Shape Optimization Approach to the Bernoulli Problem: A Lagrangian Formulation

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Abstract—**The exterior Bernoulli free boundary problem is reformulated into a shape optimization setting by tracking the Dirichlet data. The shape derivative of the corresponding cost functional is established through a Lagrangian formulation coupled with the velocity method. A numerical example using the traction method or H^1 gradient method is also provided.**

Index Terms—**Bernoulli free boundary problem, overdetermined boundary value problem, shape derivative, Lagrange method, minimax formulation.**

I. Introduction

THE exterior Bernoulli free boundary problem (in two dimension) is formulated as follows: given a bounded and connected domain $\omega \subset \mathbb{R}^2$ with a *fixed boundary* $\Gamma := \partial\omega$ and a constant $\lambda < 0$, one needs to find a bounded connected domain $B \subset \overline{U} \subset \mathbb{R}^2$ with a *free boundary* $\Sigma := \partial B$, containing the closure of ω, and an associated state function $u : \Omega \to \mathbb{R}$, where $\Omega = B \setminus \bar{\omega}$, such that the overdetermined conditions are satisfied:

$$\begin{cases} -\Delta u = 0 & \text{in } \Omega, \\ u = 1 & \text{on } \Gamma, \\ u = 0 & \text{on } \Sigma, \\ \partial_\nu u = \lambda & \text{on } \Sigma. \end{cases} \tag{1}$$

Here, ν is the outward unit normal vector to the free boundary Σ, and $\partial_\nu u := \partial u/\partial\nu$ is the normal derivative of u. The Bernoulli problem appears in various physical systems that arise or can be seen in electrochemical machining, potential flow in fluid mechanics, tumor growth, etc. (cf. [1], [17], [18]).

In this paper, we are concerned with the reformulation of the ill-posed system (1) into the following shape optimization setting:

$$\min_{\Sigma} J(\Sigma) = \min_{\Sigma} \frac{1}{2}\int_{\Sigma} u^2 \mathrm{d}s, \tag{2}$$

where $u = u(\Omega)$ satisfies the mixed boundary value problem

$$-\Delta u = 0 \text{ in } \Omega, \quad u = 1 \text{ on } \Gamma, \quad \partial_\nu u = \lambda \text{ on } \Sigma. \tag{3}$$

Same as in [25], we want to characterize the shape derivative of the cost functional J over Σ along a perturbation field $\mathbf{V}$. We, however, establish the expression for the shape derivative of J using an approach independent from those exhibited in [25]. The novelty of this work is the alternative rigorous computation of the shape derivative of J derived from a Lagrangian formulation coupled with the velocity method. The shape derivative $dJ(\Sigma;\mathbf{V})$ of J along the perturbation field $\mathbf{V}$ is obtained by going to the limit of $[J(\Sigma_t) - J(\Sigma)]/t$, where Σ_t is the result of perturbing the free boundary Σ through a non-autonomous perturbation field $\mathbf{V}$. Meanwhile, the idea behind the Lagrange method is to rewrite the cost function under consideration as the min-max of an appropriate Lagrangian; that is, a utility function plus the equality constraints. As a consequence, the differentiability of the cost functional is transferred to the differentiability of the Lagrangian with respect to a particular parameter, which is, in our case, the variable t. In this regard, one needs a theorem to differentiate a minimax or the saddle point of a Lagrangian with respect to a parameter. Fortunately, a very powerful tool to fulfil the task has already been established in [13]. Its application to shape sensitivity analysis, however, is not completely straightforward because it leads to the time dependence of the underlying function spaces appearing in the minimax formulation [15]. Nevertheless, two techniques can be employed to get around this difficulty: the function space parameterization and the function space embedding techniques (cf. [14, Section 10.2.2, p. 522–523 and Section 10.6]). It is worth noting that Lagrange methods have the advantage of providing the shape derivative of cost functionals without the need to compute the shape and material derivative of the states. Some recent studies examining the shape derivatives of cost functionals through Lagrangian methods were delivered in [9], [19], [20], [26], [28], and [29].

The rest of the paper is organized as follows. In the next section, we give the essentials of our present investigation. The Lagrangian formulation of the problem is formally presented in Section III. The minimax formulation is coupled with the function space parametrization and function space embedding technique so that a theorem on the differentiability of a saddle point (i.e., a minimax) of a Lagrangian functional with respect to a parameter can be applied. After computing the shape gradient, we give a concrete example in Section IV and numerically solve the problem using the traction method or H^1 gradient method. In Section V, we give a concluding remark regarding the present study.

II. Preliminaries

In this section, we give the requisites of our study. First, we give a brief discussion about the velocity method.

Let $\mathbf{V}$ be an element of $E^k = C([0, t_V); \mathscr{D}^k(\mathbb{R}^2, \mathbb{R}^2))$, for some integer $k \geq 2$ and a small real number $t_V > 0$,

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where $\mathscr{D}^k(\mathbb{R}^2, \mathbb{R}^2)$ denotes the space of k-times continuously differentiable functions with compact support contained in $\mathbb{R}^2$. The field $\mathbf{V}(t)(x) = \mathbf{V}(t, x)$, $x \in \mathbb{R}^2$, is an element of $\mathscr{D}^k(\mathbb{R}^2, \mathbb{R}^2)$ which may depend on $t \geq 0$. It generates the transformations $T_t(\mathbf{V})(X) := T_t(X) = x(t; X)$, $t \geq 0$, $X \in \mathbb{R}^2$, through the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t} x(t; X) = \mathbf{V}(t, x(t; X)), \qquad x(0; X) = X, \tag{4}$$

with the initial value X given. We denote the "transformed domain" $T_t(\mathbf{V})(\Omega)$ at $t \geq 0$ by $\Omega_t(\mathbf{V})$, or simply $\Omega_t =: T_t(\Omega)$. In this work, we shall consider annular domains Ω_t with boundary $\partial\Omega_t$, which is the union of two disjoint sets Γ_t and Σ_t, referred to as the fixed and free boundaries, respectively. The evolutions of the domain Ω are obtained using non-autonomous velocity fields

$$\mathbf{V}(t)(x) \in \mathcal{V} := \{\mathbf{V}(t, x) \in C^{1,1}([0, t_V] \times \overline{U}, \mathbb{R}^2) : \mathbf{V}|_{\Gamma \cup \partial U} = 0\}. \tag{5}$$

For $t \in [0, t_V]$, T_t is invertible and $T_t, T_t^{-1} \in \mathscr{D}^1(\mathbb{R}^2, \mathbb{R}^2)$ (cf. [7, Lemma 11], [8, Lemma 2.4]). In addition, the Jacobian I_t is strictly positive, i.e., $I_t = |\det DT_t(X)| > 0$, where $DT_t(X)$ is the Jacobian matrix of the transformation $T_t = T_t(\mathbf{V})$ associated with the velocity field $\mathbf{V}$. In this paper, the expressions $(DT_t)^{-1}$ and $(DT_t)^{-T}$ refer to the inverse and transpose of the the Jacobian matrix, respectively. Also, we use the notation $A_t = I_t(DT^{-1})(DT_t)^{-T}$, and $w_t = I_t|(DT_t)^{-T}\nu|$, where DT_t is the Jacobian matrix of T_t with respect to the boundary $\partial\Omega$.

For the rest of this section we state the essentials of our analysis.

Proposition 1: For a function $\varphi \in W^{1,1}_{loc}(\mathbb{R}^2)$ and $\mathbf{V} \in \mathcal{V}$, we have the following formulas

(i) $\nabla(\varphi \circ T_t) = (DT_t)^T(\nabla\varphi) \circ T_t$,

(ii) $\dfrac{\mathrm{d}}{\mathrm{d}t}(\varphi \circ T_t) = (\nabla\varphi \cdot \mathbf{V}(t)) \circ T_t$,

(iii) $\dfrac{\mathrm{d}}{\mathrm{d}t}(\varphi \circ T_t^{-1}) = -(\nabla\varphi \cdot \mathbf{V}(t)) \circ T_t^{-1}$,

(iv) $\dfrac{\mathrm{d}}{\mathrm{d}t} I_t = \mathrm{div}\mathbf{V}(t) \circ T_t I_t$,

(v) $w_t'|_{t=0} = \lim_{t \searrow 0} \frac{1}{t}(w_t - w_0) = \mathrm{div}_\Sigma \mathbf{V}(0)$,

where div_Σ denotes the surface divergence and is defined by

$$\mathrm{div}_\Sigma \mathbf{V}(0) = \mathrm{div}(\mathbf{V}(0)) - D\mathbf{V}(0)\nu \cdot \nu.$$

The above results can be found in [14], [31], and are given as properties of the transformation T_t in [7], [23], [25].

Lemma 1 ([31]): We have the following domain and boundary transformations:

(i) If $\varphi_t \in L^1(\Omega_t)$ then, $\varphi_t \circ T_t \in L^1(\Omega)$ and

$$\int_{\Omega_t} \varphi_t \, \mathrm{d}x_t = \int_\Omega \varphi_t \circ T_t I_t \, \mathrm{d}x.$$

(ii) If $\varphi_t \in L^1(\Sigma_t)$ then, $\varphi_t \circ T_t \in L^1(\Sigma)$ and

$$\int_{\Sigma_t} \varphi_t \, \mathrm{d}s_t = \int_{\Sigma_t} \varphi_t \circ T_t w_t \, \mathrm{d}s.$$

We are now ready to examine the shape derivative of J through a Lagrangian formulation in the next section.

III. Main Results

Minimax Formulation

In this section we established the shape derivative of J through a Lagrangian formulation. To begin with, we recall the variational form of system (3):

Find $u \in H^1(\Omega)$ such that

$$\int_\Omega \nabla u \cdot \nabla\varphi - \int_\Sigma \lambda\varphi = 0, \ \forall\varphi \in H^1_{\Gamma,0}(\Omega); \quad u = 1 \text{ on } \Gamma. \tag{6}$$

Since we have an essential boundary condition $u = 1$ on Γ, which is tied with the definition of the function space $H^1_{\Gamma,0}(\Omega)$, we introduce the Lagrangian multiplier $\mu \in H^{1/2}(\Gamma)$ and express the variational form (6) of (3) as follows

$$\int_\Omega \nabla u \cdot \nabla\varphi \, \mathrm{d}x - \int_\Sigma \lambda\varphi \, \mathrm{d}s + \int_\Gamma (u-1)\mu \, \mathrm{d}s = 0, \ \forall\varphi \in H^1_{\Gamma,0}(\Omega).$$

To express this equation in terms of just one variable, we take $\mu = \partial_\nu\varphi$ to obtain

$$\int_\Omega \nabla u \cdot \nabla\varphi \, \mathrm{d}x - \int_\Sigma \lambda\varphi \, \mathrm{d}s + \int_\Gamma (u-1)\partial_\nu\varphi \, \mathrm{d}s = 0, \ \forall\varphi \in H^1_{\Gamma,0}(\Omega).$$

Now, we introduce the functional

$$G(\Sigma, \varphi, \psi) = F(\Sigma, \varphi) + L(\Sigma, \varphi; \psi), \ \forall\varphi \in H^1(\Omega), \ \forall\psi \in H^1_{\Gamma,0}(\Omega), \tag{7}$$

where $F(\Omega, \varphi) := J(\varphi, \Sigma) = J(\Sigma)$, and $L(\Sigma, \varphi; \psi)$ is the Lagrangian functional given by

$$L(\Sigma, \varphi; \psi) = \int_\Omega \nabla\varphi \cdot \nabla\psi \, \mathrm{d}x - \int_\Sigma \lambda\psi \, \mathrm{d}s + \int_\Gamma (\varphi - 1)\partial_\nu\psi \, \mathrm{d}s.$$

Given this construction of G, one can easily check that

$$J(\Sigma) = \min_{\varphi \in H^1(\Omega)} \max_{\psi \in H^1_{\Gamma,0}(\Omega)} G(\Sigma, \varphi, \psi),$$

since

$$\max_{\psi \in H^1_{\Gamma,0}(\Omega)} G(\Sigma, \varphi, \psi) = \begin{cases} F(\Omega, \varphi), & \text{if } \varphi = u, \\ +\infty, & \text{otherwise.} \end{cases}$$

It is easily shown that the functional G is convex continuous with respect to φ and concave continuous with respect to ψ. Therefore, according to Ekeland and Temam [16], the functional G has a saddle point (u, p) if and only if (u, p) solves the following system

$$\begin{aligned} L(\Sigma, u; \varphi) &= 0, \quad \forall\varphi \in H^1_{\Gamma,0}(\Omega), \\ dF(\Sigma, u; \varphi) + dL(\Sigma, u, p; \varphi) &= 0, \quad \forall\varphi \in H^1_{\Gamma,0}(\Omega), \end{aligned}$$

or equivalently,

$$-\Delta u = 0 \text{ in } \Omega, \quad u = 1 \text{ on } \Gamma, \quad \partial_\nu u = \lambda \text{ on } \Sigma; \tag{8}$$

$$-\Delta p = 0 \text{ in } \Omega, \quad p = 0 \text{ on } \Gamma, \quad \partial_\nu p = -u \text{ on } \Sigma. \tag{9}$$

Similarly, the previous analysis holds in the transformed domain Ω_t under the action of the velocity field $\mathbf{V}$ for $t \geq 0$. Thus, we have

$$J(\Sigma_t) = \min_{\varphi \in H^1(\Omega_t)} \max_{\psi \in H^1_{\Gamma,0}(\Omega_t)} G(\Sigma_t, \varphi, \psi),$$

whose unique saddle point (u_t, p_t) is completely characterized by the system

$$\begin{aligned} L(\Sigma_t, u_t; \varphi) &= 0, \quad \forall\varphi \in H^1_{\Gamma,0}(\Omega_t), \\ dF(\Sigma_t, u_t; \varphi) + dL(\Sigma, u_t, p_t; \varphi) &= 0, \quad \forall\varphi \in H^1_{\Gamma,0}(\Omega_t), \end{aligned}$$

or equivalently,

$$\int_{\Omega_t} \nabla u_t \cdot \nabla\varphi \, \mathrm{d}x_t - \int_{\Sigma_t} \lambda\varphi \, \mathrm{d}s_t + \int_\Gamma (u_t - 1)\partial_\nu\varphi \, \mathrm{d}s = 0, \quad \forall\varphi \in H^1_{\Gamma,0}(\Omega_t); \tag{10}$$

$$\int_{\Omega_t} \nabla p_t \cdot \nabla\varphi \, \mathrm{d}x_t + \int_{\Sigma_t} u_t\varphi \, \mathrm{d}s_t = 0, \quad \forall\varphi \in H^1_{\Gamma,0}(\Omega_t). \tag{11}$$

Our next objective is to find the limit

$$dj(0) = \lim_{t \searrow 0} \frac{j(t) - j(0)}{t},$$

where

$$j(t) := J(\Sigma_t) = \min_{\varphi \in H^1(\Omega_t)} \max_{\psi \in H^1_{\Gamma,0}(\Omega_t)} G(\Sigma_t, \varphi, \psi).$$

Hereon, we need a theorem that would give the derivative of the minimax with respect to a parameter $t \geq 0$ at $t = 0$. Unfortunately, the Sobolev spaces $H^1(\Omega_t)$ and $H^1_{\Gamma,0}(\Omega_t)$ depend on the parameter t. To overcome this difficulty and obtain an infimum with respect to a function space that is independent of t, we can use two techniques [14], namely:

- Function space parametrization technique; and
- Function space embedding technique.

We will first use the idea of function space parametrization technique below, followed by the application of function space embedding technique afterwards.

Function Space Parametrization Technique

This section is devoted to the application of function space parametrization technique to the problem. It consists of transporting the quantities defined in the variable domain Ω_t back into the reference domain Ω. Once the technique is employed, the usual methods in differential calculus can now be applied since the functionals involved are now defined in a fixed domain Ω. The idea is to parametrize the functions in $H^1(\Omega_t)$ by elements of $H^1(\Omega)$ through the transformation $\varphi \mapsto \varphi \circ T_t^{-1} : H^1(\Omega) \to H^1(\Omega_t)$. Since T_t and T_t^{-1} are diffeomorphisms (cf. [7, Thm. 7]), it transforms the domain Ω into Ω_t and changes the boundary Σ to the boundary Σ_t of Ω_t. In particular, since $\mathbf{V} \in C^{1,1}$, we have $\varphi \circ T_t^{-1} \in H^1(\Omega_t)$ for all $\varphi \in H^1(\Omega)$, and conversely, $\psi \circ T_t \in H^1(\Omega)$ for all $\psi \in H^1(\Omega_t)$. Also, we introduce the parametrization $H^1_{\Gamma,0}(\Omega_t) = \{\varphi \circ T_t^{-1} : \varphi \in H^1_{\Gamma,0}(\Omega)\}$. These parametrizations do not affect the value of the minimum $J(\Sigma_t)$ but changes the Lagrangian functional G:

$$J(\Sigma_t) = \min_{\varphi \in H^1(\Omega)} \max_{\psi \in H^1_{\Gamma,0}(\Omega)} G(\Sigma_t, \varphi \circ T_t^{-1}, \psi \circ T_t^{-1}).$$

Given this formulation, we define a new Lagrangian

$$\tilde{G}(t, \varphi, \psi) := G(\Sigma_t, \varphi \circ T_t^{-1}, \psi \circ T_t^{-1}),$$

that is,

$$\begin{aligned}\tilde{G}(t, \varphi, \psi) = \frac{1}{2}\int_{\Sigma_t} (\varphi \circ T_t^{-1})^2 \,\mathrm{d}s_t \\ + \int_{\Omega_t} \nabla(\varphi \circ T_t^{-1}) \cdot \nabla(\psi \circ T_t^{-1}) \,\mathrm{d}x_t \\ - \int_{\Sigma_t} \lambda(\psi \circ T_t^{-1}) \,\mathrm{d}s_t \\ + \int_{\Gamma} (\varphi \circ T_t^{-1} - 1)\partial_\nu(\psi \circ T_t^{-1}) \,\mathrm{d}s, \qquad (12)\end{aligned}$$

for all $\varphi \in H^1(\Omega)$ and $\psi \in H^1_{\Gamma,0}(\Omega)$. The saddle point of this new Lagrangian is completely characterized by the following variational systems:

State equations. Find $u^t \in H^1(\Omega)$ such that

$$\begin{aligned}\int_{\Omega_t} \nabla(u^t \circ T_t^{-1}) \cdot \nabla(\varphi \circ T_t^{-1}) \,\mathrm{d}x_t - \int_{\Sigma_t} \lambda(\varphi \circ T_t^{-1}) \,\mathrm{d}s_t \\ + \int_{\Gamma} (u^t \circ T_t^{-1} - 1)\partial_\nu(\varphi \circ T_t^{-1}) \,\mathrm{d}s = 0, \quad \forall \varphi \in H^1_{\Gamma,0}(\Omega).\end{aligned} \qquad (13)$$

Adjoint state equations. Find $p^t \in H^1_{\Gamma,0}(\Omega)$ such that

$$\begin{aligned}\int_{\Omega_t} \nabla(p^t \circ T_t^{-1}) \cdot \nabla(\psi \circ T_t^{-1}) \,\mathrm{d}x_t \\ + \int_{\Sigma_t} (u^t \circ T_t^{-1})(\psi \circ T_t^{-1}) \,\mathrm{d}s_t = 0, \quad \forall \psi \in H^1_{\Gamma,0}(\Omega).\end{aligned} \qquad (14)$$

Remark 1: Comparing these expressions with the characterization of the minimizing element (u_t, p_t) of $G(\Sigma_t, \cdot, \cdot)$ on $H^1(\Omega_t) \times H^1_{\Gamma,0}(\Omega_t)$ which satisfies equations (10) and (11), we see that $u_t = u^t \circ T_t^{-1}$, $u^t = u_t \circ T_t$, $p_t = p^t \circ T_t^{-1}$ and $p^t = p_t \circ T_t$. So, (u^t, p^t) is actually the solution (u_t, p_t) of equations (10) and (11) in Ω_t transported back onto the fixed domain Ω by the change of variables induced by the transformation T_t.

Using the transformation T_t and Proposition 1(i), we can rewrite the Lagrangian (12) on Ω as

$$\begin{aligned}\tilde{G}(t, \varphi, \psi) = \frac{1}{2}\int_{\Sigma} w_t \varphi^2 \,\mathrm{d}s + \int_{\Omega} A_t \nabla\varphi \cdot \nabla\psi \,\mathrm{d}x \\ - \int_{\Sigma} w_t \lambda \psi \,\mathrm{d}s + \int_{\Gamma} w_t(\varphi - 1)\partial_\nu \psi \,\mathrm{d}s. \qquad (15)\end{aligned}$$

Furthermore, in view of Lemma 1, we find that the saddle point (u^t, p^t) of the above Lagrangian is, in fact, the solution of the following variational systems:

State equations. Find $u^t \in H^1(\Omega)$ such that

$$\begin{aligned}\int_{\Omega} A_t \nabla u^t \cdot \nabla\varphi \,\mathrm{d}x - \int_{\Sigma} w_t \lambda \varphi \,\mathrm{d}s \\ + \int_{\Gamma} w_t(u^t - 1)\partial_\nu \varphi \,\mathrm{d}s = 0, \forall \varphi \in H^1_{\Gamma,0}(\Omega). \qquad (16)\end{aligned}$$

Adjoint state equations. Find $p^t \in H^1_{\Gamma,0}(\Omega)$ such that

$$\int_{\Omega} A_t \nabla p^t \cdot \nabla\varphi \,\mathrm{d}x + \int_{\Sigma} w_t u^t \varphi \,\mathrm{d}s = 0, \ \forall \varphi \in H^1_{\Gamma,0}(\Omega). \quad (17)$$

Hereafter, a theorem concerning the differentiability of a minimax will come into play. In particular, we will apply Theorem 2 (see Appendix) due to [13] in order to get the first-order shape derivative of J. To do this, we need to verify the four assumptions (H1)–(H4) of the theorem.

Verification of Condition (H1). First, assume that $\mathbf{V} \in \mathcal{V}$. Choose a sufficiently small number $\tau > 0$ such that there exist two constants α_1, α_2 $(0 < \alpha_1 < \alpha_2)$, $\alpha_1 \leq I_t (= |I_t|) \leq \alpha_2$, for all $t \in [0, \tau]$ (cf. [7, Lem. 6]). So, we can find a number $\beta > 0$ such that $A_t \geq \beta I_2$ for all $t \in [0, \tau]$, where I_2 is the two-dimensional identity matrix (cf. [7, Lem. 11]). The existence and uniqueness of solution u^t of (13) is now easily verified as shown in [7, Sec. 4.2]. Meanwhile, the existence and uniqueness of solution p^t of (14) can also be shown by following a similar reasoning delivered in [7, Sec. 4.2], and by taking the test function $\varphi = p^t$ in (17). Hence,

$$\forall t \in [0, \tau]: \quad X(t) = \{u^t\} \neq \emptyset, \quad Y(t) = \{p^t\} \neq \emptyset.$$

Thus, (H1) is satisfied.

Verification of Condition (H2). The partial derivative of $\tilde{G}(t, \varphi, \psi)$ with respect to the parameter t is characterized by

$$\partial_t \tilde{G}(t, \varphi, p^t) = \frac{1}{2}\int_{\Sigma} w_t' \varphi^2 \,\mathrm{d}s + \int_{\Omega} A_t' \nabla\varphi \cdot \nabla\psi \,\mathrm{d}x - \int_{\Sigma} w_t' \lambda \psi \,\mathrm{d}s.$$

Since $\mathbf{V} \in \mathscr{D}^1(\mathbb{R}^2, \mathbb{R}^2)$, then $t \mapsto DT_t$ is continuous in $[0, \tau]$ (cf. [7, Lemma 11]). Hence, $\partial_t \tilde{G}(t, \varphi, \varphi)$ is well-defined and it exists everywhere on $[0, \tau]$, for all $\varphi \in H^1(\Omega)$ and $\psi \in H^1_{\Gamma,0}(\Omega)$. Thus, assumption (H2) is satisfied.

Verification of Conditions (H3) and (H4). We first show that for any sequence $\{t_n\} \subset [0, \tau]$, such that $t_n \to 0$, there exists a subsequence of $\{u^{t_n}, p^{t_n}\}$ (which is still denoted by $\{u^{t_n}, p^{t_n}\}$) such that $(u^{t_n}, p^{t_n}) \rightharpoonup (u^0, p^0) = (u, p)$ weakly in $H^1(\Omega) \times H^1_{\Gamma,0}(\Omega)$, where (u, p) is the solution of systems (8) and (9). To do this, we need to show that (u^t, p^t) is bounded in $H^1(\Omega) \times H^1_{\Gamma,0}(\Omega)$. In view of the discussion delivered in [7], one easily finds that u^t is bounded in $H^1(\Omega)$. Also, following a similar line of arguments laid out in [7, Section 4.2], we find that p^t is bounded in $H^1_{\Gamma,0}(\Omega)$. Hence, the pair (u^t, p^t) is bounded in $H^1(\Omega) \times H^1_{\Gamma,0}(\Omega)$, and so, there is a subsequence $\{u^{t_n}, p^{t_n}\}$ and a pair (z, q) in $H^1(\Omega) \times H^1_{\Gamma,0}(\Omega)$ such that $(u^{t_n}, p^{t_n}) \rightharpoonup (z, q)$ weakly in $H^1(\Omega) \times H^1_{\Gamma,0}(\Omega)$. The pair (z, q) can be characterized by passing to the limit in the variational equations

$$\begin{aligned}&\int_{\Omega} A_{t_n} \nabla u^{t_n} \cdot \nabla\varphi \,\mathrm{d}x - \int_{\Sigma} w_{t_n} \lambda \varphi \,\mathrm{d}s \\ &\quad + \int_{\Gamma} w_{t_n}(u^{t_n} - 1)\partial_\nu \varphi \,\mathrm{d}s = 0, \ \forall \varphi \in H^1_{\Gamma,0}(\Omega); \\ &\int_{\Omega} A_{t_n} \nabla p^{t_n} \cdot \nabla\varphi \,\mathrm{d}x + \int_{\Sigma} w_{t_n} u^{t_n} \varphi \,\mathrm{d}s = 0, \ \forall \varphi \in H^1_{\Gamma,0}(\Omega).\end{aligned}$$

By passing to the limit, (z, q) is characterized by

$$\int_\Omega \nabla z \cdot \nabla\varphi \,\mathrm{d}x - \int_\Sigma \lambda\varphi \,\mathrm{d}s + \int_\Gamma (z-1)\partial_\nu\varphi \,\mathrm{d}s = 0, \quad \forall\varphi \in H^1_{\Gamma,0}(\Omega);$$

$$\int_\Omega \nabla q \cdot \nabla\varphi \,\mathrm{d}x + \int_\Sigma z\varphi \,\mathrm{d}s = 0, \quad \forall\varphi \in H^1_{\Gamma,0}(\Omega).$$

By uniqueness $(z, q) = (u, p)$, where (u, p) is the solution to systems (13) and (14) at $t = 0$; that is, the pair (u, p) satisfies the system

$$\int_\Omega \nabla u \cdot \nabla\varphi \,\mathrm{d}x - \int_\Sigma \lambda\varphi \,\mathrm{d}s + \int_\Gamma (u-1)\partial_\nu\varphi \,\mathrm{d}s = 0, \quad \forall\varphi \in H^1_{\Gamma,0}(\Omega);$$

$$\int_\Omega \nabla p \cdot \nabla\varphi \,\mathrm{d}x + \int_\Sigma u\varphi \,\mathrm{d}s = 0, \quad \forall\varphi \in H^1_{\Gamma,0}(\Omega).$$

Furthermore, we can deduce the $H^1(\Omega) \times L^2(\Omega)$-strong convergence: $(u^{t_n}, p^{t_n}) \to (u, p)$. Hence, (H3)(i) and (H4)(i) are satisfied for the $H^2(\Omega) \times H^1(\Omega)$-strong topology by the classical regularity theorem (cf. [21]). Finally, assumptions (H3)(ii) and (H4)(ii) are readily satisfied in view of the strong continuity of $(t, \varphi, \psi) \mapsto \partial_t\tilde{G}(t, \varphi, \psi)$.

We have just shown that all of the four assumptions in Theorem 2 are satisfied, and so, we have the derivative

$$dJ(\Sigma; \mathbf{V}) = \partial_t\tilde{G}(t, u, p)|_{t=0} = \frac{1}{2}\int_\Sigma w_0' u^2 \,\mathrm{d}s + \int_\Omega A_0'\nabla u \cdot \nabla p \,\mathrm{d}x - \int_\Sigma w_0'\lambda p \,\mathrm{d}s. \tag{18}$$

Here $A_0' = A =: \mathrm{div}\mathbf{V} I_2 - (D\mathbf{V} + (D\mathbf{V})^T)$ and $w_0' = \mathrm{div}_\Sigma\mathbf{V}$. This expression for the shape derivative of J can be written in terms of the boundary integral. To do this, we recall the following result whose proof can be found in [1] (see also [7, Lem. 32] for an alternative proof).

Lemma 2: Let $\varphi, \psi \in H^2(\Omega)$, where Ω is a $C^{1,1}$-domain having the boundary $\partial\Omega = \Gamma \cup \Sigma$ ($\Gamma \cap \Sigma = \emptyset$), and $\mathbf{V}$ be a vector field belonging to $\mathcal{V}$. Then,

$$\int_\Omega A\nabla\varphi \cdot \nabla\psi \,\mathrm{d}x = \int_\Omega \Delta\varphi(\mathbf{V}\cdot\nabla\psi) \,\mathrm{d}x + \int_\Omega \Delta\psi(\mathbf{V}\cdot\nabla\varphi) \,\mathrm{d}x + \int_\Sigma (\nabla\varphi\cdot\nabla\psi)\mathbf{V}\cdot\nu \,\mathrm{d}s - \int_\Sigma \partial_\nu\varphi(\mathbf{V}\cdot\nabla\psi) \,\mathrm{d}s - \int_\Sigma \partial_\nu\psi(\mathbf{V}\cdot\nabla\varphi) \,\mathrm{d}s.$$

Taking φ and ψ as u and p in the previous lemma, and noting that they satisfy equations (8) and (9), respectively, we get

$$\begin{aligned}\int_\Omega A\nabla\varphi \cdot \nabla\psi \,\mathrm{d}x &= \int_\Sigma (\nabla u\cdot\nabla p)\mathbf{V}\cdot\nu \,\mathrm{d}s - \int_\Sigma \partial_\nu u(\mathbf{V}\cdot\nabla p) \,\mathrm{d}s - \int_\Sigma \partial_\nu p(\mathbf{V}\cdot\nabla u) \,\mathrm{d}s \\ &= \int_\Sigma (\nabla u\cdot\nabla p)\mathbf{V}\cdot\nu \,\mathrm{d}s - \int_\Sigma \lambda(\mathbf{V}\cdot\nabla p) \,\mathrm{d}s + \int_\Sigma u(\mathbf{V}\cdot\nabla u) \,\mathrm{d}s.\end{aligned}$$

However, $\nabla(u^2) = 2u\nabla u$, so

$$\int_\Omega A\nabla\varphi \cdot \nabla\psi \,\mathrm{d}x = \int_\Sigma (\nabla u\cdot\nabla p)\mathbf{V}\cdot\nu \,\mathrm{d}s - \int_\Sigma \lambda(\mathbf{V}\cdot\nabla p) \,\mathrm{d}s + \frac{1}{2}\int_\Sigma (\mathbf{V}\cdot\nabla u^2) \,\mathrm{d}s.$$

Therefore, the computed shape derivative (18) is equivalent to

$$dJ(\Sigma; \mathbf{V}) = \int_\Sigma \left[\mathbf{V}\cdot\nabla\left(\frac{1}{2}u^2 + \lambda p\right) + \left(\frac{1}{2}u^2 + \lambda p\right)\mathrm{div}_\Sigma\mathbf{V}\right] \mathrm{d}s + \int_\Sigma (\nabla u\cdot\nabla p)\mathbf{V}\cdot\nu \,\mathrm{d}s. \tag{19}$$

We further characterize the derivative $dJ(\Sigma; \mathbf{V})$. First, we note that the map $\mathcal{V} \ni \mathbf{V} \mapsto dJ(\Sigma; \mathbf{V})$ is linear and continuous (cf. [7]), and so $J(\Sigma)$ is indeed shape differentiable. Then, according to Hadamard-Zolésio structure theorem (cf. [14]), there is a scalar distribution $g \in \mathscr{D}^1(\Sigma)'$ such that $dJ(\Sigma; \mathbf{V}) = \int_\Sigma g_\Sigma \mathbf{V}\cdot\nu \mathrm{d}s$. If we assume that the boundary of Ω is a $C^{1,1}$, then we see that $(u, p) \in H^2(\Omega) \times (H^2(\Omega) \cap H^1_0(\Omega))$ (cf. [7, Thm. 29]). This regularity of the pair (u, p) implies that we can use the Hadamard's domain and boundary differentiation formulas [14]:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\{\int_{\Omega_t} F(t, x) \,\mathrm{d}x_t\right\}\bigg|_{t=0} = \int_\Omega \partial_t F(0, x) \,\mathrm{d}x + \int_{\partial\Omega} F(0, s)\mathbf{V}\cdot\nu \,\mathrm{d}s; \tag{20}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\{\int_{\partial\Omega_t} F(t, x) \,\mathrm{d}s_t\right\}\bigg|_{t=0} = \int_{\partial\Omega} \partial_t F(0, s) \,\mathrm{d}s + \int_{\partial\Omega} (\partial_\nu F + \kappa F(0, s))\mathbf{V}\cdot\nu \,\mathrm{d}s, \tag{21}$$

where $F : [0, \tau] \times \mathbb{R}^d \to \mathbb{R}$ is a sufficiently smooth functional. Thus, we can compute the partial derivative $\partial_t\tilde{G}(t, u, p)$ from the expression (12) using the above formulas. That is, we have

$$\partial_t\tilde{G}(0, u, p) = \frac{\mathrm{d}}{\mathrm{d}t}\left\{\mathbf{I}_1(t) + \mathbf{I}_2(t) + \mathbf{I}_3(t) + \mathbf{I}_4(t)\right\}\bigg|_{t=0},$$

where

$$\begin{aligned}\mathbf{I}_1(t) &= \frac{1}{2}\int_{\Sigma_t} (u\circ T_t^{-1})^2 \,\mathrm{d}s_t; \\ \mathbf{I}_2(t) &= \int_{\Omega_t} \nabla(u\circ T_t^{-1})\cdot\nabla(p\circ T_t^{-1}) \,\mathrm{d}x_t; \\ \mathbf{I}_3(t) &= \int_{\Gamma_t} (u\circ T_t^{-1} - 1)\partial_\nu(p\circ T_t^{-1}) \,\mathrm{d}s_t; \\ \mathbf{I}_4(t) &= -\int_{\Sigma_t} \lambda(p\circ T_t^{-1}) \,\mathrm{d}s_t.\end{aligned}$$

Taking into account Proposition 1(iii), the expressions for $\mathbf{I}_1'(0)$, $\mathbf{I}_2'(0)$, $\mathbf{I}_3'(0)$ and $\mathbf{I}_4'(0)$ are easily computed as follows. For the first integral, we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{I}_1(t)\bigg|_{t=0} &= \int_\Sigma \partial_t\left[\frac{1}{2}(u\circ T_t^{-1})^2\right]\bigg|_{t=0} \mathrm{d}s + \int_\Sigma \left[\partial_\nu\left(\frac{1}{2}u^2\right) + \kappa\frac{1}{2}u^2\right]\mathbf{V}\cdot\nu \,\mathrm{d}s \\ &= -\int_\Sigma u(\nabla u\cdot\mathbf{V}) \,\mathrm{d}s + \frac{1}{2}\int_\Sigma \left(\partial_\nu u^2 + \kappa u^2\right)\mathbf{V}\cdot\nu \,\mathrm{d}s.\end{aligned}$$

Meanwhile,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{I}_2(t)\bigg|_{t=0} &= \int_\Omega \partial_t\left\{\nabla(u\circ T_t^{-1})\cdot\nabla(p\circ T_t^{-1})\right\}\big|_{t=0} \,\mathrm{d}x + \int_{\partial\Omega} (\nabla u\cdot\nabla p)\mathbf{V}\cdot\nu \,\mathrm{d}s \\ &= \int_\Omega \partial_t\left\{\nabla(u\circ T_t^{-1})\right\}\big|_{t=0} \nabla p \,\mathrm{d}x + \int_\Omega \partial_t\left\{\nabla(p\circ T_t^{-1})\right\}\big|_{t=0} \nabla u \,\mathrm{d}x + \int_{\partial\Omega} (\nabla u\cdot\nabla p)\mathbf{V}\cdot\nu \,\mathrm{d}s \\ &= \int_\Omega \nabla(-\nabla u\cdot\mathbf{V})\nabla p \,\mathrm{d}x + \int_\Omega \nabla(-\nabla p\cdot\mathbf{V})\nabla u \,\mathrm{d}x + \int_{\partial\Omega} (\nabla u\cdot\nabla p)\mathbf{V}\cdot\nu \,\mathrm{d}s.\end{aligned}$$

We know by definition that the perturbation field $\mathbf{V}$ vanishes at the fixed boundary Γ, i.e., $\mathbf{V}|_\Gamma = 0$. Hence, by Green's first identity, we obtain the following simplification for $\mathbf{I}_2'(0)$:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{I}_2(t)\bigg|_{t=0} &= \int_\Omega \Delta p(\nabla u\cdot\mathbf{V})\,\mathrm{d}x - \int_\Sigma \partial_\nu p(\nabla u\cdot\mathbf{V})\,\mathrm{d}s\\ &\quad+\int_\Omega \Delta u(\nabla p\cdot\mathbf{V})\,\mathrm{d}x - \int_\Sigma \partial_\nu u(\nabla p\cdot\mathbf{V})\,\mathrm{d}s\\ &\quad+\int_{\partial\Sigma}(\nabla u\cdot\nabla p)\mathbf{V}\cdot\nu\,\mathrm{d}s.\end{aligned}$$

Note that u and p are solutions of systems (8) and (9), respectively. So,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{I}_2(t)\bigg|_{t=0} &= -\int_\Sigma p(\nabla u\cdot\mathbf{V})\,\mathrm{d}s - \int_\Sigma \lambda\nabla p\cdot\mathbf{V}\,\mathrm{d}s\\ &\quad+\int_\Sigma(\nabla u\cdot\nabla p)\mathbf{V}\cdot\nu\,\mathrm{d}s.\end{aligned}$$

For the third integral, we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{I}_3(t)\bigg|_{t=0} &= \int_\Gamma \partial_t\left[(u\circ T_t^{-1}-1)\partial_\nu(p\circ T_t^{-1})\right]\big|_{t=0}\,\mathrm{d}s\\ &\quad-\int_\Gamma\left[\partial_\nu((u-1)\partial_\nu p)+\kappa\lambda p\right]\mathbf{V}\cdot\nu\,\mathrm{d}s\\ &= -\int_\Gamma\left[\nabla u\cdot\mathbf{V}\partial_\nu p + u\nabla(\partial_\nu p)\cdot\mathbf{V}\right]\mathrm{d}s\\ &\quad-\int_\Gamma\left[\partial_\nu((u-1)\partial_\nu p)+\kappa\lambda p\right]\mathbf{V}\cdot\nu\,\mathrm{d}s.\end{aligned}$$

But $\mathbf{V}$ vanishes at Γ, so, $\mathbf{I}_3'(0)=0$.

Remark 2: The above computation of the derivative $\mathbf{I}_2'(0)$ provides an alternative proof of Lemma 2 which was proven in [7] and [25] in different ways.

Finally, for the fourth integral, we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{I}_4(t)\bigg|_{t=0} &= \frac{\mathrm{d}}{\mathrm{d}t}\left\{-\int_{\Sigma_t}\lambda(p\circ T_t^{-1})\,\mathrm{d}s_t\right\}\bigg|_{t=0}\\ &= -\int_\Sigma \partial_t\left[\lambda(p\circ T_t^{-1})\right]\big|_{t=0}\,\mathrm{d}s\\ &\quad-\int_\Sigma\left[\partial_\nu(\lambda p)+\kappa\lambda p\right]\mathbf{V}\cdot\nu\,\mathrm{d}s\\ &= \int_\Sigma \lambda\nabla p\cdot\mathbf{V}\,\mathrm{d}s - \int_\Sigma(\lambda\partial_\nu p+\kappa\lambda p)\,\mathbf{V}\cdot\nu\,\mathrm{d}s.\end{aligned}$$

Adding all these terms yields the desired expression for $dJ(\Sigma;\mathbf{V})$, that is,

$$\begin{aligned}&dJ(\Sigma;\mathbf{V})\\ &=\int_\Sigma\left[\frac{\partial}{\partial\nu}\left(\frac{1}{2}u^2-\lambda p\right)+\left(\frac{1}{2}u^2-\lambda p\right)\kappa+\nabla u\cdot\nabla p\right]\mathbf{V}\cdot\nu\,\mathrm{d}s.\end{aligned}$$

The above result can be obtained directly from (19). To see this, one simply employs the following result referred to as the tangential Green's formula (cf. [23, Lemma 3.3], [8, Lemma 2.15, Eq. 19]).

Lemma 3 (Tangential Green's formula): Let U be a bounded domain of class $C^{1,1}$ and $\Omega\subset U$ with boundary Γ. Also consider $\mathbf{V}\in C^{1,1}([0,t_V]\times\overline{U},\mathbb{R}^2)$ and $f\in W^{2,1}(U)$

$$\int_\Gamma(f\,\mathrm{div}_\Gamma\mathbf{V}\ +\nabla_\Gamma f\cdot\mathbf{V})\,\mathrm{d}s=\int_\Gamma\kappa f\mathbf{V}\cdot\nu\,\mathrm{d}s, \qquad (22)$$

where κ is the curvature of Γ and the tangential gradient ∇_Γ is given by

$$\nabla_\Gamma f=\nabla f|_\Gamma-(\partial_\nu f)\nu.$$

By using (19) and by taking $f=\frac{1}{2}u^2-\lambda p$ in equation (22), we get the same expression for the shape derivative $dJ(\Sigma;\mathbf{V})$. In summary, we have proven the following result differently from [25].

Theorem 1: Let $\Omega\subset\mathbb{R}^2$ be a $C^{1,1}$-bounded domain and consider the shape optimization problem (2) where the state function u is the solution of the mixed-boundary value problem (3). Then, the shape derivative of J at Σ in the direction of the perturbation field $\mathbf{V}\in\mathcal{V}$, where $\mathcal{V}$ is defined by (5), is given by

$$\begin{aligned}&dJ(\Sigma;\mathbf{V})\\ &=\int_\Sigma\left[\nabla\left(\frac{1}{2}u^2-\lambda p\right)\cdot\mathbf{V}+\left(\frac{1}{2}u^2-\lambda p\right)\,\mathrm{div}_\Sigma\mathbf{V}\right]\mathrm{d}s\\ &\quad+\int_\Sigma\left[(\nabla u\cdot\nabla p)\mathbf{V}\cdot\nu\right]\mathrm{d}s.\end{aligned}$$

Further, if Σ has C^2-regularity (or $\partial\Omega$ is $C^{1,1}$), then

$$\begin{aligned}&dJ(\Sigma;\mathbf{V})\\ &=\int_\Sigma\left[\frac{\partial}{\partial\nu}\left(\frac{1}{2}u^2-\lambda p\right)+\left(\frac{1}{2}u^2-\lambda p\right)\kappa\right]\mathbf{V}\cdot\nu\,\mathrm{d}s\\ &\quad+\int_\Sigma\left[\nabla u\cdot\nabla p\right]\mathbf{V}\cdot\nu\,\mathrm{d}s. \qquad (23)\end{aligned}$$

Here, the adjoint state $p\in H^1_{\Gamma,0}(\Omega)$ satisfies the variational equation

$$\int_\Omega\nabla p\cdot\nabla\psi\,\mathrm{d}x+\int_\Sigma u\psi\,\mathrm{d}s=0,$$

for all $\psi\in H^1_{\Gamma,0}(\Omega)$.

A. Function Space Embedding Technique

This section is devoted to the function space embedding technique. It means that the state and adjoint states are defined on a large enough domain D called a *hold-all* [14] which contains all the transformations $\{\Omega_t : 0\le t\le\tau\}$ of the reference domain Ω for some small enough number $\tau>0$.

Let $D=\mathbb{R}^2$. Then we differentiate with respect to t the minimax

$$J(\Sigma_t)=\min_{\Phi\in H^1(\mathbb{R}^2)}\max_{\Psi\in H^1_{\Gamma,0}(\mathbb{R}^2)}G(\Sigma_t,\Phi,\Psi),$$

where the new Lagrangian functional $G(\Sigma_t,\Phi,\Psi)$ is given by

$$\begin{aligned}G(t,\Phi,\Psi)&=\frac{1}{2}\int_{\Sigma_t}\Phi^2\,\mathrm{d}s_t+\int_{\Omega_t}\nabla\Phi\cdot\nabla\Psi\,\mathrm{d}x_t\\ &\quad-\int_{\Sigma_t}\lambda\Psi\,\mathrm{d}s_t+\int_\Gamma(\Phi-1)\partial_\nu\Psi. \qquad (24)\end{aligned}$$

For sufficiently smooth domain Ω_t (in our case $\partial\Omega_t$ is $C^{1,1}$), the unique solution (u_t,p_t) of systems (16) and (17) belongs to $H^2(\Omega_t)\times(H^2(\Omega_t)\cap H^1_{\Gamma,0}(\Omega_t))$ instead of $H^1(\Omega_t)\times H^1_{\Gamma,0}(\Omega_t)$. Therefore, the set $X\times Y\subset H^2(\mathbb{R}^2)\times H^2(\mathbb{R}^2)$ and the set of saddle points $S(t)=X(t)\times Y(t)$, which is not a singleton set anymore, are given by

$$\begin{aligned}X(t)&=\{\Phi\in H^2(\mathbb{R}^2):\Phi|_{\Omega_t}=u_t\};\\ Y(t)&=\{\Psi\in H^2(\mathbb{R}^2):\Psi|_{\Omega_t}=p_t\},\end{aligned}$$

where (u_t,p_t) is the unique solution in $H^2(\Omega_t)\times H^2(\Omega_t)$ to the saddle point equations (16) and (17).

We now verify the four assumptions of Theorem 2.

Verification of Condition (H1). Construct a linear and continuous extension $\Pi: H^2(\Omega)\to H^2(\mathbb{R}^2)$ and define an extension $\Pi_t: H^2(\Omega_t)\to H^2(\mathbb{R}^2)$, $\Pi(\phi)=[\Pi(\phi\circ T_t)]\circ T_t^{-1}$. We see that we can define the extensions $\Phi_t=\Pi_t u_t$ and $\Psi_t=\Pi_t p_t$ of u_t and p_t, respectively. So, $\Phi_t\in X(t)$ and $\Psi_t\in Y(t)$. These show the existence of a saddle point, i.e., $S(t)\neq\emptyset$. Thus, (H1) is satisfied.

Verification of Condition (H2). To check (H2), we compute the partial derivative of the expression (24) using Hadamard's formulas (20) and (21):

$$\begin{aligned}\partial_t G(t,\Phi,\Psi)&=\int_{\Sigma_t}\left(\frac{\partial}{\partial\nu}\left(\frac{1}{2}\Phi^2\right)+\frac{1}{2}\Phi^2\kappa\right)\mathbf{V}_t\cdot\nu_t\,\mathrm{d}s_t\\ &\quad+\int_{\Omega_t}(\nabla\Phi\cdot\nabla\Psi)\,\mathbf{V}_t\cdot\nu_t\,\mathrm{d}x_t\\ &\quad-\int_{\Sigma_t}\left(\frac{\partial(\lambda\Psi)}{\partial\nu}+\lambda\Psi\kappa\right)\mathbf{V}_t\cdot\nu_t\,\mathrm{d}s_t, \qquad (25)\end{aligned}$$

where ν_t denotes the outward unit normal to the boundary Σ_t. Since $\mathbf{V} \in \mathscr{D}^1(\mathbb{R}^2, \mathbb{R}^2)$, the expression $\partial_t G(t, \Phi, \Psi)$ exists everywhere in $[0, \tau]$ for all $(\Phi, \Psi) \in H^1(\mathbb{R}^2) \times H^1(\mathbb{R}^2)$. Hence (H2) is satisfied.

Verification of Conditions (H3) and (H4). For $C^{1,1}$-domain Ω and vector fields $\mathbf{V} \in \mathscr{D}^1(\mathbb{R}^2, \mathbb{R}^2)$, we have shown in Section III that (u^t, p^t) converges to (u_t, p_t) in the $H^2 \times H^1$-strong topology as t goes to zero. Hence, $\Phi_t \to \Phi = \Pi u_t$ and $\Psi_t \to \Psi = \Pi p_t$ strongly in $H^2(\mathbb{R}^2)$ by using the following lemma.

Lemma 4 ([14]): Given any integer $m \geq 1$, a velocity field $\mathbf{V} \in \mathscr{D}^m(\mathbb{R}^d, \mathbb{R}^d)$, and a function $\Pi \in H^m(\mathbb{R}^d)$, if $u^t \to u^0$ in $H^m(\Omega)$-strong, then $\Phi_t \to \Phi_0$ in $H^m(\Omega)$-strong, where $\Phi_t := (\Pi u^t) \circ T_t^{-1}$. One can also show that the above result also holds for the weak topology of $H^m(\mathbb{R}^d)$.

Furthermore, assumptions (H3)(i) and (H4)(i) are satisfied for the $H^2 \times H^2$-strong topology.

Now let us check (H3)(ii) and (H4)(ii). Since $(\Phi, \Psi) \in H^2(\mathbb{R}^2) \times H^2(\mathbb{R}^2)$, we can use Stoke's formula to rewrite (25) as

$$\begin{aligned}
&\partial_t G(t, \Phi, \Psi) \\
&= \int_{\Omega_t} \operatorname{div} \left\{ \left[\left(\frac{\partial}{\partial \nu} \left(\frac{1}{2} \Phi^2 \right) + \frac{1}{2} \Phi^2 \kappa \right) + (\nabla \Phi \cdot \nabla \Psi) \right] \mathbf{V}_t \right\} \mathrm{d}x_t \\
&\quad - \int_{\Omega_t} \operatorname{div} \left\{ \left[\left(\frac{\partial(\lambda \Psi)}{\partial \nu} + \lambda \Psi \kappa \right) \right] \mathbf{V}_t \right\} \mathrm{d}x_t \\
&=: \int_{\Omega_t} \operatorname{div}(F \mathbf{V}_t) \mathrm{d}x_t.
\end{aligned}$$

Here we have used the fact that $\partial \Omega_t = \Gamma \cup \Sigma_t$ and that $\mathbf{V}$ vanishes on the boundary Γ. Evidently, the map $(\Phi, \Psi) \mapsto F(\Phi, \Psi)$ is bilinear and continuous. Similarly, since $\mathbf{V} \in \mathscr{D}^1(\mathbb{R}^2, \mathbb{R}^2)$, the map

$$(t, F) \mapsto \int_\Omega (\operatorname{div} F \mathbf{V}_t) \circ T_t I_t \, \mathrm{d}x$$

from $[0, \tau] \times X \times Y$ to $\mathbb{R}$ is continuous. Therefore, (H3)(ii) and (H4)(ii) are verified. This completes the verification of the four assumptions of Theorem 2.

Consequently, we obtain

$$dJ(\Sigma; \mathbf{V}) = \min_{\Phi \in X(0)} \max_{\Psi \in Y(0)} \partial_t G(t, \Phi, \Psi)|_{t=0}. \tag{26}$$

Furthermore, we note that the expression (25) can be expressed in terms of a boundary integral on Σ (as shown in the previous section) which will not depend on (Φ, Ψ) outside of $\overline{\Omega}_t$. So, the inf and the sup in (26) can be dropped, giving us the same expression as in (23). This ends the computation.

IV. Numerical Example

The existence of optimal solution of the shape optimization problem (2)-(3) has already been studied in [10], and so we just carry out here a numerical realization of the optimization problem. To numerically solve the shape optimization problem, we employ an iterative algorithm based on the H^1 gradient method. This method was introduced in [3] and was then called the traction method (see also [4]). It was later on referred to as the H^1 gradient method in [5], and was compared with other techniques was described in [6]. The basic idea of the gradient method in a Hilbert space was presented in [27]. For more details of this method, we refer the readers to the aforementioned papers.

The optimization algorithm using the H^1 gradient method can be summarized as follows:

1) Define an initial domain Ω_0 with boundary $\partial \Omega_0 = \Gamma \cup \Sigma_0$, $\Gamma \cap \Sigma_0 = \emptyset$, and generate a finite element mesh on the given domain.
2) Solve the state equation (10) and the adjoint state equation (11) on the current domain Ω_0.
3) Compute the descent direction $\mathbf{V}_k$ by traction method, i.e., by solving the following PDE system
$$-\Delta \mathbf{V} + \mathbf{V} = 0 \text{ in } \Omega, \quad \mathbf{V} = 0 \text{ on } \Gamma, \quad \frac{\partial \mathbf{V}}{\partial \nu} = -G\nu \text{ on } \Sigma,$$
where G denotes the kernel of the shape gradient given in (23) with the domain $\Omega = \Omega_k$.
4) Modify the current domain by the perturbation field $\mathbf{V}_k$ to obtain a new domain. That is, define $\Omega_{k+1} := \{x + t_k \mathbf{V}_k(x) : x \in \Omega_k\}$, for sufficiently small $t_k > 0$, together with the nodal points of the mesh.
5) Repeat step 2-4 until the domain Ω_k converges.

For a concrete example of the problem, we consider the shape optimization reformulation (2)-(3) of (1) with $\lambda = -1$. That is, we consider the following optimization problem:

$$\min_\Sigma J(\Sigma) = \min_\Sigma \frac{1}{2} \int_\Sigma u^2 \mathrm{d}s$$

where the state variable u satisfies

$$-\Delta u = 0 \text{ in } \Omega, \quad u = 1 \text{ on } \Gamma, \quad \partial_\nu u = -1 \text{ on } \Sigma. \tag{27}$$

We consider a fixed boundary Γ constructed in an arrow-shape like figure, see Figure 1 (left). The free boundary is initially given by circle with radius three, see Figure 1 (right). Implementing the above algorithm in FreeFem++ (a free software for solving partial differential equation), figures Figure 1–Figure 4 were obtained.

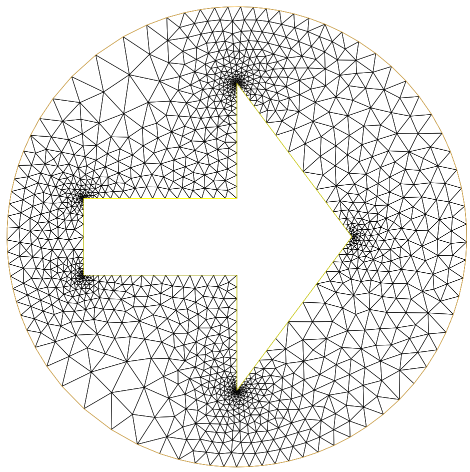

Fig. 1. Initial shape with mesh.

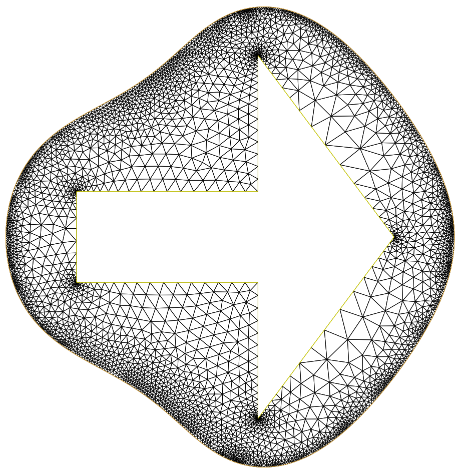

Fig. 2. Final shape with mesh.

The algorithm given above was performed in FreeFem++ with the following set-up. The step size t_k for perturbing the reference domain can be calculated through line search techniques, such as the Armijo-Goldstein line search strategy. In our implementation of the algorithm, we chose an initial step size $t_0 = 3$ and increase its value whenever the condition $J(\Omega_{k+1}) < J(\Omega_k)$ is met. Otherwise, we decrease the current step size value in half and use it for

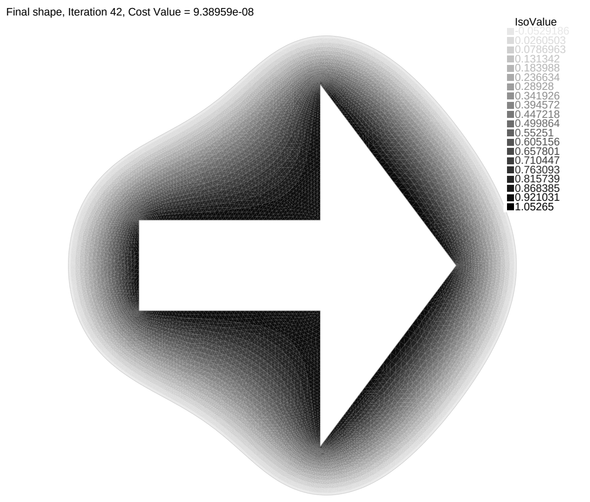

Fig. 3. State solution on final shape.

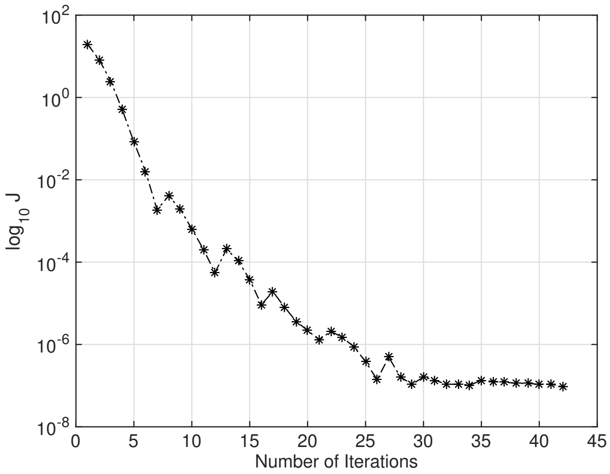

Fig. 4. Histories of the cost functional.

recalculation. Moreover, this new step size is chosen such that there are no reversed triangles within the mesh of the new domain. The iteration loop in the algorithm stops when the stopping criterion $J(\Omega_k) < 10^{-7}$ is already satisfied. This condition was met after 42 iterations with the resulting optimal shape depicted in Figure 2 with with cost value $J(\Omega_{42}) = 9 \times 10^{-8}$ as indicated in Figure 3 . The history of the cost functional values are shown in Figure 4. Notice that several fluctuations occur on the values of the cost functional as shown, for instance, in iterations 7, 8 and 9. These fluctuations occur due to the process of updating the step size t_k as described above.

V. Concluding Remark

We have successfully carried out the computation of the shape derivative of the corresponding cost functional of the tracking Dirichlet problem which is obtained through a reformulation of the exterior Bernoulli free boundary problem in a shape optimization setting. In particular, we have established the expression for the shape derivative of the cost functional through a Lagrangian formulation coupled with the velocity method. The Lagrangian is expressed as the sum of a utility function plus the equality constraints for the state variable which is actually a mixed-boundary value problem. At this juncture, we mention that another (formal) method that is often used to derive a shape derivative of a functional, which has to be used with caution because it may yield the wrong formula, is due to [12]. This method, known as *Céa's Lagrange method*, uses the same Lagrangian as the minimax formulation. However, it requires that the shape derivatives of the state and the adjoint equation exist and belong to the solution space of the PDE. Indeed, we may define $\mathcal{G}(t, \varphi, \psi) := G(\Sigma_t, \varphi, \psi)$ where G is given by (7) and assume that $\mathcal{G}$ is sufficiently differentiable with respect to t, φ and ψ. Since the strong material derivative $\dot{u}$ exists in $H^1_{\Gamma,0}(\Omega)$ (cf. [7]), then we may calculate the shape gradient as follows

$$\begin{aligned} dJ(\Sigma; \mathbf{V}) &= \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{G}(t, u^t, p)\Big|_{t=0} \\ &= \underbrace{\partial_t \mathcal{G}(t, u, p)|_{t=0}}_{\text{shape gradient}} + \underbrace{\partial_{\mathbf{u}} G(0, \mathbf{u}, \mathbf{p})[\dot{\mathbf{u}}]}_{\text{adjoint equation}}. \end{aligned}$$

The second expression on the right-hand side of the above equation vanishes due to $\dot{u} \in H^1_0(\Omega)$, and therefore we are left with $dJ(\Sigma; \mathbf{V}) = \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{G}(t, u^t, p)\big|_{t=0}$. The boundary expression of the shape derivative can be calculated without any difficulty following the line of computations in Section III. Consequently, the computed expression for the shape derivative corroborate the result in [25], and we observe that the shape derivative of the cost functional J depends on the normal component of the deformation field $\mathbf{V}$ at the free boundary Σ; that is, there exists a function g_Ω defined on the free boundary Σ such that

$$dJ(\Sigma; \mathbf{V}) = \int_\Sigma g_\Omega \mathbf{V} \cdot \nu \, \mathrm{d}s.$$

This result agrees with the Hadamard-Zolésio structure theorem (cf. [31] and [14, Remark 3.2, p. 481]). The fact that we can write the shape derivative of J in terms of a boundary integral allowed us to develop an efficient boundary variation algorithm based on the modified H^1 gradient method to numerically solve two concrete examples of the shape optimization problem (2)-(27). Even though shape optimization is, numerically, a very demanding process (cf. [11], [30]), our results show that the proposed iterative algorithm provides an (alternative) efficient numerical procedure in solving the free boundary problem through shape optimization approach.

Appendix

We first introduce some notations. Consider a functional

$$G : [0, \tau] \times X \times Y \to \mathbb{R},$$

for some $\tau > 0$ and topological spaces X and Y. For each t in $[0, \tau]$, we define

$$g(t) = \inf_{x \in X} \sup_{y \in Y} G(t, x, y) \quad \text{and} \quad h(t) = \sup_{y \in Y} \inf_{x \in X} G(t, x, y)$$

and the associated sets

$$X(t) = \left\{ \hat{x} \in X : \sup_{y \in Y} G(t, \hat{x}, y) = g(t) \right\}, \tag{28}$$

$$Y(t) = \left\{ \hat{y} \in Y : \inf_{x \in X} G(t, x, \hat{y}) = h(t) \right\}. \tag{29}$$

To complete the set of notations, we introduce the *set of saddle points*

$$S(t) = \{(\hat{x}, \hat{y}) \in X \times Y : g(t) = G(t, \hat{x}, \hat{y}) = h(t)\}, \tag{30}$$

which may be empty. In general, we always have the inequality $h(t) \le g(t)$. Further, for a fixed t in $[0, \tau]$, and for all $(x^t, y^t) = (\hat{x}, \hat{y})$ in $X(t) \times Y(t)$, $h(t) \le G(t, x^t, y^t) \le g(t)$, and when $h(t) = g(t)$, the set of saddle points $S(t)$ is exactly $X(t) \times Y(t)$.

Now, the objective of this method is to seek realistic conditions under which the existence of the limit

$$dg(0) = \lim_{t \searrow 0} \frac{g(t) - g(0)}{t}$$

is guaranteed. We are particularly interested on the situation when G admits saddle points for all t in $[0, \tau]$.

Now, we quote the improved version [14, Thm. 5.1, pp. 556–559] of the theorem of Correa and Seeger. The result also applies to situations when the state equation admits no unique solution and the Lagrangian admits saddle points. The proof of this theorem is also given in the said reference.

Theorem 2 (Correa and Seeger, [13]): Let the sets X and Y, the real number $\tau > 0$, and the functional

$$G : [0, \tau] \times X \times Y \to \mathbb{R}$$

be given. Assume that the following assumptions hold:

(H1) $S(t) \neq \emptyset$, $0 \leq t \leq \tau$;

(H2) for all $(x, y) \in [\cup\{X(t) : 0 \leq t \leq \tau\} \times Y(0)] \cup [X(t) \times \cup\{Y(t) : 0 \leq t \leq \tau\}]$, the partial derivative $\partial_t G(t, x, y)$ exists everywhere in $[0, \tau]$;

(H3) there exists a topology $\mathcal{T}_X$ on X such that for any sequence $\{t_n : 0 < t_n \leq \tau\}, t_n \to t_0 = 0$, there exist an $x^0 \in X(0)$ and a subsequence $\{t_{n_k}\}$ of $\{t_n\}$, and for each $k \geq 1$, there exists $x_{n_k} \in X(t_{n_k})$ such that

(i) $x_{n_k} \to x^0$ in the $\mathcal{T}_X$-topology, and

(ii) for all y in $Y(0)$,

$$\liminf_{\substack{t \searrow 0 \\ k \to \infty}} \partial_t G(t, x_{n_k}, y) \geq \partial_t G(0, x^0, y); \qquad (31)$$

(H4) there exists a topology $\mathcal{T}_Y$ on Y such that for any sequence $\{t_n : 0 < t_n \leq \tau\}, t_n \to t_0 = 0$, there exist $y^0 \in Y(0)$ and a subsequence $\{t_{n_k}\}$ of $\{t_n\}$, and for each $k \geq 1$, there exists $x_{n_k} \in X(t_{n_k})$ such that

(i) $y_{n_k} \to y^0$ in the $\mathcal{T}_Y$-topology, and

(ii) for all x in $X(0)$,

$$\limsup_{\substack{t \searrow 0 \\ k \to \infty}} \partial_t G(t, x, y_{n_k}) \leq \partial_t G(0, x, y^0); \qquad (32)$$

Then, there exists $(x^0, y^0) \in X(0) \times Y(0)$ such that

$$\begin{aligned} dg(0) &= \inf_{x \in X(0)} \sup_{y \in Y(0)} \partial_t G(0, x, y) = \partial_t G(0, x^0, y^0) \\ &= \sup_{y \in Y(0)} \inf_{x \in X(0)} \partial_t G(0, x, y). \end{aligned} \qquad (33)$$

Thus (x^0, y^0) is a saddle point of $\partial_t G(0, x, y)$ on $X(0) \times Y(0)$.

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