On the shape derivative for problems of Bernoulli type

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[Received 20 February 2008 and in revised form 27 November 2008]

The shape derivative of the cost functional in a Bernoulli-type problem is characterized. The calculation of the derivative of the cost does not use the shape derivative of the state variable and is achieved under mild regularity conditions on the boundary of the domain.

1. Introduction

In this note we carry out a sensitivity analysis with respect to the boundary Γ in the following shape optimization problem:

$$\min_{\Gamma} J(\Gamma) \equiv \frac{1}{2} \int_{\Gamma} \left(\frac{\partial u}{\partial n} - Q \right)^{2} d\sigma, \tag{1.1}$$

where u is the solution of the Dirichlet problem

$$-\Delta u = 0 \quad \text{on } \Omega,$$

$$u = g \quad \text{on } \Gamma_d,$$

$$u = 0 \quad \text{on } \Gamma.$$
(1.2)

Above, $\Omega \subset \mathbb{R}^2$ denotes a doubly connected, bounded domain of class $C^{1,1}$ the boundary of which consists of a fixed component Γ_d and another component Γ such that $\operatorname{dist}(\Gamma_d, \Gamma) > 0$, $Q \in \mathbb{R}$ and $g \in H^{3/2}(\Gamma_d)$.

Problems of this type arise for example in the numerical realization of Bernoulli free boundary value problems (FBVP) based on a shape optimization approach. Indeed, consider the following exterior FBVP: given a domain $\omega \subset \mathbb{R}^2$ and Q < 0 find a domain Σ with $\bar{\omega} \subset \Sigma$ and $u \colon \Sigma \setminus \bar{\omega} \to \mathbb{R}$ such that

$$-\Delta u = 0 \quad \text{on } \Sigma \setminus \bar{\omega},$$

$$u = 1 \quad \text{on } \partial \omega,$$

$$u = 0, \ \frac{\partial u}{\partial n} = Q \quad \text{on } \Gamma = \partial \Sigma.$$
(1.3)

One of the possibilities to solve (1.3) numerically is based on the following idea: since the system (1.3) is ill-posed due to the set of overdetermined boundary conditions on Γ , one of these conditions is realized in an optimization formulation. This results in an optimal shape design problem with an equality constraint involving a well posed state equation. Prescribing the Neumann data on Γ one is led to the following problem:

$$\min_{\Gamma} J(\Gamma) \equiv \frac{1}{2} \int_{\Gamma} u^2 \, d\sigma, \tag{1.4}$$

where u satisfies the mixed Dirichlet–Neumann problem

$$-\Delta u = 0 \quad \text{on } \Sigma \setminus \bar{\omega},$$

$$u = 1 \quad \text{on } \partial \omega,$$

$$\frac{\partial u}{\partial n} = Q \quad \text{on } \Gamma.$$
(1.5)

On the other hand, if the Dirichlet condition is imposed on Γ we arrive at problem (1.1) and (1.2) with $\Omega = \Sigma \setminus \bar{\omega}$, g = 1 and $\Gamma_d = \partial \omega$. The formulation (1.4) and (1.5) was used in [IKP] for the numerical realization of (1.3). The second order sensitivity analysis in [EH, EHS] reveals that the shape Hessian of J defined by (1.1) (unlike the one of (1.4)) is coercive in the corresponding energy norm, which implies the stability of the global minimizer. Another reason to prefer the formulation (1.1) and (1.2) arises from numerical considerations: since the state problem (1.2) involves only Dirichlet data on $\partial \omega \cup \Gamma$ it can be efficiently solved by an embedding domain technique based on boundary Lagrange multipliers. It can be implemented in such a way that the Lagrange multiplier represents the normal derivative $\partial u/\partial n$ on $\partial \omega \cup \Gamma$. Thus it can be used for the evaluation of (1.2) (see [HM, HKKP1]). The shape optimization approach can be used for the numerical realization of other free boundary problems of Bernoulli type. For example in [BG] the authors solved a dam problem using the cost functional (1.4). The same problem but tracking the Neumann data was considered in [HHM] using an algebraic sensitivity analysis and in [HKKP2] employing global optimization techniques for (1.1).

A formal derivation of the shape derivative of J can be found in the literature (see for example [Z]). In this paper we present a rigorous justification of the shape derivative of J with respect to Γ under what we consider minimal regularity assumptions. The technique that we employ was first suggested in [IKP] and allows one to characterize the shape derivative of the mapping $\Gamma \mapsto J(u(\Gamma))$ without recourse to the chain-rule approach. In particular, it does not involve the shape derivative of u with respect to Γ . It will be convenient to recall the main result of [IKP] without

entering the technical details. Consider a shape optimization problem of the form

$$\min J(u, \Omega, \Gamma) = \int_{\Omega} j_1(u) \, \mathrm{d}x + \int_{\Gamma} j_2(u) \, \mathrm{d}s$$
subject to $E(u, \Omega) = 0$, (1.6)

where E denotes a partial differential equation depending on a state variable u and on a reference domain Ω , and Γ stands for a codimension one manifold, which may constitute a part of the boundary of Ω or lie inside of Ω . Then the Eulerian derivative of J at Ω in the direction h is given by

$$dJ(u,\Omega,\Gamma)h = -\frac{d}{dt}\langle \tilde{E}(u,t), p\rangle \bigg|_{t=0} + \int_{\Omega} j_1(u) \operatorname{div} h \, dx + \int_{\Gamma} j_2(u) \operatorname{div}_{\Gamma} h \, ds.$$
 (1.7)

Here

$$dJ(u, \Omega, \Gamma)h = \lim_{t \to 0} \frac{1}{t} (J(u_t, \Omega_t, \Gamma_t) - J(u, \Omega, \Gamma)),$$

and $\tilde{E}(\cdot, t)$ is posed on the same reference domain Ω as E, and is related to E by means of

$$E(u_t, \Omega_t) = 0$$
 if and only if $\tilde{E}(u^t, t) = 0$,

where

$$\Omega_t = F_t(\Omega), \quad u^t = u_t \circ F_t \quad \text{and} \quad F_t = \mathrm{id} + th.$$

As already announced, the Eulerian derivative of J given in (1.7) does not depend on the shape derivative of the state. Rather it depends on the adjoint state p which is the solution of the adjoint equation

$$E_{u}^{*}(u,\Omega)p = j_{1}'(u) + \tau_{\Gamma}^{*} j_{2}'(u),$$

with τ_{Γ}^* standing for the adjoint of the trace operator onto Γ .

The regularity assumptions in [IKP] require j_i to be $C^{1,1}$ on the state space of the partial differential equation. This is not the case for the cost functional (1.1). In the present paper, however, we show that the Eulerian shape derivative of J can nevertheless be obtained using the technique developed in [IKP]. Moreover, the characterization will be accomplished under the very mild $C^{1,1}$ regularity assumption on the boundary of Ω .

Throughout the paper (\cdot, \cdot) denotes the L^2 -inner product with respect to a domain which is consistent with the context. The Euclidean product in \mathbb{R}^2 of two vectors x and y will be denoted by $x \cdot y$.

2. Continuous dependence

We embed problem (1.2) into a family of perturbed problems defined on perturbations of the reference domain Ω which are constructed by perturbing the identity. Let U be a convex bounded domain of class $C^{1,1}$ such that $\bar{\Omega} \subset U$ and let

$$\mathcal{D} = \{ V \in C^{1,1}(\bar{U}, \mathbb{R}^2) \colon V = 0 \text{ on } \partial U \cup \Gamma_d \}$$
 (2.1)

be the space of feasible deformation fields endowed with the natural norm in $C^{1,1}(\bar{U}, \mathbb{R}^2)$. Choose a fixed field $V \in \mathcal{D}$ and define for each $t \in \mathbb{R}$ the mapping $T_t : \bar{U} \to \mathbb{R}^2$ by

$$T_t = \mathrm{id} + tV. \tag{2.2}$$

Then $T_t(U) = U$ and $\{T_t\}$ is a family of $C^{1,1}$ -diffeomorphisms for |t| sufficiently small. For each $t \in \mathbb{R}$ with $|t| < \tau$ we set

$$\Omega_t = T_t(\Omega), \quad \Gamma_t = T_t(\Gamma).$$

Thus $\Omega_0 = \Omega$, $\Gamma_0 = \Gamma$, $\bar{\Omega}_t \subset U$ and $\Gamma_d = T_t(\Gamma_d)$.

The Eulerian derivative of J at Γ in the direction of the deformation field V is defined as

$$dJ(\Gamma)V = \lim_{t \to 0} \frac{1}{t} (J(\Gamma_t) - J(\Gamma)),$$

where

$$J(\Gamma_t) = \frac{1}{2} \int_{\Gamma_t} \left(\frac{\partial u_t}{\partial n_t} - Q \right)^2 d\sigma_t.$$

Above n_t stands for the outer normal unit vector to Γ_t and u_t is the solution of the perturbed Dirichlet problem

$$-\Delta u_t = 0 \quad \text{on } \Omega_t,$$

$$u_t = g \quad \text{on } \Gamma_d,$$

$$u_t = 0 \quad \text{on } \Gamma_t.$$
(2.3)

The functional J is called *shape differentiable* at Γ if $\mathrm{d}J(\Gamma)V$ exists for all $V\in\mathcal{D}$ and defines a continuous linear functional on \mathcal{D} . For an in-depth discussion of these concepts we refer to [DZ, SZ].

The variational form of (2.3) is given by:

Find $u_t \in H^1(\Omega_t)$ such that $u_t = g$ on Γ_d , $u_t = 0$ on Γ_t and

$$(\nabla u_t, \nabla v_t) = 0 \quad \text{for all } v_t \in H_0^1(\Omega_t). \tag{2.4}$$

It is known that (2.4) has a unique solution u_t which in addition satisfies $u_t \in H^2(\Omega_t)$. For t = 0 equation (2.4) represents the weak form of the reference problem (1.2). Any function $\varphi_t \colon \Omega_t \to \mathbb{R}$ can be referred to the reference domain by

$$\varphi^t = \varphi_t \circ T_t \colon \Omega \to \mathbb{R}.$$

From the chain rule it follows that the gradients of φ_t and φ^t are related by

$$\nabla \varphi_t \circ T_t = (DT_t)^{-T} \nabla \varphi^t, \tag{2.5}$$

where Df stands for the derivative of the mapping f. Let u_t denote the solution of (2.4). Then $u^t = u_t \circ T_t$ satisfies the transformed equation in Ω :

$$(A(t)\nabla u^t, \nabla \psi) = 0 (2.6)$$

for all $\psi \in H_0^1(\Omega)$, $u^t = 0$ on Γ and $u^t = g$ on Γ_d . Here and in the following we use the notation

$$I_t = \det DT_t, \quad A(t) = (DT_t)^{-1} (DT_t)^{-T} I_t, \quad w_t = I_t |(DT_t)^{-T} n|_{t}$$

where n denotes the outer normal unit vector to $\partial \Omega$ and $|\cdot|$ is the Euclidean norm of a vector in \mathbb{R}^2 or the spectral norm of a matrix in $\mathbb{R}^{2\times 2}$. By an induction argument one can prove the expansion

$$I_t(x) = 1 + t \operatorname{div} V(x) + t^2 \sum_{i=0}^{n-2} t^i f_i(DV(x)), \quad x \in \bar{U},$$
 (2.7)

with suitable polynomials f_i . This implies that for any $0 < \alpha < 1$, the inequality

$$I_t(x) \geqslant \alpha > 0, \quad x \in \bar{U},$$
 (2.8)

holds for $|t| < \tau$, with $\tau > 0$ sufficiently small. If, in addition, $\tau |DV|_{\infty} \equiv \tau \max\{|\partial_{x_j} V_i|: 1 \le i, j \le 2, x \in \bar{U}\} < 1$ then the inverse of the Jacobian DT_t can be represented by the Neumann series

$$(DT_t)^{-1} = \sum_{i=0}^{\infty} (-t)^i (DV)^i, \quad |t| < \tau,$$

which converges uniformly for $(t, x) \in [-\tau, \tau] \times \bar{U}$. For further reference we note the bound

$$|(DT_t)^{-1}|_{\infty} \leqslant \frac{1}{1 - \tau |DV|_{\infty}}.$$
 (2.9)

Let I denote the interval $[-\tau, \tau]$. Then the following regularity properties of the transformation T_t can be shown ([DZ, IKP]):

$$T_{0} = \mathrm{id}, \qquad \qquad t \mapsto T_{t} \in C^{1}(\mathbb{J}, C^{1,1}(\bar{U}, \mathbb{R}^{2})),$$

$$t \mapsto T_{t}^{-1} \in C(\mathbb{J}, C^{1}(\bar{U}, \mathbb{R}^{2})), \qquad t \mapsto I_{t} \in C^{1}(\mathbb{J}, C(\bar{U})),$$

$$t \mapsto D(T_{t})^{-T} \in C(\mathbb{J}, C(\bar{U}, \mathbb{R}^{2 \times 2})), \qquad t \mapsto w_{t} \in C(\mathbb{J}, C(\Gamma)),$$

$$\frac{\mathrm{d}}{\mathrm{d}t} T_{t} \Big|_{t=0} = V, \qquad \qquad \frac{\mathrm{d}}{\mathrm{d}t} T_{t}^{-1} \Big|_{t=0} = -V, \qquad (2.10)$$

$$\frac{\mathrm{d}}{\mathrm{d}t} D T_{t} \Big|_{t=0} = \mathrm{div} V, \qquad \qquad \frac{\mathrm{d}}{\mathrm{d}t} w_{t} \Big|_{t=0} = \mathrm{div}_{\Gamma} V.$$

The limits defining the derivatives at t = 0 exist uniformly in $x \in \bar{U}$. The surface divergence $\operatorname{div}_{\Gamma}$ is defined for $\varphi \in C^1(\bar{U}, \mathbb{R}^2)$ by

$$\operatorname{div}_{\Gamma} \varphi := \operatorname{div} \varphi|_{\Gamma} - (D\varphi \, n) \cdot n.$$

Furthermore, using (2.8) the estimate

$$(A(t)\xi,\xi) = (D(T_t)^{-T}\xi, I_t D(T_t)^{-T}\xi) \geqslant \alpha |D(T_t)^{-T}\xi|^2 \geqslant \frac{\alpha}{|D(T_t)^T|^2} |\xi|^2 \geqslant \frac{\alpha}{2} |\xi|^2$$

follows for $(\xi, x) \in \mathbb{R}^2 \times \Omega$ and τ sufficiently small, which ensures that the bilinear form in (2.6) is elliptic uniformly in $t \in \mathcal{I}$.

THEOREM 2.1 The solution u^t of equation (2.6) satisfies $u^t \in H^2(\Omega)$ for t sufficiently small. Moreover,

$$\lim_{t\to 0} \frac{1}{\sqrt{|t|}} |u^t - u|_{H^2(\Omega)} = 0,$$

where u is the weak solution of (1.2).

Proof. It suffices to show the second statement. Subtracting (2.4) with t = 0 from (2.6) one finds that $\frac{1}{t}(u^t - u)$ satisfies

$$\left(A(t)\nabla\left(\frac{1}{t}(u^t-u)\right),\nabla\psi\right)=-\left(\frac{1}{t}(A(t)-I)\nabla u,\nabla\psi\right)=\left(\operatorname{div}\left(\frac{1}{t}(A(t)-I)\nabla u\right),\psi\right)$$

for every ψ in $H^1_0(\Omega)$. Since $\frac{1}{t}(u^t-u)$ belongs to $H^1_0(\Omega)$ standard elliptic regularity theory implies $u^t-u\in H^2(\Omega)\cap H^1_0(\Omega)$ and

$$\left| \frac{1}{t} (u^t - u) \right|_{H^2(\Omega)} \le c \left| \operatorname{div} \left(\frac{1}{t} (A(t) - I) \nabla u \right) \right|_{L^2(\Omega)}$$

with a constant c > 0 which depends only on $|A(t)|_{\infty}$ and the Lipschitz constant for DV. This may be chosen independently of t (see Theorem IV-2.1 in [Ne] and the proof of Theorem 6.3.4 in [E] which is applicable to an equation on a $C^{1,1}$ -domain with $C^{0,1}$ -coefficients). The result then follows if we bound $|\frac{1}{t}D(A(t)-I)|_{\infty}$ uniformly in t. For this purpose consider any partial derivative ∂_k , k=1,2:

$$\partial_k \frac{1}{t} (A(t) - I) = \frac{1}{t} \partial_k (DT_t^{-1} - I) DT_t^{-T} I_t + \frac{1}{t} \partial_k (DT_t^{-T} - I) I_t + \frac{1}{t} \partial_k (I_t - 1) I_t$$

and observe that

$$\frac{1}{t}\partial_k(DT_t^{-1} - I) = \frac{1}{t}\partial_k(DT_t^{-1}(I - DT_t)) = -\partial_k(DT_t^{-1}DV)
= t(DT_t)^{-1}(\partial_k DV)(DT_t)^{-1}DV - DT_t^{-1}\partial_k DV.$$

By Rademacher's theorem $\partial_k DV$ exists almost everywhere in U and is bounded by the Lipschitz constant for DV. A bound uniform in t follows from (2.9). The estimate for $\partial_k \frac{1}{t}(I_t - 1)$ is similar and uses (2.7).

The above proof actually shows that the difference quotient $\frac{1}{t}|u^t - u|_{H^2(\Omega)}$ is bounded as $t \to 0$.

COROLLARY 2.1 Let u_t and u stand for the weak solution of (2.4), respectively (1.2). Then

$$\lim_{t\to 0} \frac{1}{\sqrt{|t|}} \left| \frac{\partial u_t}{\partial n_t} \circ T_t - \frac{\partial u}{\partial n} \right|_{L^2(\Gamma)} = 0.$$

Proof. Define $n^t = n_t \circ T_t$. Then

$$n^{t} = \frac{DT_{t}^{-T}n}{|DT_{t}^{-T}n|} = \frac{I_{t}}{w_{t}}DT_{t}^{-T}n$$

([DZ, Theorem 4.4]), which is meaningful because $w_t \to 1$ uniformly on Γ . As a consequence we obtain

$$\begin{split} \frac{\partial u_t}{\partial n_t} \circ T_t - \frac{\partial u}{\partial n} &= \nabla u_t \circ T_t \cdot n_t \circ T_t - \nabla u \cdot n = DT_t^{-T} \nabla u^t \cdot n^t - \nabla u \cdot n \\ &= \frac{1}{w_t} DT_t^{-T} \nabla u^t \cdot I_t DT_t^{-T} n - \nabla u \cdot n = \frac{1}{w_t} (A(t) \nabla u^t - w_t \nabla u) \cdot n \\ &= \frac{1}{w_t} \bigg((A(t) - I) \nabla u^t \cdot n + \frac{\partial}{\partial n} (u^t - u) - (w_t - 1) \frac{\partial u}{\partial n} \bigg). \end{split}$$

Now the result follows by using the differentiability of $t \mapsto A(t)$ and $t \mapsto w_t$ at t = 0, the trace theorem and Theorem 2.1.

3. Sensitivity analysis

In order to make the paper self-contained we state the main theoretical tools which will be used in the analysis below.

LEMMA 3.1 ([MS]) If $\varphi_t \in L^1(\Gamma_t)$ then $\varphi_t \circ T_t \in L^1(\Gamma)$ and

$$\int_{\Gamma_t} \varphi_t \, \mathrm{d}\sigma_t = \int_{\Gamma} \varphi_t \circ T_t \, w_t \, \mathrm{d}\sigma.$$

LEMMA 3.2 ([MS, DZ]) Let $f \in C((-\tau, \tau), W^{1,1}(U))$ and assume that $\frac{\partial f}{\partial t}(0, \cdot)$ exists in $L^1(U)$. Then

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega_t} f(t, x) \, \mathrm{d}x_t \bigg|_{t=0} = \int_{\Omega} \frac{\partial f}{\partial t}(0, x) \, \mathrm{d}x + \int_{\Gamma} f(0, x) \, V \cdot n \, \mathrm{d}\sigma.$$

LEMMA 3.3 (Tangential Green's formula) If $f \in W^{2,1}(U)$, then

$$\int_{\Gamma} (f \operatorname{div}_{\Gamma} V + \nabla_{\Gamma} f \cdot V) \, d\sigma = \int_{\Gamma} \kappa f \, V \cdot n \, d\sigma,$$

where κ denotes the curvature of Γ and the tangential gradient ∇_{Γ} is given by

$$\nabla_{\Gamma} f = \nabla f|_{\Gamma} - \frac{\partial f}{\partial n} n.$$

A proof of the tangential Green's formula can be found in [MS] (referred to as surface integration by parts formula) where it is also shown that the curvature of a $C^{1,1}$ -domain makes sense in $L^{\infty}(\Gamma)$.

Since $\Omega \in C^{1,1}$ and $g \in H^{3/2}(\Gamma_d)$, the solution u of the reference problem (1.2) belongs to $H^2(\Omega)$. Define the adjoint equation

$$-\Delta p = 0 \qquad \text{in } \Omega,$$

$$p = 0 \qquad \text{on } \Gamma_d,$$

$$p = \frac{\partial u}{\partial n} - Q \quad \text{on } \Gamma,$$
(3.1)

or equivalently

$$(\nabla p, \nabla \psi) = 0 \quad \text{for all } \psi \in H_0^1(\Omega), \tag{3.2}$$

p=0 on Γ_d and $p=\partial u/\partial n-Q$ on Γ . Since $\partial u/\partial n-Q\in H^{1/2}(\Gamma)$ equation (3.2) has a unique solution $p\in H^1(\Omega)$.

Now we turn to the shape differentiability of the cost functional (1.1).

THEOREM 3.1 Let $\Omega \in C^{1,1}$, $g \in H^{3/2}(\Gamma_d)$ and $\mathcal{D} \subset C^{1,1}(\bar{U}, \mathbb{R}^2)$ be defined by (2.1). Then the cost functional

$$J(\Gamma) = \frac{1}{2} \int_{\Gamma} \left(\frac{\partial u}{\partial n} - Q \right)^{2} d\sigma$$

is shape differentiable. For every $V \in \mathcal{D}$ its derivative in the direction V is given by

$$dJ(\Gamma)V = -\int_{\Gamma} \left(\frac{1}{2}p^2 + Qp\right) \kappa \ V \cdot n \ d\sigma - \left(\frac{\partial p}{\partial n}, \frac{\partial u}{\partial n} \ V \cdot n\right)_{\Gamma}, \tag{3.3}$$

where u and p stand for the solution of (1.2), respectively (3.2), and $\langle \cdot, \cdot \rangle_{\Gamma}$ denotes the duality pairing between $H^{-1/2}(\Gamma)$ and $H^{1/2}(\Gamma)$.

Proof. It suffices to show that the Eulerian derivative of J at Γ in the direction V can be represented in the form (3.3). Transforming the boundary integral according to Lemma 3.1 we obtain

$$J(\Gamma_t) = \frac{1}{2} \int_{\Gamma_t} \left(\frac{\partial u_t}{\partial n_t} - Q \right)^2 d\sigma_t = \frac{1}{2} \int_{\Gamma} ((\nabla u_t \cdot n_t) \circ T_t - Q)^2 w_t d\sigma.$$

In order to calculate the Eulerian derivative of J we exploit the structure of J using the identity $a^2 - b^2 = 2(a - b)b + (a - b)^2$:

$$J(\Gamma_t) - J(\Gamma) = \frac{1}{2} \int_{\Gamma} (w_t - 1) \left[\left(\frac{\partial u_t}{\partial n_t} \circ T_t - Q \right)^2 - \left(\frac{\partial u}{\partial n} - Q \right)^2 \right] d\sigma$$

$$+ \frac{1}{2} \int_{\Gamma} (w_t - 1) \left(\frac{\partial u}{\partial n} - Q \right)^2 d\sigma + \frac{1}{2} \int_{\Gamma} \left[\left(\frac{\partial u_t}{\partial n_t} \circ T_t - Q \right)^2 - \left(\frac{\partial u}{\partial n} - Q \right)^2 \right] d\sigma$$

$$= \frac{1}{2} \int_{\Gamma} (w_t - 1) \left(\frac{\partial u_t}{\partial n_t} \circ T_t - \frac{\partial u}{\partial n} \right) \left(\frac{\partial u_t}{\partial n_t} \circ T_t + \frac{\partial u}{\partial n} - 2Q \right) d\sigma$$

$$+ \frac{1}{2} \int_{\Gamma} (w_t - 1) \left(\frac{\partial u}{\partial n} - Q \right)^2 d\sigma$$

$$+ \int_{\Gamma} \left((\nabla u_t \cdot n_t) \circ T_t - \frac{\partial u}{\partial n} \right) \left(\frac{\partial u}{\partial n} - Q \right) d\sigma + \frac{1}{2} \int_{\Gamma} \left(\frac{\partial u_t}{\partial n_t} \circ T_t - \frac{\partial u}{\partial n} \right)^2 d\sigma$$

$$\equiv J_1(t) + J_2(t) + J_3(t) + J_4(t).$$

By the last equality in (2.10) and Corollary 2.1 we deduce

$$\dot{J}_1(0) = \dot{J}_4(0) = 0, \tag{3.4}$$

$$\dot{J}_2(0) = \frac{1}{2} \lim_{t \to 0} \int_{\Gamma} \frac{1}{t} (w_t - 1) \left(\frac{\partial u}{\partial n} - Q \right)^2 d\sigma = \frac{1}{2} \int_{\Gamma} \left(\frac{\partial u}{\partial n} - Q \right)^2 div_{\Gamma} V d\sigma.$$
 (3.5)

The treatment of $J_3(t)$ is more delicate. Reasoning as in the proof of Corollary 2.1 one obtains

$$\int_{\Gamma} (\nabla u_t \cdot n_t) \circ T_t \left(\frac{\partial u}{\partial n} - Q \right) d\sigma = \int_{\Gamma} A(t) \nabla u^t \cdot n \frac{1}{w_t} \left(\frac{\partial u}{\partial n} - Q \right) d\sigma,$$

which suggests writing J_3 in the following form:

$$J_3(t) = \left(\int_{\Gamma} (A(t) \nabla u^t \cdot n) \left(\frac{\partial u}{\partial n} - Q \right) d\sigma - \int_{\Gamma} \frac{\partial u}{\partial n} \left(\frac{\partial u}{\partial n} - Q \right) d\sigma \right) + \int_{\Gamma} (A(t) \nabla u^t \cdot n) \left(\frac{\partial u}{\partial n} - Q \right) (w_t^{-1} - 1) d\sigma =: J_{31}(t) + J_{32}(t).$$

Using Theorem 2.1 together with $\lim_{t\to 0} A(t) = I$ and $\lim_{t\to 0} w_t = 1$ uniformly on Γ and $J_{32}(0) = 0$ we obtain

$$\dot{J}_{32}(0) = \lim_{t \to 0} \int_{\Gamma} (A(t) - I) \nabla u^{t} \cdot n \left(\frac{\partial u}{\partial n} - Q \right) \frac{1 - w_{t}}{t w_{t}} d\sigma + \lim_{t \to 0} \int_{\Gamma} \frac{\partial u^{t}}{\partial n} \left(\frac{\partial u}{\partial n} - Q \right) \frac{1 - w_{t}}{t w_{t}} d\sigma
= - \int_{\Gamma} \frac{\partial u}{\partial n} \left(\frac{\partial u}{\partial n} - Q \right) \operatorname{div}_{\Gamma} V d\sigma.$$
(3.6)

Using the adjoint state p one can write $J_{31}(t)$ as

$$J_{31}(t) = \int_{\Gamma} A(t) \nabla u^{t} \cdot n \ p \, d\sigma - \int_{\Gamma} \frac{\partial u}{\partial n} p \, d\sigma.$$

Then Green's formula and the strong form of (2.6) imply

$$\int_{\Gamma} A(t) \nabla u^t \cdot n \ p \, d\sigma = (\operatorname{div}(A(t) \nabla u^t), \ p) + (A(t) \nabla u^t, \nabla p) = (A(t) \nabla u^t, \nabla p)$$

and analogously

$$\int_{\Gamma} \frac{\partial u}{\partial n} p \, d\sigma = (\nabla u, \nabla p).$$

From this we derive

$$J_{31}(t) = (A(t)\nabla u^t, \nabla p) - (\nabla u, \nabla p)$$

$$= (A(t)\nabla (u^t - u), \nabla p) + (A(t)\nabla u, \nabla p) - (\nabla u, \nabla p)$$

$$= ((A(t) - I)\nabla (u^t - u), \nabla p) + (\nabla (u^t - u), \nabla p) + (A(t)\nabla u, \nabla p) - (\nabla u, \nabla p)$$

$$= ((A(t) - I)\nabla (u^t - u), \nabla p) + (A(t)\nabla u, \nabla p) - (\nabla u, \nabla p),$$

where we have used the fact that $u^t - u \in H_0^1(\Omega)$ and the adjoint equation (3.2). Taking the derivative of J_{31} is complicated by the fact that p belongs to $H^1(\Omega)$ only. To overcome this difficulty we choose a sequence $(u_k)_{k=1}^{\infty} \subset C^{\infty}(\bar{\Omega})$ which approximates u in $H^2(\Omega)$ and denote by p_k the solution of the adjoint equation (3.1) with $\partial u/\partial n - Q$ replaced by $\partial u_k/\partial n - Q$. Then $p_k \in H^2(\Omega)$ and $\lim_{k\to\infty} p_k = p$ in $H^1(\Omega)$. By differentiability of $t\mapsto A(t)$ and $t\mapsto u^t$ at t=0 we find

$$\lim_{t\to 0} \left(\frac{1}{t}(A(t)-I)\nabla(u^t-u), \nabla p\right) = 0.$$

This leads to

$$\begin{split} \dot{J}_{31}(0) &= \lim_{t \to 0} \frac{1}{t} [(A(t)\nabla u, \nabla p) - (\nabla u, \nabla p)] = \lim_{t \to 0} \lim_{k \to \infty} \frac{1}{t} [(A(t)\nabla u_k, \nabla p_k) - (\nabla u_k, \nabla p_k)] \\ &= \lim_{k \to \infty} \lim_{t \to 0} \frac{1}{t} [(A(t)\nabla u_k, \nabla p_k) - (\nabla u_k, \nabla p_k)] \\ &= \lim_{k \to \infty} \frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega_t} \nabla (u_k \circ T_t^{-1}) \cdot \nabla (p_k \circ T_t^{-1}) \, \mathrm{d}x \bigg|_{t=0}. \end{split}$$

The interchange of the two limits above is justified because $\lim_{t\to 0} \frac{1}{t}(A(t)-I)$ exists uniformly in $x\in \bar{U}$. If we extend u_k and p_k to elements in $H^2(U)$, the last derivative can be calculated using Lemma 3.2 and $\frac{d}{dt}T_t^{-1}|_{t=0}=-V$:

$$\dot{J}_{31}(0) = \lim_{k \to \infty} \left[\int_{\Gamma} \nabla u_k \cdot \nabla p_k \, V \cdot n \, d\sigma + (\nabla(-\nabla u_k \cdot V), \nabla p_k) + (\nabla u_k, \nabla(-\nabla p_k \cdot V)) \right].$$

Further Green's formula combined with $\Delta p_k = 0$ in Ω and V = 0 on Γ_d leads to

$$\dot{J}_{31}(0) = \lim_{k \to \infty} \left[\int_{\Gamma} \nabla u_{k} \cdot \nabla p_{k} \, V \cdot n \, d\sigma + (\nabla u_{k} \cdot V, \Delta p_{k}) - \int_{\Gamma} \frac{\partial p_{k}}{\partial n} \nabla u_{k} \cdot V \, d\sigma \right]
+ (\Delta u_{k}, \nabla p_{k} \cdot V) - \int_{\Gamma} \frac{\partial u_{k}}{\partial n} \nabla p_{k} \cdot V \, d\sigma \right]
= \lim_{k \to \infty} \left[\int_{\Gamma} \nabla u_{k} \cdot \nabla p_{k} \, V \cdot n \, d\sigma - \int_{\Gamma} \frac{\partial p_{k}}{\partial n} \nabla u_{k} \cdot V \, d\sigma \right]
- \int_{\Gamma} \frac{\partial u_{k}}{\partial n} \nabla p_{k} \cdot V \, d\sigma + (\Delta u_{k}, \nabla p_{k} \cdot V) \right].$$
(3.7)

Collecting (3.4)–(3.7) leads to

$$\begin{split} \mathrm{d}J(\varGamma)V &= \dot{J}_1(0) + \dot{J}_2(0) + \dot{J}_3(0) + \dot{J}_4(0) \\ &= \frac{1}{2} \int_{\varGamma} \left(\frac{\partial u}{\partial n} - \mathcal{Q} \right)^2 \mathrm{div}_{\varGamma} \, V \, \mathrm{d}\sigma - \int_{\varGamma} \frac{\partial u}{\partial n} \left(\frac{\partial u}{\partial n} - \mathcal{Q} \right) \mathrm{div}_{\varGamma} \, V \, \mathrm{d}\sigma \\ &+ \lim_{k \to \infty} \left[\int_{\varGamma} \nabla u_k \cdot \nabla p_k \, V \cdot n \, \mathrm{d}\sigma - \int_{\varGamma} \frac{\partial p_k}{\partial n} \nabla u_k \cdot V \, \mathrm{d}\sigma \right. \\ &- \int_{\varGamma} \frac{\partial u_k}{\partial n} \, \nabla p_k \cdot V \, \mathrm{d}\sigma + \left(\Delta u_k, \nabla p_k \cdot V \right) \right] \\ &= \lim_{k \to \infty} \left[\frac{1}{2} \int_{\varGamma} \left(\frac{\partial u_k}{\partial n} - \mathcal{Q} \right)^2 \mathrm{div}_{\varGamma} \, V \, \mathrm{d}\sigma - \int_{\varGamma} \frac{\partial u_k}{\partial n} \left(\frac{\partial u_k}{\partial n} - \mathcal{Q} \right) \mathrm{div}_{\varGamma} \, V \, \mathrm{d}\sigma \right. \\ &+ \int_{\varGamma} \nabla u_k \cdot \nabla p_k \, V \cdot n \, \mathrm{d}\sigma - \int_{\varGamma} \frac{\partial p_k}{\partial n} \nabla u_k \cdot V \, \mathrm{d}\sigma \\ &- \int_{\varGamma} \frac{\partial u_k}{\partial n} \nabla p_k \cdot V \, \mathrm{d}\sigma + \left(\Delta u_k, \nabla p_k \cdot V \right) \right] \\ &= \lim_{k \to \infty} \left[- \int_{\varGamma} \left(\frac{1}{2} p_k^2 + \mathcal{Q} p_k \right) \mathrm{div}_{\varGamma} \, V \, \mathrm{d}\sigma + \int_{\varGamma} \nabla u_k \cdot \nabla p_k V \cdot n \, \mathrm{d}\sigma \right. \\ &- \int_{\varGamma} \frac{\partial p_k}{\partial n} \nabla u_k \cdot V \, \mathrm{d}\sigma - \int_{\varGamma} \frac{\partial u_k}{\partial n} \nabla p_k \cdot V \, \mathrm{d}\sigma \right] \end{split}$$

where we have used the equalities $p_k = \frac{\partial u_k}{\partial n} - Q$ on Γ and $\lim_{k \to \infty} \Delta u_k = 0$ in $L^2(\Omega)$ in the last step. Next we rewrite the first term using the tangential Green's formula (Lemma 3.3) and the definition of the tangential gradient $\nabla_{\Gamma} p_k$. This results in

$$\begin{split} -\int_{\Gamma} \left(\frac{1}{2} p_k^2 + Q p_k \right) \operatorname{div}_{\Gamma} V \, \mathrm{d}\sigma &= \int_{\Gamma} \nabla_{\Gamma} \left(\frac{1}{2} p_k^2 + Q p_k \right) \cdot V \, \mathrm{d}\sigma - \int_{\Gamma} \left(\frac{1}{2} p_k^2 + Q p_k \right) \kappa V \cdot n \, \mathrm{d}\sigma \\ &= \int_{\Gamma} (p_k + Q) \nabla_{\Gamma} p_k \cdot V \, \mathrm{d}\sigma - \int_{\Gamma} \left(\frac{1}{2} p_k^2 + Q p_k \right) \kappa V \cdot n \, \mathrm{d}\sigma \\ &= \int_{\Gamma} \frac{\partial u_k}{\partial n} \nabla p_k \cdot V \, \mathrm{d}\sigma - \int_{\Gamma} \frac{\partial u_k}{\partial n} \frac{\partial p_k}{\partial n} \, V \cdot n \, \mathrm{d}\sigma - \int_{\Gamma} \left(\frac{1}{2} p_k^2 + Q p_k \right) \kappa V \cdot n \, \mathrm{d}\sigma. \end{split}$$

This entails

$$dJ(\Gamma)V = \lim_{k \to \infty} \left[\int_{\Gamma} \frac{\partial u_{k}}{\partial n} \nabla p_{k} \cdot V \, d\sigma - \int_{\Gamma} \frac{\partial u_{k}}{\partial n} \frac{\partial p_{k}}{\partial n} \, V \cdot n \, d\sigma - \int_{\Gamma} \left(\frac{1}{2} \, p_{k}^{2} + Q p_{k} \right) \kappa \, V \cdot n \, d\sigma \right]$$

$$+ \int_{\Gamma} \nabla u_{k} \cdot \nabla p_{k} \, V \cdot n \, d\sigma - \int_{\Gamma} \frac{\partial p_{k}}{\partial n} \nabla u_{k} \cdot V \, d\sigma - \int_{\Gamma} \frac{\partial u_{k}}{\partial n} \nabla p_{k} \cdot V \, d\sigma \right]$$

$$= \lim_{k \to \infty} \left[-\int_{\Gamma} \left(\frac{1}{2} \, p_{k}^{2} + Q p_{k} \right) \kappa \, V \cdot n \, d\sigma - \int_{\Gamma} \frac{\partial u_{k}}{\partial n} \frac{\partial p_{k}}{\partial n} \, V \cdot n \, d\sigma \right]$$

$$+ \int_{\Gamma} \nabla u_{k} \cdot \nabla p_{k} \, V \cdot n \, d\sigma - \int_{\Gamma} \frac{\partial p_{k}}{\partial n} \nabla u_{k} \cdot V \, d\sigma \right]$$

$$= -\int_{\Gamma} \left(\frac{1}{2} \, p^{2} + Q p \right) \kappa \, V \cdot n \, d\sigma - \lim_{k \to \infty} \int_{\Gamma} \frac{\partial p_{k}}{\partial n} \frac{\partial u_{k}}{\partial n} \, V \cdot n \, d\sigma$$

$$+ \lim_{k \to \infty} \left[\int_{\Gamma} \frac{\partial u_{k}}{\partial n} \frac{\partial p_{k}}{\partial n} \, V \cdot n \, d\sigma + \int_{\Gamma} \nabla u_{k} \cdot \tau \, \nabla p_{k} \cdot \tau \, V \cdot n \, d\sigma \right]$$

$$= -\int_{\Gamma} \left(\frac{1}{2} \, p^{2} + Q p \right) \kappa \, V \cdot n \, d\sigma - \lim_{k \to \infty} \int_{\Gamma} \frac{\partial p_{k}}{\partial n} \frac{\partial u_{k}}{\partial n} \, V \cdot n \, d\sigma$$

$$+ \lim_{k \to \infty} \left[\int_{\Gamma} (\nabla p_{k} \cdot \tau) (\nabla u_{k} \cdot \tau) \, V \cdot n \, d\sigma - \int_{\Gamma} \frac{\partial p_{k}}{\partial n} (\nabla u_{k} \cdot \tau) \, V \cdot \tau \, d\sigma \right],$$

$$(3.8)$$

where τ denotes the properly oriented tangential unit vector. Since $\partial u_k/\partial n$, $\partial u/\partial n \in H^{1/2}(\Gamma)$ there exist their respective extensions $w_k, w \in H^1(\Omega)$ such that $w_k \to w$ in $H^1(\Omega)$ and the normal field $n \in C^{0,1}(\Gamma)$ can be extended to a vector field $\mathcal{N} \in C^{0,1}(\bar{\Omega})$ [GR]. Then it is readily seen that $w_k V \cdot \mathcal{N}$, $w V \cdot \mathcal{N} \in H^1(\Omega)$ and $w_k V \cdot \mathcal{N}$ converges to $w V \cdot \mathcal{N}$ in $H^1(\Omega)$ and hence $(\partial u_k/\partial n) V \cdot n$ converges to $(\partial u/\partial n) V \cdot n$ in $H^{1/2}(\Gamma)$. Since $\operatorname{div}(\nabla p_k) = \operatorname{div}(\nabla p) = 0$ in Ω , we see that ∇p_k converges to ∇p not only in $L^2(\Omega)^2$ but also in $H(\operatorname{div}, \Omega)$. Therefore the normal derivative can be extended to a bounded linear operator in $\mathcal{L}(H(\operatorname{div}, \Omega), H^{-1/2}(\Gamma))$ [GR, Theorem 2.5], enabling us to pass to the limit

$$\lim_{k \to \infty} \int_{\Gamma} \frac{\partial p_k}{\partial n} \frac{\partial u_k}{\partial n} V \cdot n \, d\sigma = \left\langle \frac{\partial p}{\partial n}, \frac{\partial u}{\partial n} V \cdot n \right\rangle_{\Gamma}.$$

Concerning the third term in (3.8) we argue similarly replacing the normal derivative by the tangential derivative in the definition of w_k . Since ∇p_k converges to ∇p also in $H(\text{curl}, \Omega)$, the tangential derivative (in \mathbb{R}^2) extends to a continuous linear operator in $\mathcal{L}(H(\text{curl}, \Omega), H^{-1/2}(\Gamma))$

[GR, Theorem 2.11]. Thus

$$\lim_{k \to \infty} \int_{\Gamma} (\nabla p_k \cdot \tau) (\nabla u_k \cdot \tau) V \cdot n \, d\sigma = \left\langle \nabla p \cdot \tau, \frac{\partial u}{\partial \tau} V \cdot n \right\rangle_{\Gamma} = 0,$$

upon making use of the boundary condition u = 0 in the last equality. Similarly one finds

$$\lim_{k \to \infty} \int_{\Gamma} \frac{\partial p_k}{\partial n} (\nabla u_k \cdot \tau) V \cdot n \, d\sigma = 0.$$

Summarizing we have shown the desired representation for the shape gradient of J:

$$dJ(\Gamma)V = -\left(\frac{\partial p}{\partial n}, \frac{\partial u}{\partial n}V \cdot n\right)_{\Gamma} - \int_{\Gamma} \left(\frac{1}{2}p^2 + Qp\right) \kappa V \cdot n \, d\sigma.$$

In the last step of the proof, the 2-dimensionality of Ω is used. In higher dimensions the representation (3.3) remains true provided that the boundary of Ω is sufficiently regular so that $u \in H^3(\Omega)$ and hence $p \in H^2(\Omega)$, in which case it is not necessary to approximate p by smoother functions p_k .

REMARK 3.1 The proof of Theorem 3.1 can be easily adapted to cover the inhomogeneous state equation

$$-\Delta u = f$$
 on Ω ,
 $u = g$ on Γ_d ,
 $u = 0$ on Γ .

Then u^t satisfies

$$(A(t)\nabla u^t, \nabla \psi) = (I_t f_t \circ T_t, \psi)$$
 for all $\psi \in H_0^1(\Omega)$,

 $u^t=0$ on Γ and $u^t=g$ on Γ_d instead of (2.6). Assuming that $f\in H^1(U)$, the shape gradient of J is then given by

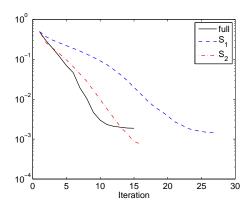
$$dJ(\Gamma)V = -\int_{\Gamma} \left(\frac{1}{2}p^2 + Qp\right) \kappa \ V \cdot n \, d\sigma - \left(\frac{\partial p}{\partial n}, \frac{\partial u}{\partial n} \ V \cdot n\right)_{\Gamma} - \int_{\Gamma} fp \ V \cdot n \, d\sigma.$$

The only changes in the proof arise in the discussion of J_{31} which has to be augmented by the term $-(I_t f_t \circ T_t - f, p)$, and in the last but one step where one has to replace $\lim_{k\to\infty} \Delta u_k = 0$ by $\lim_{k\to\infty} \Delta u_k = -f$.

4. Example

In [HKKP2] we used the analytic gradient (3.3) to solve the exterior Bernoulli problem based on the optimal shape design problem (1.1)–(1.2). The free boundary component was represented by a piecewise quadratic Bezier curve with a fixed number of Bezier arcs. For more details on the implementation and results we refer to [HKKP2]. Here we report an interesting numerical finding which is based on the observation that the shape derivative (3.3) can equivalently be written as

$$\mathrm{d}J(\Gamma)V = -\left(\frac{\partial p}{\partial n}, \frac{\partial u}{\partial n}V \cdot n\right)_{\Gamma} - \frac{1}{2} \int_{\Gamma} \left(\left(\frac{\partial u}{\partial n}\right)^{2} - Q^{2}\right) \kappa \ V \cdot n \ \mathrm{d}\sigma.$$



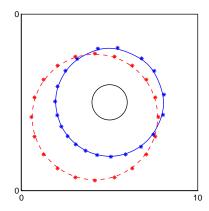


FIG. 1. Convergence history of J.

FIG. 2. Computed free boundary.

It should be noted that the second term does not depend on the adjoint variable p. This motivated us to test the "partial" gradients

$$S_1 V = -\left\langle \frac{\partial p}{\partial n}, \frac{\partial u}{\partial n} V \cdot n \right\rangle_{\Gamma}, \quad S_2 V = -\frac{1}{2} \int_{\Gamma} \left(\left(\frac{\partial u}{\partial n} \right)^2 - Q^2 \right) \kappa \ V \cdot n \, d\sigma$$

in the numerical realization of (1.1)–(1.2). Figure 1 compares the convergence history of J utilizing the full and partial gradients on a semilogarithmic scale. Figure 2 shows the computed free boundary together with the initial guess in the case of a circular fixed inner boundary with center M(5,5) and radius 1. Although it is known that for this configuration the free boundary is given by a concentric circle with radius 3, the optimization algorithm was initialized for the sake of testing by an exocentric circle. The stars indicate the position of the control nodes for the initial and final design. In Table 1 we show the average distance \bar{r} of points on the computed free boundary to M, the final value of J and the number of iterations until termination of the algorithm (in all three cases the variance for the mean radius was of the order 10^{-4}). It is noted that either gradient information—full or partial—results in a very satisfactory approximation of the free boundary. The convergence histories of J indicate that the partial gradient S_2 and the full gradient are comparable in efficiency. This behavior was not only observed in the circular case for a wide variety of initial guesses, but also in the case of an L-shaped fixed inner boundary component.

TABLE 1			
	\bar{r}	J	# iter
full	3.04	0.0018	15
S_1	3.05	0.004	27
S_2	3.04	0.00075	16

Acknowledgements

This research was supported in part by the Fonds zur Förderung der Wissenschaft und Forschung under SFB032 "Mathematical Optimization and Applications in Biomedical Sciences". The first and the third authors acknowledge the support of the project IAA100750802 of the grant agency of the Czech Republic and MSM0021620839.

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