n\rho - \beta n^2 + \alpha \rho^2}$, we check

$$1 + \frac{2R}{\beta} \leq b_n = 1 - \frac{2n\rho}{n\rho - \beta n^2 + \alpha \rho^2} \leq 1, \forall n \in \mathbb{N}$$

and see that t is solution of

$$t^{2n} \frac{n t \rho + \beta n^2 - \alpha t^2 \rho^2}{n t \rho - \beta n^2 + \alpha t^2 \rho^2} = b_n$$

or equivalently

$$t^{2n} \frac{1 + \beta \frac{n}{t\rho} - \alpha \frac{t\rho}{n}}{1 - \beta \frac{n}{t\rho} + \alpha \frac{t\rho}{n}} = b_n.$$

Setting $P_n(t) := -\beta \frac{n}{t\rho} + \alpha \frac{t\rho}{n}$, this gives

$$t^{2n}(1 - P_n(t)) = b_n(1 + P_n(t))$$

and then the equation in t at fixed ρ

$$\frac{t^{2n} - b_n}{t^{2n} + b_n} = -\beta \frac{n}{t\rho} + \alpha \frac{t\rho}{n}. \quad (3.2)$$

If there are two distinct inner radii ρ and $\tilde{\rho}$ such that the measurements g_i are the same for the annuli $B_R \setminus \overline{B_\rho}$ and $B_R \setminus \overline{B_{\tilde{\rho}}}$, then Equation (3.2) has at least two solutions one of

which is 1. We will prove that when we fix n_1 and choose n_2 sufficiently large, the only common solution of

$$\frac{t^{2n_i} - b_{n_i}}{t^{2n_i} + b_{n_i}} = -\beta \frac{n_i}{t\rho} + \alpha \frac{t\rho}{n_i} \quad i = 1, 2 \quad (3.3)$$

is $t = 1$ and then $\tilde{\rho} = \rho$. This means that only two measurements are necessary for the identifiability.

Third step: the identifiability proof. We see the solution of Equation (3.2) as the intersection in \mathbb{R}^+ of the two curves (C_1) and (C_2) where

$$(C_1) : t \mapsto h_n^1(t) := \frac{t^{2n} - b_n}{t^{2n} + b_n} \quad \text{and} \quad (C_2) : t \mapsto h_n^2(t) := -\beta \frac{n}{t\rho} + \alpha \frac{t\rho}{n} \geq -\frac{\beta}{tR}n.$$

Fix $n_1 = 1$, then Equation (3.2) is polynomial of degree 4, it has at most four solutions in \mathbb{R} , one of them is 1. Set \mathcal{S} the set of positive real solutions of (3.2) distinct of 1. It has at most three elements.

If $\mathcal{S} \neq \emptyset$, take $t \in \mathcal{S}$ and consider the sequences $h_n^i(t)$ for $i = 1, 2$. The sequence $h_n^2(t)$ clearly goes to infinity. For the sequence $h_n^1(t)$, we have to distinguish the case $t > 1$ and $t < 1$. If $t > 1$, then $h_n^1(t)$ tends to 1 since

$$|h_n^1(t) - 1| = \left| \frac{2b_n}{t^{2n} + b_n} \right| \leq \left| \frac{2}{t^{2n} + 1 + \frac{2R}{\beta}} \right|.$$

For $t < 1$, $h_n^1(t)$ goes to -1 . Hence, from the uniform in ρ bounds in the estimations for these two sequences, there is a rank n_t , such that for $n \geq n_t$, t is not solution of Equation (3.2). Taking the maximum N of n_t for $t \in \mathcal{S}$, we conclude that, for a fixed $n_1 = 1$ and $n_2 \geq N$, the unique common root of (3.3) is $t = 1$ and then that only two boundary Cauchy measurements are sufficient to identify the inner circle. \square

4 Existence of shape derivatives

In the previous section, we have proved an identifiability result in annular configurations. We want now to reconstruct the obstacle by minimizing the least squares functional (2.4) and solve the optimization problem (2.6) using shape optimization methods. Hence, we want to use the notion of shape derivatives. Thus, in this section, we prove that the solution u of Problem (2.5) is twice differentiable with respect to the shape $\omega \in \mathcal{O}_\delta$.

Let $\theta \in \mathcal{U}$. We recall that \mathcal{O}_δ is defined by (2.1), \mathcal{U} by (2.7) and that we define $\omega_\theta := (\mathbf{I} + \theta)(\omega)$. Then, we consider $u_\theta \in H^1(\Omega \setminus \overline{\omega_\theta})$ solution of

$$\begin{cases} -\Delta u_\theta = 0 & \text{in } \Omega \setminus \overline{\omega_\theta} \\ u_\theta = f & \text{on } \partial\Omega \\ \partial_{n_\theta} u_\theta + \alpha u_\theta + \beta \Delta_{\tau_\theta} u_\theta = 0 & \text{on } \partial\omega_\theta. \end{cases} \quad (4.1)$$

Notice that u_θ belongs to $H^3(\Omega \setminus \overline{\omega})$. Let us consider $F \in H^3(\Omega \setminus \overline{\omega})$ such that

$$-\Delta F = 0 \text{ in } \Omega, \quad F = f \text{ on } \partial\Omega \quad \text{and} \quad F = 0 \text{ in } \Omega_\delta.$$

Then, we define

$$v_\theta := (u_\theta - F) \circ (\mathbf{I} + \theta)$$

and the variational formulation of Problem (4.1) is then given by

$$\int_{\Omega \setminus \bar{\omega}_\theta} \nabla v_\theta \cdot \nabla \varphi_\theta + \int_{\partial \omega_\theta} (\alpha v_\theta \varphi_\theta - \beta \nabla_{\tau_\theta} v_\theta \cdot \nabla_{\tau_\theta} \varphi_\theta) = \int_{\Omega \setminus \bar{\omega}_\theta} \Delta F \varphi_\theta \quad \forall \varphi_\theta \in H_{\partial \Omega}^1(\Omega \setminus \bar{\omega}_\theta), \quad (4.2)$$

since $\int_{\partial \omega_\theta} -\beta \Delta_{\tau_\theta} v_\theta \varphi_\theta = \int_{\partial \omega_\theta} \beta \nabla_{\tau_\theta} v_\theta \cdot \nabla_{\tau_\theta} \varphi_\theta$. We will apply the general method exposed in [21, Chapter 5] using the implicit function theorem on v_θ .

4.1 Characterization of v_θ

Lemma 4.1 (Characterization of v_θ). *For $\boldsymbol{\theta} \in \mathcal{U}$, v_θ satisfies for all $\varphi \in H_{\partial \Omega}^1(\Omega \setminus \bar{\omega})$*

$$\int_{\Omega \setminus \bar{\omega}} \nabla (A(\boldsymbol{\theta})v_\theta) \cdot \nabla \varphi + \int_{\partial \omega} \alpha v_\theta \varphi w_\theta - \int_{\partial \omega} \beta (C(\boldsymbol{\theta})\nabla_\tau v_\theta) \cdot \nabla_\tau \varphi = \int_{\Omega \setminus \bar{\omega}} \Delta F \varphi J_\theta,$$

where

$$\begin{aligned} J_\theta &:= \det(\mathbf{I} + \nabla \boldsymbol{\theta}) \in W^{2,\infty}(\bar{\Omega}_\delta), \\ w_\theta &:= \det(\mathbf{I} + \nabla \boldsymbol{\theta}) \left\| {}^t(\mathbf{I} + \nabla \boldsymbol{\theta})^{-1} \mathbf{n} \right\| \in W^{2,\infty}(\bar{\Omega}_\delta), \\ A(\boldsymbol{\theta}) &:= \nu J_\theta (\mathbf{I} + \nabla \boldsymbol{\theta})^{-1} (\mathbf{I} + {}^t \nabla \boldsymbol{\theta})^{-1} \in W^{2,\infty}(\bar{\Omega}_\delta, \mathcal{M}_{d,d}), \\ C(\boldsymbol{\theta}) &:= w_\theta (\mathbf{I} + \nabla \boldsymbol{\theta})^{-1} {}^t(\mathbf{I} + \nabla \boldsymbol{\theta})^{-1} \in W^{2,\infty}(\bar{\Omega}_\delta, \mathcal{M}_{d,d}). \end{aligned}$$

Moreover, v_θ belongs to $H_{\partial \Omega}^3(\Omega \setminus \bar{\omega})$.

Remark 4.2. Hence, we characterize v_θ as the solution of

$$\begin{cases} -\operatorname{div}(A(\boldsymbol{\theta})\nabla v_\theta) = \Delta F J_\theta & \text{in } \Omega \setminus \bar{\omega} \\ v_\theta = 0 & \text{on } \partial \Omega \\ (A(\boldsymbol{\theta})\nabla v_\theta) \cdot \mathbf{n} + \alpha v_\theta w_\theta + \beta \operatorname{div}_\tau(C(\boldsymbol{\theta})\nabla_\tau v_\theta) = 0 & \text{on } \partial \omega. \end{cases}$$

Proof. Let $\varphi \in H_{\partial \Omega}^1(\Omega \setminus \bar{\omega})$. We define

$$\varphi_\theta := \varphi \circ (\mathbf{I} + \boldsymbol{\theta})^{-1} \in H_{\partial \Omega}^1(\Omega \setminus \bar{\omega}_\theta) \quad \text{and} \quad T(\boldsymbol{\theta}) := (\mathbf{I} + {}^t \nabla \boldsymbol{\theta})^{-1} \in W^{2,\infty}(\mathbb{R}^d, \mathcal{M}_{d,d}).$$

Thus, using φ_θ as a test function in the variational formulation (4.2), we obtain

$$\begin{aligned} & \int_{\Omega \setminus \bar{\omega}_\theta} \left[(T(\boldsymbol{\theta})\nabla v_\theta) \circ (\mathbf{I} + \boldsymbol{\theta})^{-1} \right] \cdot \left[(T(\boldsymbol{\theta})\nabla \varphi) \circ (\mathbf{I} + \boldsymbol{\theta})^{-1} \right] \\ & \quad + \int_{\partial \omega_\theta} \alpha \left[v_\theta \circ (\mathbf{I} + \boldsymbol{\theta})^{-1} \right] \left[\varphi \circ (\mathbf{I} + \boldsymbol{\theta})^{-1} \right] \\ & - \int_{\partial \omega_\theta} \left\{ \beta \left[(T(\boldsymbol{\theta})\nabla v_\theta) \circ (\mathbf{I} + \boldsymbol{\theta})^{-1} - (\mathbf{n} \circ (\mathbf{I} + \boldsymbol{\theta})^{-1}) \cdot \left((T(\boldsymbol{\theta})\nabla v_\theta) \circ (\mathbf{I} + \boldsymbol{\theta})^{-1} \right) \cdot (\mathbf{n} \circ (\mathbf{I} + \boldsymbol{\theta})^{-1}) \right] \right. \\ & \quad \left. \cdot \left[(T(\boldsymbol{\theta})\nabla \varphi) \circ (\mathbf{I} + \boldsymbol{\theta})^{-1} - (\mathbf{n} \circ (\mathbf{I} + \boldsymbol{\theta})^{-1}) \cdot \left((T(\boldsymbol{\theta})\nabla \varphi) \circ (\mathbf{I} + \boldsymbol{\theta})^{-1} \right) \cdot (\mathbf{n} \circ (\mathbf{I} + \boldsymbol{\theta})^{-1}) \right] \right\} \\ & \quad = \int_{\Omega \setminus \bar{\omega}_\theta} \Delta F \left(\varphi \circ (\mathbf{I} + \boldsymbol{\theta})^{-1} \right). \end{aligned}$$

Hence, using the change of variables $x = (\mathbf{I} + \boldsymbol{\theta})(y)$, we obtain

$$\begin{aligned} & \int_{\Omega \setminus \bar{\omega}} (A(\boldsymbol{\theta})\nabla v_\theta) \cdot \nabla \varphi + \int_{\partial \omega} \alpha v_\theta \varphi w_\theta \\ & \quad - \int_{\partial \omega} \beta [T(\boldsymbol{\theta})\nabla v_\theta - \mathbf{n}(T(\boldsymbol{\theta})\nabla v_\theta \cdot \mathbf{n})] \cdot [T(\boldsymbol{\theta})\nabla \varphi - \mathbf{n}(T(\boldsymbol{\theta})\nabla \varphi \cdot \mathbf{n})] w_\theta = \int_{\Omega \setminus \bar{\omega}} \Delta F \varphi J_\theta. \end{aligned}$$

Therefore, we obtain the announced result. Notice that J_θ is the volume Jacobian and w_θ is the surface Jacobian. \square

4.2 Differentiability of $\theta \mapsto v_\theta$

Lemma 4.3 (Differentiability of $\theta \mapsto v_\theta$). *The function*

$$\theta \in \mathcal{U} \mapsto v_\theta \in \mathbf{H}_{\partial\Omega}^2(\Omega \setminus \bar{\omega})$$

is differentiable in a neighborhood of $\mathbf{0}$ (and even C^∞).

Proof. Let us consider the application the application $\mathcal{F} : \mathcal{U} \times \mathbf{H}_{\partial\Omega}^2(\Omega \setminus \bar{\omega}) \rightarrow \mathbf{L}^2(\Omega \setminus \bar{\omega})$ defined for all $\varphi \in \mathbf{H}_{\partial\Omega}^1(\Omega \setminus \bar{\omega})$ by

$$\langle \mathcal{F}(\theta, v), \varphi \rangle = \int_{\Omega \setminus \bar{\omega}} (A(\theta) \nabla v) \cdot \nabla \varphi + \int_{\partial\omega} \alpha v \varphi w_\theta - \int_{\partial\omega} \beta (C(\theta) \nabla_\tau v) \cdot \nabla_\tau \varphi - \int_{\Omega \setminus \bar{\omega}} \Delta F \varphi J_\theta.$$

We have, for $\theta = \mathbf{0}$, $\mathcal{F}(\mathbf{0}, v_0) = \mathcal{F}(\mathbf{0}, u - F) = 0$. Moreover, we prove analogously to what is done in [21, Proof of Theorem 5.3.2] that the application \mathcal{F} is C^∞ . Finally, we compute for all $w, \hat{w} \in \mathbf{H}_{\partial\Omega}^1(\Omega \setminus \bar{\omega})$,

$$D_u \mathcal{F}(\mathbf{0}, u - F)(w) \cdot \hat{w} = \int_{\Omega \setminus \bar{\omega}} \nabla w \cdot \nabla \hat{w} + \int_{\partial\omega} \alpha w \hat{w} - \int_{\partial\omega} \beta \nabla_\tau w \cdot \nabla_\tau \hat{w}.$$

Thus, $D_u \mathcal{F}(\mathbf{0}, u - F)$ is an isomorphism.

Hence, the implicit function theorem applies and then there exists a C^∞ function $\theta \in \mathcal{U} \mapsto v(\theta) \in \mathbf{H}_{\partial\Omega}^2(\Omega \setminus \bar{\omega})$ such that $\mathcal{F}(\mathbf{0}, v(\theta)) = 0$ in a neighborhood of $\mathbf{0}$. Using the uniqueness of the solution of such a problem, we obtain that $\theta \in \mathcal{U} \mapsto v_\theta \in \mathbf{H}_{\partial\Omega}^2(\Omega \setminus \bar{\omega})$ is C^∞ . \square

4.3 Existence of shape derivatives

Lemma 4.4 (Differentiability of $\theta \mapsto u_\theta$). *There exists \tilde{u}_θ an extension in Ω of $u_\theta \in \mathbf{H}^1(\Omega \setminus \bar{\omega}_\theta)$ such that*

$$\theta \in \mathcal{U} \mapsto \tilde{u}_\theta \in \mathbf{H}^1(\Omega)$$

is differentiable at $\mathbf{0}$ (and even C^∞ in a neighborhood of $\mathbf{0}$).

Proof. For $\theta \in \mathcal{U}$, $u_\theta = v_\theta \circ (\mathbf{I} + \theta)^{-1} \in \mathbf{H}_{\partial\Omega}^2(\Omega \setminus \bar{\omega}_\theta)$. According to the differentiability of $\theta \mapsto v_\theta$ (see Lemma 4.3) and Stein's extension theorem (see for example [1, Theorem 5.24]), there exists \tilde{v}_θ , an extension of v_θ , such that $\theta \in \mathcal{U} \mapsto \tilde{v}_\theta \in \mathbf{H}_{\partial\Omega}^2(\Omega)$ is differentiable at $\mathbf{0}$. Moreover,

$$\theta \in \mathcal{U} \mapsto (\mathbf{I} + \theta)^{-1} - \mathbf{I} \in \mathbf{W}^{2,\infty}(\mathbb{R}^d)$$

is differentiable at $\mathbf{0}$. Thus,

$$\varphi_1 : \theta \in \mathcal{U} \mapsto (v_\theta, (\mathbf{I} + \theta)^{-1} - \mathbf{I}) \in \mathbf{H}_{\partial\Omega}^2(\Omega) \times \mathbf{W}^{2,\infty}(\mathbb{R}^d)$$

is differentiable at $\mathbf{0}$. We apply [21, Lemma 5.3.9] to get that

$$\varphi_2 : (g, \mu) \in \mathbf{H}^2(\mathbb{R}^d) \times \mathbf{W}^{2,\infty}(\Omega) \mapsto g \circ (\mathbf{I} + \mu) \in \mathbf{H}^1(\mathbb{R}^d)$$

is C^1 in a neighborhood of $\mathbf{0}$. By composition, $\theta \in \mathcal{U} \mapsto \tilde{u}_\theta := \varphi_2 \circ \varphi_1(\theta) \in \mathbf{H}_{\partial\Omega}^1(\Omega)$ is differentiable at $\mathbf{0}$. \square

Using the Fréchet differentiability given by this lemma, we obtain the Gâteaux differentiability in the direction $\mathbf{V} \in \mathcal{U}$: there exist u_t , extension in Ω of u_t such that the function $t \in [0, T) \mapsto u_t \in \mathbf{H}^1(\Omega)$ is differentiable at 0 by composition. Hence, we prove the following result:

Lemma 4.5. *The solution u of Problem (2.5) is differentiable with respect to the domain $\omega \in \mathcal{O}_\delta$. We denote by u' its derivative at 0.*

Proceeding in the same way (using $\mathbf{H}_{\partial\Omega}^3(\Omega \setminus \bar{\omega})$ instead of $\mathbf{H}_{\partial\Omega}^2(\Omega \setminus \bar{\omega})$ and $\mathbf{W}^{3,\infty}(\mathbb{R}^d)$ instead of $\mathbf{W}^{2,\infty}(\mathbb{R}^d)$), we prove the following result:

Proposition 4.6. *The solution u of Problem (2.5) is twice differentiable with respect to the domain $\omega \in \mathcal{O}_\delta$. We denote by u'' its derivative at 0.*

5 Shape calculus

Since we proved in the previous section the differentiability with respect to the domain, we can now compute the shape derivatives of the state and of the cost functional J that we want to minimize. Thus, we aim to make a sensitivity (with respect to the shape) analysis. Then, let us consider the problem on $\Omega \setminus \bar{\omega}_t$

$$\begin{cases} -\Delta u_t = 0 & \text{in } \Omega \setminus \bar{\omega}_t \\ u_t = f & \text{on } \partial\Omega \\ \partial_{\mathbf{n}_t} u_t + \alpha u_t + \beta \Delta_{\tau_t} u_t = 0 & \text{on } \partial\omega_t. \end{cases} \quad (5.1)$$

Let us remain the definition of the shape derivative in our situation (see [21] for details).

- If the mapping $\boldsymbol{\theta} \in \mathcal{U} \mapsto u_{\boldsymbol{\theta}} \circ (\mathbf{I} + \boldsymbol{\theta}) \in \mathbf{H}^1(\Omega \setminus \bar{\omega})$ is Fréchet differentiable at $\mathbf{0}$, we say that $\boldsymbol{\theta} \mapsto u_{\boldsymbol{\theta}}$ possesses a *total first variation* (or derivative) at $\mathbf{0}$. In such a case, this total first derivative at $\mathbf{0}$ in the direction $\boldsymbol{\theta}$ is denoted by $\dot{u}_{\boldsymbol{\theta}}$.
- If, for every $\mathcal{D} \subset\subset \Omega \setminus \bar{\omega}$, the mapping $\boldsymbol{\theta} \in \mathcal{U} \mapsto u_{\boldsymbol{\theta}}|_{\mathcal{D}} \in \mathbf{H}^1(\mathcal{D})$ is Fréchet differentiable at $\mathbf{0}$, we say that $\boldsymbol{\theta} \mapsto u_{\boldsymbol{\theta}}$ possesses a *local first variation* (or derivative) at $\mathbf{0}$. In such a case, this local first derivative at $\mathbf{0}$ in the direction $\boldsymbol{\theta}$ is denoted by $u'_{\boldsymbol{\theta}}$, is called *shape derivative* and is well defined in the whole domain $\Omega \setminus \bar{\omega}$:

$$u'_{\boldsymbol{\theta}} = \frac{d}{dt}(u_{t\boldsymbol{\theta}}|_{\mathcal{D}})|_{t=0} \quad \text{in each } \mathcal{D} \subset\subset \Omega \setminus \bar{\omega}.$$

We define similarly the higher order shape derivative. In the following, for $\mathbf{V} \in \mathcal{U}$, we denote by u' the local first variation $u'_{\mathbf{V}}$ which is referred as the shape derivative of the state.

We first characterize the shape derivative of the state differentiating with respect to the domain the Ventcel boundary conditions. Then, using this characterization, we compute the shape gradient of the functional J and obtain a formula with an explicit dependence with respect to the perturbation direction \mathbf{V} introducing an adapted adjoint problem. We also characterize the shape Hessian and finally prove the instability of our shape optimization problem (2.6) using a local regularity argument.

5.1 Shape derivative of the problem

Proposition 5.1 (First order shape derivative of the state). *Let $\mathbf{V} \in \mathcal{U}$. The shape derivative u' of u which belongs to $H^1(\Omega \setminus \bar{\omega})$ is the only solution of the following boundary values problem*

$$\begin{cases} -\Delta u' = 0 & \text{in } \Omega \setminus \bar{\omega} \\ u' = 0 & \text{on } \partial\Omega \\ \partial_n u' + \alpha u' + \beta \Delta_\tau u' = \xi(u, V_n) & \text{on } \partial\omega, \end{cases} \quad (5.2)$$

with

$$\begin{aligned} \xi(u, V_n) := & V_n (-\alpha \partial_n u - \alpha H u + \Delta_\tau u) + \nabla_\tau u \cdot \nabla_\tau V_n \\ & - \beta \Delta_\tau (V_n \partial_n u) - \beta \operatorname{div}_\tau (V_n H \nabla_\tau u - 2V_n D^2 b \nabla_\tau u), \end{aligned} \quad (5.3)$$

where H is the mean curvature of $\partial\omega$ and b is the signed distance.

We refer to Appendix B where we state some useful results concerning shape differential calculus (in particular concerning the signed distance b).

Proof. For $t \in [0, T)$, we consider Problem (5.1). By differentiating with respect to the shape at $t = 0$, we classically obtain (see for example [21, Chapter 5])

$$-\Delta u' = 0 \quad \text{in } \Omega \setminus \bar{\omega} \quad \text{and} \quad u' = 0 \quad \text{on } \partial\Omega.$$

Now let us compute the shape derivative of the Ventcel boundary condition $\partial_{n_t} u_t + \alpha u_t + \beta \Delta_{\tau_t} u_t = 0$ on $\partial\omega_t$ at $t = 0$. Let $\varphi \in H^2(\Omega \setminus \bar{\omega})$ compactly supported in Ω_δ . Using Stein's extension theorem, φ admits an extension in $H^2(\mathbb{R}^d)$ still denoted by φ and which is still compactly supported in Ω_δ . This extension belongs in particular to $H^2(\Omega \setminus \bar{\omega}_t)$. Using φ as a test function in the variational formulation of Problem (5.1), we have

$$\int_{\Omega \setminus \bar{\omega}_t} \nabla u_t \cdot \nabla \varphi + \int_{\partial\omega_t} (\alpha u_t \varphi - \beta \nabla_{\tau_t} u_t \cdot \nabla_{\tau_t} \varphi) = \int_{\Omega \setminus \bar{\omega}_t} \Delta F \varphi.$$

Then, by using Hadamard formulas (on the volume and on the surface: see [21, Proposition 5.4.4 and Proposition 5.4.18]), we obtain

$$\begin{aligned} & \int_{\Omega \setminus \bar{\omega}} \nabla u' \cdot \nabla \varphi + \int_{\partial\omega} \nabla u \cdot \nabla \varphi V_n \\ & + \int_{\partial\omega} \left[\alpha u' \varphi - \beta \frac{d}{dt} (\nabla_{\tau_t} u_t) \Big|_{t=0} \cdot \nabla_{\tau} \varphi - \beta \nabla_{\tau} u \cdot \frac{d}{dt} (\nabla_{\tau_t} \varphi) \Big|_{t=0} \right. \\ & \left. + V_n (\partial_n (\alpha u \varphi - \beta \nabla_{\tau} u \cdot \nabla_{\tau} \varphi) + H (\alpha u \varphi - \beta \nabla_{\tau} u \cdot \nabla_{\tau} \varphi)) \right] = \int_{\partial\omega} (\Delta F \varphi) V_n. \end{aligned}$$

Moreover,

$$\begin{aligned} \frac{d}{dt} (\nabla_{\tau_t} u_t) \Big|_{t=0} &= \frac{d}{dt} (\nabla u_t - (\nabla u_t \cdot \mathbf{n}_t) \mathbf{n}_t) \Big|_{t=0} \\ &= \nabla_{\tau} u' + (\nabla u \cdot \nabla_{\tau} V_n) \mathbf{n} + \partial_n u \nabla_{\tau} V_n, \end{aligned}$$

using the fact that $\mathbf{n}' = -\nabla_\tau V_n$ (see Proposition B.1). Hence, using the same result for $\frac{d}{dt} (\nabla_{\tau_t} \varphi) |_{t=0}$, we obtain

$$\begin{aligned} & \int_{\Omega \setminus \bar{\omega}} \nabla u' \cdot \nabla \varphi + \int_{\partial \omega} \nabla u \cdot \nabla \varphi V_n \\ & \quad + \int_{\partial \omega} \left[\alpha u' \varphi - \beta (\nabla_\tau u' + \partial_n u \nabla_\tau V_n + (\nabla u \cdot \nabla_\tau V_n) \mathbf{n}) \cdot \nabla_\tau \varphi \right. \\ & \quad \quad \left. - \beta \nabla_\tau u \cdot (\partial_n \varphi \nabla_\tau V_n + (\nabla \varphi \cdot \nabla_\tau V_n) \mathbf{n}) \right. \\ & \quad \left. + V_n (\partial_n (\alpha u \varphi - \beta \nabla_\tau u \cdot \nabla_\tau \varphi) + \mathbf{H} (\alpha u \varphi - \beta \nabla_\tau u \cdot \nabla_\tau \varphi)) \right] = \int_{\partial \omega} (\Delta F \varphi) V_n. \end{aligned}$$

Since $\nabla_\tau \varphi \cdot \mathbf{n} = 0$ and $\nabla_\tau u \cdot \mathbf{n} = 0$, this equality writes

$$\begin{aligned} & \int_{\Omega \setminus \bar{\omega}} \nabla u' \cdot \nabla \varphi + \int_{\partial \omega} \nabla u \cdot \nabla \varphi V_n \\ & \quad + \int_{\partial \omega} \left[\alpha u' \varphi - \beta (\nabla_\tau u' + \partial_n u \nabla_\tau V_n) \cdot \nabla_\tau \varphi - \beta \nabla_\tau u \cdot (\partial_n \varphi \nabla_\tau V_n) \right. \\ & \quad \left. + V_n (\partial_n (\alpha u \varphi - \beta \nabla_\tau u \cdot \nabla_\tau \varphi) + \mathbf{H} (\alpha u \varphi - \beta \nabla_\tau u \cdot \nabla_\tau \varphi)) \right] = \int_{\partial \omega} (\Delta F \varphi) V_n. \quad (5.4) \end{aligned}$$

We also have using Problem (5.1)

$$\int_{\Omega \setminus \bar{\omega}_t} \nabla u_t \cdot \nabla \varphi - \int_{\partial \omega_t} \partial_{n_t} u_t \varphi = \int_{\Omega \setminus \bar{\omega}_t} \Delta F \varphi.$$

Thus, using Hadamard formulas, we obtain

$$\begin{aligned} & \int_{\Omega \setminus \bar{\omega}} \nabla u' \cdot \nabla \varphi + \int_{\partial \omega} \nabla u \cdot \nabla \varphi V_n \\ & \quad - \int_{\partial \omega} [\partial_n u' \varphi - (\nabla u \cdot \nabla_\tau V_n) \varphi + V_n (\partial_n (\partial_n u \varphi) + \partial_n u \varphi \mathbf{H})] = \int_{\partial \omega} (\Delta F \varphi) V_n. \quad (5.5) \end{aligned}$$

Subtracting (5.4) and (5.5), we obtain

$$\begin{aligned} & \int_{\partial \omega} (\partial_n u' + \alpha u' + \beta \Delta_\tau u') \varphi = \int_{\partial \omega} \left[-\beta \operatorname{div}_\tau (\partial_n u \nabla_\tau V_n) \varphi + \beta \nabla_\tau u \cdot (\partial_n \varphi \nabla_\tau V_n) \right. \\ & \quad \left. - V_n (\partial_n (\alpha u \varphi - \beta \nabla_\tau u \cdot \nabla_\tau \varphi) + \mathbf{H} (\alpha u \varphi - \beta \nabla_\tau u \cdot \nabla_\tau \varphi)) \right] \\ & \quad \quad - \int_{\partial \omega} [-(\nabla u \cdot \nabla_\tau V_n) \varphi + V_n (\partial_n (\partial_n u \varphi) + \partial_n u \varphi \mathbf{H})]. \end{aligned}$$

Since $\partial_n (\partial_n u \varphi) = \partial_n u \partial_n \varphi + \partial_{nn}^2 u \varphi$, this leads

$$\begin{aligned} & \int_{\partial \omega} (\partial_n u' + \alpha u' + \beta \Delta_\tau u') \varphi = \int_{\partial \omega} \left[-\beta \operatorname{div}_\tau (\partial_n u \nabla_\tau V_n) \varphi + \beta \partial_n \varphi \nabla_\tau u \cdot \nabla_\tau V_n \right. \\ & \quad \left. - V_n (\alpha \partial_n u \varphi + \alpha u \partial_n \varphi - \beta \partial_n (\nabla_\tau u \cdot \nabla_\tau \varphi) + \mathbf{H} \alpha u \varphi - \mathbf{H} \beta \nabla_\tau u \cdot \nabla_\tau \varphi) \right] \\ & \quad \quad - \int_{\partial \omega} [-(\nabla u \cdot \nabla_\tau V_n) \varphi + V_n (\partial_n u \partial_n \varphi + \partial_{nn}^2 u \varphi + \mathbf{H} \partial_n u \varphi)]. \end{aligned}$$

Using an integration by part and the decomposition of the Laplace-Beltrami operator (see for example [21, Proposition 5.4.12]) given by

$$\Delta u = \Delta_\tau u + H\partial_n u + \partial_{nn}^2 u \quad \text{on } \partial\omega,$$

we obtain

$$\begin{aligned} \int_{\partial\omega} (\partial_n u' + \alpha u' + \beta \Delta_\tau u') \varphi &= \int_{\partial\omega} \left[-\beta \operatorname{div}_\tau (\partial_n u \nabla_\tau V_n) \varphi - \beta \operatorname{div}_\tau (\partial_n \varphi \nabla_\tau u) V_n \right. \\ &\quad - V_n (\alpha \partial_n u + \alpha H u - \Delta_\tau u) \varphi - V_n (\alpha u \partial_n \varphi - \beta \partial_n (\nabla_\tau u \cdot \nabla_\tau \varphi) + \partial_n u \partial_n \varphi) \\ &\quad \left. - \operatorname{div}_\tau (V_n H \beta \nabla_\tau u) \varphi + (\nabla u \cdot \nabla_\tau V_n) \varphi \right]. \end{aligned}$$

Since (see Theorem B.2)

$$\partial_n (\nabla_\tau u \cdot \nabla_\tau \varphi) + D^2 b \nabla_\tau u \cdot \nabla_\tau \varphi = \nabla_\tau (\partial_n u) \cdot \nabla_\tau \varphi + \nabla_\tau (\partial_n \varphi) \cdot \nabla_\tau u$$

and since $\partial_n u + \alpha u + \beta \Delta_\tau u = 0$ on $\partial\omega$, we have

$$\begin{aligned} &\int_{\partial\omega} \left[-\beta \operatorname{div}_\tau (\partial_n \varphi \nabla_\tau u) V_n - V_n (\alpha u \partial_n \varphi - \beta \partial_n (\nabla_\tau u \cdot \nabla_\tau \varphi) + \partial_n u \partial_n \varphi) \right] \\ &= - \int_{\partial\omega} \left[\beta \Delta_\tau u \partial_n \varphi + \beta \nabla_\tau u \cdot \nabla_\tau (\partial_n \varphi) + \alpha u \partial_n \varphi + \partial_n u \partial_n \varphi - \beta \partial_n (\nabla_\tau u \cdot \nabla_\tau \varphi) \right] V_n \\ &= - \int_{\partial\omega} \left[\beta \nabla_\tau u \cdot \nabla_\tau (\partial_n \varphi) - \beta \partial_n (\nabla_\tau u \cdot \nabla_\tau \varphi) \right] V_n \\ &= - \int_{\partial\omega} \beta \left[-\nabla_\tau (\partial_n u) \cdot \nabla_\tau \varphi + \partial_n (\nabla_\tau u \cdot \nabla_\tau \varphi) + 2D^2 b \nabla_\tau u \cdot \nabla_\tau \varphi - \partial_n (\nabla_\tau u \cdot \nabla_\tau \varphi) \right] V_n \\ &= \int_{\partial\omega} \operatorname{div}_\tau (\beta V_n (-\nabla_\tau (\partial_n u) + 2D^2 b \nabla_\tau u)) \varphi. \end{aligned}$$

Hence, we finally obtain

$$\begin{aligned} \int_{\partial\omega} (\partial_n u' + \alpha u' + \beta \Delta_\tau u') \varphi &= \int_{\partial\omega} \left[-\beta \operatorname{div}_\tau (\partial_n u \nabla_\tau V_n) \varphi - V_n (\alpha \partial_n u + \alpha H u - \Delta_\tau u) \varphi \right. \\ &\quad \left. - \operatorname{div}_\tau (V_n H \beta \nabla_\tau u) \varphi + (\nabla u \cdot \nabla_\tau V_n) \varphi + \operatorname{div}_\tau (\beta V_n (-\nabla_\tau (\partial_n u) + 2D^2 b \nabla_\tau u)) \varphi \right]. \end{aligned}$$

Then, using the density in $L^2(\partial\omega)$ of the traces on $\partial\omega$ of functions $H^2(\Omega \setminus \bar{\omega})$ with compact support in Ω_δ , we obtain

$$\begin{aligned} \partial_n u' + \alpha u' + \beta \Delta_\tau u' &= V_n (-\alpha \partial_n u - \alpha H u + \Delta_\tau u) + \nabla u \cdot \nabla_\tau V_n \\ &\quad - \beta \operatorname{div}_\tau [\partial_n u \nabla_\tau V_n + V_n H \nabla_\tau u + V_n \nabla_\tau (\partial_n u) - 2V_n D^2 b \nabla_\tau u]. \end{aligned}$$

Noticing that this equalities can be rewrite as

$$\begin{aligned} \partial_n u' + \alpha u' + \beta \Delta_\tau u' &= V_n (-\alpha \partial_n u - \alpha H u + \Delta_\tau u) + \nabla u \cdot \nabla_\tau V_n \\ &\quad - \beta \Delta_\tau (V_n \partial_n u) - \beta \operatorname{div}_\tau [V_n H \nabla_\tau u - 2V_n D^2 b \nabla_\tau u], \end{aligned}$$

we obtain the announced result using the fact that $\nabla u \cdot \nabla_\tau V_n = \nabla_\tau u \cdot \nabla_\tau V_n$ on $\partial\omega$. \square

5.2 Shape derivatives of the functional

5.2.1 First order shape derivatives of the functional

Using the previous characterization of the state, we now compute the shape gradient of the functional J in the following statement:

Proposition 5.2 (First order shape derivative of the functional). *For \mathbf{V} in \mathbf{U} , the least squares functional J is differentiable at ω in the direction \mathbf{V} with*

$$\nabla J(\omega) \cdot \mathbf{V} = - \int_{\partial\omega} \left[-\alpha \mathbf{H} u w + (-\mathbf{I} + \beta(\mathbf{H}\mathbf{I} - 2\mathbf{D}^2 b)) (\nabla_\tau u \cdot \nabla_\tau w) + \partial_n u \partial_n w \right] V_n \quad (5.6)$$

where \mathbf{H} is the mean curvature of $\partial\omega$, b is the signed distance and where $w \in \mathbf{H}^1(\Omega \setminus \bar{\omega})$ is the solution of the following boundary values problem:

$$\begin{cases} -\Delta w = 0 & \text{in } \Omega \setminus \bar{\omega} \\ w = \partial_n u - g & \text{on } \partial\Omega \\ \partial_n w + \alpha w + \beta \Delta_\tau w = 0 & \text{on } \partial\omega. \end{cases} \quad (5.7)$$

Proof. We define, for $t \in [0, T]$,

$$j(t) = J(\omega_t) := \frac{1}{2} \int_{\partial\Omega} |\partial_n u_t - g|^2,$$

where $u_t \in \mathbf{H}^1(\Omega \setminus \bar{\omega}_t)$ solves Problem (5.1). Using Hadamard's formula, we immediately obtain

$$\mathbf{D}J(\omega) \cdot \mathbf{V} = j'(0) = \int_{\partial\Omega} \partial_n u' (\partial_n u - g).$$

In order to obtain an expression of $j'(0)$ as an integral on $\partial\omega$ with an explicit dependance in the perturbation direction \mathbf{V} , let us introduce the solution $w \in \mathbf{H}^1(\Omega \setminus \bar{\omega})$ of the adjoint problem (5.7). Hence, using w as a test function in (5.2) and u' as a test function in (5.7), we use the Green's formula to obtain

$$\int_{\partial(\Omega \setminus \bar{\omega})} \partial_n u' w = \int_{\partial(\Omega \setminus \bar{\omega})} \partial_n w u'.$$

Thus, adding $\int_{\partial\omega} (\alpha u' w + \beta \Delta_\tau u' w)$ in each side of the previous equality and using the fact that $\int_{\partial\omega} \beta \Delta_\tau u' w = \int_{\partial\omega} \beta \Delta_\tau w u'$,

$$\int_{\partial\Omega} \partial_n u' w + \int_{\partial\omega} (\partial_n u' + \alpha u' + \beta \Delta_\tau u') w = \int_{\partial\Omega} \partial_n w u' + \int_{\partial\omega} (\partial_n w + \alpha w + \beta \Delta_\tau w) u'.$$

Using the boundary conditions satisfied by u' and w , we obtain the following characterization of the shape gradient of the functional

$$\mathbf{D}J(\omega) \cdot \mathbf{V} = - \int_{\partial\omega} \xi(u, V_n) w,$$

where ξ is given by (5.3). Finally, using integration by parts,

$$\begin{aligned} \mathbf{D}J(\omega) \cdot \mathbf{V} = - \int_{\partial\omega} \left[-\alpha \partial_n u w - \alpha \mathbf{H} u w + \Delta_\tau u w - \operatorname{div}_\tau (\nabla_\tau u w) \right. \\ \left. - \beta \partial_n u \Delta_\tau w + \beta (\mathbf{H} \nabla_\tau u \cdot \nabla_\tau w - 2\mathbf{D}^2 b \nabla_\tau u \cdot \nabla_\tau w) \right] V_n. \end{aligned}$$

Thus, since $-\beta \Delta_\tau w = \partial_n w + \alpha w$ on $\partial\omega$, we obtain the announced result. \square

5.2.2 Second order shape derivatives of the functional

Let us consider $\omega^* \in \mathcal{O}_\delta$ solution of the inverse problem (2.3). In order to study the stability of the optimization problem (2.6) at ω^* , we want to compute the second order shape derivative of J , *i.e.* the shape Hessian. First of all, notice that we prove in exactly the same way than we proved the existence of the shape derivative u' that the adjoint state w is differentiable with respect to the shape $\omega \in \Omega_\delta$ and we denote by w' its shape derivative. Then, we state the following result:

Proposition 5.3 (Characterization of the shape Hessian at a critical shape). *For $\mathbf{V} \in \mathbf{U}$, we have*

$$D^2J(\omega^*) \cdot \mathbf{V} \cdot \mathbf{V} = - \int_{\partial\omega^*} [-\alpha H w w' + (-I + \beta (HI - 2D^2b) (\nabla_\tau u \cdot \nabla_\tau w')) + \partial_n u \partial_n w'] V_n,$$

where H is the mean curvature of $\partial\omega^*$, b is the signed distance and where $w' \in H^1(\Omega \setminus \overline{\omega^*})$ is the solution of the following problem:

$$\begin{cases} -\Delta w' = 0 & \text{in } \Omega \setminus \overline{\omega^*} \\ w' = \partial_n u' & \text{on } \partial\Omega \\ \partial_n w' + \alpha w' + \beta \Delta_\tau w' = 0 & \text{on } \partial\omega^*. \end{cases} \quad (5.8)$$

Proof. Using Hadamard's formula, we obtain

$$j''(0) = \int_{\partial\Omega} \partial_n u'' (\partial_n u - g) + |\partial_n u'|^2.$$

We then characterize the shape derivative of the adjoint state in the same way that we characterized u' , *i.e.*

$$\begin{cases} -\Delta w' = 0 & \text{in } \Omega \setminus \overline{\omega} \\ w' = \partial_n u' & \text{on } \partial\Omega \\ \partial_n w' + \alpha w' + \beta \Delta_\tau w' = \xi(w, V_n) & \text{on } \partial\omega. \end{cases}$$

Noticing that for $\omega = \omega^*$, $\partial_n u = g$ on $\partial\Omega$ and then $w \equiv 0$ in $\Omega \setminus \overline{\omega^*}$, we obtain the characterization (5.8). Then, using the same trick than in the computation of the first order shape derivative of the functional J (with u' and w' as respective test functions in (5.8) and (5.2)), we obtain

$$\int_{\partial\Omega} |\partial_n u'|^2 = \int_{\partial\omega} -\xi(u, V_n) w'.$$

We then conclude using the same manipulations than the ones used for the computations of the shape gradient (see proof of Proposition 5.2). \square

5.3 Instability of the problem

Now let us prove the instability of the inverse problem (2.3) using the method already used in [17, 6, 14, 13]. Thus, we use a local regularity argument in order to prove the compactness of the Riesz operator corresponding to the shape Hessian at a solution $\omega^* \in \mathcal{O}_\delta$ of the inverse problem. An alternative proof could be to use the potential layers as what is done in [2].

Proposition 5.4 (Compactness at a critical point). *The Riesz operator corresponding to the shape Hessian $D^2J(\omega^*)$ defined from $\mathbf{H}^{1/2}(\partial\omega^*)$ to $\mathbf{H}^{-1/2}(\partial\omega^*)$ is compact.*

Proof. The idea of the proof is to write the shape Hessian as a composition of linear continuous operators whose one is compact (the compactness being obtained using the compactness imbedding between two Sobolev spaces).

Let us focus on the term $\int_{\partial\omega^*} \alpha H u w' V_n$ of the characterization of the shape Hessian given in Proposition 5.3. The other terms can be treated in the same way. We decompose this term as

$$\int_{\partial\omega^*} \alpha H u w' V_n = \langle K(\mathbf{V}), L(\mathbf{V}) \rangle_{\mathbf{H}^{-1/2}(\partial\omega^*), \mathbf{H}^{1/2}(\partial\omega^*)},$$

where

$$\begin{aligned} L &: \mathbf{V} \in \mathbf{H}^{1/2}(\partial\omega^*) \mapsto \alpha H u V_n \in \mathbf{H}^{1/2}(\partial\omega^*) \\ K &: \mathbf{V} \in \mathbf{H}^{1/2}(\partial\omega^*) \mapsto w' \in \mathbf{H}^{-1/2}(\partial\omega^*). \end{aligned}$$

Since u is independent of \mathbf{V} , the operator L is clearly linear continuous as multiplier by a smooth function (see [24]). Now, let us prove that the operator K is compact which will be conclude the proof.

According to the characterization (5.8) of w' , we decompose the operator K as follows: $K = K_2 \circ K_1$ with

$$\begin{aligned} K_1 &: \mathbf{V} \in \mathbf{H}^{1/2}(\partial\omega^*) \mapsto \partial_n u' \in \mathbf{H}^{1/2}(\partial\Omega) \\ K_2 &: \Psi \in \mathbf{H}^{1/2}(\partial\omega^*) \mapsto \Phi \in \mathbf{H}^{-1/2}(\partial\omega^*), \end{aligned}$$

where u' is the solution of Problem (5.2) and $\Phi \in \mathbf{H}^1(\Omega \setminus \overline{\omega^*})$ solves

$$\begin{cases} -\Delta \Phi = 0 & \text{in } \Omega \setminus \overline{\omega^*} \\ \Phi = \Psi & \text{on } \partial\Omega \\ \partial_n \Phi + \alpha \Phi + \beta \Delta_\tau \Phi = 0 & \text{on } \partial\omega^*. \end{cases} \quad (5.9)$$

The operator K_1 is clearly linear continuous. Then, we decompose the operator K_2 as $K_2 = K_{2,3} \circ K_{2,2} \circ K_{2,1}$ with

$$\begin{aligned} K_{2,1} &: \Psi \in \mathbf{H}^{1/2}(\partial\Omega) \mapsto \Phi \in \mathbf{H}^3(\Omega_\delta \setminus \overline{\omega^*}) \\ K_{2,2} &: \Phi \in \mathbf{H}^3(\Omega_\delta \setminus \overline{\omega^*}) \mapsto \Phi \in \mathbf{H}^{5/2}(\partial\omega^*) \\ K_{2,3} &: \Phi \in \mathbf{H}^{5/2}(\partial\omega^*) \mapsto \Phi \in \mathbf{H}^{-1/2}(\partial\omega^*). \end{aligned}$$

Notice that the regularity $\mathbf{H}^3(\Omega_\delta \setminus \overline{\omega^*})$ is due to a local regularity argument (as the one used in [6, 14, 13]): since the object ω^* has a C^3 boundary and since the condition on $\partial\omega^*$ is homogenous (and then smooth), the solution of Problem (5.9) is globally $\mathbf{H}^1(\Omega \setminus \overline{\omega^*})$ but locally $\mathbf{H}^3(\Omega_\delta \setminus \overline{\omega^*})$. The operators $K_{2,1}$ and $K_{2,2}$ are then linear continuous and the operator $K_{2,3}$ is the compact imbedding of $\mathbf{H}^{5/2}(\partial\omega^*)$ into $\mathbf{H}^{-1/2}(\partial\omega^*)$. Hence, we obtain the compactness result. \square

This result points out the lack of stability of the optimization problem (2.6): it means, roughly speaking, that, in a neighborhood of ω^* (*i.e.* for t small), J behaves as its second order approximation and one cannot expect an estimate of the kind $C t \leq \sqrt{J(\omega_t)}$ with a constant C uniform in \mathbf{V} . Hence, this proposition emphasizes that the gradient has not a uniform sensitivity with respect to the deformation directions: J is degenerate for highly oscillating perturbations.

6 Numerical experiments

In this section, we want to make some numerical simulations in order to confirm and complete our previous theoretical results. We use a classical shape variation descent algorithm without any regularization method in order to solve numerically the optimization problem (2.6) as what is done in the cases of Dirichlet or Neumann boundary conditions (see for example [2, 14]). Indeed, it seems that, in our case, the degeneracy of the functional does not lead to apparition of oscillations in the numerical reconstruction. This problem seems to be less unstable than the cases of classical boundary conditions.

6.1 Framework for the numerical simulations

The numerical simulations presented are made in dimension two using the finite elements library FREEFEM++ (see [20]). We use a $P2$ finite elements discretization to solve Problem (2.5) and the adjoint problem (5.7). The framework is the following: the exterior boundary is assumed to be the unit circle, the coefficients α, β are such that $\alpha = 1$, $\beta = -0.1$ and we consider the exterior Dirichlet boundary condition

$$f = \cos(\theta), \theta \in [0, 2\pi).$$

In order to have a suitable pair (*measure* g , *domain* ω^*), we use a synthetic data: we fix a shape ω^* , solve Problem (2.5) in $\Omega \setminus \overline{\omega^*}$ using another finite elements method (here a $P3$ finite elements discretization) and extract the measurement g by computing $\partial_n u$ on $\partial\Omega$.

The optimization method used for the numerical simulations is here the classical gradient algorithm. We use initially $N_{ext} := 100$ discretization points for the exterior boundary and $N_{int} := 70$ points for the interior boundary. Then, we use the function *movemesh* of FREEFEM++ in order to change the shape of the objects at each step and the function *adaptmesh* to refine and avoid degeneracy of the triangles in the meshes. In order to be completely explicit, we detail this algorithm:

Algorithm 1

1. fix a number of iterations M and an initial shape ω_0 ;
2. solve Problems (2.5) and (5.7) with $\omega = \omega_i$ (where ω_i denotes the i^{th} iterate of the approximate shape);
3. compute the kernel of $\nabla J_{KV}(\omega_i)$ in Formula (5.6);
4. move the shape using the function *movemesh*;
5. get back to the step 2. while $i < M$.

Remark 6.1. *We can notice that we have to solve only two problems (Problems (2.5) and (5.7)) to compute the descent direction. Indeed, the directional perturbations \mathbf{V} dependence is explicit in Formula (5.6).*

The stopping criterion of the algorithm is here the number of iterations. Obviously, this criterion can be modified and even improved but this simple one permits to obtain efficient results. Moreover, we precise that we stop the algorithm if the value of the residual increase between two steps.

Let us be more precise about the step 4 of the algorithm. In order to have a descent direction, we solve the following problem

$$\begin{cases} -\Delta\Phi + \Phi = 0 & \text{in } \Omega \setminus \overline{\omega} \\ \partial_n \Phi = 0 & \text{on } \partial\Omega \\ \partial_n \Phi = -[-\alpha H u w + (-I + \beta(HI - 2D^2b))(\nabla_\tau u \cdot \nabla_\tau w) + \partial_n u \partial_n w] & \text{on } \partial\omega. \end{cases}$$

where the Neumann boundary condition on $\partial\omega$ is the kernel of the shape gradient ∇J . Thus, the descent direction is given by $\nabla\Phi$. Let us precise that the step size is simply chosen testing the value of the functional: we decrease it if the value of J increases and we increase it for the next iteration if the value of J decreases.

6.2 Reconstruction of some obstacles

We first test our algorithm on simple shapes as circle or ellipse, centered or not. The results are quite efficient as showed in Figure 1. We precise here the color code that we choose

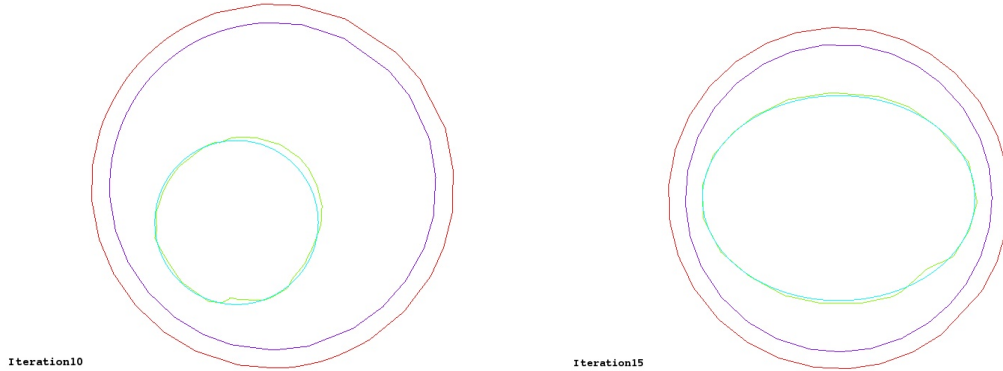


Figure 1: Reconstruction of simple shapes

and that we will use in the sequel. The exterior boundary is represented in red, the initial shape in purple, the exact shape in cyan and the obtained shape in green.

The reconstruction seems to be efficient to reconstruct "simple obstacles". Now, we aim to detect shapes with concavity or with corners. More precisely, we want to detect a square and a kite shape represented by

$$\partial\omega_1 := \left\{ \left(\begin{array}{c} 0.3 (\cos \theta + 0.65 \cos(2\theta) - 0.65) \\ 0.45 \sin \theta \end{array} \right), \theta \in [0, 2\pi) \right\}.$$

We represent the results in Figure 2 where we see that the reconstruction is again efficient.

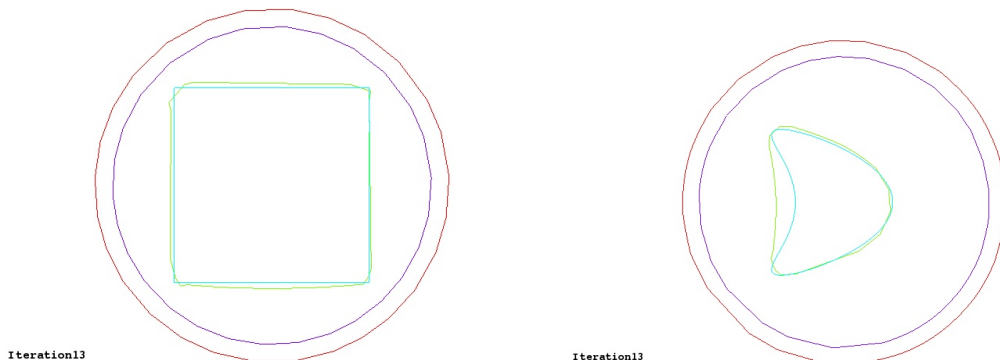


Figure 2: Reconstruction of non trivial shapes

Finally, we present in Figure 3 the reconstruction of the kite shape ω_1 with respectively 3% and 10% artificial noise. Even if the error of detection increase with the percentage of noise, we obtain reasonable results.

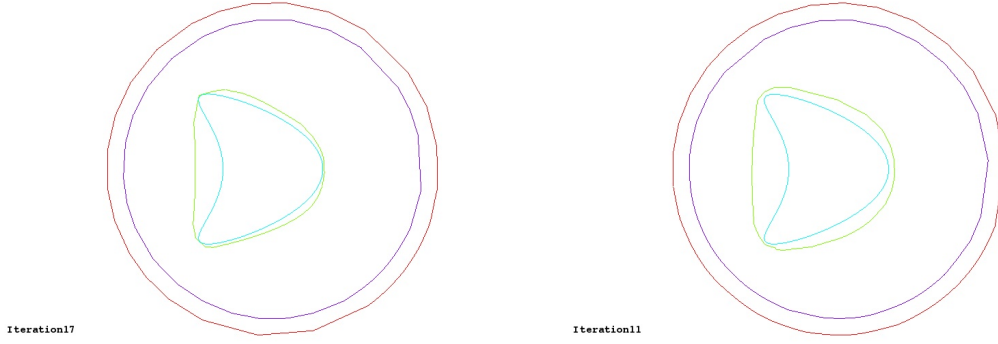


Figure 3: Reconstruction with 3% and 10% artificial noise

6.3 Influence of some parameters

Location and shape of the object. We wonder to know if our method is efficient to detect small obstacles. Thus, in Figure 4, we represent the result when we want to reconstruct a small square. We see that the detection is not good because of the object is then far away from the exterior boundary (that is where we make the measurement). It seems that, in this case, we detect efficiently the position of the obstacle but not its shape. We also see in Figure 4 that when we want to detect obstacles whose some parts are far



Figure 4: Detection non trivial shapes

away from the exterior boundary, the detection is not efficient. Here, the exact shape is represented by

$$\partial\omega_2 := \left\{ 0.5(1 + \cos(3\theta)) \begin{pmatrix} \cos \theta \\ \sin \theta \end{pmatrix}, \theta \in [0, 2\pi) \right\}.$$

It seems that, in this case, we detect only the convex hull of the object.

Measurement. The imposed Dirichlet boundary conditions f on $\partial\Omega$ seems to have an important role in the efficiency of the detection. Indeed, if we impose $f = \cos(5\theta)$ instead of $f = \cos(\theta)$ ($\theta \in [0, 2\pi)$), the result is significantly worse as represented in Figure 5, where we want to reconstruct the kite shape ω_1 .

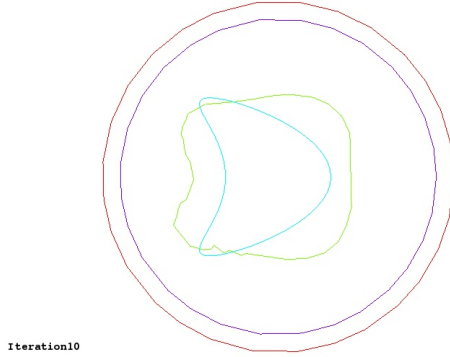


Figure 5: Detection non trivial shapes

7 Conclusion

We have partially reconstructed an obstacle immersed in a perfect fluid by minimizing a least squares functional using boundary measurements. The object ω was assumed to have a thin layer and was then modeled by using generalized boundary conditions (precisely Ventcel boundary conditions). We have first proved an identifiability result in the case of two concentric circles which claims that two pairs of measurements $(u_i|_{\partial\Omega}, \partial_n u_i|_{\partial\Omega})$, $i = 1, 2$ ensures the identification of the obstacle ω . It is a first step in the investigations of the general identifiability result. Then, we have used shape optimization methods to compute the gradient of the cost functional and the shape Hessian. Thus, we have differentiated with respect to the domain the non classical Ventcel boundary conditions on $\partial\omega$. We have then proved that this problem is unstable in the sense that the functional degenerates for the highly oscillating perturbations of the boundary. However, the numerical simulations made in the bi-dimensional case were effective even if we do not use some regularization method to reconstruct the obstacle. It seems that the generalized impedance boundary conditions of order two lead to a problem less unstable than in the cases of classical boundary conditions.

This work may be followed by some others investigations. First of all, the general identifiability result for the shape from one or several boundary measurements is still an open problem. Moreover, a natural extension would be to study the determination of both the shape and the coefficients α, β of the Ventcel boundary conditions with the use of shape derivative.

A Some results concerning Ventcel boundary conditions

For reader's convenience, we here recall some results concerning the Poisson's equation with Ventcel boundary conditions. We refer to [29] and [7] for complements (see also [28]).

Let us first state a result concerning the Laplace-Beltrami operator (see for example [29] or [28] for details).

Theorem A.1. *Let $s \in \mathbb{R}$ and ω a smooth open set. The operator*

$$-\Delta_\tau + \mathbb{I} : H^{s+1}(\partial\omega) \rightarrow H^{s-1}(\partial\omega)$$

is an isomorphism.

Now let us prove the following existence and uniqueness result:

Theorem A.2. *Let $s \in \mathbb{R}$. Let Ω and ω be two smooth bounded connected open sets of \mathbb{R}^d ($d \geq 2$ and integer) such that $\omega \subset\subset \Omega$ and $\Omega \setminus \bar{\omega}$ is connected. Let $\alpha > 0$ and $\beta < 0$ two real numbers and let $f \in \mathbf{H}^{s+2}(\partial\Omega)$ and $g \in \mathbf{H}^s(\partial\omega)$. Then there exists a unique solution $u \in \mathbf{H}^{s+\frac{5}{2}}(\Omega \setminus \bar{\omega})$ of the following boundary value problem*

$$\begin{cases} -\Delta u = 0 & \text{in } \Omega \\ u = f & \text{on } \partial\Omega \\ \partial_n u + \alpha u + \beta \Delta_\tau u = g & \text{on } \partial\omega \end{cases} \quad (\text{A.1})$$

and there exists a constant $C > 0$ such that

$$\|u\|_{\mathbf{H}^{s+\frac{5}{2}}(\Omega \setminus \bar{\omega})} \leq C \left(\|f\|_{\mathbf{H}^{s+2}(\partial\Omega)} + \|g\|_{\mathbf{H}^s(\partial\omega)} \right).$$

Proof. Let $F \in \mathbf{H}^{s+\frac{5}{2}}(\Omega)$ the unique solution of

$$\begin{cases} -\Delta F = 0 & \text{in } \Omega \\ F = f & \text{on } \partial\Omega \end{cases}$$

with $\|F\|_{\mathbf{H}^{s+\frac{5}{2}}(\Omega)} \leq C \|f\|_{\mathbf{H}^{s+2}(\partial\Omega)}$ (where $C > 0$ is a constant). Then, Problem (A.1) can be rewritten as the problem consisting of finding $\tilde{u} := u - F \in \mathbf{H}^{s+\frac{5}{2}}(\Omega)$ such that

$$\begin{cases} -\Delta \tilde{u} = 0 & \text{in } \Omega \\ \tilde{u} = 0 & \text{on } \partial\Omega \\ \partial_n \tilde{u} + \alpha \tilde{u} + \beta \Delta_\tau \tilde{u} = \tilde{g} & \text{on } \partial\omega, \end{cases} \quad (\text{A.2})$$

where $\tilde{g} := g - \partial_n F + \alpha F + \beta \Delta_\tau F$ on $\partial\omega$.

Now, let us introduce the Dirichlet-to-Neumann operator Λ_ω defined by

$$\Lambda_\omega : U \in \mathbf{H}^{s+2}(\partial\omega) \mapsto \partial_n \tilde{u} \in \mathbf{H}^{s+1}(\partial\omega)$$

where $\tilde{u} \in \mathbf{H}^{s+\frac{5}{2}}(\Omega \setminus \bar{\omega})$ is the unique solution of

$$\begin{cases} -\Delta \tilde{u} = 0 & \text{in } \Omega \\ \tilde{u} = 0 & \text{on } \partial\Omega \\ \tilde{u} = U & \text{on } \partial\omega. \end{cases}$$

This operator Λ_ω is classically well-defined (see for example [23] for details). Notice that there exists a positive constant (still denoted by C) such that

$$\|\tilde{u}\|_{\mathbf{H}^{s+\frac{5}{2}}(\Omega \setminus \bar{\omega})} \leq C \|U\|_{\mathbf{H}^s(\partial\omega)}.$$

Then, Problem (A.2) (and thus Problem (A.1)) can be rewritten as the surface equation

$$\Lambda_\omega U + \alpha U + \beta \Delta_\tau U = \tilde{g} \quad (\text{A.3})$$

where U is the trace of \tilde{u} on $\partial\omega$. Problems (A.2) and (A.3) are clearly equivalent in the sense that if \tilde{u} solves (A.2), then its trace on $\partial\omega$ solves (A.3) and, conversely, if U solves (A.3), then its harmonic extension defined through Λ_ω solves (A.2).

Hence, we obtain the announced result if this surface equation (A.3) admits a unique solution in $\mathbf{H}^{s+2}(\partial\omega)$ and if there exists a constant $C > 0$ such that

$$\|U\|_{\mathbf{H}^{s+2}(\partial\omega)} \leq C \|\tilde{g}\|_{\mathbf{H}^s(\partial\omega)},$$

which is proved in the following lemma. □

Lemma A.3. *The surface equation (A.3) admits a unique solution $U \in \mathbf{H}^{s+2}(\partial\omega)$ and there exists a constant $C > 0$ such that*

$$\|U\|_{\mathbf{H}^{s+2}(\partial\omega)} \leq C \|\tilde{g}\|_{\mathbf{H}^s(\partial\omega)}.$$

Proof. Let us begin by considering the simplest situation $s = -1$. Then, the variational formulation of problem (A.3) is given by

$$\int_{\partial\omega} \Lambda_\omega U \phi + \alpha \int_{\partial\omega} U \phi - \beta \int_{\partial\omega} \nabla_\tau U \cdot \nabla_\tau \phi = \int_{\partial\omega} \tilde{g} \phi \quad \forall \phi \in \mathbf{H}^1(\partial\omega).$$

Applying Lax-Milgram theorem to the bilinear form

$$a(U, V) := \int_{\partial\omega} \Lambda_\omega U V + \alpha \int_{\partial\omega} U V - \beta \int_{\partial\omega} \nabla_\tau U \cdot \nabla_\tau V,$$

we prove the existence of a unique solution of Problem (A.3) for $s = -1$ with the corresponding estimate. Indeed, the bilinear symmetric continuous form a is coercive since

$$\begin{aligned} a(U, U) &= \int_{\partial\omega} \Lambda_\omega U U + \alpha \|U\|_{\mathbf{L}^2(\partial\omega)}^2 - \beta \|\nabla_\tau U\|_{\mathbf{L}^2(\partial\omega)}^2 \\ &\geq \|\nabla \tilde{u}\|_{\mathbf{L}^2(\Omega \setminus \bar{\omega})}^2 + \alpha \|U\|_{\mathbf{L}^2(\partial\omega)}^2 - \beta \|\nabla_\tau U\|_{\mathbf{L}^2(\partial\omega)}^2 \\ &\geq c \|\tilde{u}\|_{\mathbf{H}^1(\Omega \setminus \bar{\omega})}^2 + \alpha \|U\|_{\mathbf{L}^2(\partial\omega)}^2 - \beta \|\nabla_\tau U\|_{\mathbf{L}^2(\partial\omega)}^2 \\ &\geq c \|U\|_{\mathbf{L}^2(\partial\omega)}^2 + \alpha \|U\|_{\mathbf{L}^2(\partial\omega)}^2 - \beta \|\nabla_\tau U\|_{\mathbf{L}^2(\partial\omega)}^2 \\ &\geq C \|u\|_{\mathbf{H}^1(\partial\omega)}^2, \end{aligned}$$

where $C := \min(c + \alpha, -\beta) > 0$, since $\|U\|_{\mathbf{L}^2(\partial\omega)}^2 + \|\nabla_\tau U\|_{\mathbf{L}^2(\partial\omega)}^2$ is (the square of) an equivalent norm in $\mathbf{H}^1(\partial\omega)$.

Consider now the case $s > -1$. Problem (A.3) admits a unique solution $U \in \mathbf{H}^1(\partial\omega)$ using the previous step. Moreover

$$-\Delta_\tau U + U = \frac{1}{-\beta} (\tilde{g} - \Lambda_\omega U + (-\beta - \alpha)U) \in \mathbf{H}^{\min\{s, 0\}}(\partial\omega).$$

Hence, according to Theorem A.1, $U \in \mathbf{H}^{\min\{s+2, 2\}}$. Consequently, by a bootstrap argument, we obtain $U \in \mathbf{H}^{s+2}(\partial\omega)$. The estimate is obtained using the Closed Graph Theorem since the operator

$$\mathcal{V} := \Lambda_\omega + \alpha \mathbf{I} + \beta \Delta_\tau : \mathbf{H}^{s+2}(\partial\omega) \rightarrow \mathbf{H}^s(\partial\omega)$$

is bounded and since we just proved that it is bijective.

To conclude, let us treat the case $s < -1$ by transposition. The operator \mathcal{V} continuously maps $\mathbf{H}^{s+2}(\partial\omega)$ into $\mathbf{H}^s(\partial\omega)$ for all $s \in \mathbb{R}$. Its adjoint is \mathcal{V} himself which maps $\mathbf{H}^{-s}(\partial\omega)$ into $\mathbf{H}^{-s-2}(\partial\omega)$, which is bijective according to above since $-s - 2 > -1$. Hence, we conclude as in the previous case. \square

B Shape differential calculus

In this section, we recall some elements that are useful to compute shape derivatives. For more details on the shape calculus, the reader can consult the books [16] and [21] of Delfour *et al.* and of Henrot *et al.* In the sequel Ω will denote an open bounded set of \mathbb{R}^d ($d \geq 2$) with a C^1 boundary.

B.1 Tangential differentiation

Given $h \in C^1(\partial\Omega)$, we define the tangential gradient $\nabla_\tau h$ of h by

$$\nabla_\tau h := \left(\nabla \tilde{h} - \partial_n \tilde{h} \mathbf{n} \right) \Big|_{\partial\Omega} \quad \text{on } \partial\Omega,$$

where $\tilde{h} \in C^1(\mathbb{R}^d)$ is an extension of h . It is shown that the definition does not depend on the extension. Moreover, we extend this definition by density to the functions $h \in W^{1,1}(\partial\Omega)$.

Given a vector field $\mathbf{W} \in C^1(\partial\Omega)$, we define the tangential divergence $\operatorname{div}_\tau \mathbf{W}$ of \mathbf{W} by

$$\operatorname{div}_\tau \mathbf{W} := \left(\operatorname{div} \widetilde{\mathbf{W}} - \left(\left[\widetilde{\mathbf{W}}' \right] \mathbf{n} \right) \cdot \mathbf{n} \right) \Big|_{\partial\Omega} \quad \text{on } \partial\Omega,$$

where $\widetilde{\mathbf{W}} \in C^1(\mathbb{R}^d)$ is an extension of \mathbf{W} and $\left[\widetilde{\mathbf{W}}' \right]$ is the Jacobian matrix of $\widetilde{\mathbf{W}}$. It is shown that the definition does not depend on the extension. Moreover, we extend this definition by density to the functions $\mathbf{W} \in \mathbf{W}^{1,1}(\partial\Omega)$.

Assume that Ω has a C^2 boundary. We define the Laplacian-Beltrami operator $\Delta_\tau h$ of a function $h \in W^{2,1}(\partial\Omega)$ by

$$\Delta_\tau h := \operatorname{div}_\tau(\nabla_\tau h) \quad \text{on } \partial\Omega.$$

Let $u \in H^3(\Omega)$. It is known (see for example [21, Proposition 5.4.12]) that the relation between Δ and Δ_τ is given by

$$\Delta u = \Delta_\tau u + H \partial_n u + \partial_{nn}^2 u \quad \text{on } \partial\Omega,$$

where

$$\partial_{nn}^2 u := (\mathbf{D}^2 u \mathbf{n}) \cdot \mathbf{n} = \sum_{i,j=1}^d \frac{\partial^2 u}{\partial x_i \partial x_j} n_i n_j$$

and where H is the mean curvature of $\partial\Omega$ defined by $H := \operatorname{div}_\tau \mathbf{n}$.

B.2 Shape derivative of functionals

We essentially need the result concerning the shape derivative of boundary integral that we recall here (see [21, Proposition 5.4.18]). Assume that Ω has a C^3 boundary. We consider the functional $J(\partial\Omega) = \int_{\partial\Omega} \Psi$, where Ψ belongs to $W^{2,1}(\partial\Omega)$. The shape derivative of J in an admissible perturbation direction $\mathbf{V} \in \mathbf{W}^{1,\infty}(\mathbb{R}^d)$ is given by

$$dJ(\partial\Omega, \mathbf{V}) = \int_{\partial\Omega} \Psi' + \int_{\partial\Omega} (\partial_n \Psi + H \Psi) (\mathbf{V} \cdot \mathbf{n}),$$

where Ψ' is the shape derivative of Ψ .

B.3 Shape tangential derivation

When $\partial\Omega$ is subject to a deformation, we have to define an extension of the exterior unit normal \mathbf{n} to a no variable domain. This can be done with the signed distance to $\partial\Omega$. Then, we recall an important result that we need to compute shape derivative of the least squares functional.

For $x \in \mathbb{R}^d$, we define $b(x, \partial\Omega)$ the signed distance to $\partial\Omega$ by

$$b(x, \partial\Omega) := \begin{cases} d(x, \partial\Omega) & \text{if } x \in \mathbb{R}^d \setminus \overline{\Omega} \\ 0 & \text{if } x \in \partial\Omega \\ -d(x, \partial\Omega) & \text{if } x \in \Omega. \end{cases}$$

In [21, page 198–199], it is shown that $\nabla b(x, \partial\Omega)$ is a smooth extension of the exterior unit normal \mathbf{n} . Furthermore, we have

$$\mathbf{n} = \nabla b(x, \partial\Omega)|_{\partial\Omega} \quad \text{on } \partial\Omega$$

and $D^2b = \nabla n = \nabla_\tau n$ is symmetric in a tubular neighborhood of \mathbb{R}^d . We can resume the needed result on b in the following two results.

Proposition B.1. *The shape derivative of \mathbf{n} is*

$$\mathbf{n}' = -\nabla_\tau(\mathbf{V} \cdot \mathbf{n}),$$

where \mathbf{V} represents a perturbed direction.

Proof. Since $\nabla b \cdot \nabla b = 1$, we have $(|\nabla b|^2)' = 0$, i.e. $\nabla b' \cdot \nabla b = 0$. Hence

$$\nabla b'|_{\partial\Omega} = \nabla_\tau b'|_{\partial\Omega} + (\nabla b' \cdot \mathbf{n}) \mathbf{n} = \nabla_\tau b'|_{\partial\Omega}.$$

Since $b' = -\mathbf{V} \cdot \mathbf{n}$ on $\partial\Omega$, we have $\mathbf{n}' = \nabla_\tau b'|_{\partial\Omega} = -\nabla_\tau(\mathbf{V} \cdot \mathbf{n})|_{\partial\Omega}$. □

Theorem B.2. *Given $u, \varphi \in C^2(\overline{\Omega})$, we have*

$$\partial_n(\nabla_\tau u \cdot \nabla_\tau \varphi) = \nabla_\tau(\partial_n u) \cdot \nabla_\tau \varphi + \nabla_\tau \varphi \cdot \nabla_\tau(\partial_n u) - 2D^2b \nabla_\tau u \cdot \nabla_\tau \varphi,$$

where b is the signed distance to $\partial\Omega$.

Proof. We have, on $\partial\Omega$,

$$\begin{aligned} \partial_n(\nabla_\tau u \cdot \nabla_\tau \varphi) &= \nabla(\nabla_\tau u \cdot \nabla_\tau \varphi) \cdot \mathbf{n} \\ &= \nabla(\nabla u \cdot \nabla \varphi - \partial_n u \partial_n \varphi) \cdot \mathbf{n} \\ &= D^2u \nabla \varphi \cdot \mathbf{n} + D^2\varphi \nabla u \cdot \mathbf{n} - \partial_{nn}^2 u \partial_n \varphi - \partial_{nn}^2 \varphi \partial_n u \\ &= \partial_n \varphi (D^2u \mathbf{n}) \cdot \mathbf{n} + (D^2u \nabla_\tau \varphi) \cdot \mathbf{n} + \partial_n u D^2\varphi \mathbf{n} \cdot \mathbf{n} \\ &\quad + D^2\varphi \nabla_\tau u \cdot \mathbf{n} - \partial_{nn}^2 u \partial_n \varphi - \partial_{nn}^2 \varphi \partial_n u \\ &= (D^2u \nabla_\tau \varphi) \cdot \mathbf{n} + (D^2\varphi \nabla_\tau u) \cdot \mathbf{n}. \end{aligned} \tag{B.1}$$

Moreover, since $\nabla \mathbf{n} = D^2b$, we have

$$\nabla(\nabla u \cdot \mathbf{n}) \cdot \nabla_\tau \varphi = (D^2u \mathbf{n}) \cdot \nabla_\tau \varphi + (D^2b \nabla u) \cdot \nabla_\tau \varphi$$

and since $D^2b \mathbf{n} = 0$, it comes

$$\nabla(\nabla u \cdot \mathbf{n}) \cdot \nabla_\tau \varphi = (D^2u \mathbf{n}) \cdot \nabla_\tau \varphi + (D^2b \nabla_\tau u) \cdot \nabla_\tau \varphi.$$

Hence,

$$(D^2u \nabla_\tau \varphi) \cdot \mathbf{n} = \nabla_\tau(\partial_n u) \cdot \nabla_\tau \varphi - D^2b \nabla_\tau u \cdot \nabla_\tau \varphi. \tag{B.2}$$

Reporting in (B.1), we get the announced result (since (B.2) is also valid interchanging the role of u and φ). □

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