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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 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.

Keywords: Shape derivative; Bernoulli problem; Level set

1. Introduction

In this paper we consider the shape optimization problem

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

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where $u = u(\Gamma)$ is a solution of the mixed boundary value problem

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

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

We shall characterize the shape derivative $dJ(\Gamma, h)$ of $J(\Gamma)$ with respect to perturbations of the domain Ω defined by a vector field h. Subsequently we solve (1.1) numerically by means of a level set implementation. For this procedure 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 Γ.

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

$$
\min \quad J(\Gamma_t) \equiv \frac{1}{2}\int_{\Gamma_t} u_t^2 \, d\Gamma_t \tag{1.3}
$$

$$
\text{subject to} \quad e(u_t) = 0. \tag{1.4}
$$

Here e represents the equality constraints due to the partial differential equation (1.2) and u_t denotes the weak solution of (1.2) on the perturbed domain $\Omega_t = F_t(\Omega)$, where $F_t : \Omega \to \mathbb{R}^2$ is the transformation given by $F_t(x) = x + t\,h(x)$ for $t \in \mathbb{R}$. The most common approach for computing the Eulerian derivative $dJ(\Gamma, h) = \lim_{t\to 0^+} \frac{1}{t}(J(\Gamma_t) - J(\Gamma))$ is based on the chain rule. Considering u_t as a function of the domain—the dependence on the domain being encoded in the scalar parameter t—$dJ(\Gamma, h)$ can be represented as

$$
dJ(\Gamma, h) = \int_\Gamma u u'(\Gamma, h)\, d\Gamma + \frac{1}{2}\int_\Gamma \left(\frac{\partial u^2}{\partial n} + \kappa u^2\right) h \cdot n \, d\Gamma, \tag{1.5}
$$

where κ is the curvature of Γ and $u'(\Gamma, h)$ is the shape derivative of u in the direction h. Following [16], $u'(\Gamma, h)$ is defined in terms of the material derivative $\dot{u}(\Gamma, h)$ of u at Γ in the direction h,

$$
\dot{u}(\Gamma, h) = \lim_{t\to 0^+} \frac{1}{t}(u_t \circ F_t - u). \tag{1.6}
$$

Once the material derivative $\dot{u}(\Gamma, h)$ is available, one defines the shape derivative

$$
u'(\Gamma, h) = \dot{u}(\Gamma, h) - \nabla_\Gamma u \cdot h, \tag{1.7}
$$

using the tangential gradient ∇_Γ. Frequently an equation for $u'(\Gamma, h)$ can be derived by formally differentiating $e(u) = 0$ with respect to the domain. For system (1.2) one would find that $u' \equiv u'(\Gamma, h)$ satisfies

$$
\begin{aligned}
&-\Delta u' = 0 \quad \text{in } \Omega,\\
&u' = 0 \quad \text{on } \Gamma_d,\\
&\frac{\partial u'}{\partial n} = \operatorname{div}_\Gamma (h \cdot n \nabla_\Gamma u) + \left(f + \frac{\partial g}{\partial n} + \kappa g \right) h \cdot n \quad \text{on } \Gamma,
\end{aligned}
\tag{1.8}
$$

where $\operatorname{div}_\Gamma$ denotes the tangential divergence and u is the solution of (1.2) on Ω. This formal step must be justified by verifying the identity (1.7). This in itself is a nontrivial task. Introducing a suitably defined adjoint variable and using (1.8), the first term on the right-hand side of (1.5) can be manipulated in such a way that $dJ(\Gamma, h)$ can be represented in the form assured by the Zolesio–Hadamard structure theorem [4]

$$
dJ(\Gamma, h) = \int_\Gamma G h \cdot n \, d\Gamma.
$$

Note that the kernel G does not involve the shape derivative $u'(\Gamma, h)$ any more.

The Eulerian derivative of J can also be obtained by considering both the state variable u and the geometric variable Ω 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 [5,6], strongly depends on sophisticated differentiability properties of saddle point problems.

In the approach that we employ for characterizing $dJ(\Gamma, h)$ we avoid the disadvantages of the "chain rule" approach as well as those of the Lagrangian technique. Again, we consider the state variable u as a dependent variable. However, differently from the "chain rule" approach, we bypass steps (1.6)–(1.8) by exploiting the special structure of the cost functional and a consistent use of the adjoint variable. On the technical level the existence of the material derivative $\dot{u}(\Gamma, h)$ can be replaced by Hölder continuity of the state with exponent greater than $\frac{1}{2}$ with respect to the deformation of the shape, see Proposition 3.1. Since this approach does not utilize the shape derivative of the state it has the potential of allowing the characterization of the shape gradient of J under weaker regularity assumptions. For example, $u \in H^2(\Omega)$ is not sufficient to ensure that the solution of (1.8) is an element of $H^1(\Omega)$. In our analysis, however, we only need $u \in H^2(\Omega)$ for the characterization of the shape derivative.

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. 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 Appendix A.

2. Formulation of the problem

Consider the shape optimization problem

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

subject to the mixed boundary value problem

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

where the boundary $\partial\Omega$ is the disjoint union of a fixed part Γ_d and an unknown part Γ 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 $g \in H^2(U)$. 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 Γ will be described below.

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

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

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

Let us define the Hilbert space

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

endowed with the norm

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

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

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

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 Γ *without* taking the shape derivative of u. The admissible set of free boundaries is described by a particular class of perturbations of the domain Ω. Let $\mathcal{H}$ denote the set

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

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

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

One can verify that F_t is injective for $|t| < t_h^{-1}$, $t_h = \max\{|Dh(x)|:\ x \in \bar{U}\}$ and defines a $C^{1,1}$-diffeomorphism from Ω 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 Γ_d and $\Gamma_t \equiv F_t(\Gamma)$.

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

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

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 $dJ(\Gamma, h)$ exists for all $h \in \mathcal{H}$ and the mapping $h \to dJ(\Gamma, h)$ 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 τ:

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

The tangential vector is oriented such that Ω lies on the left of τ.

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 Ω and the choice of the vector field h but is independent of t. We recall from [16] 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*

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

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

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

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

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 the following regularity*:

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

and the properties listed below:

(1) $I_t = 1 + t \operatorname{div} h + t^2 \det Dh$,
(2) *there are positive constants α_0, α_1 and β such that $0 < \alpha_0 \leqslant I_t(x) \leqslant \alpha_1$ and $A_t(x) \geqslant \beta I$ 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 [12]. *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*:

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

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

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

Lemma 3.4. *For any $f \in L^p(U)$, $p \geqslant 1$, 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_ε on $\bar{U}$, one obtains the estimates

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

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

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

Lemma 3.5. *Let $\varphi \in W^{2,p}(U)$, $p \geqslant 1$. 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 $L^p(\Omega)$,

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

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

$$\begin{aligned} &\left| \varphi \circ F_t - \varphi - t \int_0^1 D\varphi(\cdot + sth) h\, ds \right|_{L^p(\Omega)} \\ &\quad \leqslant |\varphi \circ F_t - \varphi_\varepsilon \circ F_t|_{L^p(\Omega)} + |\varphi_\varepsilon - \varphi|_{L^p(\Omega)} \\ &\qquad + \left| \varphi_\varepsilon \circ F_t - \varphi_\varepsilon - t \int_0^1 D\varphi_\varepsilon(\cdot + sth) h\, ds \right|_{L^p(\Omega)} \\ &\qquad + \left| t \int_0^1 \bigl| D\varphi_\varepsilon(\cdot + sth) - D\varphi(\cdot + sth) \bigr|\, ds \right|_{L^p(\Omega)} |h|_\infty. \end{aligned}$$

As a consequence of (3.2), one obtains

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

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

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

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

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

$$= \int_{\Omega} \int_0^1 \big[h^T(x) D^2\varphi\big(x + sth(x)\big)\big(I + st\,Dh(x)\big)_i + D\varphi\big(x + sth(x)\big)\big(Dh(x)\big)_i\big]\, ds\, \chi(x)\, dx.$$

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

$$\left| D\left(\frac{1}{t}(\varphi \circ F_t - \varphi) - D(D\varphi h)\right)\right|^p_{L^p(\Omega)} \leqslant \int_{\Omega} \int_0^1 \big|h^T(x)\big[D^2\varphi\big(x + sth(x)\big)\big(I + st\,Dh(x)\big) - D^2\varphi(x)\big]\big|^p\, ds\, dx + \int_{\Omega} \int_0^1 \big|\big(D\varphi\big(x + sth(x)\big) - D\varphi(x)\big)Dh(x)\big|^p\, ds\, dx.$$

Now the proof of the lemma follows using the smoothness of φ and Lemma 3.4. □

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

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

The Sobolev embedding theorem [12, 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 Lemmas 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 $q \geqslant 1$ from the continuous embedding of $H^{1/2}(\Gamma)$ into $L^q(\Gamma)$.

Now we turn to the discussion of Eq. (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 $f^t = f \circ F_t$ and $g^t = g \circ F_t$.

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

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

which by Lemma 3.1 implies

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

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 Eq.* (3.4) *are uniformly bounded in $H^1(\Omega)$ for $t \in J$. Moreover, for $f \in H^1(U)$,*

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

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

Proof. Let $G_d \in H^1(U)$ be an extension of g_d from Γ_d to U. Since $u^t - G_d \in H^1_{\Gamma_d,0}(\Omega)$, Eq. (3.4) together with the uniform positivity of $A_t(x)$ for $x \in \Omega$ implies the estimate

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

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

$$\begin{aligned}
|I_t f^t|_{L^2(\Omega)}^2 &= \int_\Omega \big(I_t \circ F_t^{-1}\big) \circ F_t(x) f^2 \circ F_t(x) I_t(x)\,dx \\
&= \int_{\Omega_t} I_t \circ F_t^{-1} f^2\,dx \leqslant \alpha_1 |f|_{L^2(U)}^2
\end{aligned}$$

entails the bound

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

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

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

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

$$|u^t - G_d|_1 \leqslant c\big(|f|_{L^2(U)} + |g|_{H^1(U)} + |A|_\infty |G_d|_{H^1(U)}\big),$$

which implies the boundedness of u^t in $H^1(\Omega)$ for $t \in J$. In order to prove (3.5), subtract (2.5) from (3.4) to obtain for $\chi \in H^1_{\Gamma_{d,0}}(\Omega)$,

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

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

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

As a consequence, one concludes

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

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

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

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

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

which implies (3.5) using Lemmas 3.2, 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 Γ. At first we assume $f \in H^1(U)$. This assumption will be weakened later on. In view of Lemma 3.1 one obtains

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

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 $\operatorname{div}_\Gamma h \in C(\Gamma)$ (which follows from $x \to n(x) \in C^{0,1}(\Gamma)$) gives

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

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

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

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

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

using Lemma 3.2, Corollaries 3.1 and 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, ∇u and ∇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*

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

Proof. The identity

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

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

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

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

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

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

$$\begin{aligned}
\dot J_3(0) &= (h\cdot\nabla u, u)_\Gamma + (fp, h\cdot n)_\Gamma - (\nabla u\cdot\nabla p, h\cdot n)_\Gamma \\
&\quad + (g, h\cdot\nabla p)_\Gamma + (h\cdot\nabla g + g\operatorname{div}_\Gamma h, p)_\Gamma \\
&= \left(\nabla\left(\frac12 u^2 + gp\right), h\right)_\Gamma + (fp, h\cdot n)_\Gamma + (g\operatorname{div}_\Gamma h, p)_\Gamma \\
&\quad - (\nabla u\cdot\nabla p, h\cdot n)_\Gamma.
\end{aligned}$$

Combining the last result with (4.2), one obtains

$$\begin{aligned}
dJ(\Gamma, h) &= \int_\Gamma \left[h\cdot\nabla\left(\frac12 u^2 + gp\right) + \left(\frac12 u^2 + gp\right)\operatorname{div}_\Gamma h\right] d\Gamma \\
&\quad + (fp - \nabla u\cdot\nabla p, n\cdot h)_\Gamma.
\end{aligned} \tag{4.9}$$

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

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

[16, Formula (2.144)]. A sufficient condition is C^2-regularity of Γ.

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 Ω 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*

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

where κ denotes the mean curvature of Γ.

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

$$|u|_{H^2(\Omega)} \leqslant c\big(|f|_{L^2(\Omega)} + |u_d|_{H^{3/2}(\Gamma_d)} + |g|_{H^{1/2}(\Gamma)}\big),$$
$$|p|_{H^2(\Omega)} \leqslant c|u|_{H^{1/2}(\Gamma)},$$

with a constant $c > 0$ which just depends on Ω, 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

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

Furthermore, in order to assure the required regularity of u and p one has to impose the condition that Γ_d and Γ meet at an angle less than π.

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 [13] 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 [15]. We formally present the basic idea and represent a family of domains Ω_t, $t \in [0, T]$, by a single level set function $\psi : \mathbb{R}^2 \times [0, T] \to \mathbb{R}$ such that for all $t \in [0, T]$,

$$\Omega_t = \big\{x \in \mathbb{R}^2\colon \ \psi(x, t) < 0\big\}, \qquad \Gamma_t = \big\{x \in \mathbb{R}^2\colon \ \psi(x, t) = 0\big\}$$

((Ω_0, Γ_0) corresponds to the pair (Ω, Γ) of the previous section). Here we are interested in the case of Ω_t being a small deformation of a given reference domain Ω_0 specified by

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

The function ψ is determined by the requirement

$$X \in \Gamma_0 \quad \Longrightarrow \quad x(t; X) \in \Gamma_t, \quad t \in (0, T],$$

which can be equivalently expressed by the identity

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

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 ψ_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

$$dJ(\Gamma, h) = \int_\Gamma G(h \cdot n)\, d\Gamma,$$

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 Γ_0 may serve as a descent direction for J at Γ_0. Since (5.3) determines the deformation field h only on Γ_0, the kernel G still needs to be defined off Γ_0. Let G_{ext} denote a suitable extension of G and insert

$$h(x) = -G_{\text{ext}}(x)\frac{\nabla\psi(x, t)}{|\nabla\psi(x, t)|} \tag{5.4}$$

into (5.2) to obtain the Hamilton–Jacobi equation

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

Evaluating J at Ω_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 Ω_0,
(2) compute the kernel G,
(3) compute the extension G_{ext},
(4) solve the HJ-equation (5.5) for ψ,
(5) update Ω_0 by $\Omega_T = \{x \in \mathbb{R}^2\colon\ \psi(x, T) < 0\}$.

Since Γ_t, $t \in (0, T]$, and Γ_0 are close for T sufficiently small, ψ and consequently G_{ext} need only be known on a neighborhood N of Γ_0 [2]. For the extension of G to N we use the fast marching method of [3]. 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 Ω_0. It is noted that the solution of the HJ-equation (5.5) remains a signed distance function if ψ_0 is replaced by $\tilde{\psi}_0$ [3]. Therefore, integrating (5.5) over $[0, T]$, we obtain using $|\nabla\psi(\cdot,t)| = 1$, $t \in (0, T]$,

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

This representation for ψ is used in the neighborhood N. Alternatively, (5.5) may be solved applying one of the ENO schemes discussed in [13–15]. 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

$$J(\Gamma_T) \simeq J(\Gamma_0) + dJ(\Gamma_0, h)T = J(\Gamma_0) - \|G\|^2_{L^2(\Gamma_0)} T,$$

where u_t denotes the solution of (2.2) on Ω_t, $t \in [0, T]$. The requirement

$$J(\Gamma_T) = \alpha J(\Gamma_0)$$

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

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

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

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

where Γ_d is the fixed inner, and Γ the unknown outer boundary component of Ω. It is known that (5.6) has a solution (Ω, u) if g is a negative constant and Γ_d is Lipschitz continuous [1]. A survey of the Bernoulli problem can be found in [7].

Example 1. First we consider the case where Γ_d is given by the circle

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

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

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

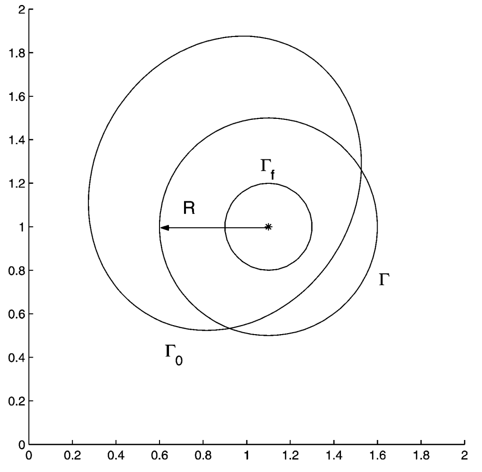

Fig. 1.

Table 1

Iter.	$J(\Gamma_T)$	$\|G\|^2_{L^2(\Gamma_T)}$	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		

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 Fig. 1.

Table 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 [9,10] on a rectangular grid with mesh size $h = \frac{2}{49}$. The parameter α was set to $\alpha = 0.1$. The algorithm terminated after 6 iterations by the condition $\|G\|^2_{L^2(\Gamma_t)} < \mathrm{tol}_g$, $\mathrm{tol}_g = 10^{-4}$. 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 size $h = \frac{2}{99}$ using the more stringent termination parameter $\mathrm{tol}_g = 10^{-6}$. Figure 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 $\log_{10} J(\Gamma_T)$. The restart increases the initial cost, however the optimization terminates after only 3 additional

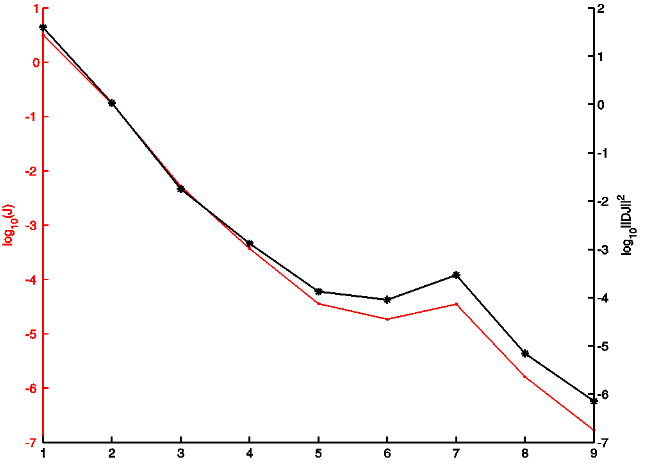

Fig. 2.

Table 2

Iter.	$J(\Gamma_T)$	$\|G\|^2_{L^2(\Gamma_T)}$	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		

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 2. We experimented with other initial guesses such as concentric/excentric circles and ellipses. In any case the algorithm terminated after a modest number of iterations at a domain which was graphically indistinguishable from the true solution.

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. Fig. 3. In this case the solution of the Bernoulli problem is not explicitly known. Fig. 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 $h = 0.2$ 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 3 and Fig. 4.

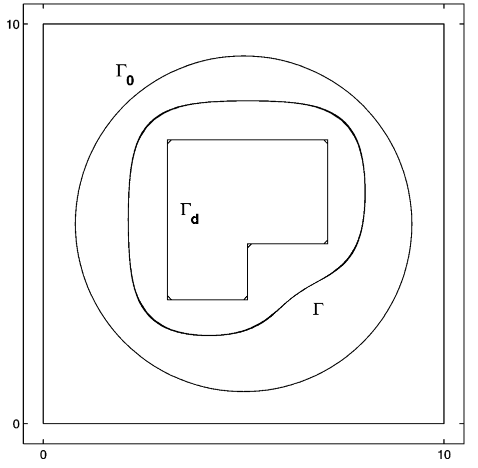

Fig. 3.

Table 3

Iter.	$J(\Gamma_T)$	$\|DJ\|^2$	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

This example was also solved in [8] by a completely different technique. There, we formulated the optimization problem

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

subject to the Dirichlet problem

$$-\Delta u = 0 \quad \text{on } \Omega,$$
$$u = 1 \quad \text{on } \Gamma_d,$$
$$u = 0 \quad \text{on } \Gamma.$$

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

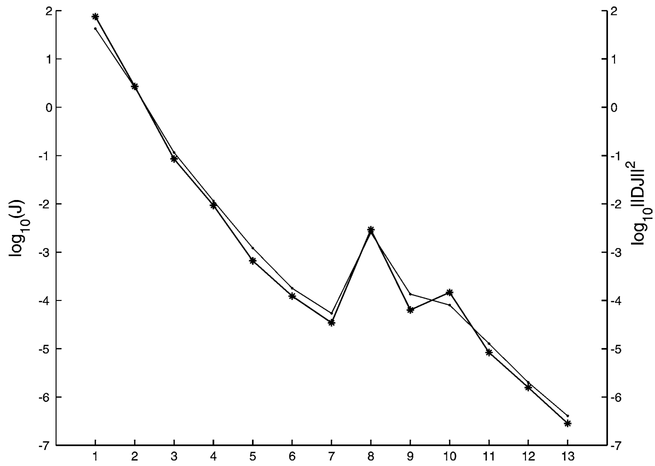

Fig. 4.

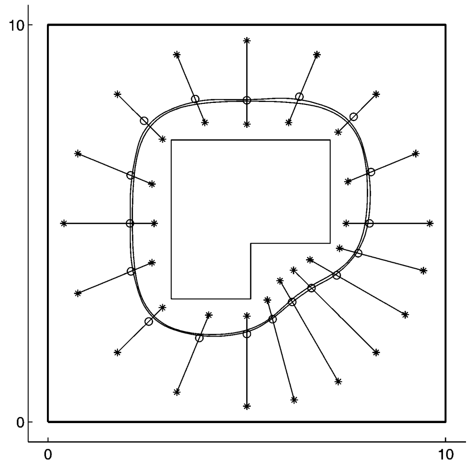

Fig. 5.

by a derivative free global method. Figure 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 10 000 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 [8].

Appendix A

Proof of Lemma 3.1. Let $\varphi : T \to V$ 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 $f : M \to \mathbb{R}$ 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

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

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

Lemma A.1 [11]. *Given independent vectors $x_1, \ldots, x_{n-1}$ in $\mathbb{R}^n$, let X be the $n \times n-1$ matrix $X = [x_1, \ldots, x_{n-1}]$ and let n denote the vector with coordinates*

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

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

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

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

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

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

Define $B_0 = \{\xi' \in \mathbb{R}^{n-1}\colon\ \|\xi'\| \leqslant 1\}$ and let $\tilde{h}_i : B_0 \to \Gamma \cap O_i$ stand for the restriction of $h_i = c_i^{-1}$ to $\{\xi \in B(0,1)\colon\ \xi_n = 0\}$. Then $\tilde{h}_i : B_0 \to \Gamma \cap O_i$ determines a local patch of Γ, hence $F_t \circ \tilde{h}_i : F_t(\Gamma) \cap F_t(O_i)$ 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

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

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

$$\det Dh(Dh)^{-T} e_n = (\operatorname{adj} Dh)^T e_n \equiv \tilde{n} \circ h, \tag{A.2}$$

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 ith coordinate of $\tilde{n} \circ h$ is given by

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

From Lemma A.1 we infer that $\tilde{n} \circ h$ is a normal vector to Γ of length

$$\|\tilde{n} \circ h\| = |\det Dh| \big\|(Dh)^{-T} e_n\big\| = \big[\det(D_{\xi'} \tilde{h}^T D_{\xi'} \tilde{h})\big]^{1/2}. \tag{A.3}$$

Using the chain rule and (A.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 Ω. Inserting this result and (A.3) with h replaced by $F_t \circ h$ into (A.2) results in

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

which is the desired transformation rule. Finally we point out that in view of (A.3) we have for $f \in L^1(\Gamma)$, $\operatorname{supp} f \subset O_i \cap \Gamma$,

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

which is the definition of the surface integral given in [16]. □

References

[1] H.W. Alt, L.A. Cafarelli, Existence and regularity for a minimum problem with free boundary, J. Reine Angew. Math. 325 (1981) 105–144.

[2] D. Adalsteinsson, J.A. Sethian, A fast level set method for propagating interfaces, J. Comput. Phys. 118 (1995) 269–277.

[3] D. Adalsteinsson, J.A. Sethian, The fast construction of extension velocities in level set methods, J. Comput. Phys. 148 (1999) 2–22.

[4] M.C. Delfour, J.P. Zolesio, Shapes and Geometries, SIAM, 2001.

[5] M.C. Delfour, J.P. Zolesio, Shape sensitivity analysis via min-max differentiability, SIAM J. Control Optim. 26 (1988) 834–862.

[6] M.C. Delfour, J.P. Zolesio, Velocity method and Lagrangian formulation for the computation of the shape Hessian, SIAM J. Control Optim. 29 (1991) 1414–1442.

[7] M. Flucher, M. Rumpf, Bernoulli's free-boundary problem, qualitative theory and numerical approximation, J. reine angew. Math. 486 (1997) 165–204.

[8] J. Haslinger, T. Kozubek, K. Kunisch, G. Peichl, Shape optimization and fictitious domain approach for solving free-boundary value problems of Bernoulli type, Comput. Optim. Appl. 26 (2003) 231–251.

[9] R.J. LeVeque, Z. Li, The immersed interface method for elliptic equations with discontinuous coefficients and singular sources, SIAM J. Numer. Anal. 31 (1994) 1019–1044.
[10] Z. Li, The immersed interface method—A numerical approach for partial differential equations with interfaces, PhD thesis, University of Washington, 1994.
[11] J. Munkres, Analysis on Manifolds, Addison–Wesley, 1991.
[12] J. Neĉas, Les Méthodes directes en Theorie des Équations Elliptiques, Masson, 1967.
[13] S. Osher, J. Sethian, Fronts propagating with curvature dependent speed: Algorithms based on Hamilton–Jacobi formulations, J. Comput. Physics 56 (1988) 12–49.
[14] F. Santosa, A level-set approach for inverse problems involving obstacles, ESAIM: Control, Optimisation and Calculus of Variations 1 (1996) 17–33.
[15] J.A. Sethian, Level Set Methods and Fast Marching Methods, Cambridge Univ. Press, 1999.
[16] J. Sokolowski, J. Zolesio, Introduction to Shape Optimization, Springer-Verlag, Berlin, 1991.