# VARIATIONAL APPROACH TO SHAPE DERIVATIVES FOR A CLASS OF BERNOULLI PROBLEMS

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ABSTRACT. The shape derivative of a functional related to a Bernoulli problem is derived without using the the shape derivative of the state. The gradient information is combined with level set ideas in a steepest descent algorithm. Numerical examples show the feasibility of the approach.

## 1. INTRODUCTION

In this paper we consider the shape optimization problem

$$\min_{\Gamma} J(u,\Gamma) \equiv \min_{\Gamma} \frac{1}{2} \int_{\Gamma} u^2 d\,\Gamma \tag{1.1}$$

subject to the mixed boundary value problem

$$\begin{array}{rcccl} -\Delta u & = & f & \text{in} & \Omega, \\ u & = & g_d & \text{on} & \Gamma_d, \\ \frac{\partial u}{\partial n} & = & g & \text{on} & \Gamma, \end{array} \tag{1.2}$$

where the boundary $\partial\Omega$ of the domain $\Omega \subset \mathbb{R}^2$ is the disjoint union of a fixed part $\Gamma_d$ and an unknown part $\Gamma$ both with nonempty relative interior.

We shall characterize the shape derivative $\delta J(u,\Gamma)h$ of $J(u,\Gamma)$ with respect to perturbations of the domain $\Omega$ defined by a vector field $h$. Once the shape derivative is available we proceed to solve (1.1) numerically by means of a level set implementation. The shape derivative is used to update the level set equation during an iterative minimization technique and the zero-level-set of the level set function represents the desired boundary $\Gamma_d$.

The approach that we utilize for computing the shape gradient appears to differ from the commonly employed techniques. To put it into a perspective with other methods we proceed formally and consider the family of perturbed problems,

$$\begin{array}{l} \min\ \frac{1}{2} \displaystyle\int_{\Sigma_t} |u_t - z_t|^2 d\Sigma_t \\ \text{subject to}\ \ e(u_t) = 0, \ \ \text{with } u_t \in \mathcal{F}(\Omega_t). \end{array} \tag{$P_t$}$$

Here $e$ represents the equality constraints due to the partial differential equation and boundary conditions, $\mathcal{F}(\Omega_t)$ denotes a function space over $\Omega_t$, and $\Omega_t = F_t(\Omega)$, where

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$F_t\colon \Omega \to \mathbb{R}^2$ is the transformation given by $F_t(x) = x + t\, h(x)$, for $t \in \mathbb{R}$. Moreover $z_t\colon \Omega_t \to \mathbb{R}$ are given and $\Sigma_t$ are subsets of $\Omega_t$. Typically $\Sigma_t = \Omega_t$ or $\Sigma_t = \Gamma_t$ which arises in case we consider the perturbed form of (1.1) – (1.2). Henceforth, if we use no index for the variables $u, \Sigma, z$ it is understood to represent their values with $t = 0$. The most common approach for computing $\delta J(u, \Sigma)h = \lim_{t\to 0} \frac{1}{t}(J(u_t, \Sigma_t) - J(u, \Sigma))$ is based on the chain rule, i.e. $u$ is considered as a function of the domain, and the "chain rule" is applied $t \to J(u_t, \Sigma_t)$. In optimal control of partial differential equations this is referred to as the approach based on the "reduced" functional. In the present context it requires to compute the shape derivative of the cost $J$ with respect to the domain and the state $u$, followed by the shape derivative of $u$. Alternatively both the state variable $u$ and the geometric variable can be interpreted as independent variables. Then the equality constraint $e(u) = 0$ can be imposed by means of a Lagrangian approach. The associated Lagrange multiplier becomes the state variable of the adjoint equation. This technique which was investigated in [DZ1, DZ2], strongly depends on sophisticated differentiability properties of saddle point problems. Differently from the "chain rule" approach, the Lagrangian (or saddle-point) technique does not require the shape derivative of the state variable and as a consequence it has the potential of allowing the characterization of the shape gradient of the cost functional under weaker regularity assumptions.

In the technique that we employ for characterizing the gradient we again consider the state variable $u$ as a dependent variable. However, differently from the "chain rule" approach, we avoid using the strong shape derivative of the state variable. Rather the shape derivative of the state variable is only required in variational, i.e. in weak, form, allowing a characterization of the shape derivative of the cost functional under weak regularity assumptions. We next explain formally the main step of the proof for the existence of a shape derivative of the cost $J(u, \Sigma)$. The integrals on $\Sigma_t$ are transformed to a reference geometry $\Sigma$ by transforming functions $v_t$ defined on $\Sigma_t$ and $\Omega_t$ to functions $v^t$ defined on $\Sigma$ and $\Omega$ by means of $v^t = v_t \circ F_t$. Let $w_t$ denote the element which transforms the infinitesimal elements $d\Sigma$ and $d\Sigma_t$, i.e. $d\Sigma_t = w_t\, d\Sigma$. Then we have

$$
\begin{aligned}
&J(u_t, \Sigma_t) - J(u, \Sigma) = \frac{1}{2}\int_{\Sigma_t} |u_t - z_t|^2 d\Sigma_t - \frac{1}{2}\int_{\Sigma} |u - z|^2 d\Sigma \\
&= \frac{1}{2}\int_{\Sigma} [|u^t - z^t|^2 w_t - |u - z|^2] d\Sigma \\
&= \frac{1}{2}\int_{\Sigma} [(w_t - 1)(|u^t - z^t|^2 - |u - z|^2) + (w_t - 1)|u - z|^2 \\
&+ 2(u^t - u)(u - z) + |u^t - u|^2] d\Sigma = J_1(t) + J_2(t) + J_3(t) + J_4(t).
\end{aligned}
$$

Assuming that

$$\lim_{t\to 0}|u^t - z^t| = |u - z|, \quad |u^t - u|^2 \sim o(t) \tag{1.3}$$

$$\lim_{t\to 0} \tfrac{1}{t}(w_t - 1) \text{ exists} \tag{1.4}$$

$$\lim_{t\to 0} \tfrac{1}{t} \int_\Sigma (u^t - u)(u - z)d\Sigma \text{ exists,} \tag{1.5}$$

we have $\dot{J}_1(0) = \dot{J}_4(0)$ and $\lim_{t\to 0} \frac{1}{t}(J(u_t, \Sigma_t) - J(u, \Sigma))$ exists. The treatment of $J_3$ will suggest the form of the adjoint equation. On the technical level Hlder continuity of the state with exponent greater than $\frac{1}{2}$ with respect to the deformation of the shape is needed, see Proposition 3.5.

Let us turn to a brief description of the organization of this paper. The short Section 2 gives the precise problem formulation. In Section 3 we gather necessary tools from shape analysis and verify (1.3) - (1.5) in a precisely defined sense for problem (1.1) - (1.2). The existence of a shape derivative and its analytic expression are proven in Section 4. In Section 5 a level set approach, its implementation and numerical examples are described. The proofs of some technical results used in Section 3 are postponed to an Appendix.

## 2. Formulation of the problem

Consider the shape optimization problem

$$\min_\Gamma J(u,\Gamma) \equiv \min_\Gamma \frac{1}{2}\int_\Gamma u^2 \, d\Gamma \tag{2.1}$$

subject to the mixed boundary value problem

$$\begin{aligned} -\Delta u &= f, && \text{in } \Omega, \\ u &= u_d, && \text{on } \Gamma_d, \\ \frac{\partial u}{\partial n} &= g, && \text{on } \Gamma, \end{aligned} \tag{2.2}$$

where the boundary $\partial\Omega$ is the disjoint union of a fixed part $\Gamma_d$ and an unknown part $\Gamma$ both being nonempty and such that $\operatorname{dist}(\Gamma_d, \Gamma) > 0$. We assume that there is a fixed convex bounded open set $U \subset \mathbb{R}^2$ such that $\bar{\Omega} \subset U$. We require $u_d \in H^{3/2}(\Gamma_d)$, $f \in H^s(U)$, $s > \frac{1}{2}$ and that $g$ is the trace on $\Gamma$ of a given function $G \in H^2(U)$. Furthermore we assume that the shape optimization problem (2.1) – (2.2) has a solution which is smooth enough to ensure $\Omega \in C^{1,1}$. The class of feasible boundaries $\Gamma$ will be described below.

The optimization problem (2.1), (2.2) arises for example in free boundary problems of Bernoulli type: Find $(u, \Gamma)$ such that

$$
\begin{aligned}
-\Delta u &= f, && \text{in } \Omega, \\
u &= u_d, && \text{on } \Gamma_d, \\
u = 0 \quad \text{and} \quad \frac{\partial u}{\partial n} &= g && \text{on } \Gamma,
\end{aligned}
\tag{2.3}
$$

Note, that a solution $(u, \Gamma)$ of (2.3) provides a global minimizer for (2.1) corresponding to vanishing cost. Conversely, if there exists an optimal shape such that $J(u, \Gamma) = 0$, any such optimum determines a solution of (2.3).

Let us define the Hilbertspace

$$
H^1_{\Gamma_{d,0}}(\Omega) = \{\varphi \in H^1(\Omega) \colon \varphi|_{\Gamma_d} = 0\}
\tag{2.4}
$$

endowed with the norm

$$
|\varphi|_1 = (\nabla\varphi, \nabla\varphi)_\Omega^{1/2},
$$

where $(\cdot, \cdot)_S$ denotes the inner product in $L^2(S)$ for any measurable set $S$. Similarly, we define for $v \in H^{1/2}(\Gamma_d)$ the linear manifold

$$
H^1_{\Gamma_{d,v}}(\Omega) = \{\varphi \in H^1(\Omega) \colon \varphi|_{\Gamma_d} = v\}.
$$

It is known that (2.2) has a unique solution $u \in H^1_{\Gamma_{d,u_d}}(\Omega)$ which can be characterized by the variational equation

$$
(\nabla u, \nabla\varphi)_\Omega - (f, \varphi)_\Omega - (g, \varphi)_\Gamma = 0
\tag{2.5}
$$

for all $\varphi \in H^1_{\Gamma_{d,0}}(\Omega)$.

The objective of this paper is to calculate directly the shape derivative of the cost functional in (2.1) at a domain $\Omega \in C^{1,1}$ with respect to the boundary shape $\Gamma$ *without* taking the shape derivative of $u$. The admissible set of free boundaries is described by a particular class of perturbations of the domain $\Omega$. Let $\mathcal{H}$ denote the set

$$
\mathcal{H} = \{h \in C^{1,1}(\bar{U})^2 \colon h|_{\Gamma_d} = 0\}
\tag{2.6}
$$

and define for each $h \in \mathcal{H}$ and $t \in \mathbb{R}$ the transformation $F_t \colon \bar{\Omega} \to \mathbb{R}^2$

$$
F_t(x) = x + th(x).
\tag{2.7}
$$

One can verify that $F_t$ is injective for $|t| < t_h^{-1}$, $t_h = \max\{|Dh(x)| \colon x \in \bar{U}\}$ and defines a $C^{1,1}$–diffeomorphism from $\Omega$ onto $\Omega_t \equiv F_t(\Omega)$. For such $t$ one obtains $\Omega_t \in C^{1,1}$ and $\bar{\Omega}_t \subset U$. The boundary $\partial\Omega_t$ is the disjoint union of $\Gamma_d$ and $\Gamma_t \equiv F_t(\Gamma)$.

The Eulerian derivative of the cost functional $J$ in (2.1) at $\Omega$ in the direction of the vector field $h$ is defined as

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

where $u_t \in H^1_{\Gamma, u_d}(\Omega_t)$ satisfies

$$
(\nabla u_t, \nabla\varphi_t)_{\Omega_t} - (f, \varphi_t)_{\Omega_t} - (g, \varphi_t)_{\Gamma_t} = 0
\tag{2.8}
$$

for all $\varphi_t \in H^1_{\Gamma_{d,0}}(\Omega_t)$. The Eulerian derivative is called shape derivative if $\delta J(u,\Gamma)h$ exists for all $h \in \mathcal{H}$ and the mapping $h \to \delta J(u,\Gamma)h$ is linear and continuous with respect to the topology of $C^{1,1}(\bar\Omega)^2$.

In the discussion below we shall frequently use the notation

$$\varphi^t = \varphi \circ F_t. \tag{2.9}$$

We also introduce the unit outward normal vector $n$ and the unit tangential vector $\tau$

$$n = \begin{pmatrix} n_1 \\ n_2 \end{pmatrix} \qquad \text{and} \qquad \tau = \begin{pmatrix} -n_2 \\ n_1 \end{pmatrix}. \tag{2.10}$$

The tangential vector is oriented such that $\Omega$ lies on the left of $\tau$.

## 3. Analysis of the state equation on the perturbed domain

In this section we utilize the method of mapping to compare the solution $u_t$ of (2.8) to the solution $u$ of (2.5). We shall use $c$ to indicate a generic positive constant which may depend on the geometry of $\Omega$ and the choice of the vector field $h$ but is independent of $t$. We recall from [SZ] the following transformation theorems:

**Lemma 3.1.** *1) Let $\varphi_t \in L^1(\Omega_t)$ then $\varphi_t \circ F_t \in L^1(\Omega)$ and*

$$\int_{\Omega_t} \varphi_t \, dx_t = \int_{\Omega} \varphi_t \circ F_t \, \det DF_t \, dx.$$

*2) Let $h_t \in L^1(\Gamma_t)$ then $h_t \circ F_t \in L^1(\Gamma)$ and*

$$\int_{\Gamma_t} h_t \, d\Gamma_t = \int_{\Gamma} h_t \circ F_t \, \det DF_t \, |(DF_t)^{-T} n| \, d\Gamma.$$

In the formulation of the transformation formula for volume integrals we used $\det DF_t(x) > 0$ on $\Omega$ for $|t|$ sufficiently small. A proof of the transformation theorem for surface integrals will be given in the Appendix.

Above we have used the abbreviation $(DF_t)^{-T} = ((DF_t)^T)^{-1}$. The following notation simplifies the discussion below.

$$\begin{aligned} I_t(x) &= \det DF_t(x), \\ A_t(x) &= (DF_t(x))^{-1}(DF_t(x))^{-T} \, I_t(x), \qquad x \in \bar\Omega \\ w_t(x) &= I_t(x) \, |(DF_t(x))^{-T} n(x)|, \qquad x \in \Gamma \end{aligned} \tag{3.1}$$

We collect some useful properties of the functions defined in (3.1):

**Lemma 3.2.** *Consider a fixed vector field $h \in \mathcal{H}$ and let the transformation $F_t$ be defined by* (2.7)*. Then there is $t_h > 0$ such that the functions defined in* (3.1) *restricted to $\mathcal{J} = (-t_h, t_h)$ have following regularity*

$$\begin{aligned} t &\to F_t \in C^1(\mathcal{J}, C^1(\bar\Omega)), &\qquad t &\to F_t^{-1} \in C(\mathcal{J}, C^1(\bar U)), \\ t &\to I_t \in C^1(\mathcal{J}, C(\bar\Omega)), &\qquad t &\to A_t \in C^1(\mathcal{J}, C(\bar\Omega)), \\ t &\to w_t \in C^1(\mathcal{J}, C(\bar\Gamma)), \end{aligned}$$

*and the properties listed below:*

(1) $I_t = 1 + t \operatorname{div} h + t^2 \det Dh$,
(2) *There are positive constants* $\alpha_0$, $\alpha_1$ *and* $\beta$ *such that* $0 < \alpha_0 \leq I_t(x) \leq \alpha_1$ *and* $A_t(x) \geq \beta I$ *for* $x \in \Omega$,
(3) $\frac{d}{dt} F_t|_{t=0} = h$,
(4) $\frac{d}{dt} DF_t|_{t=0} = Dh$ *and* $\frac{d}{dt}(DF_t)^{-1}|_{t=0} = -Dh$,
(5) $\frac{d}{dt} I_t|_{t=0} = \operatorname{div} h$,
(6) $\frac{d}{dt} A_t|_{t=0} = \operatorname{div} h I - (Dh + (Dh)^T) \equiv A$,
(7) $\lim_{t\to 0} w_t = 1$ *and* $\frac{d}{dt} w_t|_{t=0} = \operatorname{div}_\Gamma h$,

*where the surface divergence* $\operatorname{div}_\Gamma$ *is defined by*

$$\operatorname{div}_\Gamma h = \operatorname{div} h|_\Gamma - (Dh\, n)\cdot n.$$

In particular the difference quotients defining the above derivatives with respect to $t$ exist uniformly in $x \in \Omega$ respectively $x \in \Gamma$.

**Lemma 3.3** ([Ne])**.** *For* $h \in \mathcal{H}$ *we have* $\varphi_t \in H^1(\Omega_t)$ *if and only if* $\varphi^t = \varphi_t \circ F_t \in H^1(\Omega)$. *Moreover the following inequality holds*

$$|\varphi^t|_{H^1(\Omega)} \leq \frac{1 + |t_h|\,|Dh|_\infty}{\sqrt{\alpha_0}}\,|\varphi_t|_{H^1(\Omega_t)}$$

In particular if $\varphi_t = \varphi|_{\Omega_t}$ for some $\varphi \in H^1(U)$ we have

$$|\varphi_t \circ F_t|_{H^1(\Omega)} \leq c|\varphi|_{H^1(U)}.$$

**Lemma 3.4.** *For any* $f \in L^p(U)$, $p \geq 1$, *we have* $\lim_{t\to 0} f\circ F_t = f$ *in* $L^p(\Omega)$.

*Proof.* For $\varepsilon > 0$ choose $f_\varepsilon \in C^1(\bar{U})$ such that $|f - f_\varepsilon|_{L^p(U)} < \varepsilon$. Using Lemma 3.1 and the uniform continuity of $f_\varepsilon$ on $\bar{U}$ one obtains the estimates

$$|f\circ F_t - f_\varepsilon \circ F_t|_{L^p(\Omega)} \leq \frac{1}{\alpha_0^{1/p}} |f - f_\varepsilon|_{L^p(U)}$$
$$|f_\varepsilon \circ F_t - f_\varepsilon|_{L^p(\Omega)} \leq \varepsilon |\Omega|^{1/p},$$

the last one of which holds for all $t$ sufficiently small. Then the claim follows from

$$\begin{aligned}|f\circ F_t - f|_{L^p(\Omega)} &\leq |f\circ F_t - f_\varepsilon\circ F_t|_{L^p(\Omega)} + |f_\varepsilon\circ F_t - f_\varepsilon|_{L^p(\Omega)} + |f_\varepsilon - f|_{L^p(\Omega)} \\ &\leq \frac{1}{\alpha_0^{1/p}}|f - f_\varepsilon|_{L^p(U)} + \varepsilon|\Omega|^{1/p} + \varepsilon.\end{aligned}$$

□

**Lemma 3.5.** *Let* $\varphi \in W^{2,p}(U)$, $p \geq 1$. *Then the mapping* $t \to \varphi\circ F_t$ *from* $\mathcal{J} \to W^{1,p}(\Omega)$ *is differentiable at* $t = 0$ *and the derivative is given by*

$$\lim_{t\to 0} \frac{1}{t}(\varphi\circ F_t - \varphi) = D\varphi\, h.$$

*Proof.* At first we establish the expansion in $L^p(\Omega)$

$$\varphi\circ F_t(x) - \varphi(x) = t\int_0^1 D\varphi(x + sth(x))h(x)\,ds. \tag{3.2}$$

Choose any $\varphi_\varepsilon \in C^1(\bar U)$ such that $|\varphi - \varphi_\varepsilon|_{W^{1,p}(U)} < \varepsilon$. Then (3.2) follows from the estimate

$$|\varphi\circ F_t - \varphi - t\int_0^1 D\varphi(\cdot + sth)h\,ds|_{L^p(\Omega)}$$
$$\leq |\varphi\circ F_t - \varphi_\varepsilon\circ F_t|_{L^p(\Omega)} + |\varphi_\varepsilon - \varphi|_{L^p(\Omega)} + |\varphi_\varepsilon\circ F_t - \varphi_\varepsilon - t\int_0^1 D\varphi_\varepsilon(\cdot + sth)|\,ds|_{L^p(\Omega)}|h|_\infty$$
$$+ |t\int_0^1 |D\varphi_\varepsilon(\cdot + sth) - D\varphi(\cdot + sth)|\,ds|_{L^p(\Omega)}|h|\infty.$$

As a consequence of (3.2) one obtains

$$\int_\Omega |\frac{1}{t}(\varphi\circ F_t(x) - \varphi(x)) - D\varphi(x)h(x)|^p dx$$
$$= \int_\Omega |\int_0^1 D\varphi(x + sth(x))h(x)\,ds - D\varphi(x)h(x)|^p dx$$
$$\leq \int_\Omega\int_0^1 |D\varphi(x + sth(x)) - D\varphi(x)|^p|h(x)|^p\,dsdx$$

which invoking Lemma 3.4 and the Lebesgue dominated convergence theorem ensures the differentiability of $t \to \varphi\circ F_t$ at $t = 0$ with respect to the topology of $L^p(\Omega)$.

Since by Lemma 3.3 the lefthand side of (3.2) defines a function in $W^{1,p}(\Omega)$ the same regularity holds for the righthand side. We show that its distributional derivative for fixed $t \in J$ is determined by

$$D\int_0^1 D\varphi(\cdot + sth)h\,ds = \int_0^1 [h^T D^2\varphi(\cdot + sth)(I + stDh) + D\varphi(\cdot + sth)Dh]\,ds. \tag{3.3}$$

Choose $\chi \in \mathcal{D}(\Omega)$. Then using Fubini's theorem and integrating by parts the distributional partial derivative $\frac{\partial}{\partial x_i}$ is given by

$$\langle\frac{\partial}{\partial x_i}\int_0^1 D\varphi(\cdot + sth)h\,ds, \chi\rangle = -\int_\Omega\int_0^1 D\varphi(x + sth(x))h(x)\,ds\,\frac{\partial}{\partial x_i}\chi(x)\,dx$$
$$= -\int_0^1\int_\Omega D\varphi(x + sth(x))h(x)\frac{\partial}{\partial x_i}\chi(x)\,dxds$$
$$= \int_0^1\int_\Omega [\sum_{k=1}^2\sum_{j=1}^2 \frac{\partial^2}{\partial x_k\partial x_j}\varphi(x + sth(x))(\delta_{ij} + st\frac{\partial}{\partial x_i}h_j(x))h_k(x)$$

$$
\begin{aligned}
&+\sum_{k=1}^{2}\frac{\partial\varphi}{\partial x_k}(x+sth(x))\frac{\partial}{\partial x_i}h_k(x)\big]\,\chi(x)\,dxds\\
&=\int_0^1\int_\Omega\big[h^T(x)D^2\varphi(x+sth(x))(I+stDh(x))_i\\
&\quad+D\varphi(x+sth(x))(Dh(x))_i\big]\chi(x)\,dxds\\
&=\int_\Omega\int_0^1\big[h^T(x)D^2\varphi(x+sth(x))(I+stDh(x))_i\\
&\quad+D\varphi(x+sth(x))(Dh(x))_i\big]\,ds\chi(x)\,dx.
\end{aligned}
$$

Note that (3.3) is valid also for $t=0$. As a consequence we obtain

$$
\begin{aligned}
&|D(\frac{1}{t}(\varphi\circ F_t-\varphi)-D(D\varphi h))|^p_{L^p(\Omega)}\\
&\quad\le\int_\Omega\int_0^1|h^T(x)\big[D^2\varphi(x+sth(x))(I+stDh(x))-D^2\varphi(x)\big]|^p dsdx\\
&\quad\quad+\int_\Omega\int_0^1|\big(D\varphi(x+sth(x))-D\varphi(x)\big)Dh(x)|^p dsdx.
\end{aligned}
$$

Now the proof of the lemma follows using the smoothness of $\varphi$ and Lemma 3.4. $\square$

**Corollary 3.1.** *Let $\varphi\in H^1(U)$. Then the mapping $t\to I_t\,\varphi\circ F_t$ from $J$ to $L^2(\Omega)$ is differentiable at $t=0$ and the derivative is given by*

$$\lim_{t\to 0}\frac{1}{t}(I_t\,\varphi\circ F_t-\varphi)=\operatorname{div}(\varphi h).$$

*Proof.* The result is a consequence of

$$\frac{1}{t}(I_t\,\varphi\circ F_t-\varphi)=\frac{1}{t}((I_t-1)\varphi^t+\frac{1}{t}(\varphi^t-\varphi)\underset{t\to 0}{\to}\varphi\operatorname{div}h+D\varphi\,h=\operatorname{div}(h\varphi).$$

$\square$

The Sobolev embedding theorem ([Ne, Theorem II.5.5]) implies the following corollary.

**Corollary 3.2.** *Let $\varphi\in W^{2,p}(U)$, $p>1$. Then the mapping $t\to\varphi\circ F_t|_\Gamma$ from $J$ to $W^{1-1/p,p}(\Gamma)$ is differentiable at $t=0$.*

**Corollary 3.3.** *Let $\varphi\in H^2(U)$. Then the map $t\to w_t\,\varphi\circ F_t|_\Gamma$ from $J$ to $H^{1/2}(\Gamma)$ is differentiable at $t=0$ and the derivative is given by*

$$\lim_{t\to 0}\frac{1}{t}(w_t\,\varphi\circ F_t-\varphi)=\varphi\operatorname{div}_\Gamma h+D\varphi\,h.$$

*Proof.* The result follows from Lemma 3.2, 3.5

$$\frac{1}{t}(w_t\varphi\circ F_t-\varphi)=\frac{1}{t}((w_t-1)\varphi^t+\frac{1}{t}(\varphi^t-\varphi)\underset{t\to 0}{\to}\varphi\operatorname{div}h+D\varphi\cdot h$$

and the trace theorem. □

For $p = 2$ in particular we infer the differentiability of $t \to \varphi \circ F_t$ at $t = 0$ in $L^q(\Gamma)$ for arbitrary $q \geq 1$ from the continuous embedding of $H^{1/2}(\Gamma)$ into $L^q(\Gamma)$.

Now we turn to the discussion of equation (2.8). It can be shown that $u^t = u_t \circ F_t$ satisfies

$$(A_t \nabla u^t, \nabla \varphi)_\Omega - (I_t f^t, \varphi)_\Omega - (w_t g^t, \varphi)_\Gamma = 0 \tag{3.4}$$

for all $\varphi \in H^1_{\Gamma_d,0}(\Omega)$. Above we have set $f^t = f \circ F_t$.

In fact, the chain rule for $u_t = u^t \circ F_t^{-1}$ entails

$$Du_t = Du^t \circ F_t^{-1}(DF_t^{-1}) = Du^t \circ F_t^{-1}(DF_t \circ F_t^{-1})^{-1} = (Du^t(DF_t)^{-1}) \circ F_t^{-1}$$

which by Lemma 3.1 implies

$$\begin{aligned}
(\nabla u_t, \nabla \psi_t)_{\Omega_t} &= \int_{\Omega_t} (Du_t)(x_t)\,(D\psi_t)^T(x_t)\,dx_t \\
&= \int_{\Omega_t} (Du^t(DF_t)^{-1}) \circ F_t^{-1}(x_t)\,(D\psi^t(DF_t)^{-1})^T \circ F_t^{-1}(x_t)\,dx_t \\
&= \int_\Omega Du^t(DF_t)^{-1}\,(D\psi^t(DF_t)^{-1})^T I_t(x)\,dx \\
&= \int_\Omega Du^t(DF_t)^{-1}(DF_t)^{-T} I_t (D\psi^t)^T\,dx = (A_t \nabla u^t, \nabla \psi^t)_\Omega.
\end{aligned}$$

Apply Lemma 3.1 to obtain

$$(f, \psi_t)_{\Omega_t} = \int_{\Omega_t} f(x_t)\psi_t(x_t)\,dx_t = \int_\Omega f \circ F_t \psi^t I_t\,dx = (I_t f^t, \psi^t)_\Omega$$

and

$$(g, \psi_t)_{\Gamma_t} = \int_{\Gamma_t} g \circ F_t \psi^t w_t\,d\Gamma = (w_t g^t, \psi^t)_\Gamma.$$

Hence (2.8) is transformed into

$$(A_t \nabla u^t, \nabla \psi^t)_\Omega - (I_t f^t, \psi^t)_\Omega - (w_t g^t, \psi^t)_\Gamma = 0$$

for all $\psi^t \in H^1_{\Gamma_d,0}(\Omega)$. Now, the result follows from Lemma 3.3.

**Proposition 3.1.** *The solutions $u^t$ of equation* (3.4) *are uniformly bounded in $H^1(\Omega)$ for $t \in J$. Moreover,*

$$\lim_{t \to 0^+} \frac{1}{\sqrt{t}} |(u^t - u)|_{H^1(\Omega)} = 0 \tag{3.5}$$

*holds, where $u$ is the solution of* (2.5).

*Proof.* The uniform positivity of $A_t(x)$ for $x \in \Omega$ and (3.4) imply the estimate

$$\begin{aligned}\beta|u^t|_1^2 &\le (A_t\nabla u^t, \nabla u^t)_\Omega = (I_t f^t, u^t)_\Omega + (w_t g^t, u^t)_\Gamma \\ &\le |I_t f^t|_{L^2(\Omega)}|u^t|_{L^2(\Omega)} + |w_t g^t|_{L^2(\Gamma)}|u^t|_{L^2(\Gamma)} \\ &\le c\,(|I_t f^t|_{L^2(\Omega)} + |w_t g^t|_{L^2(\Gamma)})|u^t|_1,\end{aligned}$$

where $c$ depends on the embedding constant of $H^1(\Omega)$ into $L^2(\partial\Omega)$ and the constant appearing in the equivalence of $|\cdot|_1$ and the full $H^1$ norm, but is independent of $t$. The following calculation

$$|I_t f^t|^2_{L^2(\Omega)} = \int_\Omega (I_t \circ F_t^{-1})\circ F_t(x) f^2 \circ F_t(x)\, I_t(x)\, dx = \int_{\Omega_t} I_t \circ F_t^{-1}\, f^2\, dx \le \alpha_1 |f|^2_{L^2(U)}$$

entails the bound

$$|I_t f^t|^2_{L^2(\Omega)} \le \alpha_1 |f|^2_{L^2(U)}.$$

Concerning $|w_t g^t|_{L^2(\Gamma)}$ one argues

$$|w_t g^t|_{L^2(\Gamma)} \le \omega |g \circ F_t|_{L^2(\Gamma)} \le \omega c\, |G \circ F_t|_{H^1(\Omega)} \le \omega c |G|_{H^1(U)},$$

with $\omega = \max_{x\in\bar\Gamma} |w_t(x)|$, and where the last inequality follows by Lemma 3.3. Summarizing we obtain the a priori estimate

$$|u^t|_1 \le c\,(|f|_{L^2(U)} + |G|_{H^1(U)}).$$

In order to prove (3.5) subtract (2.5) from (3.4) to obtain for $\chi \in H^1_{\Gamma_{d,0}}(\Omega)$

$$\begin{aligned}(\nabla(u^t - u), \nabla\chi)_\Omega &= -((A_t - I)\nabla u^t, \nabla\chi)_\Omega + (A_t \nabla u^t, \nabla\chi)_\Omega - (\nabla u, \nabla\chi)_\Omega \\ &= -((A_t - I)\nabla u^t, \nabla\chi)_\Omega + (I_t f^t - f, \chi)_\Omega + (w_t g^t - g, \chi)_\Gamma.\end{aligned}$$

Since $u^t - u \in H^1_{\Gamma_{d,0}}(\Omega)$ one may choose $\chi = u^t - u$ which gives

$$\begin{aligned}|u^t - u|_1^2 = &-((A_t - I)\nabla u^t, \nabla(u^t - u))_\Omega + (I_t f^t - f, u^t - u)_\Omega \\ &+ (w_t g^t - g, u^t - u)_\Gamma.\end{aligned} \tag{3.6}$$

As a consequence one concludes

$$|u^t - u|_1 \le c(|(A_t - I)\nabla u^t|_{L^2(\Omega)} + |I_t f^t - f|_{L^2(\Omega)} + |w_t g^t - g|_{L^2(\Gamma)}),$$

which in view of Lemma 3.2, Lemma 3.4, Corollary 3.2 and the boundedness of $u^t$, $g^t$ in $H^1(\Omega)$, respectively $L^2(\Gamma)$ implies

$$\lim_{t\to 0} u^t = u \quad \text{in } H^1(\Omega). \tag{3.7}$$

Boundedness of $g^t$ follows from $|g^t|_{L^2(\Gamma)} = |G \circ F_t|_{L^2(\Gamma)} \leq c\,|G \circ F_t|_{H^1(\Omega)} \leq c\,|G|_{H^1(U)}$. Finally dividing (3.6) by $t$ results in

$$\begin{aligned}\frac{1}{t}|u^t - u|_1^2 = -(&\frac{1}{t}(A_t - I)\nabla u^t, \nabla(u^t - u))_\Omega \\ &+ (\frac{1}{t}(I_t - 1)f^t, u^t - u)_\Omega + (\frac{1}{t}(f^t - f), u^t - u)_\Omega + \\ &+ (\frac{1}{t}(w_t - 1)g^t, u^t - u)_\Gamma + (\frac{1}{t}(g^t - g), u^t - u)_\Gamma,\end{aligned}$$

which implies (3.5) using Lemma 3.2, Lemma 3.5, Corollary 3.2 and (3.7). □

## 4. The shape derivative

In this section we turn to the calculation of the Eulerian derivative of the cost functional in (2.1) which will turn out to be a shape derivative. We point out that we do not use the shape derivative of $u_t$ with respect to $\Gamma$. At first we assume $f \in H^1(U)$. This assumption will be weakened later on. In view of Lemma 3.1 one obtains

$$\begin{aligned}J(u_t, \Gamma_t) - J(u, \Gamma) &= \frac{1}{2}\int_{\Gamma_t} |u_t|^2\, d\Gamma_t - \frac{1}{2}\int_\Gamma |u|^2\, d\Gamma \\ &= \frac{1}{2}\int_\Gamma [w_t|u^t|^2 - |u|^2]\, d\Gamma \\ &= \frac{1}{2}\int_\Gamma \left[(w_t - 1)(|u^t|^2 - |u|^2) + (w_t - 1)\,|u|^2 + |u^t|^2 - |u|^2\right] d\Gamma \\ &= \frac{1}{2}\int_\Gamma \left[(w_t - 1)(|u^t|^2 - |u|^2) + (w_t - 1)\,|u|^2\right. \\ &\qquad \left. + 2(u^t - u)u + |u^t - u|^2\right] d\Gamma \\ &\equiv J_1(t) + J_2(t) + J_3(t) + J_4(t).\end{aligned}$$

Lemma 3.2 and Proposition 3.1 entail

$$\dot{J}_1(0) = \dot{J}_4(0) = 0. \tag{4.1}$$

Another application of Lemma 3.2 and the observation $\mathrm{div}_\Gamma\, h \in C(\Gamma)$ (which follows from $x \to n(x) \in C^{0,1}(\Gamma)$) gives

$$\dot{J}_2(0) = \frac{1}{2}\int_\Gamma |u|^2\, \mathrm{div}_\Gamma\, h\, d\Gamma. \tag{4.2}$$

Let $p \in H^1_{\Gamma_{d,0}}(\Omega)$ satisfy the adjoint equation

$$(\nabla p, \nabla\psi)_\Omega - (u, \psi)_\Gamma = 0 \tag{4.3}$$

for all $\psi \in H^1_{\Gamma_{d,0}}(\Omega)$. Then $J_3$ can be written as

$$J_3(t) = (\nabla(u^t - u), \nabla p)_\Omega.$$

Proceeding as in the derivation above (3.6) one finds

$$J_3(t) = -\big((A_t - I)\nabla u^t, \nabla p\big)_\Omega + (I_t f^t - f, p)_\Omega + (w_t g^t - g, p)_\Gamma$$

which implies

$$\dot{J}_3(0) = -\,(A\nabla u, \nabla p)_\Omega + (\operatorname{div}(hf), p)_\Omega + (h\cdot\nabla g + g \operatorname{div}_\Gamma h, p)_\Gamma \tag{4.4}$$

using Lemma 3.2, Corollary 3.1 and Corollary 3.3. Note that so far $u \in H^1_{\Gamma_{d,0}}(\Omega)$ was sufficient to justify the derivatives. Since $\Omega \in C^{1,1}$ elliptic regularity theory implies $u$,$p \in H^2(\Omega)$.

The first term in (4.4) will be manipulated using the formalism for the curl-operator in $\mathbb{R}^3$. For this purpose we embed $h$, $n$, $\nabla u$ and $\nabla p$ into $\mathbb{R}^3$ by appending a zero third coordinate.

**Lemma 4.1.** *The term* $-(A\nabla u, \nabla p)_\Omega$ *can be represented as*

$$-(A\nabla u, \nabla p)_\Omega = (\nabla(h\cdot\nabla u), \nabla p)_\Omega - (h\Delta u, \nabla p)_\Omega - (\nabla u\cdot\nabla p, h\cdot n)_\Gamma + (\frac{\partial u}{\partial n}, h\cdot\nabla p)_\Gamma.$$

*Proof.* The identity

$$((D\chi)^T - D\chi)\xi = \xi \times \operatorname{curl}\chi, \tag{4.5}$$

which holds for $\chi \in H^1(\Omega)^3$ and $\xi \in \mathbb{R}^3$, suggests to separate the skew symmetric part of $Dh$ in $A$ as

$$\begin{aligned} -A\nabla u &= 2Dh\nabla u + (Dh^T - Dh)\nabla u - \operatorname{div} h\,\nabla u \\ &= 2Dh\nabla u - \operatorname{div} h\,\nabla u + \operatorname{curl}(u \operatorname{curl} h) - u \operatorname{curl}\operatorname{curl} h. \end{aligned}$$

In the last step we used (4.5) together with

$$\operatorname{curl}(\chi v) = v \operatorname{curl}\chi + \nabla v \times \chi \tag{4.6}$$

which holds for all $(\chi, v) \in H^1(\Omega)^3 \times H^1(\Omega)$. Applying (4.6) once more with $v = u$ and $\chi = \operatorname{curl} h$ one obtains

$$-A\nabla u = B - \operatorname{curl}(\nabla u \times h),$$

where we have set

$$B = 2Dh\nabla u - \operatorname{div} h\nabla u + \operatorname{curl}\operatorname{curl}(uh) - u\operatorname{curl}\operatorname{curl} h.$$

Using $\operatorname{curl}\operatorname{curl}\chi = \operatorname{grad}\operatorname{div}\chi - \Delta\chi$ twice one finds

$$\begin{aligned} B &= -\Delta(uh) + \nabla(\operatorname{div}(uh)) - u\operatorname{curl}\operatorname{curl} h + 2Dh\nabla u - \operatorname{div} h\,\nabla u \\ &= -h\Delta u - u\Delta h - 2Dh\nabla u + \nabla(u\operatorname{div} h + h\cdot\nabla u) \\ &\quad - u\operatorname{curl}\operatorname{curl} h + 2Dh\nabla u - \operatorname{div} h\,\nabla u \\ &= -u(\operatorname{curl}\operatorname{curl} h + \Delta h - \nabla\operatorname{div} h) - h\Delta u + \nabla(h\cdot\nabla u) \\ &= -h\Delta u + \nabla(h\cdot\nabla u), \end{aligned}$$

which implies

$$-A\nabla u = -h\Delta u + \nabla(h\cdot\nabla u) - \operatorname{curl}(\nabla u\times h). \tag{4.7}$$

Let $z = (\nabla u \times h)_3$ denote the third (nontrivial) coordinate of $\nabla u \times h$. Then Green's theorem implies

$$\begin{aligned}(\operatorname{curl}(\nabla u\times h),\nabla p)_\Omega &= \int_\Omega (z_{x_2}p_{x_1} - z_{x_1}p_{x_2})\,dx\\ &= \int_\Omega z(p_{x_2x_1} - p_{x_1x_2})\,dx + \int_{\partial\Omega} z(p_{x_1}n_2 - p_{x_2}n_1)\,d\Gamma\\ &= -\int_\Gamma (\nabla u\times h, n\times\nabla p)\,d\Gamma\\ &= -(\nabla u\cdot n, h\cdot\nabla p)_\Gamma + (\nabla u\cdot\nabla p, h\cdot n)_\Gamma \end{aligned}\tag{4.8}$$

where we used the Lagrange identity

$$(a\times b, c\times d) = (a,c)(b,d) - (a,d)(b,c)$$

for $a$, $b$, $c$, $d\in\mathbb{R}^3$. The Lemma follows now from (4.7) and (4.8). □

Since $h\cdot\nabla u \in H^1_{\Gamma_{d,0}}(\Omega)$ it may serve as a test function in the adjoint equation (4.3). Hence Lemma 4.1, (2.2), (4.3) and the divergence theorem together with $h|_{\Gamma_d} = 0$ imply

$$\begin{aligned}-(A\nabla u,\nabla p)_\Omega &= (h\cdot\nabla u, u)_\Gamma + (fh,\nabla p)_\Omega - (\nabla u\cdot\nabla p, h\cdot n)_\Gamma + (g, h\cdot\nabla p)_\Gamma\\ &= (h\cdot\nabla u, u)_\Gamma + (fp, h\cdot n)_\Gamma - (\operatorname{div}(fh), p)_\Omega\\ &\quad - (\nabla u\cdot\nabla p, h\cdot n)_\Gamma + (g, h\cdot\nabla p)_\Gamma.\end{aligned}$$

Inserting this expression into (4.4) gives

$$\begin{aligned}\dot J_3(0) &= (h\cdot\nabla u, u)_\Gamma + (fp, h\cdot n)_\Gamma - (\nabla u\cdot\nabla p, h\cdot n)_\Gamma\\ &\quad + (g, h\cdot\nabla p)_\Gamma + (h\cdot\nabla g + g\operatorname{div}_\Gamma h, p)_\Gamma\\ &= (\nabla(\tfrac{1}{2}u^2 + gp), h)_\Gamma + (fp, h\cdot n)_\Gamma + (g\operatorname{div}_\Gamma h, p)_\Gamma - (\nabla u\cdot\nabla p, h\cdot n)_\Gamma.\end{aligned}$$

Combining the last result with (4.2) one obtains

$$\delta J(u,\Gamma)h = \int_\Gamma \left[h\cdot\nabla(\frac{1}{2}u^2 + gp) + (\frac{1}{2}u^2 + gp)\operatorname{div}_\Gamma h\right] d\Gamma + (fp - \nabla u\cdot\nabla p, n\cdot h)_\Gamma. \tag{4.9}$$

It is apparent that the Eulerian derivative is in fact a shape derivative. The representation (4.9) can be further simplified if the integration by parts formula holds

$$\int_\Gamma (\nabla b\cdot V + b\operatorname{div}_\Gamma V)\,d\Gamma = \int_\Gamma (\frac{\partial b}{\partial n} + b\operatorname{div}_\Gamma n)\, n\cdot V\,d\Gamma \tag{4.10}$$

([SZ, Formula (2.144)]). A sufficient condition is $C^2$-regularity of $\Gamma$.

**Theorem 4.1.** *Let $\Omega \in C^{1,1}$ and $f \in H^s(U)$, $s > \frac{1}{2}$. Then the shape derivative of $J$ at $\Omega$ with respect to $h \in \mathcal{H}$ is given by* (4.9)*. If the integration by parts formula* (4.10) *holds the shape derivative of $J$ can be represented as*

$$\delta J(u,\Gamma)h = \frac{1}{2}\int_\Gamma \big[\frac{\partial}{\partial n}(\frac{1}{2}u^2 + gp) + (\frac{1}{2}u^2 + gp)\kappa + fp - \nabla u\cdot\nabla p\big]\, n\cdot h\, d\Gamma, \tag{4.11}$$

*where $\kappa$ denotes the mean curvature of $\Gamma$.*

*Proof.* At first we show that (4.9) is valid for $f \in H^s(U)$, $s > \frac{1}{2}$. This is a consequence of the continuous dependence on the data of the solution of the state equation as well as the adjoint equation

$$\begin{aligned} |u|_{H^2(\Omega)} &\le c(|f|_{L^2(\Omega)} + |u_d|_{H^{3/2}(\Gamma_d)} + |g|_{H^{1/2}(\Gamma)}),\\ |p|_{H^2(\Omega)} &\le c|u|_{H^{1/2}(\Gamma)}, \end{aligned}$$

with a constant $c > 0$ which just depends on $\Omega$, the continuity of the trace operator from $H^s(\Omega) \to H^{s-1/2}(\Gamma)$, $s < \frac{1}{2}$, and the density of $H^1(\Omega)$ in $H^s(\Omega)$.

The representation (4.11) follows from (4.9) and (4.10) setting $b = \frac{1}{2}u^2 + gp$ together with the observation that

$$\operatorname{div} n = \kappa,$$

holds in $\mathbb{R}^2$. □

*Remark* 4.1. The derivation of the shape derivative of $J$ used the fact that dist $(\Gamma_d, \Gamma) > 0$ in the embedding properties of $H^{1/2}(\Gamma)$ and the regularity of $u$ and $p$. If $\partial\Omega$ is connected $H^{1/2}(\Gamma)$ should be replaced by the space

$$H^{1/2}_{00}(\Gamma) = \{\phi \in H^{1/2}(\partial\Omega) \colon \phi = 0 \text{ on } \partial\Omega \setminus \Gamma\}.$$

Furthermore, in order to assure the required regularity of $u$ and $p$ one has to impose the condition that $\Gamma_d$ and $\Gamma$ meet at an angle less than $\pi$.

## 5. Numerical Results

In this section we indicate how the derivative information in (4.11) can be combined with level set ideas to obtain an efficient algorithm for the solution of the shape optimization problem (2.1)-(2.2). The level set technique was introduced in [OSe] to track moving interfaces. Meanwhile this technique is well known and used for a wide range of applications. A thorough discussion of the method and many applications can be found in the monograph [Se]. The basic idea is to represent a family of domains $\Omega_t$, $t \in [0,T]$, by a single level set function $\psi \colon \mathbb{R}^2 \times [0,T] \to \mathbb{R}$ such that for all $t \in [0,T]$

$$\begin{aligned} \Omega_t &= \{x \in \mathbb{R}^2 \colon \psi(x,t) < 0\},\\ \Gamma_t &= \{x \in \mathbb{R}^2 \colon \psi(x,t) = 0\}, \end{aligned}$$

$(\Omega_0, \Gamma_0)$ corresponds to the pair $(\Omega, \Gamma)$ of the previous section). Here we are interested in the case of $\Omega_t$ being a small deformation of a given reference domain $\Omega_0$ specified by

$$\Omega_t = \{x(t;X) = X + th(X), X \in \Omega_0, t \in (0,T]\}. \tag{5.1}$$

The function $\psi$ is determined by the requirement

$$X \in \Gamma_0 \Rightarrow x(t;X) \in \Gamma_t, \qquad t \in (0,T],$$

which can be equivalently expressed by the identity

$$\psi(x(t;X),t) = 0, \qquad t \in (0,T]$$

for all $X \in \Gamma_0$. A formal differentiation leads to the level set equation

$$\begin{aligned} &\psi_t + \nabla\psi \cdot h = 0, \\ &\psi(\cdot, 0) = \psi_0, \end{aligned} \tag{5.2}$$

where $\psi_0$ is any function such that $\Omega_0 = \{x \in \mathbb{R}^2 \colon \psi_0(x) < 0\}$. The representation of the shape derivative of $J$

$$\delta J(u,\Gamma)h = \int_\Gamma G\,(h \cdot n)\,d\Gamma,$$

with a kernel $G$ being determined by (4.11) suggests that any vector field $h$ satisfying

$$h(x) = -G(x)n(x) = -G(x)\frac{\nabla\psi(x,0)}{|\nabla\psi(x,0)|} \tag{5.3}$$

for all $x$ on the boundary $\Gamma_0$ may serve as a descent direction for $J$ at $\Gamma_0$. Since (5.3) determines the deformation field $h$ only on $\Gamma_0$ the kernel $G$ still needs to be defined off $\Gamma_0$. Let $G_{ext}$ denote a suitable extension of $G$ and insert

$$h(x) = -G_{ext}(x)\frac{\nabla\psi(x,t)}{|\nabla\psi(x,t)|}, \quad t \in [0,T], \tag{5.4}$$

into (5.2) to obtain the Hamilton-Jacobi equation

$$\begin{aligned} &\psi_t - G_{ext}|\nabla\psi| = 0, \\ &\psi(\cdot, 0) = \psi_0. \end{aligned} \tag{5.5}$$

Evaluating $J$ at $\Omega_T$ for $T$ sufficiently small this choice of $h$ ensures a decrease of $J$ by construction. Summarizing, the proposed level set based steepest descent algorithm requires at each iteration the following steps:

(1) solve the state equation (2.2) and the adjoint equation (4.3) on the current domain $\Omega_0$,
(2) compute the kernel $G$,
(3) compute the extension $G_{ext}$,
(4) solve the HJ-equation (5.5) for $\psi$,
(5) update $\Omega_0$ by $\Omega_T = \{x \in \mathbb{R}^2 \colon \psi(x,T) < 0\}$.

Since $\Gamma_t$, $t \in (0,T]$, and $\Gamma_0$ are close for $T$ sufficiently small, $\psi$ and consequently $G_{ext}$ need only be known on a neighborhood $N$ of $\Gamma_0$, ([ASe1]). For the extension of $G$ to $N$ we use the fast marching method of [ASe2]. As a by-product the signed distance function

$$\tilde{\psi}_0(x) = \begin{cases} \operatorname{dist}(x, \Gamma_0) & x \in N \setminus \Omega_0 \\ -\operatorname{dist}(x, \Gamma_0) & x \in N \cap \Omega_0 \end{cases}$$

is constructed by solving the eikonal equation

$$|\nabla \tilde{\psi}_0| = 1$$

on $N$. Hence $\tilde{\psi}_0$ also serves as a level set function to represent $\Omega_0$. It is noted that the solution of the HJ-equation (5.5) remains a signed distance function if $\psi_0$ is replaced by $\tilde{\psi}_0$ ([ASe2]). Therefore, integrating (5.5) over $[0,T]$ we obtain using $|\nabla\psi(\cdot,t)| = 1$, $t \in (0,T]$,

$$\psi(\cdot, T) = \tilde{\psi}_0 + G_{ext} \int_0^T |\nabla \psi(\cdot, s)|\, ds = \tilde{\psi}_0 + G_{ext} T.$$

This representation for $\psi$ is used in the neighborhood $N$. Alternatively, (5.5) may be solved applying one of the ENO schemes discussed in [OSe, Se, Sa]. The choice of the final time $T$ is a delicate issue. We determine $T$ according to the following heuristic which is inspired by the Armijo-Goldstein line search strategy. Using (5.1) and (5.4) a formal expansion gives

$$\begin{aligned} J(u_T, \Gamma_T) &\simeq J(u_0, \Gamma_0) + \delta J(u_0, \Gamma_0) h T \\ &= J(u_0, \Gamma_0) - ||G||^2_{L^2(\Gamma_0)} T \end{aligned}$$

where $u_t$ denotes the solution of (5.5) on $\Omega_t$, $t \in [0,T]$. The requirement

$$J(u_T, \Gamma_T) = \alpha J(u_0, \Gamma_0)$$

for some $\alpha \in (0,1)$ then suggests the choice

$$T = \frac{J(u_0, \Gamma_0)}{||G||^2_{L^2(\Gamma_0)}}(1-\alpha).$$

We demonstrate the feasibility of this approach by means of the outer Bernoulli problem: find a domain $\Omega$ and a function $u \in H^1(\Omega)$ such that

$$\begin{aligned} \Delta u &= 0, && \text{in } \Omega, \\ u &= 1, && \text{on } \Gamma_d, \\ u &= 0, && \text{on } \Gamma, \\ \frac{\partial u}{\partial n} &= g, && \text{on } \Gamma, \end{aligned} \tag{5.6}$$

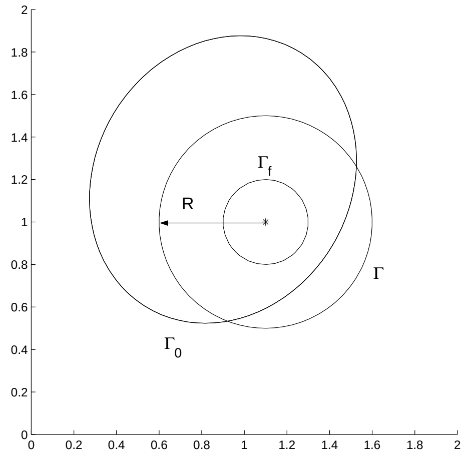


FIGURE 5.1

| $iter$ | $J(u_T, \Gamma_T)$ | $\|\|G\|\|^2_{L^2(\Gamma_T)}$ | $T$ |
|---|---|---|---|
| 1 | 3.15340 | 39.28927 | 0.0722 |
| 2 | 0.17410 | 1.07601 | 0.1456 |
| 3 | 0.00521 | 0.01775 | 0.2641 |
| 4 | 0.00037 | 0.00132 | 0.2521 |
| 5 | 0.00004 | 0.00013 | 0.2414 |
| 6 | 0.00002 | 0.00009 | 0.1858 |
| mean radius | | 0.4983 | |
| variance | | 0.0008 | |
| $\|u_c - u_{ex}\|_\infty$ | | 0.0021 | |

TABLE 5.1

where $\Gamma_d$ is the fixed inner, and $\Gamma$ the unknown outer boundary component of $\Omega$. It is known that (5.6) has a solution $(\Omega, u)$ if $\lambda < 0$ and $\Gamma_d$ is Lipschitz continuous ([AC]). A survey of the Bernoulli problem can be found in [FR].

5.1. **Example 1.** First we consider the case where $\Gamma_d$ is given by the circle

$$\Gamma_d = \{(x, y) \colon (x - 1.1)^2 + (y - 1)^2 = r_d^2\}.$$

In this case the free boundary is a concentric circle with radius $R$ which is determined by

$$R = r_d e^{-\frac{1}{gR}}$$

and $u$ is given by

$$u(x, y) = \frac{1}{2} gR \log \frac{(x - 1.1)^2 + (y - 1)^2}{r_d}.$$

In the numerical example below we set $r_d = 0.2$, $R = 0.5$ and calculate $g$ from $u$. As an initial guess for the free boundary we choose an excentric ellipse with axes of length 0.7, respectively 0.6, rotated counterclockwise by $\frac{\pi}{3}$ and center at $(0.9, 1.2)$, see Figure 5.1.

Table 5.1 shows the convergence history of a numerical realization of the proposed algorithm. The state and adjoint equation are solved by a variant of immersed interface techniques which were introduced by Z. Li and R. Leveque ([Li, LeLi]) on a rectangular grid with mesh size $h = \frac{2}{49}$. The parameter $\alpha$ was set to $\alpha = 0.1$. The algorithm terminated after 6 iterations by the condition $||G||^2_{L^2(\Gamma_t)} < tol_g$, $tol_g = 10^{-4}$. The intercepts of the computed free boundary are located approximately on a circle with center $(1.1, 1)$ and mean radius $R_m = 0.4983$ with variance 0.0008. The error of the computed solution at interior grid points is $||u - u_c||_\infty \simeq 0.0021$. We restart the optimization at the previously obtained interface interpolated on a grid with mesh

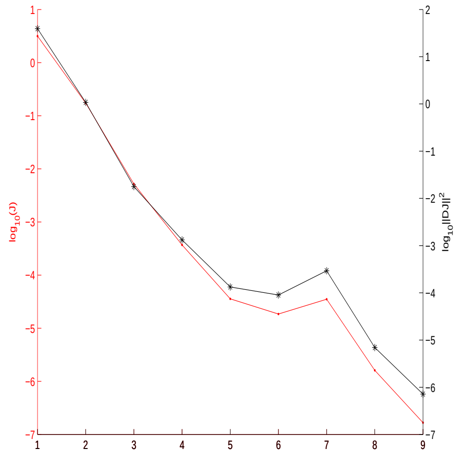


FIGURE 5.2

| *iter* | $J(u_T, \Gamma_T)$ | $\|\|G\|\|^2_{L^2(\Gamma_T)}$ | $T$ |
|---|---|---|---|
| 1 | 0.0000352 | 0.0002924 | 0.1082 |
| 2 | 0.0000016 | 0.0000069 | 0.2088 |
| 3 | 0.0000002 | 0.0000007 | 0.2094 |
| mean radius | | 0.4998 | |
| variance | | 0.0002 | |
| $\|\|u_c - u_{ex}\|\|_\infty$ | | 0.0009 | |

TABLE 5.2

size $h = \frac{2}{99}$ using the more stringent termination parameter $tol_g = 10^{-6}$. Figure 5.2 shows the combined convergence history on a logarithmic scale: the solid line refers to $\log_{10} ||G||^2_{L^2(\Gamma_T)}$, the dashed line illustrates $\log_{10} J(u_T, \Gamma_T)$. The restart increases the initial cost, however the optimization terminates after only 3 additional iterations at a significantly reduced cost, improved mean radius and variance. The error of the computed solution $u_c$ is reduced by a factor 2, cf. Table 5.2.

5.2. **Example 2.** We again consider the outer Bernoulli problem. Now the fixed boundary is L-shaped as specified by the list of corners $(3.1, 3.1)$, $(5.1, 3.1)$, $(5.1, 4.5)$, $(7.1, 4.5)$, $(7.1, 7.1)$, $(3.1, 7.1)$, cf. Figure 5.3. In this case the solution of the Bernoulli problem is not explicitly known. Figure 5.3 shows the free boundaries computed by the 2 level optimization strategy sketched above: first we solve the problem on a grid with mesh size $h = .2$ on the computational domain $[0, 10] \times [0, 10]$ starting from the circle $(x-5)^2 + (y-5)^2 = 4.2^2$ as initial guess. Then the resulting level set function is interpolated on a 3 times finer grid and used as an initial guess for the second run. The computed free boundaries are almost indistinguishable. Nevertheless, the 6 additional iterations on the finer grid, however, reduce the cost as well as $||G||^2_{L^2(\Gamma_t)}$ by two orders of magnitude, cf. Table 5.3 and Figure 5.4.

This example was also solved in [HKKP] by a completely different technique. There, we formulated the optimization problem

$$\min_{\Gamma} \frac{1}{2} \int_{\Gamma} (\frac{\partial u}{\partial n} - g)^2 \, d\Gamma$$

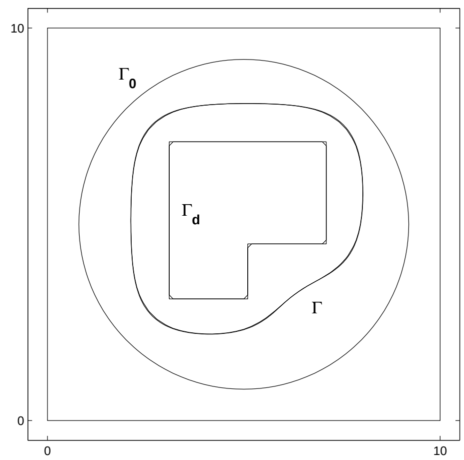


FIGURE 5.3

| *iter* | *cost* | $\|\|DJ\|\|^2$ | $t$ |
|---|---|---|---|
| 1 | 42.5073820 | 75.6076829 | 0.5060 |
| 2 | 2.5646458 | 2.6962668 | 0.8561 |
| 3 | 0.1157191 | 0.0848614 | 1.2273 |
| 4 | 0.0115121 | 0.0092944 | 1.1147 |
| 5 | 0.0012156 | 0.0006600 | 1.6576 |
| 6 | 0.0001781 | 0.0001228 | 1.3057 |
| 7 | 0.0000540 | 0.0000345 | 1.4101 |
| 1 | 0.0025375 | 0.0029234 | 0.7812 |
| 2 | 0.0001348 | 0.0000636 | 1.9079 |
| 3 | 0.0000803 | 0.0001466 | 0.4929 |
| 4 | 0.0000128 | 0.0000084 | 1.3723 |
| 5 | 0.0000020 | 0.0000016 | 1.1400 |
| 6 | 0.0000004 | 0.0000003 | 1.2876 |

TABLE 5.3

subject to the Dirichlet problem

$$\begin{aligned} -\Delta u &= 0, && \text{on } \Omega \\ u &= 1, && \text{on } \Gamma_d, \\ u &= 0, && \text{on } \Gamma. \end{aligned}$$

The free boundary was represented by a piecewise quadratic Bezier spline, the state equation was solved by an embedding domain technique and the optimization was carried out by a derivative free global method. Figure 5.5 shows a comparison of the free boundary obtained by the composite level set technique after 13 iterations with the result of the global method after 10000 function evaluations. The circles mark the final position of the control nodes of the Bezier splines which were allowed to move only on the indicated segments. A complete discussion can be found in [HKKP].

## 6. Appendix

*Proof of Lemma 3.1.* Let $\varphi\colon T \to V$ be a local patch for an $n-1$-dimensional manifold $M$ in $\mathbb{R}^n$, $T$ being open in $\mathbb{R}^n$, $V$ open in $M$. Let $f\colon M \to \mathbb{R}$ satisfy $\operatorname{supp} f \subset V$. Recall that $f$ is integrable over $V$ if $t \to f\circ\varphi\,[\det(D\varphi^T(t)D\varphi(t)]^{1/2}$ is integrable over $T$. One then defines

$$\int_M f(x)\,dM = \int_T f\circ\varphi(t)\,[\det(D\varphi^T(t)D\varphi(t)]^{1/2}\,dt.$$

We also note the following result which is useful in the manipulation of the surface element.

**Lemma 6.1** ([M])**.** *Given independent vectors $x_1, \dots, x_{n-1}$ in $\mathbb{R}^n$, let $X$ be the $n \times n-1$ matrix $X = [x_1, \dots, x_{n-1}]$ and let $n$ denote the vector with coordinates*

$$n_i = (-1)^{i-1} \det X(1, \dots, \hat{i}, \dots, n),$$

*where $\hat{i}$ indicates deletion of the $i$-th row in $X$. Then $n$ is a normal to the hyperplane determined by $x_1, \dots, x_{n-1}$ of length*

$$||n|| = \sqrt{\det(X^T X)}.$$

*(Hence $||n||$ gives the volume of the parallelepiped spanned by $x_1, \dots, x_{n-1}$.)*

Since $\Omega \in C^{1,1}$ there exists a family $O_1, \dots, O_m$ of open sets in $\mathbb{R}^n$ covering $\Gamma$ and $C^{1,1}$-diffeomorphisms $c_i \colon O_i \to B(0,1)$ such that

$$c_i(\Omega \cap O_i) = \{\xi \in B(0,1) \colon \xi_n \le 0\},$$
$$c_i(\Gamma \cap O_i) = \{\xi \in B(0,1) \colon \xi_n = 0\}.$$

Define $B_0 = \{\xi' \in \mathbb{R}^{n-1} \colon ||\xi'|| \le 1\}$ and let $\tilde{h}_i \colon B_0 \to \Gamma \cap O_i$ stand for the restriction of $h_i = c_i^{-1}$ to $\{\xi \in B(0,1) \colon \xi_n = 0\}$. Then $\tilde{h}_i \colon B_0 \to \Gamma \cap O_i$ determines a local patch of $\Gamma$, hence $F_t \circ \tilde{h}_i \colon F_t(\Gamma) \cap F_t(O_i)$ is a local patch of $\Gamma_t = F_t(\Gamma)$. Using a suitable partition of unity we may consequently assume $\operatorname{supp} f_t \subset F_t(\Gamma) \cap F_t(O_i)$. To simplify notation we subsequently omit the index $i$. By definition of the surface integral we have

$$\int_{\Gamma_t} f_t(x_t)\, d\Gamma_t = \int_{B_0} f_t \circ (F_t \circ \tilde{h}) [\det \left( D_{\xi'}(F_t \circ \tilde{h})^T D_{\xi'}(F_t \circ \tilde{h}) \right)]^{1/2}\, d\xi'. \tag{6.1}$$

From the relation relating the inverse of a matrix to its algebraic complement we obtain

$$\det Dh\, (Dh)^{-T} e_n = (\operatorname{adj} Dh)^T e_n \equiv \tilde{n} \circ h, \tag{6.2}$$

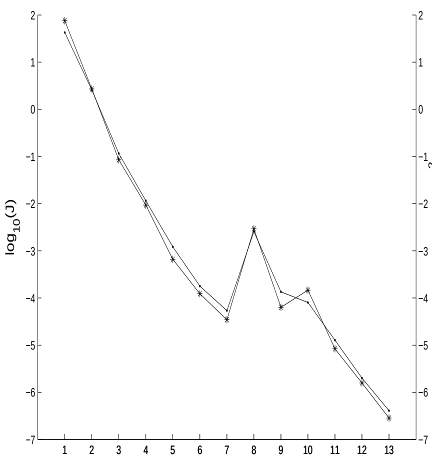


FIGURE 5.4

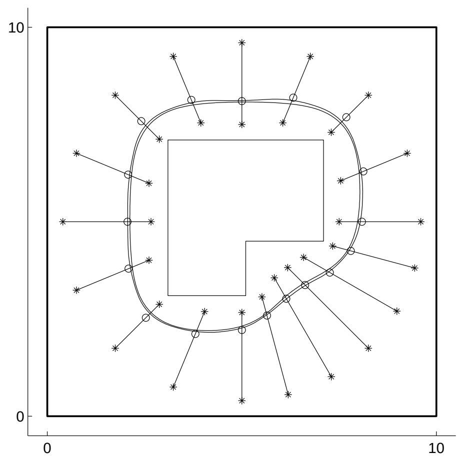


FIGURE 5.5

which is to be evaluated at $(\xi', 0)$, $\xi' \in B_0$. Therefore $\tilde{n}\circ h = \tilde{n}\circ\tilde{h}$. Observe that the $i$-th coordinate of $\tilde{n}\circ h$ is given by

$$(\tilde{n}\circ h)_i = (-1)^{n+i-1} \det(D_{\xi'} h(1, \ldots, \hat{i}, \ldots, n)), \quad i = 1, \ldots, n.$$

From Lemma 6.1 we infer that $\tilde{n}\circ h$ is a normal vector to $\Gamma$ of length

$$||\tilde{n}\circ h|| = |\det Dh|\, ||(Dh)^{-T} e_n|| = [\det \big(D_{\xi'}\tilde{h}^T D_{\xi'}\tilde{h}\big)]^{1/2}. \tag{6.3}$$

Using the chain rule and (6.2) we furthermore obtain

$$\begin{aligned} D(F_t\circ h)^{-T} e_n &= (DF_t)^{-T}\circ h\, (Dh)^{-T} e_n = (\det Dh)^{-1} (DF_t)^{-T} \circ h \tilde{n}\circ h \\ &= (\det Dh)^{-1} \big((DF_t)^{-T} n\big)\circ h\, ||\tilde{n}||\circ h \end{aligned}$$

where $n$ denotes the normalized vector $\tilde{n}$ oriented such that it points to the exterior of $\Omega$. Inserting this result and (6.3) with $h$ replaced by $F_t\circ h$ into (6.2) results in

$$\begin{aligned} \int_{\Gamma_t} f_t(x_t)\, d\Gamma_t &= \int_{B_0} f_t\circ(F_t\circ\tilde{h}) \det(DF_t\circ h)\, ||D(F_t\circ h)^{-T} e_n||\, d\xi' \\ &= \int_{B_0} f_t\circ(F_t\circ\tilde{h}) \det(DF_t\circ h)\, (\det Dh)^{-1} ||(DF_t)^{-T} n||\circ h\, ||\tilde{n}||\circ h\, d\xi' \\ &= \int_{B_0} f_t\circ(F_t\circ\tilde{h}) \det(DF_t\circ h)\, (\det Dh)^{-1} ||(DF_t)^{-T} n||\circ h [\det \big(D_{\xi'}\tilde{h}^T D_{\xi'}\tilde{h}\big)]^{1/2}\, d\xi' \\ &= \int_{B_0} (f_t\circ F_t)\circ\tilde{h} \det(DF_t)\circ h\, ||(DF_t)^{-T} n||\circ h\, [\det \big(D_{\xi'} h^T D_{\xi'}\tilde{h}\big)]^{1/2}\, d\xi' \\ &= \int_{\Gamma} f_t\circ F_t \det DF_t\, ||(DF_t)^{-T} n||\, d\Gamma, \end{aligned}$$

which is the desired transformation rule. Finally we point out that in view of (6.3) we have for $f \in L^1(\Gamma)$, $\operatorname{supp} f \subset O_i \cap \Gamma$

$$\begin{aligned} \int_{\Gamma} f\, d\Gamma &= \int_{B_0} f\circ h [\det \big(D_{\xi'} h^T D_{\xi'}\tilde{h}\big)]^{1/2}\, d\xi' \\ &= \int_{B_0} f\circ h |\det Dh|\, ||(Dh)^{-T} e_n||\, d\xi', \end{aligned}$$

which is the definition of the surface integral given in [SZ]. □

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