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VARIATIONAL APPROACH TO SHAPE DERIVATIVES *

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Abstract. A general framework for calculating shape derivatives for optimization problems with partial differential equations as constraints is presented. The proposed technique allows to obtain the shape derivative of the cost without the necessity to involve the shape derivative of the state variable. In fact, the state variable is only required to be Lipschitz continuous with respect to the geometry perturbations. Applications to inverse interface problems, and shape optimization for elliptic systems and the Navier-Stokes equations are given.

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1. Introduction

We propose a framework for characterizing the shape derivative for optimization problems of the form

$$\begin{cases} \min J(u,\Omega,\Gamma) \\ \text{subject to } E(u,\Omega)=0, \end{cases} \tag{1.1}$$

where E denotes a partial differential equation depending on a state variable u and a reference domain Ω, and J stands for a cost functional depending, besides u and Ω, on a codimension one manifold Γ, which may constitute part of the boundary of Ω or lie inside of Ω. This topic has been widely analyzed in the past and is covered in the well-know lecture notes [12] and in the monographs [6,9,10,13,16], for example.

The method for computing the shape derivative that we propose is quite elementary and more direct than most common techniques. A widely used approach relies on differentiating the reduced functional $\hat{J} = J(u(\Omega,\Gamma),\Omega,\Gamma)$, which is treated as a composite mapping consisting of $(\Omega,\Gamma) \to u(\Omega,\Gamma)$ and $(u,\Omega,\Gamma) \to J(u,\Omega,\Gamma)$. As a consequence shape differentiability of the state variable is essential in this method. In an alternative approach the partial differential equation is realized in a Lagrangian formulation, see [6], for example.

In short, our approach can be described as follows. We pass to the limit with respect to the class of admissible perturbations in an efficiently arranged version of the difference quotient of the cost J with respect

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to the geometry perturbation. The constraint $E(u,\Omega)=0$ is observed by introducing an appropriately defined adjoint equation. In this process, differentiability of the state with respect to the geometric quantities is not used. In fact, we only require Hölder continuity with exponent greater $\frac{1}{2}$ of u with respect to the geometric data. On a technical level we utilize well-known results from the method of mapping and on the differentiation of functionals with respect to geometric quantities.

For comparison we briefly discuss an example using the "chain rule" approach. Consider the cost functional

$$\min_{\Gamma} J(u,\Omega,\Gamma) \equiv \min_{\Gamma} \frac{1}{2}\int_{\Gamma} u^2 \,\mathrm{d}\Gamma \tag{1.2}$$

subject to the constraint $E(u,\Omega)=0$ which is given by the mixed boundary value problem

$$-\Delta u = f, \qquad \text{in } \Omega, \tag{1.3}$$

$$u = 0, \qquad \text{on } \Gamma_0, \tag{1.4}$$

$$\frac{\partial u}{\partial n} = g, \qquad \text{on } \Gamma. \tag{1.5}$$

Here the boundary $\partial\Omega$ of the domain Ω is the disjoint union of a fixed part Γ_0 and the unknown part Γ. A formal differentiation leads to the shape derivative of the cost functional

$$dJ(u,\Omega,\Gamma)h = \int_{\Gamma} u u'_{\Omega} \,\mathrm{d}\Gamma + \frac{1}{2}\int_{\Gamma}\left(\frac{\partial u^2}{\partial n} + \kappa u^2\right) h\cdot n \,\mathrm{d}\Gamma \tag{1.6}$$

where u'_{Ω} denotes the shape derivative of the solution u of (1.3) at Ω with respect to a deformation field h which realizes the feasible perturbations of the reference domain Ω and κ stands for the curvature of Γ. For a thorough discussion of the details we refer to [6,13]. Differentiating formally the constraint $E(u,\Omega)=0$ with respect to the domain one obtains that u'_{Ω} satisfies

$$\begin{aligned} -\Delta u'_{\Omega} &= 0, && \text{in } \Omega,\\ u'_{\Omega} &= 0, && \text{on } \Gamma_0,\\ \frac{\partial u'_{\Omega}}{\partial n} &= \mathrm{div}_{\Gamma}(h\cdot n\,\nabla_{\Gamma} u) + \left(f + \frac{\partial g}{\partial n} + \kappa g\right) h\cdot n, && \text{on } \Gamma, \end{aligned} \tag{1.7}$$

where div_{Γ}, ∇_{Γ} stand for the tangential divergence, respectively the tangential gradient. Introducing a suitably defined adjoint variable and using (1.7) the first term on the right hand side of (1.6) can be manipulated in such a way that $dJ(u,\Omega,\Gamma)h$ can be represented in the form required by the Zolesio-Hadamard structure theorem [6]

$$dJ(u,\Omega,\Gamma)h = \int_{\Gamma} G h\cdot n \,\mathrm{d}\Gamma. \tag{1.8}$$

We emphasize that the kernel G does not involve the shape derivative u'_{Ω} any more. Although u'_{Ω} is only an intermediate quantity a rigorous analysis requires to justify the formal steps in the preceding discussion. In addition one has to verify that the solution of (1.7) actually is the shape derivative of u in the sense of the definition in [13]. These in itself are nontrivial tasks. Furthermore, $u \in H^2(\Omega)$ is not sufficient to justify the formal calculations rendering (1.6) into (1.8). In our approach, however, we utilize only $u \in H^2(\Omega)$ for the characterization of the shape derivative of $J(u,\Omega,\Gamma)$. We return to this example in Section 3.3.

In Section 3.5 we provide an example for the situation where the standard chain rule approach is not applicable due to lack of shape differentiability of the state variable, but our approach allows a rigorous computation of the cost with respect to perturbations of the domain.

In summary, the method that we develop enables us to directly calculate the shape derivative of the cost functional without utilizing the shape derivative of the state u with respect to the geometric variable. Its main ingredients include the weak formulation of the state-equation constraint, the method of mappings and the shape derivatives of the cost functionals. As we shall demonstrate in Section 3 it can readily be applied to a general class of shape optimization problems.

In Section 2 we present the proposed general framework to compute the shape derivative for (1.1). Section 3 contains applications to shape optimization constrained by linear elliptic systems, inverse interface problems, the Bernoulli problem, and shape optimization for the Navier Stokes equations.

2. Shape derivative

Consider the shape optimization problem

$$\min J(u,\Omega,\Gamma) \equiv \int_\Omega j_1(u)\,\mathrm{d}x + \int_\Gamma j_2(u)\,\mathrm{d}s + \int_{\partial\Omega\setminus\Gamma} j_3(u)\,\mathrm{d}s \tag{2.1}$$

subject to the constraint

$$E(u,\Omega) = 0 \tag{2.2}$$

which represents a partial differential equation posed on a domain Ω with boundary $\partial\Omega$. Further Γ is a closed co-dimension one manifold which represents part of $\partial\Omega$ or is strictly inside Ω. We focus on sensitivity analysis of (2.1)–(2.2) with respect to Ω and Γ. The perturbations of Ω will be such that $\partial\Omega\setminus\Gamma$ remains fixed.

To describe the admissible class of geometries, let $U \subset \mathbb{R}^d$ be a fixed bounded domain with $C^{1,1}$-boundary ∂U, or convex and Lipschitzean boundary, and let D be a domain with $C^{1,1}$-boundary $\Gamma := \partial D$, satisfying $\bar{D} \subset U$. For the reference domain Ω we admit either of three cases

(i) $\Omega = D$
(ii) $\Omega = U$
(iii) $\Omega = U\setminus\bar{D}$.

Note that

$$\partial\Omega = (\partial\Omega\cap\Gamma)\,\dot{\cup}\,(\partial\Omega\setminus\Gamma) \subset U\,\dot{\cup}\,\partial U. \tag{2.3}$$

Thus the boundary $\partial\Omega$ for cases (i)–(iii) is given by

(i)' $\partial\Omega = \Gamma\cup\emptyset = \Gamma$
(ii)' $\partial\Omega = \emptyset\cup\partial U = \partial U$
(iii)' $\partial\Omega = \Gamma\cup\partial U$.

To introduce the admissible class of perturbations let $h \in C^{1,1}(\bar{U},\mathbb{R}^d)$ with $h|\partial U = 0$ and define for, $t\in\mathbb{R}$, the mappings $F_t : U \to \mathbb{R}^d$ by the perturbation of identity

$$F_t = id + th. \tag{2.4}$$

Then there exists $\tau > 0$ such that $F_t(U) = U$ and F_t is a diffeomorphism for $|t| < \tau$. Defining the perturbed domains

$$\Omega_t = F_t(\Omega)$$

and the perturbed manifolds as

$$\Gamma_t = F_t(\Gamma),$$

it follows that Γ_t is of class $C^{1,1}$ and $\bar{\Omega}_t \subset U$ for $|t| < \tau$. Note that since $h|\partial U = 0$ the boundary of U remains fixed as t varies, and hence by (2.3)

$$(\partial\Omega)_t\setminus\Gamma_t = \partial\Omega\setminus\Gamma, \quad \text{for} \quad |t| < \tau.$$

Alternatively to (2.4) the perturbations could be described as the flow determined by the initial value problem

$$\dot{\xi}(t) = h(\xi(t))$$
$$\xi(0) = x,$$

with $F_t(x) = \xi(t;0,x)$, *i.e.* by the velocity method.

The Eulerian derivative of J at Ω in the direction of the deformation field h is defined as

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

where u_t satisfies the constraint

$$E(u_t,\Omega_t) = 0. \tag{2.5}$$

The functional J is called shape differentiable at Ω if $dJ(u,\Omega,\Gamma)h$ exists for all $h \in C^{1,1}(\bar{U},\mathbb{R}^d)$ and defines a continuous linear functional on $C^{1,1}(\bar{U},\mathbb{R}^d)$. Using the method of mappings one transforms the perturbed state constraint (2.5) to the fixed domain Ω. For this purpose define

$$u^t = u_t \circ F_t.$$

Then $u^t\colon \Omega \to \mathbb{R}^l$ satisfies an equation on the reference domain Ω which we express as

$$\tilde{E}(u^t,t) = 0, \quad |t| < \tau. \tag{2.6}$$

We suppress the dependence of $\tilde{E}$ on h, because h will denote a fixed vector field throughout. Because of $F_0 = id$ one obtains $u^0 = u$ and

$$\tilde{E}(u^0,0) = E(u,\Omega). \tag{2.7}$$

We axiomatize the above description and impose the following assumptions on $\tilde{E}$, respectively E.

(H1) There is a Hilbert space X and a C^1-function $\tilde{E} : X \times (-\tau,\tau) \to X^*$ such that $E(u_t,\Omega_t) = 0$ is equivalent to

$$\tilde{E}(u^t,t) = 0 \text{ in } X^*,$$

with $\tilde{E}(u,0) = E(u,\Omega)$ for all $u \in X$.

(H2) There exists $0 < \tau_0 \le \tau$ such that for $|t| < \tau_0$ there exists a unique solution $u^t \in X$ to $\tilde{E}(u^t,t) = 0$ and

$$\lim_{t\to 0} \frac{|u^t - u^0|_X}{|t|^{1/2}} = 0.$$

(H3) $E_u(u,\Omega) \in \mathcal{L}(X,X^*)$ satisfies

$$\langle E(v,\Omega) - E(u,\Omega) - E_u(u,\Omega)(v-u), \psi\rangle_{X^*\times X} = \mathcal{O}(|v-u|_X^2)$$

for every $\psi \in X$, where $u, v \in X$.

(H4) $\tilde{E}$ and E satisfy

$$\lim_{t\to 0} \frac{1}{t}\langle \tilde{E}(u^t,t) - \tilde{E}(u,t) - E(u^t,\Omega) + E(u,\Omega), \psi\rangle_{X^*\times X} = 0$$

for every $\psi \in X$, where u^t and u are the solutions of (2.6), respectively (2.2).

In applications (H4) typically results in an assumption on the regularity of the coefficients in the partial differential equation and on the vector-field h. We assume throughout that $X \hookrightarrow L^2(\Omega,\mathbb{R}^l)$ and, in the case that j_2, j_3 are non-trivial, that the elements of X admit traces in $L^2(\Gamma,\mathbb{R}^l)$, respectively $L^2(\partial\Omega \setminus \Gamma,\mathbb{R}^l)$. Typically X will be a subspace of $H^1(\Omega,\mathbb{R}^l)$ for some $l \in \mathbb{N}$.

With regards to the cost functional J we require:

(H5) $j_i \in C^{1,1}(\mathbb{R}^l, \mathbb{R})$, $i = 1, 2, 3$.

As a consequence of (H1)–(H2) we infer that equation (2.5) has a unique solution u_t which is given by $u_t = u^t \circ F_t^{-1}$. Condition (H5) implies that $j_1(u) \in L^2(\Omega)$, $j_1'(u) \in L^2(\Omega)^l$, $j_2(u) \in L^2(\Gamma)$, $j_2'(u) \in L^2(\Gamma)^l$ and $j_3(u) \in L^2(\partial\Omega\backslash\Gamma)$, $j_3'(u) \in L^2(\partial\Omega\backslash\Gamma)^l$ for $u \in X$. Hence the cost functional $J(u, \Omega, \Gamma)$ is well defined for every $u \in X$.

Lemma 2.1. *There is a constant $c > 0$, such that*

$$|j_i(v) - j_i(u) - j_i'(u)(v-u)|_{L^1} \le c|v-u|_X^2$$

hold for all v, $u \in X$, $i = 1, 2, 3$.

Proof. For j_1 the claim follows from

$$\begin{aligned}\int_\Omega |j_1(v) - j_1(u) - j_1'(u)(v-u)|\,\mathrm{d}x &\le \int_\Omega \int_0^1 |j_1'\big(u(x) + s(v(x)-u(x))\big) - j_1'(u(x))|\,\mathrm{d}s|v(x)-u(x)|\,\mathrm{d}x \\ &\le \frac{L}{2}|v-u|_{L^2}^2 \le c|v-u|_X^2,\end{aligned}$$

where $L > 0$ is the Lipschitz constant for j_1'. The same argument is valid also for j_2 and j_3. □

Subsequently we use the following notation

$$\begin{aligned} I_t &= \det DF_t, \qquad A_t = (DF_t)^{-T}, \\ w_t &= I_t|A_t n|, \end{aligned}$$

where DF_t is the Jacobian of F_t and n denotes the outer normal unit vector to Ω. We require additional regularity properties of the transformation F_t. Let $\mathcal{I} = [-\tau_0, \tau_0]$ with τ_0 sufficiently small.

$$\begin{aligned}
&F_0 = id && t \to F_t \in C(\mathcal{I}, C^{1,1}(\bar{U}, \mathbb{R}^d)) \\
&t \to F_t \in C^1(\mathcal{I}, C^1(\bar{U}, \mathbb{R}^d)) && t \to F_t^{-1} \in C(\mathcal{I}, C^1(\bar{U}, \mathbb{R}^d)) \\
&t \to I_t \in C^1(\mathcal{I}, C(\bar{U})) && t \to A_t \in C(\mathcal{I}, C(\bar{U}, \mathbb{R}^{d\times d})) \\
&t \to w_t \in C(\mathcal{I}, C(\Gamma)) && \qquad (2.8) \\
&\frac{\mathrm{d}}{\mathrm{d}t} F_t|_{t=0} = h && \frac{\mathrm{d}}{\mathrm{d}t} F_t^{-1}|_{t=0} = -h \\
&\frac{\mathrm{d}}{\mathrm{d}t} DF_t|_{t=0} = Dh && \frac{\mathrm{d}}{\mathrm{d}t} DF_t^{-1}|_{t=0} = \frac{\mathrm{d}}{\mathrm{d}t}(A_t)^T|_{t=0} = -Dh \\
&\frac{\mathrm{d}}{\mathrm{d}t} I_t|_{t=0} = \operatorname{div} h && \frac{\mathrm{d}}{\mathrm{d}t} w_t|_{t=0} = \operatorname{div}_\Gamma h.
\end{aligned}$$

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

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

The properties (2.8) are easily verified if F_t is specified by perturbing the identity. As a consequence of (2.8) there exists $\alpha > 0$ such that

$$I_t(x) \ge \alpha, \qquad x \in \bar{U}. \tag{2.9}$$

We furthermore recall the following transformation theorem where we already utilize (2.9).

Lemma 2.2. (1) *Let* $\varphi_t \in L^1(\Omega_t)$*, then* $\varphi_t \circ F_t \in L^1(\Omega)$ *and*

$$\int_{\Omega_t} \varphi_t \, \mathrm{d}x_t = \int_\Omega \varphi_t \circ F_t \, \det DF_t \, \mathrm{d}x.$$

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

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

As the main result of this paper we now formulate the representation of the Eulerian derivative of J.

Theorem 2.1. *Assume that* (H1)–(H5) *hold, that* F *satisfies* (2.8) *and that the adjoint equation*

$$\langle E_u(u,\Omega)\psi, p\rangle_{X^*\times X} - (j_1'(u),\psi)_\Omega - (j_2'(u),\psi)_\Gamma - (j_3'(u),\psi)_{\partial\Omega\setminus\Gamma} = 0, \qquad \psi \in X, \tag{2.10}$$

admits a unique solution $p \in X$*, where* u *is the solution to* (2.2)*. Then the Eulerian derivative of* J *at* Ω *in the direction* $h \in C^{1,1}(\bar U, \mathbb{R}^d)$ *exists and is given by*

$$dJ(u,\Omega,\Gamma)h = -\frac{\mathrm{d}}{\mathrm{d}t}\langle \tilde E(u,t), p\rangle_{X^*\times X}|_{t=0} + \int_\Omega j_1(u) \,\mathrm{div}\, h \,\mathrm{d}x + \int_\Gamma j_2(u)\,\mathrm{div}_\Gamma\, h\,\mathrm{d}s. \tag{2.11}$$

Proof. Referring to (H2) let u^t, $u \in X$ satisfy

$$\tilde E(u^t, t) = E(u,\Omega) = 0 \tag{2.12}$$

for $|t| < \tau_0$. Then $u_t = u^t \circ F_t$ is the solution of (2.5). Utilizing Lemma 2.2 one therefore obtains

$$\begin{aligned}
\frac{1}{t}(J(u_t,\Omega_t,\Gamma_t) - J(u,\Omega,\Gamma)) &= \frac{1}{t}\int_\Omega \big(I_t j_1(u^t) - j_1(u)\big)\,\mathrm{d}x + \frac{1}{t}\int_\Gamma \big(w_t j_2(u^t) - j_2(u)\big)\,\mathrm{d}s \\
&\quad + \frac{1}{t}\int_{\partial\Omega\setminus\Gamma} (j_3(u^t) - j_3(u))\mathrm{d}s \\
&= \frac{1}{t}\int_\Omega \big(I_t(j_1(u^t) - j_1(u) - j_1'(u)(u^t-u)) + (I_t - 1)j_1'(u)(u^t-u) \\
&\quad + j_1'(u)(u^t-u) + (I_t-1)j_1(u)\big)\,\mathrm{d}x \\
&\quad + \frac{1}{t}\int_\Gamma \big(w_t(j_2(u^t) - j_2(u) - j_2'(u)(u^t-u)) + (w_t-1)j_2'(u)(u^t-u) \\
&\quad + j_2'(u)(u^t-u) + (w_t-1)j_2(u)\big)\,\mathrm{d}s \\
&\quad + \frac{1}{t}\int_{\partial\Omega\setminus\Gamma} (j_3(u^t) - j_3(u) - j_3'(u)(u^t-u))\mathrm{d}s \\
&\quad + \frac{1}{t}\int_{\partial\Omega\setminus\Gamma} j_3'(u)(u^t-u)\mathrm{d}s.
\end{aligned} \tag{2.13}$$

Lemma 2.1 and (2.8) result in the estimates

$$\left|\int_\Omega I_t(j_1(u^t)-j_1(u)-j_1'(u)(u^t-u))\,\mathrm{d}x\right|\le c|u^t-u|_X^2$$
$$\left|\int_\Gamma w_t(j_2(u^t)-j_2(u)-j_2'(u)(u^t-u))\,\mathrm{d}s\right|\le c|u^t-u|_X^2,$$
$$\left|\int_{\partial\Omega\setminus\Gamma}(j_3(u^t)-j_3(u)-j_3'(u)(u^t-u))\mathrm{d}s\right|\le c|u^t-u|_X^2 \tag{2.14}$$

where $c>0$ does not depend on t. Employing the adjoint state p one obtains

$$\begin{aligned}(j_1'(u),u^t-u)_\Omega+(j_2'(u),u^t-u)_\Gamma+(j_3'(u),u^t-u)_{\partial\Omega\setminus\Gamma}&=\langle E_u(u,\Omega)(u^t-u),p\rangle_{X^*\times X}\\&=-\langle E(u^t,\Omega)-E(u,\Omega)-E_u(u,\Omega)(u^t-u),p\rangle_{X^*\times X}\\&\quad-\langle\tilde E(u^t,t)-\tilde E(u,t)-E(u^t,\Omega)+E(u,\Omega),p\rangle_{X^*\times X}\\&\quad-\langle\tilde E(u,t)-\tilde E(u,0),p\rangle_{X^*\times X},\end{aligned}\tag{2.15}$$

where we used (2.12). We estimate the ten additive terms on the right hand side of (2.13). Terms one, five and nine converge to zero by (2.14) and (H2). Terms two and six converge to 0 by (2.8) and (H2). For terms four and eight ones uses (2.8). The claim (2.11) now follows by passing to the limit in terms three, seven and ten using (2.15), (H3), (H2), (H4) and (H1). □

Remark 2.1. The proof of Theorem 2.1 reveals that the assumption (H1) can be considerably weakened. In fact all that is needed is the following.

(H1') There is a Hilbert space X and a function $\tilde E: X\times(-\tau,\tau)\to X^*$ such that
  (a) $E(u_t,\Omega_t)=0$ is equivalent to

$$\tilde E(u^t,t)=0 \text{ in } X^*,$$

  with $\tilde E(u,0)=E(u,\Omega)$ for all $u\in X$.
  (b) The mapping $v\to\langle\tilde E(v,0),p\rangle_{X^*\times X}$ is differentiable at $v=u$ and $t\to\langle\tilde E(u,t),p\rangle_{X^*\times X}$ is differentiable at $t=0$, where u is the solution of $E(u,\Omega)=0$ and p satisfies the adjoint equation (2.10).

To check (H2) in specific applications the following result will be useful. It relies on

$$\text{(H6)}\quad\begin{cases}\text{the linearized equation}\\ \langle E_u(u,\Omega)\delta u,\psi\rangle_{X^*\times X}=\langle f,\psi\rangle_{X^*\times X},\qquad \psi\in X\\ \text{admits a unique solution } \delta u\in X \text{ for every } f\in X^*.\end{cases}$$

Note that this condition is more stringent than the assumption of solvability of the adjoint equation in Theorem 2.1 which requires solvability only for a specific right hand side.

Proposition 2.1. *Assume that* (2.2) *admits a unique solution* u *and that* (H6) *is satisfied. Then* (H2) *holds.*

Proof. Let $u\in X$ be the unique solution of (2.2). In view of

$$\tilde E_u(u,0)=E_u(u,\Omega)$$

(H6) implies that $\tilde E_u(u,0)$ is bijective. The claim follows from the implicit function theorem. □

Computing the derivative $\frac{\mathrm{d}}{\mathrm{d}t}\langle\tilde{E}(u,t),p\rangle_{X^*\times X}|_{t=0}$ in (2.11) can be facilitated by transforming the expressions $\tilde{E}(u,t)$ and p back to $E(u\circ F_t^{-1},\Omega_t)$ and $p\circ F_t^{-1}$, and utilizing the following well known differentiation rules:

Lemma 2.3 [6]**.** (1) *Let $f\in C(\mathcal{I},W^{1,1}(U))$ and assume that $f_t(0)$ exists in $L^1(U)$, then*

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_t} f(t,x)\,\mathrm{d}x|_{t=0}=\int_\Omega f_t(0,x)\,\mathrm{d}x+\int_\Gamma f(0,x)\,h\cdot n\,\mathrm{d}s.$$

(2) *Let $f\in C(\mathcal{I},W^{2,1}(U))$ and assume that $f_t(0)$ exists in $W^{1,1}(U)$. Then*

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Gamma_t} f(t,x)\,\mathrm{d}s|_{t=0}=\int_\Gamma f_t(0,x)\,\mathrm{d}s+\int_\Gamma\left(\frac{\partial}{\partial n}f(0,s)+\kappa f(0,s)\right)\,h\cdot n\,\mathrm{d}s,$$

where κ stands for the additive curvature of Γ.

The first part of the theorem is valid also for domains Ω with Lipschitz continuous boundary. The additional $C^{1,1}$ regularity is used as sufficient condition in [6] for (2).

In the examples below $f(t,\cdot)$ will be typically given by expressions of the form

$$\mu v\circ F_t^{-1},\quad \mu\partial_i(v\circ F_t^{-1})\partial_j(w\circ F_t^{-1}),\quad v\circ F_t^{-1}w\circ F_t^{-1}\partial_i(z\circ F_t^{-1})$$

where $\mu\in H^1(U)$ and v, z and $w\in H^2(U)$ are extensions of elements in $H^2(\Omega)$. The assumptions of Lemma 2.3 can be verified using the following result.

Lemma 2.4 [13]**.** (1) *Let $u\in L^p(U)$ then $t\to u\circ F_t^{-1}\in C(\mathcal{I},L^p(U))$, $1\le p<\infty$.*
(2) *Let $u\in H^2(U)$ then $t\to u\circ F_t^{-1}\in C(\mathcal{I},H^2(U))$.*
(3) *Let $u\in H^2(U)$ then $\frac{\mathrm{d}}{\mathrm{d}t}(u\circ F_t^{-1})|_{t=0}$ exists in $H^1(U)$ and is given by*

$$\frac{\mathrm{d}}{\mathrm{d}t}(u\circ F_t^{-1})|_{t=0}=-(Du)\,h.$$

As a consequence we note that $\frac{\mathrm{d}}{\mathrm{d}t}\partial_i\big((u\circ F_t^{-1})\big)|_{t=0}$ exists in $L^2(U)$ and is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\partial_i\big((u\circ F_t^{-1})\big)|_{t=0}=-\partial_i(Du\,h),\qquad i=1,\dots,d.$$

In the next section ∇u stands for $(Du)^T$ where u is either a scalar or vector valued function. To enhance readability we use two symbols for the inner product in $\mathbb{R}^d$, (x,y) respectively $x\cdot y$. The latter will only be utilized in the case of nested inner products.

3. Examples

Throughout the examples section it is assumed that (H5) is satisfied and that the regularity assumptions of Section 2 for D, Ω and U hold. If J does not depend on Γ we write $J(u,\Omega)$ in place of $J(u,\Omega,\Gamma)$.

3.1. Elliptic Dirichlet boundary value problem

As a first example we consider the volume functional

$$J(u,\Omega)=\int_\Omega j_1(u)\,\mathrm{d}x$$

subject to the constraint

$$(\mu\nabla u,\nabla\psi)_\Omega-(f,\psi)_\Omega=0, \tag{3.1}$$

where $X = H_0^1(\Omega)$, $f \in H^1(U)$ and $\mu \in C^1(\bar{U}, \mathbb{R}^{d\times d})$ such that $\mu(x)$ is symmetric and uniformly positive definite. Here $\Omega = D$ and $\Gamma = \partial\Omega$. Thus $E(u,\Omega) : X \to X^*$ is given by

$$\langle E(u,\Omega), \psi\rangle_{X^*\times X} = (\mu\nabla u, \nabla\psi)_\Omega - (f,\psi)_\Omega.$$

The equation on the perturbed domain is determined by

$$\begin{aligned}\langle E(u_t,\Omega_t), \psi_t\rangle_{X_t^*\times X_t} &= \int_{\Omega_t} (\mu\nabla u_t, \nabla\psi_t)\,\mathrm{d}x_t - \int_{\Omega_t} f\psi_t\,\mathrm{d}x_t \\ &= \int_\Omega (\mu^t A_t\nabla u^t, A_t\nabla\psi^t) I_t\,\mathrm{d}x - \int_\Omega f^t\psi^t I_t\,\mathrm{d}x \equiv \langle \tilde{E}(u^t,t), \psi^t\rangle_{X^*,X},\end{aligned} \tag{3.2}$$

for any $\psi_t \in X_t$, with $u^t = u_t \circ F_t$, $\mu^t = \mu\circ F_t$, $f^t = f\circ F_t$ and $X_t = H_0^1(\Omega_t)$. Here we used that $\nabla u_t = (A_t\nabla u^t)\circ F_t^{-1}$ and Lemma 2.3. (H1) is a consequence of (2.8), (3.2) and the smoothness of μ and f. Since (3.1) admits a unique solution and (H6) holds, Proposition 2.1 implies (H2). Since $\tilde{E}$ is linear in u assumption (H3) follows. For the verification of (H4) observe that

$$\begin{aligned}\langle \tilde{E}(u^t,t) - \tilde{E}(u,t) - E(u^t,\Omega) + E(u,\Omega), \psi\rangle_{X^*\times X} &= ((\mu^t I_t A_t - \mu)\nabla(u^t-u), A_t\nabla\psi)_\Omega \\ &\quad + (\mu\nabla(u^t-u), (A_t - I)\nabla\psi).\end{aligned}$$

Hence (H4) follows from differentiability of μ, (2.8) and (H2).

In view of Theorem 2.1 we have to compute $\frac{\mathrm{d}}{\mathrm{d}t}\langle\tilde{E}(u,t),p\rangle_{X^*\times X}|_{t=0}$ for which we use the representation on Ω_t in (3.2). Recall that the solution u of (3.1) as well as the adjoint state p, defined by

$$(\mu\nabla p, \nabla\psi)_\Omega = (j_1'(u), \psi)_\Omega, \qquad \psi \in H_0^1(\Omega) \tag{3.3}$$

belong to $H^2(\Omega)\cap H_0^1(\Omega)$. Since $\Omega \in C^{1,1}$ (actually Lipschitz continuity of the boundary would suffice), u as well as p can be extended to functions in $H^2(U)$, which we again denote by the same symbol. Therefore Lemma 2.3(1) and Lemma 2.4 entail that

$$\begin{aligned}&\tfrac{\mathrm{d}}{\mathrm{d}t}\langle\tilde{E}(u,t),p\rangle_{X^*\times X}|_{t=0} = \tfrac{\mathrm{d}}{\mathrm{d}t}\big(\textstyle\int_{\Omega_t}(\mu\nabla(u\circ F_t^{-1}), \nabla(p\circ F_t^{-1}))\,\mathrm{d}x_t - \int_{\Omega_t} fp\circ F_t^{-1}\mathrm{d}x_t\big)|_{t=0} \\ &= \textstyle\int_\Gamma (\mu\nabla u, \nabla p)\,(h,n)\,\mathrm{d}s + \int_\Omega \big((\mu\nabla(-\nabla u\cdot h), \nabla p) + \big(\mu\nabla u, \nabla(-\nabla p\cdot h)\big) + f(\nabla p, h)\,\big)\,\mathrm{d}x.\end{aligned} \tag{3.4}$$

Note that $\nabla u\cdot h$ as well as $\nabla p\cdot h$ do not belong to $H_0^1(\Omega)$ but they are elements of $H^1(\Omega)$. Therefore Green's theorem implies

$$\begin{aligned}\int_\Omega \big((\mu\nabla(-\nabla u\cdot h), \nabla p) + (\mu\nabla u, \nabla(-\nabla p\cdot h)) + f(\nabla p,h)\big)\,\mathrm{d}x &= \int_\Omega \mathrm{div}(\mu\nabla p)\,(\nabla u,h)\,\mathrm{d}x - \int_\Gamma (\mu\nabla p,n)(\nabla u,h)\,\mathrm{d}s \\ &\quad + \int_\Omega (\mathrm{div}(\mu\nabla u)+f)\,(\nabla p,h)\,\mathrm{d}x - \int_\Gamma (\mu\nabla u,n)\,(\nabla p,h)\,\mathrm{d}s \\ &= -\int_\Omega j_1'(u)\,(\nabla u,h)\,\mathrm{d}x - 2\int_\Gamma (\mu n,n)\frac{\partial u}{\partial n}\frac{\partial p}{\partial n}\,(h,n)\,\mathrm{d}s.\end{aligned} \tag{3.5}$$

Above we used the strong form of (3.1) and (3.3) in $L^2(\Omega)$ as well as the identities

$$(\mu\nabla u, n) = (\mu n,n)\frac{\partial u}{\partial n} \qquad (\nabla u, h) = \frac{\partial u}{\partial n}(h,n)$$

(together with the ones with u and p interchanged) which follow from $u,\, p \in H_0^1(\Omega)$. Applying Theorem 2.1 results in

$$\begin{aligned} dJ(u,\Omega)h &= -\frac{\mathrm{d}}{\mathrm{d}t}\langle \tilde{E}(u,t), p\rangle_{X^*,X}|_{t=0} + \int_\Omega j_1(u)\,\mathrm{div}\, h\,\mathrm{d}x \\ &= \int_\Gamma (\mu n, n)\frac{\partial u}{\partial n}\frac{\partial p}{\partial n}\,(h,n)\,\mathrm{d}s + \int_\Omega (j_1'(u)(\nabla u, h) + j_1(u)\,\mathrm{div}\, h)\,\mathrm{d}x \\ &= \int_\Gamma (\mu n, n)\frac{\partial u}{\partial n}\frac{\partial p}{\partial n}\,(h,n)\,\mathrm{d}s + \int_\Omega \mathrm{div}(j_1(u)h)\,\mathrm{d}x, \end{aligned}$$

and the Stokes theorem yields the final result

$$dJ(u,\Omega)h = \int_\Gamma \Big((\mu n, n)\frac{\partial u}{\partial n}\frac{\partial p}{\partial n} + j_1(u)\Big)\,(h,n)\,\mathrm{d}s.$$

Remark 3.1. If we were to be content with a representation of the shape variation in terms of volume integrals we could take the expression for $\frac{\mathrm{d}}{\mathrm{d}t}\tilde{E}(u,t)|_{t=0}$ given in (3.4) and bypass the use of Green's theorem in (3.5). The regularity requirement on the domain then results from $u \in H^2(\Omega)$, $p \in H^2(\Omega)$. In [1] the shape derivative in terms of the volume integral is referred to as the weak shape derivative, whereas the final form in terms of the boundary integrals is called the strong shape derivative.

3.2. **Inverse interface problem**

We consider an inverse interface problem which is motivated by electrical impedance tomography. Let $U = \Omega = (-1,1)\times(-1,1)$ and $\partial U = \partial\Omega$. Further let the domain $D = \Omega^-$, with $\bar{\Omega}^- \subset U$, represent the inhomogeneity of the conducting medium and set $\Omega^+ = U \setminus \bar{\Omega}^-$. We assume that Ω^- is a simply connected domain of class $C^{1,1}$ with boundary Γ which represents the interface between Ω^- and Ω^+. The inverse problem consists of identifying the unknown interface Γ from measurements z which are taken on the boundary ∂U. This can be formulated as

$$\min J(u,\Omega) \equiv \int_{\partial U} (u-z)^2\,\mathrm{d}s \tag{3.6}$$

subject to the constraint

$$\begin{aligned} &-\mathrm{div}(\mu\nabla u) = 0, && \text{in } \Omega^-\cup\Omega^+, \\ &[u] = 0, \quad \left[\mu\frac{\partial u}{\partial n^-}\right] = 0 && \text{on } \Gamma, \\ &\frac{\partial u}{\partial n} = g, && \text{on } \partial U, \end{aligned} \tag{3.7}$$

where $g \in H^{1/2}(\partial U)$, $z \in L^2(\partial U)$, with $\int_{\partial U} g = \int_{\partial U} z = 0$, with $[v] = v^+ - v^-$ on Γ and $n^{+/-}$ standing for the unit outer normals to $\Omega^{+/-}$. The conductivity μ is given by

$$\mu(x) = \begin{cases} \mu^- & x\in\Omega^-, \\ \mu^+ & x\in\Omega^+, \end{cases}$$

for some positive constants μ^- and μ^+. In the context of the general framework of Section 2 we have $j_1 = j_2 = 0$ and $j_3 = (u-z)^2$. Clearly (3.7) admits a unique solution $u \in H^1(U)$ with $\int_{\partial U} u = 0$. Its restrictions to Ω^+ and Ω^- will be denoted by u^+ and u^-, respectively. It turns out that the regularity of $u^\pm$ is better than the one of u.

Proposition 3.1. *Let Ω and $\Omega^{\pm}$ be as described above. Then the solution $u \in H^1(U)$ of (3.7) satisfies*

$$u^{\pm} \in H^2(\Omega^{\pm}).$$

Proof. Let Γ_H be the smooth boundary of a domain Ω_H with

$$\overline{\Omega^-} \subset \Omega_H \subset \overline{\Omega_H} \subset U.$$

Then $u|\Gamma_H \in H^{3/2}\left(\Gamma_H\right)$. The problem

$$\begin{cases} -\operatorname{div}(\mu^+ \nabla u_H) = 0 & \text{in} \quad U \backslash \overline{\Omega_H} \\ \frac{\partial u_H}{\partial n} = g \quad \text{on} \quad \partial U, \quad u_H = u|\Gamma_H & \text{on} \quad \Gamma_H, \end{cases}$$

has a unique solution $u_H \in H^2(U \backslash \overline{\Omega_H})$ with $u^H = u^+|_{\Omega_H}$. Therefore,

$$b := u|\partial U = u_H|\partial U \in H^{3/2}(\partial U).$$

Then the solution u to (3.7) coincides with the solution to

$$\begin{cases} -\operatorname{div}(\mu \nabla u) = 0, & \text{in} \quad \Omega^- \cup \Omega^+, \\ [u] = 0, \ [\mu \frac{\partial u}{\partial n^-}] = 0 & \text{on } \Gamma, \\ u = b, & \text{on} \quad \partial U. \end{cases}$$

We now argue that $u^{\pm} \in H^2(\Omega^{\pm})$. Let $u_b \in H^2(U)$ denote the solution to

$$\begin{cases} -\Delta u_b = 0 & \text{in } U \\ u_b = b & \text{on } \partial U. \end{cases}$$

Define $w \in H_0^1(U)$ as the unique solution to the interface problem

$$\begin{cases} -\operatorname{div}(\mu \nabla w) = 0 \quad \text{in} \quad \Omega \\ [w] = 0, \quad [\mu \frac{\partial w}{\partial n^-}] = -[\mu \frac{\partial u_b}{\partial n^-}] \quad \text{on} \quad \Gamma. \\ w = 0 \quad \text{on} \quad \partial U. \end{cases} \tag{3.8}$$

Then $u_b \in H^2(\Omega)$ implies $[\mu \frac{\partial u_b}{\partial n^-}] \in H^{1/2}(\Gamma)$. By [2] equation (3.8) has a unique solution $w \in H_0^1(U)$ with the additional regularity $w^{\pm} \in H^2(\Omega^{\pm})$. Consequently $u = w + u_b$ satisfies $u|\partial\Omega = g$ and $u^{\pm} \in H^2(\Omega^{\pm})$, as desired. In an analogous way $p^{\pm} \in H^2(\Omega^{\pm})$. □

To consider the inverse problem (3.6), (3.7) within the general framework of Section 2 we set $X = \{v \in H^1(U) \colon \int_{\partial U}^{v} = 0\}$ and define

$$\langle E(u, \Omega), \psi \rangle_{X^* \times X} = (\mu \nabla u, \nabla \psi)_U - (g, \psi)_{\partial U},$$

respectively

$$\begin{aligned} &\langle \tilde{E}(u, t), \psi \rangle_{X^* \times X} = (\mu^t A_t \nabla u, A_t \nabla \psi I_t)_U - (g, \psi)_{\partial U} \\ &= (\mu^+ \nabla(u \circ F_t^{-1}), \nabla(\psi \circ F_t^{-1}))_{\Omega_t^+} + (\mu^- \nabla(u \circ F_t^{-1}), \nabla(\psi \circ F_t^{-1}))_{\Omega_t^-} - (g, \psi)_{\partial U}. \end{aligned}$$

Note that the boundary term is not affected by the transformation F_t since the deformation field h vanishes on ∂U. The adjoint state is given by

$$\begin{aligned} &-\operatorname{div}(\mu\nabla p) = 0, && \text{in } \Omega^- \cup \Omega^+, \\ &[p] = 0, \quad \left[\mu\frac{\partial p}{\partial n^-}\right] = 0 && \text{on } \Gamma, \\ &\frac{\partial p}{\partial n} = 2(u-z) && \text{on } \partial U, \end{aligned} \tag{3.9}$$

respectively

$$(\mu\nabla p, \nabla\psi)_U = 2(u-z,\psi)_{\partial U}, \qquad \text{for } \psi \in X. \tag{3.10}$$

Assumption (H4) requires us to consider

$$\begin{aligned} \frac{1}{t}|\langle \tilde{E}(u^t-u,t) - E(u^t-u,\Omega),\psi\rangle| &\le \frac{1}{t}\int_{\Omega^+} |(\mu^+ I_t A_t\nabla(u^t-u), A_t\nabla\psi) - (\mu^+\nabla(u^t-u),\nabla\psi)|\,\mathrm{d}x \\ &\quad + \frac{1}{t}\int_{\Omega^-} |(\mu^- I_t A_t\nabla(u^t-u), A_t\nabla\psi) - (\mu^+\nabla(u^t-u),\nabla\psi)|\,\mathrm{d}x \\ &\le \mu^+\int_{\Omega^+}\left|\left(\frac{1}{t}(I_tA_t - I)\nabla(u^t-u), A_t\nabla\psi\right)\right|\,\mathrm{d}x \\ &\quad + \mu^+\int_{\Omega^+}|(\nabla(u^t-u), \frac{1}{t}(A_t-I)\nabla\psi)|\,\mathrm{d}x \\ &\quad + \mu^-\int_{\Omega^-}\left|\left(\frac{1}{t}(I_tA_t - I)\nabla(u^t-u), A_t\nabla\psi\right)\right|\,\mathrm{d}x \\ &\quad + \mu^-\int_{\Omega^-}|(\nabla(u^t-u), \frac{1}{t}(A_t-I)\nabla\psi)|\,\mathrm{d}x. \end{aligned}$$

The right hand side of this inequality converges to 0 as $t \to 0$ by (2.8). The remaining assumptions can be verified as in Example 3.1 and thus Theorem 2.1 is applicable. By Proposition 3.1 the restrictions $u^\pm = u|_{\Omega^\pm}$, $p^\pm = p|_{\Omega^\pm}$ satisfy $u^\pm$, $p^\pm \in H^2(\Omega^\pm)$. Using Lemma 2.3 we find that

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle\tilde{E}(u,t),p\rangle_{X^*\times X}|_{t=0} &= \int_{\partial\Omega^+}(\mu^+\nabla u^+,\nabla p^+)(h,n^+)\,\mathrm{d}s - \int_{\Omega^+}(\mu^+\nabla(\nabla u^+\cdot h),\nabla p^+)\,\mathrm{d}x \\ &\quad - \int_{\Omega^+}(\mu^+\nabla u^+,\nabla(\nabla p^+\cdot h))\,\mathrm{d}x + \int_{\partial\Omega^-}(\mu^-\nabla u^-,\nabla p^-)(h,n^-)\,\mathrm{d}s \\ &\quad - \int_{\Omega^-}(\mu^-\nabla(\nabla u^-\cdot h),\nabla p^-)\,\mathrm{d}x - \int_{\Omega^-}(\mu^-\nabla u^-,\nabla(\nabla p^-\cdot h))\,\mathrm{d}x \\ &= \int_\Gamma[\mu\nabla u,\nabla p](h,n^+)\,\mathrm{d}s - \int_{\Omega^+}\mu^+\big(\nabla(\nabla u^+\cdot h),\nabla p^+) + (\nabla u^+,\nabla(\nabla p^+\cdot h)\big)\,\mathrm{d}x \\ &\quad - \int_{\Omega^-}\mu^-\big(\nabla(\nabla u^-\cdot h),\nabla p^-) + (\nabla u^-,\nabla(\nabla p^-\cdot h)\big)\,\mathrm{d}x. \end{aligned}$$

Applying Green's formula as in Example 3.1 (observe that $(\nabla u, h)$, $(\nabla p, h) \notin H^1(U)$) together with (3.9) results in

$$
\begin{aligned}
-\int_{\Omega^+} (\mu^+(\nabla(\nabla u^+ \cdot h), \nabla p^+))\,\mathrm{d}x - \int_{\Omega^-} (\mu^-(\nabla(\nabla u^- \cdot h), \nabla p^-))\,\mathrm{d}x \\
= \int_{\Omega^+} \operatorname{div}(\mu^+\nabla p^+)(\nabla u^+, h)\,\mathrm{d}x + \int_{\Omega^-} \operatorname{div}(\mu^-\nabla p^-)(\nabla u^-, h)\,\mathrm{d}x \\
- \int_{\partial\Omega^+} (\mu^+\nabla p^+, n^+)(\nabla u^+, h)\,\mathrm{d}s - \int_{\partial\Omega^-} (\mu^-\nabla p^-, n^-)(\nabla u^-, h)\,\mathrm{d}s \\
= -\int_\Gamma \left[\mu \frac{\partial p}{\partial n^+}(\nabla u, h)\right]\,\mathrm{d}s.
\end{aligned}
$$

In the last step we utilize $h = 0$ on ∂U. Similarly we obtain

$$
-\int_{\Omega^+} (\mu^+(\nabla u^+, \nabla(\nabla p^+ \cdot h)))\,\mathrm{d}x - \int_{\Omega^-} (\mu^-(\nabla u^-, \nabla(\nabla p^- \cdot h)))\,\mathrm{d}x = -\int_\Gamma \left[\mu \frac{\partial u}{\partial n^+}(\nabla p, h)\right]\,\mathrm{d}s.
$$

Collecting terms results in

$$
dJ(u,\Omega)h = -\int_\Gamma [\mu(\nabla u, \nabla p)]\,(h, n^+)\,\mathrm{d}s + \int_\Gamma \left(\left[\mu \frac{\partial p}{\partial n^+}(\nabla u, h)\right] + \left[\mu \frac{\partial u}{\partial n^+}(\nabla p, h)\right]\right)\,\mathrm{d}s.
$$

The identity

$$
[ab] = [a]b^+ + a^-[b] = a^+[b] + [a]b^-
$$

implies

$$
[ab] = 0 \qquad \text{if } [a] = [b] = 0.
$$

Hence the transition conditions

$$
\begin{aligned}
\left[\mu \frac{\partial u}{\partial n^+}\right] &= \left[\frac{\partial u}{\partial \tau}\right] = 0 \\
\left[\mu \frac{\partial p}{\partial n^+}\right] &= \left[\frac{\partial p}{\partial \tau}\right] = 0,
\end{aligned}
\tag{3.11}
$$

where $\frac{\partial}{\partial \tau}$ stands for the tangential derivative imply

$$
\begin{aligned}
\left[\mu \frac{\partial p}{\partial n^+}(\nabla u, h)\right] &= \left[\mu \frac{\partial p}{\partial n^+}\frac{\partial u}{\partial n^+}(h, n^+) + \mu \frac{\partial p}{\partial n^+}\frac{\partial u}{\partial \tau}(h, \tau)\right] \\
&= \left[\mu \frac{\partial p}{\partial n^+}\frac{\partial u}{\partial n^+}(h, n^+)\right] + \left[\mu \frac{\partial p}{\partial n^+}\frac{\partial u}{\partial \tau}(h, \tau)\right] \\
&= \left[\mu \frac{\partial p}{\partial n^+}\frac{\partial u}{\partial n^+}\right](h, n^+),
\end{aligned}
$$

and analogously

$$
\left[\mu \frac{\partial u}{\partial n^+}(\nabla p, h)\right] = \left[\mu \frac{\partial p}{\partial n^+}\frac{\partial u}{\partial n^+}\right](h, n^+),
$$

which entails

$$
\begin{aligned}
dJ(u,\Omega)h &= -\int_\Gamma [\mu(\nabla u,\nabla p)]\,(h,n^+)\,\mathrm{d}s + 2\int_\Gamma \left[\mu\frac{\partial p}{\partial n^+}\frac{\partial u}{\partial n^+}\right](h,n^+)\,\mathrm{d}s\\
&= -\int_\Gamma \left[\mu\frac{\partial u}{\partial \tau}\frac{\partial p}{\partial \tau}\right](h,n^+)\,\mathrm{d}s + \int_\Gamma \left[\mu\frac{\partial u}{\partial n^+}\frac{\partial p}{\partial n^+}\right](h,n^+)\,\mathrm{d}s\\
&= -\int_\Gamma [\mu]\frac{\partial u}{\partial \tau}\frac{\partial p}{\partial \tau}\,(h,n^+)\,\mathrm{d}s + \int_\Gamma \left[\mu\frac{\partial u}{\partial n^+}\frac{\partial p}{\partial n^+}\right](h,n^+)\,\mathrm{d}s.
\end{aligned}
$$

In view of (3.11) this can be rearranged as

$$
\begin{aligned}
&-[\mu]\frac{\partial u}{\partial \tau}\frac{\partial p}{\partial \tau} + \left[\mu\frac{\partial u}{\partial n^+}\frac{\partial p}{\partial n^+}\right]\\
&= -\mu^+\frac{\partial u}{\partial \tau}\frac{\partial p}{\partial \tau} + \mu^-\frac{\partial u}{\partial \tau}\frac{\partial p}{\partial \tau} + \mu^+\frac{\partial u^+}{\partial n^+}\frac{\partial p^+}{\partial n^+} - \mu^-\frac{\partial u^-}{\partial n^+}\frac{\partial p^-}{\partial n^+}\\
&= -\mu^+\left(\frac{\partial u}{\partial \tau}\frac{\partial p}{\partial \tau} + \frac{1}{2}\left(\frac{\partial u^+}{\partial n^+}\frac{\partial p^-}{\partial n^+} + \frac{\partial u^-}{\partial n^+}\frac{\partial p^+}{\partial n^+}\right)\right)\\
&\quad + \mu^-\left(\frac{\partial u}{\partial \tau}\frac{\partial p}{\partial \tau} + \frac{1}{2}\left(\frac{\partial u^-}{\partial n^+}\frac{\partial p^+}{\partial n^+} + \frac{\partial u^+}{\partial n^+}\frac{\partial p^-}{\partial n^+}\right)\right)\\
&= -\frac{1}{2}[\mu]\left((\nabla u^+,\nabla p^-) + (\nabla u^-,\nabla p^+)\right)
\end{aligned}
$$

which gives the representation

$$
\begin{aligned}
dJ(u,\Omega,\Gamma)h &= -\frac{1}{2}\int_\Gamma [\mu]\big((\nabla u^+,\nabla p^-) + (\nabla u^-,\nabla p^+)\big)\,(h,n^+)\,\mathrm{d}s\\
&= -\int_\Gamma [\mu](\nabla u^+,\nabla p^-)\,(h,n^+)\,\mathrm{d}s.
\end{aligned}
$$

3.3. **Elliptic systems**

Here we consider a domain $\Omega = U\setminus D$, where $\bar{D}\subset U$ and the boundaries ∂U and $\Gamma = \partial D$ are assumed to be $C^{1,1}$ regular.

We consider the optimization problem

$$
\min J(u,\Omega,\Gamma) \equiv \int_\Omega j_1(u)\,\mathrm{d}x + \int_\Gamma j_2(u)\,\mathrm{d}s
$$

where u is the solution of the elliptic system

$$
\langle E(u,\Omega),\psi\rangle_{X^*\times X} = \int_\Omega \big(a(x,\nabla u,\nabla\psi) - (f,\psi)\big)\,\mathrm{d}x - \int_\Gamma (g,\psi)\,\mathrm{d}s = 0 \tag{3.12}
$$

in $X = \{v\in H^1(\Omega)^l : v|_{\partial U} = 0\}$. Above ∇u stands for $(Du)^T$. We require $f\in H^1(U)^l$ and that g is the trace of a given function $G\in H^2(U)^l$. Furthermore we assume that $a\colon \bar{U}\times\mathbb{R}^{d\times d}\times\mathbb{R}^{d\times d}$ satisfies

(1) $a(\cdot,\xi,\eta)$ is continuously differentiable on $\bar{U}$ for every $\xi,\eta\in\mathbb{R}^{d\times d}$.
(2) $a(x,\cdot,\cdot)$ defines a bilinear form on $\mathbb{R}^{d\times d}\times\mathbb{R}^{d\times d}$ which is uniformly bounded in $x\in\bar{U}$.
(3) $a(x,\cdot,\cdot)$ is uniformly coercive for all $x\in\bar{U}$.

In the case of linear elasticity a is given by

$$
a(x,\nabla u,\nabla\psi) = \lambda\,\mathrm{tr}\,e(u)\,\mathrm{tr}\,e(\psi) + 2\mu\,e(u):e(\psi),
$$

where $e(u) = \frac{1}{2}(\nabla u + (\nabla u)^T)$, and λ, μ are the positive Lamé coefficients. In this case a is symmetric, and (3.12) admits a unique solution in $X \cap H^2(\Omega)^l$ for every $f \in L^2(\Omega)^l$ and $g \in H^{\frac{1}{2}}(\partial U)^l$, see *e.g.* [3].

The method of mapping suggests to define

$$\begin{aligned}\langle \tilde{E}(u,t), \psi\rangle_{X^* \times X} &= \int_\Omega \big(a(F_t(x), A_t\nabla u, A_t \nabla\psi) - (f^t, \psi)\big) I_t \,\mathrm{d}x - \int_\Gamma (g^t, \psi) w_t \,\mathrm{d}s \\ &= \int_{\Omega_t} \big(a(x, \nabla(u\circ F_t^{-1}), \nabla(\psi\circ F_t^{-1})) - (f, \psi\circ F_t^{-1})\big)\,\mathrm{d}x - \int_{\Gamma_t} (g, \psi\circ F_t^{-1})\,\mathrm{d}s. \end{aligned} \tag{3.13}$$

The adjoint state is determined by the equation

$$\langle E_u(u,\Omega)\psi, p\rangle_{X^*\times X} = \int_\Omega \big(a(x,\nabla\psi,\nabla p) - j_1'(u)\psi\big)\,\mathrm{d}x - \int_\Gamma j_2'(u)\psi\,\mathrm{d}s = 0, \tag{3.14}$$

$\psi \in X$. Under the regularity assumptions on a equation (3.12) admits a unique solutions in $X \cap H^2(\Omega)^l$ [15]. Moreover the adjoint equation admits a solution for any right hand side in X^* so that Proposition 2.1 is applicable. Assumptions (H1)–(H4) can then be argued as in Section 3.1.

Employing Lemma 2.3 we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle \tilde{E}(u,t), p\rangle_{X^*\times X}|_{t=0} = &-\int_\Omega \big(a(x, \nabla(\nabla u^T h), \nabla p) + a(x, \nabla u, \nabla(\nabla p^T h))\,\mathrm{d}x \\ &+ \int_\Gamma a(x,\nabla u,\nabla p)\,(h,n)\,\mathrm{d}s + \int_\Omega (f, \nabla p^T h)\,\mathrm{d}x - \int_\Gamma (f,p)\,(h,n)\,\mathrm{d}s \\ &+ \int_\Gamma (g, \nabla p^T h)\,\mathrm{d}s - \int_\Gamma \left(\frac{\partial}{\partial n}(g,p) + \kappa(g,p)\right)(h,n)\,\mathrm{d}s.\end{aligned}$$

Since $\nabla u^T h \in X$ and $\nabla p^T h \in X$ this expression can be simplified using (3.12) and (3.14)

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle \tilde{E}(u,t), p\rangle_{X^*\times X}|_{t=0} = &-\int_\Omega j_1'(u)\nabla u^T h\,\mathrm{d}x - \int_\Gamma j_2'(u)\nabla u^T h\,\mathrm{d}s \\ &+ \int_\Gamma \big(a(x,\nabla u,\nabla p) - (f,p)\big)\,(h,n)\,\mathrm{d}s - \int_\Gamma \left(\frac{\partial}{\partial n}(g,p) + \kappa(g,p)\right)(h,n)\,\mathrm{d}s,\end{aligned}$$

which implies

$$\begin{aligned}dJ(u,\Omega,\Gamma)h = &\int_\Omega j_1'(u)\nabla u^T h\,\mathrm{d}x + \int_\Omega j_1(u)\,\mathrm{div}\,h\,\mathrm{d}x \\ &+ \int_\Gamma j_2'(u)\nabla u^T h\,\mathrm{d}s + \int_\Gamma j_2(u)\,\mathrm{div}_\Gamma\,h\,\mathrm{d}s \\ &+ \int_\Gamma \big(-a(x,\nabla u,\nabla p) + (f,p) + \frac{\partial}{\partial n}(g,p) + \kappa(g,p)\big)\,(h,n)\,\mathrm{d}s.\end{aligned}$$

For the third and fourth term the tangential Green's formula, see *e.g.* [12], (or the Appendix of the internal technical report for this paper for a detailed proof in the case of a $C^{1,1}$ boundary only),

$$\int_\Gamma j_2'(u)\nabla u^T h\,\mathrm{d}s + \int_\Gamma j_2(u)\,\mathrm{div}_\Gamma\,h\,\mathrm{d}s = \int_\Gamma \big(\frac{\partial}{\partial n} j_2(u) + \kappa j_2(u)\big)\,(h,n)\,\mathrm{d}s.$$

The first and second term can be combined using the Stokes theorem. Summarizing we finally obtain

$$dJ(u,\Omega,\Gamma)h = \int_\Gamma \big(-a(x,\nabla u,\nabla p) + (f,p) + j_1(u) + \frac{\partial}{\partial n}\big(j_2(u)+(g,p)\big) + \kappa(j_2(u)+(g,p))\big)\,(h,n)\,\mathrm{d}s. \tag{3.15}$$

This example also comprises the shape optimization problem of Bernoulli type

$$\min J(u,\Omega) \equiv \min_\Gamma \int_\Gamma u^2\,\mathrm{d}s$$

where u is the solution of the mixed boundary value problem

$$\begin{array}{cccc} -\Delta u & = & f & \text{in} & \Omega, \\ u & = & 0 & \text{on} & \partial U, \\ \frac{\partial u}{\partial n} & = & g & \text{on} & \Gamma \end{array}$$

which was analyzed with a similar approach in [11]. Here the boundary $\partial\Omega$ of the domain $\Omega \subset \mathbb{R}^2$ is the disjoint union of a fixed part ∂U and an unknown part Γ both with nonempty relative interior. Let the state space X be given by

$$X = \{\varphi \in H^1(\Omega)\colon \varphi = 0 \text{ on } \partial U\}.$$

Then the Eulerian derivative of J is given by (3.15) which reduces to

$$dJ(u,\Omega,\Gamma)h = \int_\Gamma \big(-(\nabla u,\nabla p) + fp + \frac{\partial}{\partial n}(u^2+gp) + \kappa(u^2+gp)\big)\,(h,n)\,\mathrm{d}s.$$

This result coincides with the representation obtained in [11]. The present derivation however is considerably simpler due to a better arrangement of terms in the proof of Theorem 2.1. It is straightforward to adapt the framework to shape optimization problems associated with the exterior Bernoulli problem.

3.4. **Navier-Stokes system**

Consider the stationary Navier-Stokes equations

$$\begin{aligned} -\nu\,\Delta u + (u\cdot\nabla)u + \nabla p = f, &\qquad \text{in } \Omega,\\ \operatorname{div} u = 0, &\qquad \text{in } \Omega,\\ u = 0, &\qquad \text{on } \partial U, \end{aligned} \tag{3.16}$$

on a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 2,3$, with $\nu > 0$ and $f \in H^1(U)$. In the context of the general framework we set $\Omega = D$ and $\Gamma = \partial\Omega$. The variational formulation of (3.16) is given by

Find $(u,p) \in X \equiv H_0^1(\Omega)^d \times L^2(\Omega)/\mathbb{R}$ such that

$$\begin{aligned} \langle E\big((u,p),\Omega\big),(\psi,\chi)\rangle_{X^*\times X} \equiv{}& \nu(\nabla u,\nabla\psi)_\Omega + ((u\cdot\nabla)u,\psi)_\Omega \\ &- (p,\operatorname{div}\psi)_\Omega - (f,\psi)_\Omega + (\operatorname{div} u,\chi)_\Omega = 0 \end{aligned} \tag{3.17}$$

holds for all $(\psi,\chi) \in X$. Let the cost functional J be given by

$$J(u,\Omega) = \int_\Omega j_1(u)\,\mathrm{d}x.$$

Considering (3.17) on a perturbed domain Ω_t mapping the equation back to the reference domain Ω yields the form of $\tilde{E}(u,t)$. Concerning the transformation of the divergence we note that for $\psi_t \in H_0^1(\Omega_t)^d$ and $\psi^t = \psi_t \circ F_t \in H_0^1(\Omega)^d$ one obtains

$$\operatorname{div} \psi_t = (D\psi_i^t A_t^T e_i) \circ F_t^{-1} = ((A_t)_i \nabla \psi_{t,i}) \circ F_t^{-1},$$

where e_i stands for the i-th canonical basis vector in $\mathbb{R}^d$ and $(A_t)_i$ denotes the i-th row of $A_t = (DF_t)^{-T}$. We follow the convention to sum over indices which occur at least twice in a term. Thus one obtains

$$\begin{aligned}\langle \tilde{E}\big((u^t,p^t),t\big),(\psi,\chi)\rangle_{X^*\times X} = \nu(I_t A_t \nabla u^t, A_t \nabla \psi)_\Omega + \big((u^t \cdot A_t \nabla)u^t, I_t \psi\big)_\Omega \\ - \big(p^t, I_t (A_t)_k \nabla \psi_k\big)_\Omega - (f^t I_t, \psi)_\Omega + \big(I_t (A_t)_k \nabla u_k^t, \chi\big)_\Omega = 0,\end{aligned}$$

for all $(\psi,\chi) \in X$.

The adjoint state $(\lambda, q) \in X$ is given by the solution to

$$\langle E'\big((u,p),\Omega\big)(\psi,\chi),(\lambda,q)\rangle_{X^*\times X} = (j_1'(u),\psi)_\Omega$$

which amounts to

$$\nu(\nabla\psi,\nabla\lambda)_\Omega + ((\psi\cdot\nabla)u + (u\cdot\nabla)\psi,\lambda)_\Omega - (\chi,\operatorname{div}\lambda)_\Omega + (\operatorname{div}\psi,q)_\Omega = (j_1'(u),\psi)_\Omega, \tag{3.18}$$

for all $(\psi,\chi) \in X$. Integrating by parts one obtains

$$((u\cdot\nabla)\psi,\lambda)_\Omega = -\int_\Omega \psi\cdot\lambda \operatorname{div} u \,\mathrm{d}x - \int_\Omega \psi\cdot((u\cdot\nabla)\lambda)\,\mathrm{d}x + \int_\Gamma (\psi\cdot\lambda)\,(u\cdot n)\,\mathrm{d}s = -(\psi,(u\cdot\nabla)\lambda)_\Omega$$

because $u \in H_0^1(\Omega)^d$ and $\operatorname{div} u = 0$. Therefore

$$((\psi\cdot\nabla)u + (u\cdot\nabla)\psi,\lambda)_\Omega = (\psi,(\nabla u)\lambda - (u\cdot\nabla)\lambda)_\Omega \tag{3.19}$$

holds for all $\psi \in H^1(\Omega)^d$. As a consequence the adjoint equation can be interpreted as

$$\begin{aligned}&-\nu\Delta\lambda + (\nabla u)\lambda - (u\cdot\nabla)\lambda - \nabla q = j_1'(u),\\ &\operatorname{div}\lambda = 0,\end{aligned} \tag{3.20}$$

where the first equation holds in $L^2(\Omega)^d$, the second one in $L^2(\Omega)$.

For the evaluation of $\frac{\mathrm{d}}{\mathrm{d}t}\langle \tilde{E}\big((u,p),t\big),(\lambda,q)\rangle_{X^*\times X}|_{t=0}$, (u,p), $(\lambda,q) \in X$ being the solution of (3.17), respectively (3.18), we transform this expression back to Ω_t which gives

$$\begin{aligned}\langle \tilde{E}\big((u,p),t\big),(\lambda,q)\rangle_{X^*\times X} &= \nu(\nabla(u\circ F_t^{-1}),\nabla(\lambda\circ F_t^{-1}))_{\Omega_t} \\ &+ \big((u\circ F_t^{-1}\cdot\nabla)u\circ F_t^{-1},\lambda\circ F_t^{-1}\big)_{\Omega_t} - (\operatorname{div}(\lambda\circ F_t^{-1}),p\circ F_t^{-1})_{\Omega_t} \\ &- (f,\lambda\circ F_t^{-1})_{\Omega_t} + (\operatorname{div}(u\circ F_t^{-1}),q\circ F_t^{-1})_{\Omega_t}.\end{aligned}$$

To verify conditions (H1)–(H4) we introduce the continuous trilinear form $c\colon H_0^1(\Omega)^d \times H_0^1(\Omega)^d \times H_0^1(\Omega)^d$ by $c(u,v,w) = ((u\cdot\nabla)v,w)$ and assume that

$$\nu^2 > \mathcal{N}|f|_{H^{-1}} \text{ and } \nu > \mathcal{M} \tag{3.21}$$

where $\mathcal{N} = \sup_{u,v,w\in H_0^1} \frac{c(u,v,w)}{|u|_{H_0^1}|v|_{H_0^1}|w|_{H_0^1}}$ and $\mathcal{M} = \sup_{v\in H_0^1} \frac{c(v,v,u)}{|v|_{H_0^1}^2}$, with u the solution to (3.16). Condition (H1) is satisfied by construction. If ν is sufficiently large so that the first inequality in (3.21) is satisfied, existence of a unique solution $(u,p) \in H_0^1(\Omega)^d \times L^2(\Omega)/\mathbb{R}$ to (3.16) is guaranteed, see *e.g.* [4,5,14]. The second condition in (3.21) ensures the bijectivity of the linearized operator $E'(u,p)$ [5], and thus (H6) holds. In particular this implies that (H2) holds and that the adjoint equation admits a unique solution. To verify (H3) we consider for arbitrary $(v,q) \in X$ and $(\psi,\chi) \in X$

$$\langle E((v,q),\Omega) - E((u,p),\Omega) - E'((u,p),\Omega)((v,q)-(u,p)),(\psi,\chi)\rangle_{X^*,X} \\ = ((v-u)\cdot\nabla)(v-u),\psi) \le K|\psi|_{H_0^1(\Omega)}|v-u|^2_{H_0^1(\Omega)},$$

where K is an embedding constant, independent of $(v,q) \in X$ and $(\psi,\chi) \in X$. Verifying (H4) requires us to consider the quotient of the following expression with t and taking the limit as $t \to 0$:

$$\nu[(I_tA_t\nabla(u^t-u),A_t\nabla\psi) - (\nabla(u^t-u),\nabla\psi)] + [((u^t\cdot A_t\nabla)u^t,I_t\psi) - ((u^t\cdot\nabla)u^t,\psi) - ((u\cdot A_t\nabla)u,I_t\psi) \\ + ((u\cdot\nabla)u,\psi)] - [(I_t(A_t)_k\nabla\psi_k,p^t-p) + (\operatorname{div}\psi,p^t-p)] \\ + [(I_t(A_t)_k\nabla\ (u_k^t-u_k),\chi) - (\operatorname{div}(u^t-u),\chi)],$$

for $(\psi,\chi) \in X$. The first two term in square brackets can be treated by analogous estimates as in Examples 3.1 and 3.2. Noting that the third and forth square bracket can be estimated quite similarly to each other we give the estimate for the last one:

$$((I_t-1)(A_t)_k\nabla(u_k^t-u_k),\chi) + (((A_t)_k-e_k)\nabla(u_k^t-u_k),\chi)(e_k\nabla(u_k^t-u_k) - \operatorname{div}(u^t-u),\chi)$$

which, upon division by t, tends to 0 for $t \to 0$.

In the following calculation we utilize that (u,p), $(\lambda,q) \in H^2(\Omega)^d \times H^1(\Omega)$, which is satisfied if Γ is C^2, see *e.g.* [4]. Applying Lemma 2.3 results in

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\tilde{E}\big((u,p),t\big),(\lambda,q)\rangle_{X^*\times X}|_{t=0} = \nu(\nabla(-\nabla u^Th),\nabla\lambda)_\Omega + \nu(\nabla u,\nabla(-\nabla\lambda^Th))_\Omega + \nu\int_\Gamma(\nabla u,\nabla\lambda)\,(h,n)\,\mathrm{d}s \\ + \Big(\big((-\nabla u^Th)\cdot\nabla\big)u,\lambda\Big)_\Omega + \big((u\cdot\nabla)(-\nabla u^Th),\lambda\big)_\Omega \\ + \big((u\cdot\nabla)u,-\nabla\lambda^Th\big)_\Omega + \int_\Gamma\big((u\cdot\nabla)u,\lambda\big)\,(h,n)\,\mathrm{d}s \\ - (-\nabla p^Th,\operatorname{div}\lambda)_\Omega - (p,\operatorname{div}(-\nabla\lambda^Th))_\Omega - \int_\Gamma p\operatorname{div}\lambda\,(h,n)\,\mathrm{d}s \\ - (f,-\nabla\lambda^Th)_\Omega - \int_\Gamma f\lambda\,(h,n)\,\mathrm{d}s \\ + (\operatorname{div}(-\nabla u^Th),q)_\Omega + (\operatorname{div}u,-\nabla q^Th)_\Omega + \int_\Gamma q\operatorname{div}u\,(h,n)\,\mathrm{d}s.$$

Since $\operatorname{div}u = \operatorname{div}\lambda = 0$ and u, $\lambda \in H_0^1(\Omega)^d$ this expression simplifies to

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\tilde{E}\big((u,p),t\big),(\lambda,q)\rangle_{X^*\times X}|_{t=0} = \nu(\nabla u,\nabla\psi_\lambda)_\Omega + ((u\cdot\nabla)u,\psi_\lambda)_\Omega - (p,\operatorname{div}\psi_\lambda)_\Omega - (f,\psi_\lambda)_\Omega \\ + \nu(\nabla\psi_u,\nabla\lambda)_\Omega + ((\psi_u\cdot\nabla)u + (u\cdot\nabla)\psi_u,\lambda)_\Omega + (\operatorname{div}\psi_u,q)_\Omega \\ + \nu\int_\Gamma(\nabla u,\nabla\lambda)\,(h,n)\,\mathrm{d}s,$$

where we have used the abbreviation

$$\psi_u = -(\nabla u)^Th, \qquad \psi_\lambda = -(\nabla\lambda)^Th.$$

Note that ψ_u, $\psi_\lambda \in H^1(\Omega)^d$ but not in $H_0^1(\Omega)^d$. Green's formula together with (3.16), (3.20) entails

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\langle \tilde{E}\big((u,p),t\big),(\lambda,q)\rangle_{X^*\times X}|_{t=0} &= (-\nu\Delta u + (u\cdot\nabla u)u + \nabla p - f, \psi_\lambda)_\Omega + \int_\Gamma \nu\left(\frac{\partial u}{\partial n},\psi_\lambda\right)\,\mathrm{d}s + \int_\Gamma p\,(\psi_\lambda,n)\,\mathrm{d}s \\
&\quad + (\psi_u, -\nu\Delta\lambda + (\nabla u)\lambda - (u\cdot\nabla)\lambda - \nabla q)_\Omega + \int_\Gamma \nu\left(\frac{\partial\lambda}{\partial n},\psi_u\right)\,\mathrm{d}s \\
&\quad + \int_\Gamma q\,(\psi_u,n)\,\mathrm{d}s + \nu\int_\Gamma (\nabla u,\nabla\lambda)\,(h,n)\,\mathrm{d}s \\
&= -\int_\Gamma \nu\left(\frac{\partial u}{\partial n},(\nabla\lambda)^T h\right)\,\mathrm{d}s - \int_\Gamma p\,((\nabla\lambda)^T h,n)\,\mathrm{d}s - \int_\Gamma \nu\left(\frac{\partial\lambda}{\partial n},(\nabla u)^T h\right)\,\mathrm{d}s \\
&\quad - \int_\Gamma q\,((\nabla u)^T h,n)\,\mathrm{d}s + \nu\int_\Gamma (\nabla u,\nabla\lambda)\,(h,n)\,\mathrm{d}s - (j_1'(u),(\nabla u)^T h)_\Omega \\
&= -\int_\Gamma \left(\nu\left(\frac{\partial u}{\partial n},\frac{\partial\lambda}{\partial n}\right) + p\left(\frac{\partial\lambda}{\partial n},n\right) + q\left(\frac{\partial u}{\partial n},n\right)\right)(h,n)\,\mathrm{d}s \\
&\quad - (j_1'(u),(\nabla u)^T h)_\Omega.
\end{aligned}$$

Arguing as in example 3.3 one eventually obtains by Theorem 2.1

$$\begin{aligned}
dJ(u,\Omega,\Gamma)h &= \int_\Gamma \left(\nu\left(\frac{\partial u}{\partial n},\frac{\partial\lambda}{\partial n}\right) + p\left(\frac{\partial\lambda}{\partial n},n\right) + q\,(\frac{\partial u}{\partial n},n)\right)(h,n)\,\mathrm{d}s \\
&\quad + \int_\Omega (j_1(u)\,\mathrm{div}\,h + j_1'(u)\nabla u^T h)\,\mathrm{d}x \\
&= \int_\Gamma \left(\nu\left(\frac{\partial u}{\partial n},\frac{\partial\lambda}{\partial n}\right) + p\left(\frac{\partial\lambda}{\partial n},n\right) + q\,(\frac{\partial u}{\partial n},n) + j_1(u)\right)(h,n)\,\mathrm{d}s.
\end{aligned}$$

3.5. **Lack of shape differentiability of the state variable**

We provide an example where the chain rule approach to obtain the shape derivative of the cost functional with respect to perturbations of the domain is not applicable, whereas the technique presented in this paper guarantees shape differentiability of the cost.

We consider the volume functional

$$J(u,\Omega) = \int_\Omega |\nabla u|^2\,\mathrm{d}x \tag{3.22}$$

subject to the constraint

$$\langle E(u,\Omega),\psi\rangle_{X^*\times X} = (\nabla u,\nabla\psi)_\Omega - (f,\psi)_\Omega = 0, \tag{3.23}$$

where $X = H_0^1(\Omega)$. Differently from the previous examples we assume that $\Omega \subset \mathbb{R}^3$ is of class $C^{2,1}$ and $f \in W^{1,q}(\Omega)$ with $q \in (1,\frac{6}{5})$. As a consequence we obtain $u \in W^{3,q}(\Omega)$ [7]. The equation on the perturbed domain is the same as in (3.2), whereas the adjoint equation is given by

$$\langle E_u(u,\Omega)\psi,p\rangle_{X^*\times X} = (\nabla\psi,\nabla p)_\Omega - 2(\nabla u,\nabla\psi)_\Omega = 0, \qquad \psi\in X, \tag{3.24}$$

which can be interpreted as

$$\begin{aligned}
\Delta p &= 2\Delta u, \quad &&\text{in } \Omega,\\
p &= 0, &&\text{on } \Gamma.
\end{aligned} \tag{3.25}$$

Since $u \in W^{3,q}(\Omega)$ we obtain $\Delta u \in W^{1,q}(\Omega)$ which entails $p \in W^{3,q}(\Omega)$. Sobolev's embedding theorem then implies ∇u, $\nabla p \in L^3(\Omega)^3$ and Δu, $\Delta p \in L^{3/2}(\Omega)$ for each $q \geq 1$. Thus the last term in (3.24) is well defined.

Since $u \in W^{3,q}(\Omega)$ we have $\frac{\partial u}{\partial n} \in W^{2-\frac{1}{q},q}(\Gamma)$ and since Γ is a two-dimensional manifold it follows that $\frac{\partial u}{\partial n} \in L^2(\Gamma)$. Similarly $\frac{\partial p}{\partial n} \in L^2(\Gamma)$.

If the shape derivative of u existed in $H^1(\Omega)$, then it is the variational solution to

$$\begin{aligned} \Delta u' &= 0, \qquad \text{in } \Omega, \\ u' &= -\frac{\partial u}{\partial n}(h,n), \quad \text{on } \Gamma. \end{aligned} \tag{3.26}$$

Let us choose h such that $h|_\Gamma = n$. Due to the assumption that $q \in (1, \frac{6}{5})$ the space $W^{2-\frac{1}{q},q}(\Gamma)$ is not embedded in $H^{\frac{1}{2}}(\Gamma)$ [8]. Hence there exists $g \in W^{2-\frac{1}{q},q}(\Gamma) \setminus H^{\frac{1}{2}}(\Gamma)$. Since the mapping $f \to \frac{\partial u}{\partial n}$ is a homeomorphism from $W^{1,q}(\Omega)$ to $W^{2-\frac{1}{q},q}(\Gamma)$, see [8], [7] (Chap. 1), there exists $f \in W^{1,q}(\Omega)$ such that $\frac{\partial u}{\partial n} = g$. Since the Dirichlet solution operator of (3.26) is a homeomorphism from $H^1(\Omega) \to H^{\frac{1}{2}}(\Gamma)$ it follows from (3.26), with $(h,n) = 1$ on Γ, that u cannot be shape differentiable with shape derivative $u' \in H^1(\Omega)$ for this choice of f. As a side remark we mention that (3.26) admits a very weak solution $u' \in L^2(\Omega)$ since $\frac{\partial u}{\partial n}(h,n) \in L^2(\Gamma)$.

Next we use the technique of Theorem 2.1 to argue that the shape derivative of J for problem (3.22) and (3.23) exists and we compute its form. This computation holds for any perturbation characterized by $h \in C^{2,1}(\bar{U}, \mathbb{R}^3)$. Theorem 2.1 is not directly applicable since the functionals in (2.1) do not include derivatives of the state. We therefore give an independent proof following the lines of the proof of Theorem 2.1. We first address (H1'), (H2)–(H4). Conditions (H3) and (H4) follow by the same arguments as in the example of Section 3.1. To verify (H1') of Remark 2.1 it suffices to verify the existence of $\frac{\mathrm{d}}{\mathrm{d}t}\langle \tilde{E}(u,t), p\rangle_{X^* \times X}|_{t=0}$ where u and p stand for the solutions of (3.23), respectively (3.24). This follows from

$$\begin{aligned} \langle \tilde{E}(u,t), p\rangle_{X^* \times X} &= \int_\Omega (A_t \nabla u, A_t \nabla p)\, I_t \,\mathrm{d}x - \int_\Omega f^t I_t p \,\mathrm{d}x \\ &= \int_\Omega (A_t \nabla u, A_t \nabla p)\, I_t \,\mathrm{d}x - \int_{\Omega_t} f\,(p \circ F_t^{-1}) \,\mathrm{d}x \end{aligned}$$

(2.8) and Lemma 2.3. To verify (H2) note that

$$\left| \frac{1}{t}(f^t - f) \right|_{L^q(\Omega)} \quad \text{is bounded for } t \to 0^+,$$

if $f \in W^{1,q}(U)$. Since $u^t - u \in W^{3,q}(\Omega) \subset L^\infty(\Omega)$,

$$\left| \frac{1}{t}(I_t f^t - f, u^t - u) \right| \le M$$

for some constant M independent of $t > 0$, thus $\frac{1}{t}|u^t - u|_X^2 \le M$ and hence $u^t \to u$ in X as $t \to 0$. Then,

$$\left| \frac{1}{t}(I_t f^t - f, u^t - u) \right| \le \left(\left| \frac{I_t - 1}{t} \right|_{L^\infty} |f^t|_{L^q} + \left| \frac{f^t - f}{t} \right|_{L^q} \right) |u^t - u|_{L^p},$$

where $\frac{1}{q} + \frac{1}{p} = 1$, and thus $p > 6$. Now,

$$|u^t - u|_{L^p} = |u^t - u|_{L^\infty}^{1-\alpha} (|u^t - u|_{L^{p\alpha}})^\alpha \le C |u^t - u|_{L^\infty}^{1-\alpha} |u^t - u|_X^\alpha,$$

where $p\alpha = 6$ and C is the embedding constant of X into $L^6(\Omega)$. Thus,

$$\left| \frac{1}{t}(I_t f^t - f, u^t - u) \right| \to 0$$

and

$$\frac{1}{t}|u^t - u|_X^2 \to 0,$$

which implies (H2).

The difference of the cost function at Ω_t and Ω can be written as

$$\begin{aligned} J(u_t,\Omega_t) - J(u,\Omega) &= \int_{\Omega_t} |\nabla u_t|^2 \, \mathrm{d}x - \int_\Omega |\nabla u|^2 \, \mathrm{d}x \\ &= \int_\Omega (I_t|\nabla u^t|^2 - |\nabla u|^2) \, \mathrm{d}x + \int_\Omega I_t(|A_t\nabla u^t|^2 - |\nabla u^t|^2) \, \mathrm{d}x \\ &= R(t) + S(t). \end{aligned}$$

The first term corresponds to Theorem 2.1 with $j_2 = j_3 = 0$ and $j_1(u(x))$ replaced by $|\nabla u(x)|^2$. Hence we obtain as before

$$\begin{aligned} R(t) &= \int_\Omega I_t|\nabla(u^t - u)|^2 \, \mathrm{d}x + \int_\Omega (I_t - 1)(2\nabla u, \nabla(u^t - u)) \, \mathrm{d}x + \int_\Omega (2\nabla u, \nabla(u^t - u)) \, \mathrm{d}x + \int_\Omega (I_t - 1)|\nabla u|^2) \, \mathrm{d}x \\ &= R_1(t) + R_2(t) + R_3(t) + R_4(t). \end{aligned}$$

As in the proof of Theorem 2.1 we argue

$$\lim_{t\to 0} R_i(t) = 0, \qquad i = 1, 2$$

and use the adjoint equation in $R_3(t)$

$$\begin{aligned} R_3(t) &= (2\nabla u, \nabla(u^t - u))_\Omega = (\nabla(u^t - u), \nabla p)_\Omega \\ &= \langle E(u^t,\Omega) - E(u,\Omega), p\rangle_{X^*\times X} \\ &= -\langle \tilde{E}(u^t,t) - \tilde{E}(u,t) - E(u^t,\Omega) + E(u,\Omega), p\rangle_{X^*\times X} \\ &\quad - \langle \tilde{E}(u,t) - \tilde{E}(u,0), p\rangle_{X^*\times X}, \end{aligned}$$

which by (H4) and (H1') gives

$$\lim_{t\to 0} \frac{1}{t} R_3(t) = -\frac{\mathrm{d}}{\mathrm{d}t} \langle \tilde{E}(u,t), p\rangle_{X^*\times X}|_{t=0}.$$

It turns out to be advantageous to replace u^t in $S(t)$ by the fixed solution u. This motivates the following splitting (norms and inner products are taken in $\mathbb{R}^3$)

$$\begin{aligned} |A_t\nabla u^t|^2 - |\nabla u^t|^2 &= |A_t\nabla(u^t - u) + A_t\nabla u|^2 - |\nabla(u^t - u) + \nabla u|^2 \\ &= \big((A_t - I)\nabla(u^t - u), (A_t + I)\nabla(u^t - u)\big) \\ &\quad + 2\big((A_t - I)\nabla(u^t - u), A_t\nabla u\big) + 2\big(\nabla(u^t - u), (A_t - I)\nabla u\big) \\ &\quad + |A_t\nabla u|^2 - |\nabla u|^2, \end{aligned}$$

and this results in

$$\begin{aligned} S(t) &= \big(I_t(A_t - I)\nabla(u^t - u), (A_t + I)\nabla(u^t - u)\big)_\Omega \\ &\quad + 2\big(I_t(A_t - I)\nabla(u^t - u), A_t\nabla u\big)_\Omega + 2\big(I_t\nabla(u^t - u), (A_t - I)\nabla u\big)_\Omega \\ &\quad + \int_\Omega I_t(|A_t\nabla u|^2 - |\nabla u|^2) \, \mathrm{d}x = S_1(t) + S_2(t) + S_3(t) + S_4(t). \end{aligned}$$

In view of (H2) and (2.8) we conclude

$$\lim_{t\to 0}\frac{1}{t}S_i(t)=0;\qquad i=1,2,3.$$

Concerning S_4 we argue

$$\begin{aligned}S_4(t)&=\int_\Omega I_t(|A_t\nabla u|^2-|\nabla u|^2)\,\mathrm{d}x=\int_\Omega (I_t|A_t\nabla u|^2-|\nabla u|^2)\,\mathrm{d}x-R_4(t)\\&=S_5(t)-R_4(t).\end{aligned}$$

Since $\nabla^2 u\in L^{3/2}(\Omega,\mathbb{R}^{3\times 3})$ and $\nabla u\in L^3(\Omega)^3$ we infer that $|\nabla u|^2\in W^{1,1}(\Omega)$. Therefore Lemma 2.3 can be applied to obtain

$$\begin{aligned}\lim_{t\to 0}\frac{1}{t}S_5(t)&=\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega_t}|\nabla(u\circ F_t^{-1})|^2\,\mathrm{d}x|_{t=0}\\&=\int_\Gamma|\nabla u|^2\,(h,n)\,\mathrm{d}s+2\int_\Omega(\nabla u,\nabla(-\nabla u\cdot h))\,\mathrm{d}x\\&=\int_\Gamma\left(\frac{\partial u}{\partial n}\right)^2\,(h,n)\,\mathrm{d}s+2\int_\Omega(\nabla u,\nabla(-\nabla u\cdot h))\,\mathrm{d}x.\end{aligned}$$

The boundary term above is integrable since $\nabla u\in W^{2,1}(\Omega)^3$ implies $\nabla u\in L^2(\Gamma)^3$, hence $\frac{\partial u}{\partial n}\in L^2(\Gamma)$. Collecting terms results in

$$\begin{aligned}dJ(u,\Omega)h=&-\frac{\mathrm{d}}{\mathrm{d}t}\langle\tilde{E}(u,t),p\rangle_{X^*\times X}|_{t=0}+\int_\Gamma\left(\frac{\partial u}{\partial n}\right)^2\,(h,n)\,\mathrm{d}s\\&+2\int_\Omega(\nabla u,\nabla(-\nabla u\cdot h))\,\mathrm{d}x\end{aligned}\tag{3.27}$$

(note the cancellation of $R_4(t)$). Using Proposition 2.37 in [13] the derivative above is calculated as in Example 3.1:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle\tilde{E}(u,t),p\rangle_{X^*\times X}|_{t=0}&=\frac{\mathrm{d}}{\mathrm{d}t}\left(\int_{\Omega_t}(\nabla(u\circ F_t^{-1}),\nabla(p\circ F_t^{-1}))\,\mathrm{d}x-\int_{\Omega_t}f(p\circ F_t^{-1})\,\mathrm{d}x\right)|_{t=0}\\&=\int_\Gamma\frac{\partial u}{\partial n}\frac{\partial p}{\partial n}\,(h,n)\,\mathrm{d}x+(\nabla(-\nabla u\cdot h),\nabla p)_\Omega+(\nabla u,\nabla(-\nabla p\cdot h))_\Omega+(f,\nabla p\cdot h)_\Omega\\&=(\nabla(-\nabla u\cdot h),\nabla p)_\Omega,\end{aligned}$$

where we used Green's theorem and $-\Delta u=f$ in the last step. Another application of Green's theorem combined with (3.25) shows

$$\begin{aligned}(\nabla(-\nabla u\cdot h),\nabla p)_\Omega&=(\Delta p,\nabla u\cdot h)_\Omega-\int_\Gamma\frac{\partial u}{\partial n}\frac{\partial p}{\partial n}\,(h,n)\,\mathrm{d}x\\&=2(\Delta u,\nabla u\cdot h)_\Omega-\int_\Gamma\frac{\partial u}{\partial n}\frac{\partial p}{\partial n}\,(h,n)\,\mathrm{d}x\end{aligned}$$

which implies

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\tilde{E}(u,t),p\rangle_{X^*\times X}|_{t=0}=2(\Delta u,\nabla u\cdot h)_\Omega-\int_\Gamma\frac{\partial u}{\partial n}\frac{\partial p}{\partial n}\,(h,n)\,\mathrm{d}x.$$

Inserting this expression into (3.27) and applying Green's theorem one more time we are eventually led to

$$\begin{aligned} dJ(u,\Omega)h &= 2(\Delta u, -\nabla u\cdot h)_\Omega + 2(\nabla u, \nabla(-\nabla u\cdot h))_\Omega \\ &\quad + \int_\Gamma \frac{\partial u}{\partial n}\frac{\partial p}{\partial n}\,(h,n)\,\mathrm{d}x + \int_\Gamma \left(\frac{\partial u}{\partial n}\right)^2 (h,n)\,\mathrm{d}s \\ &= \int_\Gamma \frac{\partial u}{\partial n}\frac{\partial p}{\partial n}\,(h,n)\,\mathrm{d}x - \int_\Gamma \left(\frac{\partial u}{\partial n}\right)^2 (h,n)\,\mathrm{d}s. \end{aligned} \tag{3.28}$$

Note that such a functional is not covered by Theorem 2.1.

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