Shape Differentiability Under Non-linear PDE Constraints

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Abstract We review available methods to compute shape sensitivities and apply these methods to a semi-linear model problem. This will reveal the difficulties of each method and will help to decide which approach should be used for a concrete applications.

Keywords Lagrange method · Shape derivative · Non-linear PDE · Material derivative · Céa's method · Minimax formulation

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1 Introduction

The objective of this manuscript is to give readers an overview on methods that allow to derive the shape differentiability of PDE (partial differential equation) constrained shape functions. There are several methods available to prove the shape differentiability of shape functions depending on the solution of a PDE. In the recent past two new methods have been proposed: the rearrangement method [14] and an approach using a novel adjoint equation [19]. Other more established methods comprise the material/shape derivative method [18] (also called 'chain rule' approach), the min approach for energy cost functions [7], the minimax approach of [9] and an interesting penalization method [8] to derive sensitivities for a class of variational inequalities. The approach of Céa [5] is frequently used to derive the formulas for the shape derivative, but itself gives no proof for the shape differentiability. Indeed, there are cases where Céa's method fails; cf. [17, 19]. For linear partial differential equations and (semi)-convex cost functions all mentioned methods (except Céa's Lagrange method in some cases) work and the necessary assumptions are readily

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verified. But for non-linear PDEs the situation is quite different as we will see in the presented example. After reading this article the reader may decide which method is suited for his or her problem in hand .

In particular the presented methods are:

- The material derivative method analyzes the sensitivity of the solution of the PDE with respect to the domain. This procedure is similar to the direct approach used in PDE constraint optimal control [21]. Here, the solution of the PDE depends on a control function, which belongs to a usually convex set. The main objective when deriving the necessary optimality conditions is the investigation of the control-solution operator. In shape optimization we have to investigate the "domain-state" operator. The investigation of shape function is more involved, since spaces of shapes admit no vector space structure.
- The rearrangement method exploits a first order expansion of the PDE and the cost function with a remainder which tends to zero with order two. This expansion is combined with the Hölder continuity of the domain-state operator. The main challenge of this method constitute the proof of the Hölder continuity, but more importantly the first order expansion.
- In the minimax approach the cost function is expressed as a minimax of the Lagrangian associated to the optimization problem. By definition a Lagrangian is a function that is the sum of a utility function and a state equation. The problem of the differentiability of the cost function is shifted to the differentiability of a minimax function. The Theorem of Correa-Seeger [6] can be applied to prove the differentiability if (among other requirements) the Lagrangian admits saddle points. A special case of this approach is when the cost function is itself a minimum of an energy. In this case the minimax of the Lagrangian is replaced by the min of the energy and we have to investigate the differentiability of the min function to prove the shape differentiability.
- The averaged adjoint approach can also be seen as a proof for the differentiability of a minimax function. Unlike the Theorem of Correa-Seeger it requires no saddle point assumption. Therefore it constitutes an extension of the Theorem of Correa-Seeger for the special class of Lagrangian functions.

The manuscript is organized as follows:

Section 2, the basic notation is introduced and basic tools from shape optimization, including the Zolésio-Hadamard structure theorem, are recalled. We introduce the basic model problem and make some basic assumptions.

Section 3, the existence of the strong material derivatives associated to this equation is shown under suitable assumption. This proves then the shape differentiability of the cost function.

Section 4, the minimax formulation is reviewed for the particular example. Then the Theorem of Correa-Seeger is applied to prove the differentiability of the minimax function with respect to a parameter, that is, the shape differentiability of the cost function.

Section 5, the rearrangement method is employed to derive the shape differentiability of the semi-linear model problem.

Section 6, the shape differentiability of a special cost function, that is the energy associated to the PDE, is proved. In this case the minimax differentiability reduces to the differentiability of a min function.

Section 7, a recently proposed approach of the averaged adjoint equation is presented and applied to the semi-linear problem.

2 Notations and Problem Description

2.1 Notation

Let E and F be Banach spaces and $U \subset E$ an open subset. We denote by $C(U; F)$ the space of all continuous functions $f : U \to F$. We call a function $f : U \to F$ differentiable in $x \in U$ if it is Fréchet differentiable at x and denote the derivative by $\partial f(x)$. The function is called differentiable if it is differentiable at every point $x \in U$. For $k \geq 1$, the space of all k-times continuously differentiable functions $f : U \to F$ is denoted by $C^k(U; F)$. The directional derivative of f at x in direction v is denoted by $df(x; v)$. When $F = \mathbf{R}$ and $E = \mathbf{R}^d$, we adopt the notation $C^k(\overline{U}; \mathbf{R}^d)$ of [23] for all those functions $f \in C^k(U; F)$ that admit extendable partial derivative $\partial^\alpha f$ to $\overline{U}$ for all indices $\alpha = (\alpha_1, \ldots, \alpha_d)$ with $|\alpha| \leq k$. Also, we identify the derivative $\partial f(x) : \mathbf{R}^d \to \mathbf{R}$ via the Riesz representation theorem by the gradient $\nabla f(x)$, which is for each point $x \in \mathbf{R}^d$ a vector in $\mathbf{R}^d$. For $p \geq 1$, the space of all measurable functions $f : \Omega \to \mathbf{R}$ for which $\|f\|_{L_p(\Omega)} := \left(\int_\Omega |f|^p \, dx\right)^{1/p} < \infty$ is denoted by $L_p(\Omega)$. The space of functions of bounded variations on D is denoted by $BV(D)$. For the one-sided limit (t approaches zero from the right) we write $\lim_{t \searrow 0}$. The right derivative in zero of a function $f : U \subset \mathbf{R} \to \mathbf{R}$ is denoted $f(0^+) := \lim_{t \searrow 0}(f(t) - f(0))/t$.

2.2 The Problem Description

Let $d \in \mathbf{N}^+$. Throughout this manuscript, we consider the following semi-linear **state equation**

$$-\Delta u + \varrho(u) = f \ \text{ in } \Omega, \quad u = 0 \ \text{ on } \partial\Omega. \tag{2.1}$$

on a domain $\Omega \subset \mathbf{R}^d$. The function $u : \Omega \to \mathbf{R}$ is called **state** and $f : D \to \mathbf{R}$ is a function specified below. Without loss of generality, we may assume $\varrho(0) = 0$ otherwise consider $\tilde{\varrho}(x) := \varrho(x) - \varrho(0)$ with right hand side $\tilde{f}(x) := f(x) - \varrho(0)$. To simplify the exposition, we choose as objective function

$$J(\Omega) := \int_\Omega |u - u_r|^2 \, dx, \tag{2.2}$$

where $u_r : \overline{D} \to \mathbf{R}$ is given and $|\ |$ denotes the absolute value. The task is now to derivative the shape derivative of the cost function (2.2) by employing different techniques.

Throughout this manuscript we suppose that the following assumption is satisfied.

Assumption (*Data*)

(i) Let $\Omega \subset D \subset \mathbf{R}^d$ be two simply connected domains with Lipschitz boundaries $\partial\Omega$ and ∂D, respectively.
(ii) The functions $u_r, f : \overline{D} \to \mathbf{R}$ are continuously differentiable.
(iii) The vector field θ belongs to $C_c^2(D, \mathbf{R}^d)$.

For any $k \geq 1$, we define the space

$$\mathcal{C}_c^k(D, \mathbf{R}^d) := \{\theta \in C^k(\mathbf{R}^d; \mathbf{R}^d) : \ \mathrm{supp}(\theta) \subset D\}$$

and set $\mathcal{C}_c^\infty(D, \mathbf{R}^d) = \bigcap_{n\in\mathbf{N}} \mathcal{C}_c^n(D, \mathbf{R}^d)$. The **flow** of a vector field $\theta \in \mathcal{C}_c^k(D, \mathbf{R}^d)$ is defined for each $x_0 \in D$ by $\Phi_t^\theta(x_0) := x(t)$, where $x : [0, \tau] \to \mathbf{R}^d$ solves

$$\dot{x}(t) = \theta(x(t)) \quad \text{in } (0, \tau), \quad x(0) = x_0.$$

In the sequel, we write Φ_t instead of Φ_t^θ.

2.3 Compositions of Functions with Flows

In the following let $\theta \in C_c^1(D, \mathbf{R}^d)$ be a given vector field and $\Phi_t = \Phi_t^\theta$ its associated flow. First, note that by the chain rule $\partial\Phi^{-1}(t, \Phi(t, x)) = (\partial\Phi(t, x))^{-1}$ or briefly $(\partial(\Phi_t^{-1})) \circ \Phi_t = (\partial\Phi_t)^{-1} =: \partial\Phi_t^{-1}$, which implies[1]

$$(\nabla f) \circ \Phi_t = \partial\Phi_t^{-T} \nabla(f \circ \Phi_t).$$

Subsequently the following abbreviations are used

$$\xi(t) := \det(\partial\Phi_t), \qquad A(t) := \xi(t)\partial\Phi_t^{-1}\partial\Phi_t^{-T}, \quad B(t) := \partial\Phi_t^{-T}, \tag{2.3}$$

where $\det : \mathbf{R}^{d,d} \to \mathbf{R}$ denotes the determinant. Step-by-step, we will derive properties of the quantities ξ, B and A.

[1] For any scalar function $f \in H^1(\mathbf{R}^d)$, we have for all $v \in \mathbf{R}^d$ and all $x \in D$

$$\partial(f(\Phi_t(x))v = \partial f(\Phi_t(x))\partial\Phi_t(x)v = \nabla f(\Phi_t(x)) \cdot \partial\Phi_t(x)v = (\partial\Phi_t(x))^T \nabla(f(\Phi_t(x))) \cdot v.$$

Proposition 2.1 *Let a continuous mapping $A \in C([0,\tau]; C(\overline{D}; \mathbf{R}^{d,d}))$ and a function $\xi \in C([0,\tau]; C(\overline{D}))$ be given and assume $A(0) = I$ and $\xi(0) = 1$. Then there are constants $\gamma_1, \gamma_2, \delta_1, \delta_2 > 0$ and $\tau > 0$ such that*

$$\forall \zeta \in \mathbf{R}^d,\ \forall t \in [0,\tau]: \quad \gamma_1|\zeta|^2 \le \zeta \cdot A(t)\zeta \le \gamma_2|\zeta|^2, \qquad (a)$$
$$\delta_1 \le \xi(t) \le \delta_2. \qquad (b)$$

Proof (a) We can estimate

$$\begin{aligned} |\eta|^2 &= (I - A(t))\eta \cdot \eta + A(t)\eta \cdot \eta \\ &\le \|I - A(t)\|_{C(D;\mathbf{R}^{d,d})}\eta \cdot \eta + A(t)\eta \cdot \eta. \end{aligned}$$

By continuity of $t \mapsto A(t)$ there exists for all $\varepsilon > 0$, a $\delta > 0$ such that for all $t \in [0,\delta]$ we have $\|I - A(t)\|_{C(D;\mathbf{R}^{d,d})} \le \varepsilon$. From this the claim follows.
(b) This is clear. □

Proposition 2.2 *Let $B : [0,\tau] \to \mathbf{R}^{d,d}$ be a bounded mapping such that $\|B^{-1}(t)\|_{C(\overline{D};\mathbf{R}^{d,d})} \le C$ for all $t \in [0,\tau]$ for some constant $C > 0$. Then for any $p \ge 1$ there is a constant $C > 0$ such that*

$$\forall t \in [0,\tau],\ \forall f \in W^1_p(D): \ \|\nabla f\|_{L_p(D;\mathbf{R}^d)} \le C\|B(t)\nabla f\|_{L_p(D;\mathbf{R}^d)}$$

Proof Estimating

$$\|\nabla f\|_{L_p(D;\mathbf{R}^d)} = \|(B(t))^{-1}B(t)\nabla f\|_{L_p(D;\mathbf{R}^d)} \le C\,\|B(t)\nabla f\|_{L_p(D;\mathbf{R}^d)}$$

gives the first inequality. □

Lemma 2.3 *Let $\theta \in C^1([0,\tau]; C^1_c(D,\mathbf{R}^d))$ be vector field and Φ its flow. The functions $t \mapsto A(t) := \xi(t)\partial\Phi_t^{-1}\partial\Phi_t^{-T}$, $t \mapsto \xi(t) := \det(\partial\Phi_t)$ and $t \mapsto B(t) := \partial\Phi_t^{-T}$ are differentiable on $[0,\tau]$ and satisfy the following ordinary differential equations*

$$\begin{aligned} B'(t) &= -B(t)(\partial\theta^t)^T B(t) \\ \xi'(t) &= tr(\partial\theta^t B^T(t))\xi(t) \\ A'(t) &= tr(\partial\theta^t B^T(t))A(t) - B^T(t)\partial\theta^t A(t) - (B^T(t)\partial\theta^t A(t))^T, \end{aligned}$$

where $\theta^t(x) := \theta(t,\Phi_t(x))$ and $' := \frac{d}{dt}$.

Proof (i) Let E, F be two Banach spaces. In [2, p. 222. Satz 7.2] it is proved that

$$\mathrm{inv} : \mathcal{L}\mathrm{is}(E;F) \to \mathcal{L}(F;E), \quad A \mapsto A^{-1}$$

is infinitely continuously differentiable with derivative $\partial\mathrm{inv}(A)(B) = -A^{-1}BA^{-1}$. Now by the fundamental theorem of calculus, we have

$$\Phi_t(x) = x + \int_0^t \theta(s, \Phi_s(x))\, ds \ \Rightarrow\ \partial\Phi_t(x) = I + \int_0^t \partial\theta(s, \Phi_s(x)))\, ds,$$

where $I \in \mathbf{R}^{d,d}$ denotes the identity matrix. Therefore $t \mapsto \partial\Phi_t(x)$ is differentiable for each $x \in \overline{D}$ with derivative

$$\frac{d}{dt}(\partial\Phi_t(x)) = \partial\theta^t(x) = \partial\theta(t, \Phi_t(x))\partial\Phi_t(x).$$

Thus if we let $E = F = \mathbf{R}^{d,d}$ and take into account the previous equation, we get by the chain rule

$$\frac{d}{dt}(\mathrm{inv}(\partial\Phi_t(x))) = -(\partial\Phi_t(x))^{-1}\partial\theta^t(x)(\partial\Phi_t(x))^{-1}.$$

(ii) A proof may be found in [22, p. 215, Proposition 10.6].
(iii) Follows from the product rule together with (i) and (ii). □

Remark 2.4 Note that equation (i) can also be proved by differentiating the identity $\partial\Phi_t\partial\Phi_t^{-1} = I$, where I is the identity matrix in $\mathbf{R}^d$. That the inverse $t \mapsto \partial\Phi_t^{-1}$ is differentiable can also be seen by the well known formula $\partial\Phi_t^{-1} = (\det(\partial\Phi_t))^{-1}(\mathrm{cofac}(\partial\Phi_t))^T$, where cofac denotes the cofactor matrix.

Lemma 2.5 *Let $D \subset \mathbf{R}^d$ be an open, bounded set and $p \geq 1$ a real number. Denote by Φ_t the flow of $\theta \in C_c^1(D, \mathbf{R}^d)$.*

(i) For any $f \in L_p(D)$, we have

$$\lim_{t \searrow 0} \|f \circ \Phi_t - f\|_{L_p(D)} = 0 \quad \textit{and} \quad \lim_{t \searrow 0} \|f \circ \Phi_t^{-1} - f\|_{L_p(D)} = 0.$$

(ii) For any $f \in W_p^1(D)$, we have

$$\lim_{t \searrow 0} \|f \circ \Phi_t - f\|_{W_p^1(D)} = 0. \tag{2.4}$$

(iii) For $p \geq 1$ a real number, $k \in \{1, 2\}$ and any $f \in W_p^k(D)$, we have

$$\lim_{t \searrow 0} \left\| \frac{f \circ \Phi_t - f}{t} - \nabla f \cdot \theta \right\|_{W_p^{k-1}(D)} = 0.$$

(iv) Fix $p \geq 1$ and let $t \to u_t : [0, \tau] \to W_p^1(D)$ be a continuous function in 0. Set $u := u_0$. Then $t \mapsto u_t \circ \Phi_t : [0, \tau] \to W_p^1(D)$ is continuous in 0 and

$$\lim_{t \searrow 0} \|u_t \circ \Phi_t - u\|_{W_p^1(D)} = 0.$$

Proof (i) A proof can be found in [10, p. 529].
(ii) In order to prove (2.4) it is sufficient to show

$$\lim_{t\searrow 0}\|\nabla(f\circ\Phi_t - f)\|_{L_p(D)} = \lim_{t\searrow 0}\|\partial\Phi_t^T((\nabla f)\circ\Phi_t - \nabla f)\|_{L_p(D)} = 0.$$

By the triangle inequality, we have

$$\|\partial\Phi_t^T((\nabla f)\circ\Phi_t - \nabla f)\|_{L_p(D)} \le \|(\nabla f)\circ\Phi_t - \nabla f)\|_{L_p(D)} + \|(\partial\Phi_t^T - I)\nabla f)\|_{L_p(D)}.$$

For the first term on the right hand side we can use (i) and the second term tends to zero since $\partial\Phi_t^T \to I$ in $C(\overline{D};\mathbf{R}^{d,d})$.
(iii) A proof can be found in [14, p. 6, Lemma 3.6].
(iv) By the triangle inequality, we get

$$\|u_t\circ\Phi_t - u\|_{W_p^1(D)} \le \|u_t\circ\Phi_t - u\circ\Phi_t\|_{W_p^1(D)} + \|u\circ\Phi_t - u\|_{W_p^1(D)}.$$

The last term on the right hand side converges to zero as $t\to 0$ due to (ii). For the second inequality note that

$$\begin{aligned}\|u_t\circ\Phi_t - u\circ\Phi_t\|_{W_p^1(D)} &= \left(\int_D \xi^{-1}(t)|u_t - u|^p + \xi^{-1}(t)|B(t)\nabla(u_t - u)|^p\right)^{1/p}\\ &\le C\left(\int_D |u_t - u|^p + |\nabla(u_t - u)|^p\right)^{1/p}\end{aligned}$$

and the right hand side converges to zero. □

Definition 2.6 (*Eulerian semi-derivative*) Let $\Omega\subset D$ and $k\ge 1$ be given. Suppose we are given a shape function $J : \Xi(\Omega)\to\mathbf{R}$ on the set $\Xi(\Omega) := \cup_{t\in[0,\tau]}\{\Phi_t(\Omega)|\,\theta\in\mathcal{C}_c^k(D,\mathbf{R}^d)\}$. Then the **Eulerian semi-derivative** of J at Ω in the direction θ is defined as the limit (if it exists)

$$dJ(\Omega)[\theta] := \lim_{t\searrow 0}\frac{J(\Omega_t) - J(\Omega)}{t}.$$

Moreover, if the Eulerian semi-derivative $dJ(\Omega)[\theta]$ exists for all $\theta\in\mathcal{C}_c^\infty(D,\mathbf{R}^d)$ and the map $\theta\mapsto dJ(\Omega)[\theta] : \mathcal{C}_c^\infty(D,\mathbf{R}^d)\to\mathbf{R}$, is linear and continuous, then J is called **shape differentiable** at Ω.

Finally, we state the following theorem from [10, pp. 483–484], which will be used to compute the boundary expression of the shape derivative.

Theorem 2.7 *Let $\theta\in\mathcal{C}_c^k(D,\mathbf{R}^d)$, where $k\ge 1$. Fix $\tau > 0$ and let $\varphi\in C(0,\tau;W_{loc}^{1,1}(\mathbf{R}^d))\cap C^1(0,\tau;L_{loc}^1(\mathbf{R}^d))$ and an bounded domain Ω with Lipschitz boundary Γ be given. The right sided derivative of the function $f(t) := \int_{\Omega_t}\varphi(t)\,dx$ at $t = 0$ is given by*

$$f'(0^+) = \int_\Omega \varphi'(0)\, dx + \int_\Gamma \varphi(0)\, \theta_n\, ds.$$

In the following, we prove the shape differentiability of J defined in (2.2) by the following methods: the material and shape derivative method, the min-max formulation of Correa-Seeger and the rearrangement method. We present a modification of Céa's Lagrange method which allows a rigorous derivation of the shape derivative in the case of existence of material derivatives.

3 Material and Shape Derivative Method

3.1 Material Derivative Method

In order to compute the Eulerian semi-derivative of J given by (2.2) via material derivative method (chain rule approach), we make the following assumption:

Assumption ($\mathcal{A}$) The function $\varrho : \mathbf{R} \to \mathbf{R}$ is continuously differentiable, bounded and monotonically increasing.

We call $u \in H_0^1(\Omega)$ a **weak solution** of (2.1) if

$$\int_\Omega \nabla u \cdot \nabla \psi\, dx + \int_\Omega \varrho(u)\, \psi\, dx = \int_\Omega f \psi\, dx \quad \text{for all } \psi \in H_0^1(\Omega). \tag{3.1}$$

The weak solution of the previous equation characterizes the unique minimum of the energy $E(\Omega, \cdot) : H_0^1(\Omega) \to \mathbf{R}$ defined by

$$E(\Omega, \varphi) := \frac{1}{2} \int_\Omega |\nabla \varphi|^2 + \hat{\varrho}(\varphi)\, dx - \int_\Omega f \varphi\, dx,$$

where $\hat{\varrho}(s) := \int_0^s 2\, \varrho(s')\, ds'$. In the following, we denote by

$$d_\varphi E(\Omega, \varphi; \psi) := \lim_{t \searrow 0} \frac{E(\Omega, \varphi + t\, \psi) - E(\Omega, \varphi)}{t}$$

$$d_\varphi^2 E(\Omega, \varphi; \psi, \tilde{\psi}) := \lim_{t \searrow 0} \frac{d_\varphi E(\Omega, \varphi + t\, \tilde{\psi}; \psi) - d_\varphi E(\Omega, \varphi; \psi)}{t}$$

the first and second order directional derivative of E at φ in the direction ψ and $(\psi, \tilde{\psi})$, respectively. Then we may write (3.1) as $d_\varphi E(\Omega, u; \psi) = 0$ for all $\psi \in H_0^1(\Omega)$.

Lemma 3.1 *Assume that ϱ is continuously differentiable. Then the mapping*

$$s \mapsto \int_{\Omega} \varrho(\varphi + s\tilde{\varphi})\psi \, dx$$

is continuously differentiable on $\mathbf{R}$ *for all* $\varphi, \tilde{\varphi} \in L_\infty(\Omega)$ *and* $\psi \in H_0^1(\Omega)$.

Proof Let $\varphi, \tilde{\varphi} \in H_0^1(\Omega) \cap L_\infty(\Omega)$ and $\psi \in H_0^1(\Omega)$. Put $z^s(x) := \varrho(\varphi(x) + s\tilde{\varphi}(x))\psi(x)$. We have for almost all $x \in \Omega$

$$\frac{z^{s+h}(x) - z^s(x)}{h} \to = \varrho'(\varphi(x) + s\tilde{\varphi}(x))\tilde{\varphi}(x)\psi(x) \quad \text{as } h \to 0,$$
$$\left| \frac{d}{ds} z^s(x) \right| \leq C|\psi(x)||\tilde{\varphi}(x)|.$$

Then it holds

$$\begin{aligned} \left| \frac{z^{s+h}(x) - z^s(x)}{h} \right| &= \left| \frac{1}{h} \int_s^{s+h} \frac{d}{ds'} z^{s'}(x) ds' \right| \\ &\leq C|\psi(x)||\tilde{\varphi}(x)| \frac{1}{h} \int_{s'}^{s'+h} ds' \\ &= C|\psi(x)||\tilde{\varphi}(x)|. \end{aligned}$$

Therefore applying Lebesgue's dominated convergence theorem we conclude

$$\frac{d}{ds} \int_{\Omega} z^s(x) \, dx = \int_{\Omega} \varrho'(\varphi(x) + s\tilde{\varphi}(x))\tilde{\varphi}(x)\psi(x) \, dx.$$

As a consequence of the previous lemma, we get the differentiability of $s \mapsto d_\varphi E(\Omega, \varphi + s\tilde{\varphi}, \psi)$. Moreover, we conclude by the monotonicity of ϱ

$$d_\varphi^2 E(\Omega, \varphi; \psi, \psi) = \int_{\Omega} |\nabla \psi|^2 + \varrho'(\varphi)\psi^2 \, dx \geq C\|\psi\|^2_{H_0^1(\Omega)}$$

for all $\varphi \in H_0^1(\Omega) \cap L_\infty(\Omega)$ and $\psi \in H_0^1(\Omega)$. We now want to calculate the shape derivative of (2.2). For this purpose, we consider the perturbed cost function $J(\Omega_t) = \int_{\Omega_t} |u_t - u_r|^2 \, dx$, where u_t denotes the weak solution of (3.1) on the domain $\Omega_t := \Phi_t(\Omega)$, that is, $u_t \in H_0^1(\Omega_t)$ solves

$$\int_{\Omega_t} \nabla u_t \cdot \nabla \hat{\psi} \, dx + \int_{\Omega_t} \varrho(u_t)\hat{\psi} \, dx = \int_{\Omega_t} f\hat{\psi} \, dx \quad \text{for all } \hat{\psi} \in H_0^1(\Omega_t). \tag{3.2}$$

It would be possible to compute the derivative of $u_t : \Omega_t \to \mathbf{R}$ pointwise by

$$du(x) := \lim_{t\searrow 0} \frac{u_t(x) - u(x)}{t} \quad \text{for all } x \in \left(\bigcap_{t\in[0,\tau]} \Omega_t\right) \cap \Omega.$$

In the literature this derivative is referred to as *local shape derivative of u* in direction θ; cf. [12]. Nevertheless, we go another way and use the change of variables $\Phi_t(x) = y$ to rewrite $J(\Omega_t)$ as

$$J(\Omega_t) = \int_\Omega \xi(t)|u^t - u_r \circ \Phi_t|^2\, dx, \tag{3.3}$$

where $u^t := \Psi_t(u_t) : \Omega \to \mathbf{R}$ is a function on the fixed domain Ω. We introduce the mapping $\Psi_t(\varphi) := \varphi \circ \Phi_t$ with inverse $\Psi^t(\hat{\varphi}) := \Psi_t^{-1}(\hat{\varphi}) = \hat{\varphi} \circ \Psi_t^{-1}$. To study the differentiability of (3.3), we can study the function $t \mapsto u^t$. Notice that $u_0 = u^0 = u$ is nothing but the weak solution of (3.1).

The limit $\dot{u} := \lim_{t\searrow 0}(u^t - u)/t$ is called **strong material derivative** if we consider this limit in the norm convergence in $H_0^1(\Omega)$ and **weak material derivative** if we consider the weak convergence in $H_0^1(\Omega)$.

The crucial observation of [23, Theorem 2.2.2, p. 52] is that Ψ_t constitutes an isomorphism from $H^1(\Omega_t)$ into $H^1(\Omega)$. Hence using a change of variables in (3.2) shows that u^t satisfies

$$\int_\Omega A(t)\nabla u^t \cdot \nabla\psi\, dx + \int_\Omega \xi(t)\, \varrho(u^t)\psi\, dx = \int_\Omega \xi(t) f^t \psi\, dx \quad \text{for all } \psi \in H_0^1(\Omega), \tag{3.4}$$

where we used the notation from (2.3). The previous equation characterizes the unique minimum of the convex energy $\tilde{E} : [0, \tau] \times H_0^1(\Omega) \to \mathbf{R}$[2]

$$\tilde{E}(t, \varphi) := \frac{1}{2}\int_\Omega \xi(t)|B(t)\nabla\varphi|^2 + \xi(t)\hat{\varrho}(\varphi)\, dx - \int_\Omega \xi(t) f^t \varphi\, dx. \tag{3.5}$$

By standard regularity theory (see e.g. [15]) it follows that $u^t \in C(\overline{\Omega})$ for all $t \in [0, \tau]$. Moreover, the proof of [4, Theorem 3.1] shows that there is a constant $C > 0$ such that

$$\|u^t\|_{C(\overline{\Omega})} + \|u^t\|_{H^1(\Omega)} \leq C \quad \text{for all } t \in [0, \tau].$$

As before using Lebesque's dominated convergence theorem it is easy to verify that for fixed $t \in [0, \tau]$ the second order directional derivative $d_\varphi^2 \tilde{E}(t, \varphi; \psi, \eta)$ exists for all $\varphi \in L_\infty(\Omega) \cap H_0^1(\Omega)$ and $\psi, \eta \in H_0^1(\Omega)$. Taking into account Proposition 2.1, we see that

$$C\|\psi\|^2_{H^1(\Omega;\mathbf{R}^d)} \leq d_\varphi^2 \tilde{E}(t, \varphi; \psi, \psi). \tag{3.6}$$

[2] Here we mean convex with respect to φ for each $t \in [0, \tau]$.

or all *varphi* $\in L_\infty(\Omega) \cap H_0^1(\Omega)$, $\psi \in H_0^1(\Omega)$ and for all $t \in [0, \tau]$, Note that $d_\varphi \tilde{E}(t, \varphi; \psi)$ is also differentiable with respect to t and Lemma 2.3 shows:

$$\begin{aligned} \partial_t d_\varphi \tilde{E}(t, \varphi; \psi) = & \int_\Omega A'(t)\nabla\varphi \cdot \nabla\psi + \xi'(t)\varrho(\varphi)\,\psi\,dx \\ & - \int_\Omega (\xi'(t) f^t + \xi(t)B(t)\nabla f^t)\varphi\,dx \\ & \leq C(1 + \|\varphi\|_{H^1(\Omega)})\|\psi\|_{H^1(\Omega)}, \end{aligned} \tag{3.7}$$

for all $t \in [0, \tau]$, where $C > 0$ is a constant. By the coercivity property (3.6) of the second order derivative of $\tilde{E}$

$$C\|\nabla(u^t - u)\|^2_{L_2(\Omega;\mathbf{R}^d)} \leq \int_0^1 d_\varphi^2 \tilde{E}(t, su^t + (1-s)u; u^t - u, u^t - u) \tag{3.8}$$

$$= d_\varphi \tilde{E}(t, u^t; u^t - u) - d_\varphi \tilde{E}(t, u; u^t - u) \tag{3.9}$$

$$= -(d_\varphi \tilde{E}(t, u; u^t - u) - d_\varphi \tilde{E}(0, u; u^t - u)) \tag{3.10}$$

$$= -t\partial_t d_\varphi \tilde{E}(\eta_t\, t, u; u^t - u) \tag{3.11}$$

$$\leq Ct\,\|\nabla(u^t - u)\|_{L_2(\Omega;\mathbf{R}^d)}. \tag{3.12}$$

In step (3.8)–(3.9), we applied the mean value theorem in integral form, in step (3.9)–(3.10), we used that $d_\varphi \tilde{E}(t, u^t; u^t - u) = d_\varphi \tilde{E}(0, u; u^t - u) = 0$, and in step from (3.10)–(3.11), we applied the mean value theorem which yields $\eta_t \in (0, 1)$. In the last step (3.12), we employed the estimate (3.7). Finally, by the Poincaré inequality, we conclude that there is $c > 0$ such that $\|u^t - u\|_{H^1(\Omega)} \leq ct$ for all $t \in [0, \tau]$. From this estimate we deduce that for any real sequence $(t_n)_{n\in\mathbf{N}}$ with $t_n \searrow 0$ as $n \to \infty$, the quotient $w^n := (u^{t_n} - u)/t_n$ converges weakly in $H_0^1(\Omega)$ to some element $\dot{u}$ and by compactness there is a subsequence $(t_{n_k})_{k\in\mathbf{N}}$ such that $(w^{n_k})_{k\in\mathbf{N}}$ converges strongly in $L_q(\Omega)$ to some v, where $0 < q < \frac{2d}{d-2}$; (cf. [11, p. 270, Theorem 6]).[3] Extracting a further subsequence we may assume that $w^{t_k}(x) \to \dot{u}(x)$ as $k \to \infty$ for almost every $x \in \Omega$. Notice that the limit $\dot{u}$ depends on the sequence $(t_{n_k})_{k\in\mathbf{N}}$. However, we will see that this limit is the same for any sequence $(t_n)_{n\in\mathbf{N}}$ converging to zero.

Subtracting (3.4) at $t > 0$ and $t = 0$ yields

$$\begin{aligned} & \int_\Omega A(t)\nabla(u^t - u)\cdot\nabla\psi\,dx + \int_\Omega \xi(t)(\varrho(u^t) - \varrho(u))\,\psi\,dx \\ & = \int_\Omega (\xi(t) - 1)\,\varrho(u)\,\psi\,dx - \int_\Omega (A(t) - I)\nabla u \cdot \nabla\psi\,dx \\ & \quad + \int_\Omega (\xi(t) - 1) f^t\psi\,dx + \int_\Omega (f^t - f)\psi\,dx. \end{aligned} \tag{3.13}$$

[3] When $d = 2$ this means $H^1(\Omega)$ is compactly embedded into $L_p(\Omega)$ for arbitrary $p > 1$. When $d = 3$ we get that $H^1(\Omega)$ compactly embeds into $L_{6-\varepsilon}(\Omega)$ for any small $\varepsilon > 0$.

We choose $t = t_{n_k}$ in the previous equation and want to pass to the limit $k \to \infty$. The only difficult term in (3.13) is

$$\int_\Omega \xi(t) \frac{\varrho(u^t) - \varrho(u)}{t} \psi \, dx = \int_\Omega \xi(t) \left[\int_0^1 \varrho'(u_s^t) \, ds \right] \left(\frac{u^t - u}{t} \right) \psi \, dx.$$

From the strong convergence of $(u^{t_{n_k}} - u)/t_{n_k}$ to $\dot{u}$ in $L_2(\Omega)$ and the pointwise convergence $\xi(t_{n_k}) \to 1$ and $\varrho'(u_s^{t_{n_k}}) \to \varrho'(u)$, we infer that

$$\int_\Omega \xi(t_{n_k}) \frac{\varrho(u^{t_{n_k}}) - \varrho(u)}{t_{n_k}} \psi \, dx \longrightarrow \int_\Omega \varrho'(u) \, \dot{u} \, \psi \, dx \quad \text{as } k \to \infty.$$

Therefore, choosing $t = t_{n_k}$ in (3.13) and dividing by t_{n_k}, we may pass to the limit:

$$\begin{aligned} &\int_\Omega \nabla \dot{u} \cdot \nabla \psi + \varrho'(u) \, \dot{u} \, \psi \, dx + \int_\Omega A'(0) \nabla u \cdot \nabla \psi \, dx \\ &\quad + \int_\Omega \operatorname{div} \theta \varrho(u) \psi \, dx = \int_\Omega \operatorname{div}(\theta) f \psi \, dx + \int_\Omega \nabla f \cdot \theta \, \psi \, dx. \end{aligned} \tag{3.14}$$

for all $\psi \in H_0^1(\Omega)$. The function $\dot{u}$ is the unique solution of (3.14). Hence for every sequence $(t_n)_{n \in \mathbf{N}}$ converging to zero there exists a subsequence $(t_{n_k})_{k \in \mathbf{N}}$ such that $w^{t_k} \to \dot{u}$ as $k \to \infty$. Moreover,

$$\int_\Omega \xi(t) \frac{\varrho(u^t) - \varrho(u)}{t} \psi \, dx \longrightarrow \int_\Omega \varrho'(u) \, \dot{u} \, \psi \, dx \quad \text{as } t \searrow 0$$

and

$$\int_\Omega A(t) \nabla \frac{u^t - u}{t} \cdot \nabla \psi \, dx \longrightarrow \int_\Omega \nabla \dot{u} \cdot \nabla \psi \, dx \quad \text{as } t \searrow 0.$$

We now show that the strong material derivative exists. For this subtract (3.14) from (3.13) to obtain

$$\begin{aligned} &\int_\Omega A(t) \nabla \left(\frac{u^t - u}{t} - \dot{u} \right) \cdot \nabla \psi \, dx + \int_\Omega \xi(t) \left[\int_0^1 \varrho'(u_s^t) \, ds \right] \left(\frac{u^t - u}{t} - \dot{u} \right) \psi \, dx \\ &= \int_\Omega (A(t) - I) \nabla \dot{u} \cdot \nabla \psi \, dx + \int_\Omega (\xi(t) - 1) \left[\int_0^1 \varrho'(u_s^t) \, ds \right] \dot{u} \, \psi \, dx \\ &\quad + \int_\Omega \left[\int_0^1 \varrho'(u_s^t) - \varrho'(u) \, ds \right] \dot{u} \, \psi \, dx - \int_\Omega \left(\frac{A(t) - I}{t} - A'(0) \right) \nabla u \cdot \nabla \psi \, dx \\ &\quad + \int_\Omega \left(\frac{\xi(t) - 1}{t} - \operatorname{div}(\theta) \right) \varrho(u) \, \psi \, dx + \int_\Omega \left(\frac{\xi(t) - 1}{t} - \operatorname{div}(\theta) \right) f^t \psi \, dx \\ &\quad + \int_\Omega \left(\frac{f^t - f}{t} - \nabla f \cdot \theta \right) \psi \, dx. \end{aligned}$$

Now we insert $\psi = w^t - \dot{u}$ as test function into the previous equation. Using Proposition 2.1 and the fact that $\xi(t) > 0$, $\varrho' \geq 0$ we get

$$
\begin{aligned}
\gamma_1 \|\nabla(w^t - \dot{u})\|^2_{L_2(\Omega)} \leq & \int_\Omega (A(t) - I)\nabla \dot{u} \cdot \nabla(w^t - \dot{u})\, dx \\
& + \int_\Omega (\xi(t) - 1) \int_0^1 \varrho'(u_s^t)\, ds\, \dot{u}\, (w^t - \dot{u})\, dx \\
& + \int_\Omega \int_0^1 (\varrho'(u_s^t) - \varrho'(u)\, ds)\, \dot{u}\, (w^t - \dot{u})\, dx \\
& - \int_\Omega \left(\frac{A(t) - I}{t} - A'(0) \right) \nabla u \cdot \nabla(w^t - \dot{u})\, dx \\
& + \int_\Omega \left(\frac{\xi(t) - 1}{t} - \operatorname{div}(\theta) \right) (\varrho(u)\, (w^t - \dot{u}) + f^t\, (w^t - \dot{u}))\, dx \\
& + \int_\Omega \left(\frac{f^t - f}{t} - \nabla f \cdot \theta \right) (w^t - \dot{u})\, dx.
\end{aligned}
$$

Using the convergences $A(t) \to I$, $(A(t) - I)/t - A'(0) \to 0$, $(f^t - f)/t - \nabla f \cdot \theta \to 0$, $\xi(t) \to 1$ and $(\xi(t) - 1)/t - \operatorname{div}(\theta)$ in $C(\overline{\Omega})$, and the uniform boundedness of $\|w^t - \dot{u}\|_{H^1(\Omega)}$ and $\|\dot{u}\|_{H^1(\Omega)}$ yields

$$
\|w^t - \dot{u}\|_{H^1(\Omega)} \to 0 \quad \text{as } t \searrow 0.
$$

We are now in the position to calculate the volume expression of the shape derivative. First, we differentiate (3.3) with respect to t

$$
dJ(\Omega)[\theta] = \int_\Omega \operatorname{div}(\theta)|u - u_r|^2\, dx - \int_\Omega 2(u - u_r)\nabla u_r \cdot \theta\, dx + \int_\Omega 2(u - u_r)\dot{u}\, dx.
$$

Note that for the previous calculation it was enough to have $\|u^t - u\|_{H^1(\Omega)} \leq ct$ for all $t \in [0, \tau]$. This is sufficient to differentiate the L_2 cost function. Nevertheless, for a cost function that involves gradients of u such as

$$
\tilde{J}(\Omega) := \int_\Omega \|\nabla u - \nabla u_r\|^2\, dx,
$$

this is not true anymore. Now in order to eliminate the material derivative in the last equation, the so-called adjoint equation is introduced

$$
\text{Find } p \in H_0^1(\Omega): \quad d_\varphi E(\Omega, u; p, \psi) = -2 \int_\Omega (u - u_r)\, \psi\, dx \quad \text{for all } \psi \in H_0^1(\Omega). \tag{3.15}
$$

The function p is called *adjoint state*. Finally, testing the adjoint equation with $\dot{u}$ and the material derivative Eq. (3.14) with p, we arrive at the volume expression

$$
\begin{aligned}
dJ(\Omega)[\theta] &\overset{(3.15)}{=} \int_\Omega \operatorname{div}(\theta)|u-u_r|^2\,dx \\
&\quad - \int_\Omega 2(u-u_r)\nabla u_r\cdot\theta\,dx - d_\varphi E(\Omega,u;p,\dot u) \\
&\overset{(3.14)}{=} \int_\Omega \operatorname{div}(\theta)|u-u_r|^2\,dx - \int_\Omega 2(u-u_r)\nabla u_r\cdot\theta\,dx \\
&\quad + \int_\Omega A'(0)\nabla u\cdot\nabla p + \operatorname{div}(\theta)\varrho(u)p\,dx - \int_\Omega \operatorname{div}(\theta f)p\,dx. \qquad (3.16)
\end{aligned}
$$

Note that the volume expression already makes sense when $u, p \in H^1_0(\Omega)$. Assuming higher regularity of the state and adjoint (e.g. $u, p \in H^2(\Omega)\cap H^1_0(\Omega)$) would allow us to rewrite the previous volume expression into a boundary expression, that is, an integral over the boundary $\partial\Omega$.

3.2 Shape Derivative Method

Assuming that the solutions u, p and the boundary $\partial\Omega$ are smooth, say C^2, we may transform the volume expression (3.16) into an integral over $\partial\Omega$. This can be accomplished by integration by parts or in the following way. Instead of transporting the cost function back to Ω, one may directly differentiate $J(\Omega_t) = \int_{\Omega_t}|\Psi^t(u^t) - u_r|^2\,dx$ by invoking Theorem 2.7, to obtain

$$
dJ(\Omega)[\theta] = \int_{\partial\Omega}|u-u_r|^2\theta_n ds + \int_\Omega 2\,(u-u_r)(\dot u - \partial_\theta u)\,dx. \qquad (3.17)
$$

The function $u' := \dot u - \partial_\theta u$ is called **shape derivative** of u at Ω in direction θ associated with the parametrization Ψ_t. It is linear with respect to θ. Note that since $\Psi^0 = id$, we have $\Psi^t\circ\Psi^{-t} = \Psi^0 = id_{H^1_0(\Omega)}$ and $\Psi^{-t}\circ\Psi^t = \Psi^0 = id_{H^1_0(\Omega_t)}$. Note that setting $u^t := \Psi_t(u_t)$, we can write

$$
u' = \frac{d}{dt}\Psi^t(u^t)|_{t=0} = \frac{d}{dt}(u^t\circ\Phi_t^{-1})|_{t=0}.
$$

Therefore the shape derivative decomposes into two parts, namely

$$
u' = \underbrace{\partial_t\Psi^t(u^t)_{|t=0}}_{\in L_2(\Omega)} + \underbrace{\Psi^0(\dot u)}_{\in H^1_0(\Omega)},
$$

where $\partial_t\Psi^t(u^t)|_{t=0} := \lim_{t\searrow 0}(\Psi^t(u^t) - \Psi^0(u^t))/t = -\partial_\theta u$. Assuming that the solution u belongs to $u\in H^1_0(\Omega)\cap H^2(\Omega)$, we have

$$u' = \underbrace{\partial_t \Psi^t(u^t)_{|t=0}}_{\in H^1(\Omega)} + \underbrace{\Psi^0(\dot{u})}_{\in H_0^1(\Omega)\cap H^2(\Omega)}$$

The perturbed state equation (3.2) can be rewritten as

$$\int_{\Omega_t} \nabla(\Psi^t(u^t)) \cdot \nabla(\Psi^t(\varphi)) \,+\, \varrho(\Psi^t(u^t))\,(\Psi^t(\varphi))\,dx = \int_{\Omega_t} f\,\Psi^t(\varphi)\,dx$$

for all $\varphi \in H_0^1(\Omega)$. Suppose that $u, p \in H^2(\Omega) \cap H_0^1(\Omega)$. Hence by formally differentiating the last equation using the transport Theorem 2.7:

$$\begin{aligned}&\int_\Omega \nabla u' \cdot \nabla\varphi + \varrho'(u)u'\,\varphi\,dx - \int_\Omega \nabla u \cdot \partial_\theta\varphi + \varrho(u)\,\partial_\theta\varphi\,dx \\ &\quad + \int_{\partial\Omega} (\nabla u \cdot \nabla\varphi + \varrho(u)\,p)\,\theta_n ds = \int_{\partial\Omega} f\varphi\,\theta_n ds - \int_\Omega f\,\partial_\theta\varphi\,dx\end{aligned} \tag{3.18}$$

for all $\varphi \in H^2(\Omega) \cap H_0^1(\Omega)$, where $\theta_n := \theta \cdot n$ and $\partial_\theta := \theta \cdot \nabla$. Note that the adjoint state p vanishes on Γ. This equation can also be derived from (3.14) by partial integration.

Remark 3.2 Note that u' does not belong to $H_0^1(\Omega)$, but only to $H^1(\Omega)$. As the shape derivative does not belong to the solution space of the state equation, it may lead to false or incomplete formulas for the boundary expression. This seems to be first observed in [17].

Note that $u = 0$ on Γ implies that $\nabla_\Gamma u = 0$ and hence $\nabla u|_\Gamma = (\partial_n u)n$. Then integrating by parts in (3.18) and using that u is a strong solution yields

$$\begin{aligned}\int_\Omega \nabla\dot{u} \cdot \nabla\varphi \,+\, \varrho'(u)\dot{u}\,\varphi\,dx &= \int_{\partial\Omega} (\partial_n u\,\partial_n\varphi - 2\,\partial_n u\,\partial_n\varphi)\,\theta_n\,ds \\ &\quad + \int_\Omega \partial_\theta u\,(-\Delta\varphi + \varrho'(u)\,\varphi)\,dx.\end{aligned} \tag{3.19}$$

Now, one can eliminate $\dot{u}$ in $dJ(\Omega)[\theta]$ given by (3.17) using the previous equation and the adjoint state equation

$$\begin{aligned}dJ(\Omega)[\theta] &\overset{(3.15)}{=} \int_{\partial\Omega} |u - u_r|^2\,\theta_n\,ds + \int_\Omega \nabla\dot{u} \cdot \nabla p + \varrho'(u)\,\dot{u}\,p\,dx \\ &\quad + \int_\Omega \partial_\theta u\,2(u - u_r)\,dx \\ &\overset{(3.19)}{=} \int_{\partial\Omega} |u - u_r|^2\,\theta_n\,ds - \int_{\partial\Omega} 2\partial_n u\,\partial_n p\,\theta_n ds \\ &\quad + \int_\Omega (-\Delta p + \varrho'(u)\,p + 2(u - u_r))\partial_\theta u\,dx.\end{aligned}$$

Finally, assuming that p solves the adjoint equation in the strong sense, we get

$$dJ(\Omega)[\theta] = \int_{\partial\Omega} (|u - u_r|^2 - \partial_n u \, \partial_n p) \, \theta_n \, ds. \tag{3.20}$$

What we observe in the calculations above is that there is no material derivative $\dot{u}$ or shape derivative u' in the final expression (3.16) or (3.20). This suggests that there might be a way to obtain this formula without the computation of $\dot{u}$. In the next section, we get to know one possible way to avoid the material derivatives.

4 The Min-Max Formulation of Correa and Seeger

In this section, we want to discuss the minimax formulation of shape optimization problems and a theorem of Correa and Seeger [6] that gives a powerful tool to differentiate a minimax function with respect to a parameter. The cost function for many optimal control problems can be rewritten as the min-max of a Lagrangian function $\mathcal{L}$, that is, an utility function plus the equality constraints, i.e.,

$$J(u) = \inf_{\varphi \in A} \sup_{\psi \in B} \mathcal{L}(u, \varphi, \psi).$$

Therefore, the directional differentiation of the cost function is equivalent to the differentiation of the inf-sup with respect to u. This method has clear restrictions, but still it is applicable to many commonly used cost functions and to a certain class of non-linear partial differential equations. This method is in particular applicable to linear partial differential equations and convex cost functions.

4.1 Saddle Points and Their Characterization

For the convenience of the reader we recall here the definition of saddle points and their characterization.

Definition 4.1 Let A, B be sets and $G : A \times B \to \mathbf{R}$ a map. Then a pair $(u, p) \in A \times B$ is said to be a **saddle point** on $A \times B$ if

$$G(u, \psi) \le G(u, p) \le G(\varphi, p) \quad \text{for all } \varphi \in A, \quad \text{for all } \psi \in B.$$

We have the following equivalent condition for (u, p) being a saddle point.

Lemma 4.2 *A pair $(u, p) \in A \times B$ is a saddle point of $G(,)$ if and only if*[4]

$$\min_{\hat{\varphi}\in A} \sup_{\hat{\psi}\in B} G(\hat{\varphi}, \hat{\psi}) = \max_{\hat{\psi}\in B} \inf_{\hat{\varphi}\in A} G(\hat{\varphi}, \hat{\psi}),$$

and it is equal to $G(u, p)$, where u being the attained minimum and p the attained maximum, respectively.

Proof A proof can be found in [20, p. 166–167].

4.2 Min-Max Formulation for the Semi-linear Equation

Let $\varphi, \psi \in H_0^1(\Omega)$ be two functions. Instead of differentiating the cost function and the state equation separately, we incorporate both in the Lagrangian

$$\mathcal{L}(\Omega, \varphi, \psi) := \int_\Omega |\varphi - u_r|^2\, dx + \int_\Omega \nabla\varphi \cdot \nabla\psi\, dx + \int_\Omega \varrho(\varphi)\psi\, dx - \int_\Omega f\psi\, dx.$$

The point of departure for the **min-max formulation** is the observation that

$$J(\Omega) = \min_{\varphi\in H_0^1(\Omega)} \sup_{\psi\in H_0^1(\Omega)} \mathcal{L}(\Omega, \varphi, \psi),$$

since for any $\varphi \in H_0^1(\Omega)$

$$\sup_{\psi\in H_0^1(\Omega)} \mathcal{L}(\Omega, \varphi, \psi) = \begin{cases} J(\Omega) & \text{when } \varphi = u \text{ solves (3.1)} \\ +\infty & \text{else .} \end{cases}$$

In order to apply the **theorem of Correa-Seeger** to the Lagrangian $\mathcal{L}$, we have to show that it admits saddle points. Reasonable conditions to ensure the existence of saddle points for our specific example is to assume that $\mathcal{L}$ is convex and differentiable with respect to φ.

Assumption $(\mathcal{C})$ The function ϱ is linear, that is, $\varrho(x) = ax$, where $a \in \mathbf{R}$.

Since for every open set $\Omega \subset \mathbf{R}^d$ the Lagrangian $\mathcal{L}$ is convex and differentiable with respect to φ, and concave and differentiable with respect to ψ, we know from [20, Proposition 1.6, p. 169–170] that the saddle points can be characterized by

$$\begin{aligned} u \in H_0^1(\Omega) : \quad & \partial_\psi \mathcal{L}(\Omega, u, p)(\hat{\psi}) = 0 \quad \text{for all } \hat{\psi} \in H_0^1(\Omega) \\ p \in H_0^1(\Omega) : \quad & \partial_\varphi \mathcal{L}(\Omega, u, p)(\hat{\varphi}) = 0 \quad \text{for all } \hat{\varphi} \in H_0^1(\Omega). \end{aligned}$$

[4] Here the min and max indicate that the infimum and supremum is attained, respectively.

The last equations are exactly the state equation (3.1) and the adjoint Eq. (3.15). To compute the shape derivative of J, we consider for $t > 0$

$$
\begin{aligned}
J(\Omega_t) &= \min_{\hat{\varphi}\in H_0^1(\Omega_t)} \sup_{\hat{\psi}\in H_0^1(\Omega_t)} \mathcal{L}(\Omega_t, \hat{\varphi}, \hat{\psi}) \\
&= \min_{\varphi\in H_0^1(\Omega)} \sup_{\psi\in H_0^1(\Omega)} \mathcal{L}(\Omega_t, \Psi^t(\varphi), \Psi^t(\psi)),
\end{aligned}
\tag{4.1}
$$

where the saddle points of $\mathcal{L}(\Omega_t, \cdot, \cdot)$ are again given by the solutions of (3.1) and (3.15), but the domain Ω has to be replaced by Ω_t. By definition of a saddle point

$$
\mathcal{L}(\Omega_t, u_t, \hat{\psi}) \le \mathcal{L}(\Omega_t, u_t, p_t) \le \mathcal{L}(\Omega_t, \hat{\varphi}, p_t) \quad \text{for all } \hat{\psi}, \hat{\varphi} \in H_0^1(\Omega_t). \tag{4.2}
$$

Since $\Psi_t : H_0^1(\Omega_t) \to H_0^1(\Omega)$ is a bijection it is easily seen that the saddle points of $G(t, \varphi, \psi) := \mathcal{L}(\Omega_t, \Psi^t(\varphi), \Psi^t(\psi))$ are given by $u^t = \Psi_t(u_t)$ and $p^t = \Psi_t(p_t)$. It can also be verified that the function u^t solves (3.4) and applying the change of variables $\Phi_t(x) = y$ to (3.15) shows that p^t solves

$$
\int_\Omega A(t)\nabla\psi \cdot \nabla p^t + \xi(t)\, \varrho'(u^t)\, p^t\, \psi\, dx = -2\int_\Omega \xi(t)(u^t - u_r^t)\psi\, dx \tag{4.3}
$$

for all $\psi \in H_0^1(\Omega)$. Moreover, the functions u^t, p^t satisfy

$$
G(t, u^t, \psi) \le G(t, u^t, p^t) \le G(t, \varphi, p^t) \quad \text{for all } \psi, \varphi \in H_0^1(\Omega),
$$

where G takes, after applying the change of variables $\Phi_t(x) = y$, the explicit form

$$
G(t, \varphi, \psi) = \int_\Omega \xi(t)|\varphi - u_r^t|^2\, dx + \int_\Omega A(t)\nabla\varphi \cdot \nabla\psi + \xi(t)\varrho(\varphi)\,\psi\, dx - \int_\Omega \xi(t) f^t \psi\, dx. \tag{4.4}
$$

From Lemma 4.2 and the definition of a saddle point (u^t, p^t) of $G(t,)$, we conclude

$$
g(t) := \min_{\varphi\in H_0^1(\Omega)} \sup_{\psi\in H_0^1(\Omega)} G(t, \varphi, \psi) = G(t, u^t, p^t). \tag{4.5}
$$

Moreover, we have the relation

$$
g(t) = G(t, u^t, \psi) \quad \text{for all } \psi \in H_0^1(\Omega), \tag{4.6}
$$

since u^t solves (3.4). In view of (4.1), we can obtain the shape derivative $dJ(\Omega)[\theta]$ by calculating the derivative of $g(t)$ at $t = 0$. In order to use (4.5), we have to find conditions which show that we are allowed to differentiate the min-max of the function G with respect to t at $t = 0$. On the other hand the relation (4.6) shows that $dJ(\Omega)[\theta] = \frac{d}{dt}G(t, u^t, \psi)_{|_{t=0}}$ for all $\psi \in H_0^1(\Omega)$, that means the differentiability of the min-max of G is equivalent to the differentiability of $G(t, u^t, \psi)$ and it is independent of ψ. Sufficient conditions for the differentiability are provided by the Theorem of Correa-Seeger (Theorem 4.5). Note the relation (4.5) is also true for a general function G when u^t, p^t are saddle points, but the relation (4.6) only for the special structure (4.4) of G. It is clear that if the functions u^t and G are sufficiently differentiable the derivative $\frac{d}{dt}(g(t))_{t=0}$ exists. The purpose of the reformulation of the cost function as an inf-sup is to avoid the material derivatives $\dot{u}$. Note that when the state equation has no unique solution the cost function is not well-defined, but the the function g is. Without a computation of the material derivative $\dot{u}$ or $\dot{p}$, we can show (cf. also the Theorem 4.5) that $dJ(\Omega)[\theta] = \partial_t G(0, u, p)$. Clearly the functions $t \mapsto u^t$, $t \mapsto p^t$ and G have to satisfy some additional conditions. Let us sketch the proof of this fundamental result when G is given by (4.4). To be more precise we want to establish the following.

Proposition 4.3 *Let $\psi \in H^1_0(\Omega)$. Then the function $[0, \tau] \to \mathbf{R} : \ t \mapsto G(t, u^t, \psi)$ is differentiable from the right side in 0. Moreover, we have the following*

$$\frac{d}{dt} G(t, u^t, \psi)|_{t=0} = \partial_t G(0, u, p) \tag{4.7}$$

for arbitrary $\psi \in H^1_0(\Omega)$. Here, $p \in H^1_0(\Omega)$ solves the adjoint Eq. (3.15).

Proof By definition of a saddle point (u^t, p^t)

$$G(t, u^t, p^t) \le G(t, u, p^t), \quad G(0, u, p) \le G(0, u^t, p)$$

and therefore setting $\Delta(t) := G(t, u^t, p^t) - G(0, u, p)$ gives

$$G(t, u^t, p) - G(0, u^t, p) \le \Delta(t) \le G(t, u, p^t) - G(0, u, p^t).$$

Using the mean value theorem, we find for each $t \in [0, \tau]$ numbers $\zeta_t, \eta_t \in (0, 1)$ such that

$$t\partial_t G(t\zeta_t, u^t, p) \le \Delta(t) \le t\partial_t G(t\eta_t, u, p^t), \tag{4.8}$$

where the derivative of G with respect to t is given by

$$\begin{aligned} \partial_t G(t, \varphi, \psi) = & \int_\Omega \xi'(t)|\varphi - u^t_r|^2 - 2\xi(t)(\varphi - u^t_r)B(t)\nabla u^t_r \cdot \theta^t \, dx \\ & + \int_\Omega A'(t)\nabla\varphi \cdot \nabla\psi + \xi'(t)\varrho(\varphi)\,\psi - \xi'(t)\, f^t \psi - B(t)\nabla f^t \cdot \theta^t \psi \, dx \end{aligned} \tag{4.9}$$

and the derivatives ξ' and A' are given by Lemma 2.3. It can be verified from this formula that $(t, \varphi) \mapsto \partial_t G(t, \varphi, p)$ is strongly continuous and $(t, \psi) \mapsto \partial_t G(t, u, \psi)$ is even weakly continuous. Moreover, from (3.4) and (4.3) it can be inferred that $t \mapsto u^t$ and $t \mapsto p^t$ are bounded in $H^1_0(\Omega)$ and therefore for any sequence $(t_n)_{n\in\mathbf{N}}$ we get $u^{t_n} \rightharpoonup w$, $p^{t_n} \rightharpoonup v$ for two elements $w, v \in H^1_0(\Omega)$. Passing to the limit in

(3.4) and (4.3) and taking into account Lemma 2.5, we see that w solves the state equation and v the adjoint equation. By uniqueness of the state and adjoint equation we get $w = u$ and $v = p$. Selecting a further subsequence $(t_{n_k})_{k\in\mathbf{N}}$ yields that $u^{t_{n_k}}$ converges strongly in $L_2(\Omega)$. Thus we conclude from (4.8)

$$\liminf_{t\searrow 0} \Delta(t)/t \geq \partial_t G(0,u,p), \quad \limsup_{t\searrow 0} \Delta(t)/t \leq \partial_t G(0,u,p),$$

which leads to $\limsup_{t\searrow 0} \Delta(t)/t = \liminf_{t\searrow 0} \Delta(t)/t$. This finishes the proof of (4.7) and hence we have shown the shape differentiability of J.

Evaluating the derivative $\partial_t G(t,u,p)|_{t=0}$ leads to the formula (3.16). Note that when $\partial\Omega$ is C^2 then we may extend $u, p \in H^2(\Omega)\cap H^1_0(\Omega)$ to global H^2 functions $\tilde{u}, \tilde{p} \in H^2(\mathbf{R}^d)$. Then the boundary expression is obtained by applying the transport theorem (Theorem 2.7) to $\frac{d}{dt}\mathcal{L}(\Omega_t, \Psi^t(\tilde{u}), \Psi^t(\tilde{p}))|_{t=0}$:

$$\begin{aligned} dJ(\Omega)[\theta] = &\int_\Gamma (|u-u_r|^2 + \nabla u\cdot\nabla p + \varrho(u)\,p)\theta_n\,ds + \int_\Omega \nabla\mathring{u}\cdot\nabla p + \varrho'(u)\,\mathring{u}\,p\,dx \\ &+ \int_\Omega (u-u_r)\mathring{u}\,dx + \int_\Omega \nabla u\cdot\nabla\mathring{p} + \varrho(u)\,\mathring{p}\,dx - \int_\Omega f\,\mathring{p}\,dx, \end{aligned}$$

where $\mathring{u} = \partial_t(\Psi^t(\tilde{u}))|_{t=0} = -\nabla u\cdot\theta$, $\mathring{p} = \partial_t(\Psi^t(\tilde{p}))|_{t=0} = -\nabla p\cdot\theta$. To rewrite the equation into an integral over Γ, we integrate by parts and obtain

$$\begin{aligned} dJ(\Omega)[\theta] = &\int_\Gamma (|u-u_r|^2 + \nabla u\cdot\nabla p + \varrho(u)\,p)\,\theta_n\,ds \\ &+ \int_{\partial\Omega} \mathring{u}\;\partial_n p\,ds + \int_{\partial\Omega} \partial_n u\;\mathring{p}\,ds \\ &- \int_\Omega \mathring{u}\,\big(-\Delta p + \varrho'(u)\,p + 2(u-u_r)\big)\,dx \\ &- \int_\Omega \mathring{p}\,(-\Delta u + \varrho(u) - f)\,dx. \end{aligned}$$

Finally, using the strong solvability of u and p, and taking into account $\nabla u = (\partial_n u)n$ on $\partial\Omega$, we arrive at (3.20).

Remark 4.4 We point out that the inequalities (4.2) are the key to avoid the material derivatives. Nevertheless, without the assumption of convexity of G with respect to φ it is difficult to prove this inequality.

4.3 The Theorem of Correa-Seeger

Finally, we quote the Theorem of Correa-Seeger, which applies in situations when the state equation admits no unique solution and the Lagrangian admits saddle points.

The proof is similar to the proof of Proposition 4.3. Let a real number $\tau > 0$ and vector spaces E and F be given. We consider a mapping

$$G : [0, \tau] \times E \times F \to \mathbf{R}.$$

For each $t \in [0, \tau]$ we define

$$g(t) := \inf_{u \in E} \sup_{p \in F} G(t, u, p), \qquad h(t) := \sup_{p \in F} \inf_{u \in E} G(t, u, p)$$

and the associated sets

$$E(t) = \left\{ \hat{\varphi} \in E : \sup_{p \in F} G(t, \hat{\varphi}, p) = g(t) \right\}$$
$$F(t) = \left\{ \hat{\psi} \in F : \inf_{u \in E} G(t, u, \hat{\psi}) = h(t) \right\}.$$

For fixed t they are the points in E respectively F where inf respectively the sup are attained in $g(t)$ respectively $h(t)$. We know that if $g(t) = h(t)$ then the set of saddle points is given by

$$S(t) := E(t) \times F(t).$$

Theorem 4.5 (R. Correa and A. Seeger, [9]) *Let the function G and the vector spaces E, F be as before. Suppose the following conditions:*

(HH1) *For all $t \in [0, \tau]$ assume $S(t) \neq \emptyset$.*
(HH2) *The partial derivative $\partial_t G(t, u, p)$ exists for all $(t, u, p) \in [0, \tau] \times E \times F$.*
(HH3) *For any sequence $(t_n)_{n \in \mathbf{N}}$ with $t_n \searrow 0$ there exists a subsequence $(t_{n_k})_{k \in \mathbf{N}}$ and an element $u_0 \in E(0)$, $u_{t_{n_k}} \in E(t_{n_k})$ such that for all $p \in F(0)$*

$$\lim_{\substack{k \to \infty \\ t \searrow 0}} \partial_t G(t, u_{n_k}, p) = \partial_t G(0, u_0, p).$$

(HH4) *For any sequence $(t_n)_{n \in \mathbf{N}}$ with $t_n \searrow 0$ there exists a subsequence $(t_{n_k})_{k \in \mathbf{N}}$ and an element $p_0 \in F(0)$, $p_{t_{n_k}} \in F(t_{n_k})$ such that for all $u \in E(0)$*

$$\lim_{\substack{k \to \infty \\ t \searrow 0}} \partial_t G(t, u, p_{t_{n_k}}) = \partial_t G(0, u, p_0).$$

Then there exists $(u_0, p_0) \in E(0) \times F(0)$ such that

$$\frac{d}{dt} g(t)|_{t=0} = \partial_t G(0, u_0, p_0).$$

4.4 Céa's Classical Lagrange Method and a Modification

Let the function G be defined by (4.4). Assume that G is sufficiently differentiable with respect to t, φ and ψ. Additionally, assume that the strong material derivative $\dot{u}$ exists in $H_0^1(\Omega)$. Then we may calculate as follows

$$dJ(\Omega)[\theta] = \frac{d}{dt}(G(t, u^t, p))|_{t=0} = \underbrace{\partial_t G(t, u, p)|_{t=0}}_{\text{shape derivative}} + \underbrace{\partial_\varphi G(0, u, p)(\dot{u})}_{\text{adjoint equation}},$$

and due to $\dot{u} \in H_0^1(\Omega)$ it implies

$$dJ(\Omega)[\theta] = \partial_t G(t, u, p)|_{t=0}.$$

Therefore, we can follow the lines of the calculation of the previous section to obtain the boundary and volume expression of the shape derivative.

In the original work [5], it was calculated as follows

$$dJ(\Omega)[\theta] = \partial_\Omega \mathcal{L}(\Omega, u, p) + \partial_\varphi \mathcal{L}(\Omega, u, p)(u') + \partial_\psi \mathcal{L}(\Omega, u, p)(p'), \quad (4.10)$$

where $\partial_\Omega \mathcal{L}(\Omega, u, p) := \lim_{t \searrow 0}(\mathcal{L}(\Omega_t, u, p) - \mathcal{L}(\Omega, u, p))/t$. Then it was assumed that u' and p' belong to $H_0^1(\Omega)$, which has as consequence that $\partial_\varphi \mathcal{L}(\Omega, u, p)(u') = \partial_\psi \mathcal{L}(\Omega, u, p)(p') = 0$. Thus (4.10) leads to the wrong formula

$$dJ(\Omega)[\theta] = \int_\Gamma (|u - u_r|^2 + \partial_n u\, \partial_n p)\, \theta_n \, ds.$$

This can be fixed by noting that $u' = \dot{u} - \partial_\theta u$ and $p' = \dot{p} - \partial_\theta p$ with $\dot{u}, \dot{p} \in H_0^1(\Omega)$:

$$dJ(\Omega)[\theta] = \partial_\Omega \mathcal{L}(\Omega, u, p) - \partial_\varphi \mathcal{L}(\Omega, u, p)(\partial_\theta u) - \partial_\psi \mathcal{L}(\Omega, u, p)(\partial_\theta p),$$

which gives the correct formula. Finally, note that for Maxwell's equations a different parametrization than $v \mapsto v \circ \Phi_t$ of the function space is necessary since the differential operator is modified differently. This leads then to a different definition of the shape derivative and also the formulas will be different. This is well-known from the finite element analysis of Maxwell's equations; cf. [1, 3, 13, 16].

5 Rearrangement of the Cost Function

The rearrangement method introduced in [14] avoids the material derivative and is applicable to a wide class of elliptic problems. We describe the method at hand of our semi-linear example and write subsequently the perturbed cost function (3.3) as

$$J(\Omega_t) = \int_\Omega j(t, u^t)\, dx, \quad j(t, v) := \xi(t)|v - u_r^t|^2. \tag{5.1}$$

In order to derive the shape differentiability, we make the following assumptions:

Assumption $(\mathcal{R})$ Assume that $\varrho \in C^2(\mathbf{R}) \cap L_\infty(\mathbf{R})$, $\varrho'' \in L_\infty(\mathbf{R})$ and $\varrho'(x) \geq 0$ for all $x \in \mathbf{R}$.

Instead of requiring the Lipschitz continuity of $t \mapsto u^t$, we claim that the following holds: there exist constants $c, \tau, \varepsilon > 0$ such that $\|u^t - u\|_{H_0^1(\Omega)} \leq ct^{1/2+\varepsilon}$ for all $t \in [0, \tau]$.

Theorem 5.1 *Let Assumption* $(\mathcal{R})$ *be satisfied and let* $\theta \in C_c^2(D, \mathbf{R}^d)$. *Then* $J(\Omega_t)$ *given by* (5.1) *is differentiable with derivative:*

$$dJ(\Omega)[\theta] = \partial_t G(0, u, p),$$

where u, p *are solutions of the state and adjoint state equation.*

Proof The main idea is to rewrite the difference $J(\Omega_t) - J(\Omega)$ and use a first order expansions of the PDE and the cost function with respect to the unknown together with Hölder continuity of $t \mapsto u^t$. To be more precise, write

$$\begin{aligned}
\frac{J(\Omega_t) - J(\Omega)}{t} &= \underbrace{\frac{1}{t}\int_\Omega (j(t, u^t) - j(t, u) - j'(t, u)(u^t - u))\, dx}_{B_1(t)} \\
&+ \underbrace{\frac{1}{t}\int_\Omega (j(t, u) - j(0, u))\, dx}_{B_2(t)} \\
&+ \underbrace{\frac{1}{t}\int_\Omega (j'(t, u) - j'(0, u))(u^t - u)\, dx}_{B_3(t)} \\
&+ \underbrace{\frac{1}{t}\int_\Omega j'(0, u)(u^t - u)\, dx}_{B_4(t)},
\end{aligned} \tag{5.2}$$

where $j' := \partial_u j$ and $u_s^t := su^t + (1-s)u$. Using the mean value theorem in integral form entails for some constant $C > 0$

$$\begin{aligned}
\int_\Omega (j(t, u^t) - j(t, u) - j'(t, u)(u^t - u))\, dx &= \int_0^1 (1 - s) j''(t, u_s^t)(u^t - u)^2\, dx \\
&\leq C\|u^t - u\|_{L_2(\Omega)}^2 \quad \text{for all } t \in [0, \tau].
\end{aligned}$$

Using the $\lim_{t\searrow 0}\|u^t-u\|_{H^1_0(\Omega)}/\sqrt{t}=0$, we see that B_1 tends to zero as $t\searrow 0$. Let $\tilde{E}(t,\varphi)$ be defined by (3.5). Then the fourth term in (5.2) can be written by using the adjoint Eq. (3.15) as follows

$$\begin{aligned}\int_\Omega j'(0,u)(u^t-u)\,dx &= d_\varphi\tilde{E}(0,u^t;p)-d_\varphi\tilde{E}(0,u;p)-d^2_\varphi\tilde{E}(0,u;u^t-u,p)\\ &\quad + d_\varphi\bar{E}(t,u^t;p)-d_\varphi\bar{E}(t,u;p)\\ &\quad - (d_\varphi\tilde{E}(0,u^t;p)-d_\varphi\tilde{E}(0,u;p))\\ &\quad + d_\varphi\tilde{E}(t,u;p)-d_\varphi\tilde{E}(0,u;p).\end{aligned} \tag{5.3}$$

By standard elliptic regularity theory, we may assume that $p\in H^1_0(\Omega)\cap L_\infty(\Omega)$. Therefore by virtue of Taylor's formula in Banach spaces (cf. [2, p. 193, Theorem 5.8]) the first line in (5.3) on the right hand side can be written as

$$\begin{aligned}&d_\varphi\tilde{E}(0,u^t;p)-d_\varphi\tilde{E}(0,u;p)-d^2_\varphi\tilde{E}(0,u;u^t-u,p)\\ &=\int_0^1(1-s)d^3\tilde{E}(0,u^t_s;u^t-u,u^t-u,p)\,ds,\end{aligned}$$

where the remainder can be estimated as follows

$$\begin{aligned}\int_0^1(1-s)d^3_\varphi\tilde{E}(0,u^t_s;u^t-u,u^t-u,p)\,ds &= \int_0^1(1-s)\varrho''(u^t_s)(u^t-u)^2\,p\,ds\\ &\le \frac{1}{2}\|p\|_{L_\infty(\Omega)}\|\varrho''\|_{L_\infty(\mathbf{R})}\|u^t-u\|_{L_2(\Omega)}.\end{aligned}$$

Using $d_\varphi\tilde{E}(t,u^t;p)-d_\varphi\tilde{E}(0,u;p)=0$, and the differentiability of $t\mapsto\tilde{E}(t,u)$ yields

$$\begin{aligned}\lim_{t\searrow 0}\frac{d_\varphi\tilde{E}(t,u^t;p)-d_\varphi\tilde{E}(t,u;p)}{t} &= \lim_{t\searrow 0}\frac{1}{t}(d_\varphi\tilde{E}(0,u^t;p)-d_\varphi\tilde{E}(0,u;p)),\\ \lim_{t\searrow 0}\frac{d_\varphi\tilde{E}(t,u;p)-d_\varphi\tilde{E}(0,u;p)}{t} &= \int_\Omega A'(0)\nabla u\cdot\nabla p-\operatorname{div}(\theta)fp-\nabla f\cdot\theta\,p\,dx.\end{aligned}$$

Thus from (5.3), we infer

$$\begin{aligned}&\lim_{t\searrow 0}\frac{1}{t}\int_\Omega j'(0,u)(u^t-u)\,dx\\ &=\int_\Omega A'(0)\nabla u\cdot\nabla p+\operatorname{div}(\theta)\varrho(u)p-\operatorname{div}(\theta)fp-\nabla f\cdot\theta\,p\,dx.\end{aligned}$$

Therefore we may pass to the limit in (5.2) and obtain

$$\lim_{t\searrow 0} \frac{J(\Omega_t) - J(\Omega)}{t} = \int_\Omega \partial_t j(0,u)\,dx + \partial_t d_\varphi \tilde{E}(0,u;\,p).$$

This finishes the proof and shows that $dJ(\Omega)[\theta] = \partial_t G(0,u,\,p)$. □

6 Differentiability of Energy Functionals

If it happens that the cost function J is the energy of the PDE (2.1), that is,

$$J(\Omega) := \min_{\varphi \in H_0^1(\Omega)} E(\Omega,\varphi),$$

then it is easy to show the shape differentiability of J by using a result from [10, p. 524, Theorem 2.1], see also [7, pp. 139]. First note that $J(\Omega_t) = \min_{\varphi \in H_0^1(\Omega)} \tilde{E}(t,\varphi)$. By definition of the minimum u^t of $\tilde{E}(t,\cdot)$ and u of $\tilde{E}(0,\cdot)$, respectively, we have

$$\tilde{E}(0,u^t) - \tilde{E}(0,u) \geq 0, \qquad \tilde{E}(t,u) - \tilde{E}(0,u) \leq 0$$

and thus

$$\begin{aligned} J(\Omega_t) - J(\Omega) &= \tilde{E}(t,u^t) - \tilde{E}(0,u^t) + \tilde{E}(0,u^t) - \tilde{E}(0,u) \\ &\geq \tilde{E}(t,u^t) - \tilde{E}(0,u^t) \\ J(\Omega_t) - J(\Omega) &= \tilde{E}(t,u^t) - \tilde{E}(t,u) + \tilde{E}(t,u) - \tilde{E}(0,u) \\ &\leq \tilde{E}(t,u) - \tilde{E}(0,u). \end{aligned}$$

Using the mean value theorem, we conclude the existence of numbers $\eta_t, \zeta_t \in (0,1)$ such that

$$t\,\partial_t \tilde{E}(\eta_t\, t, u^t) \leq J(\Omega_t) - J(\Omega) \leq t\,\partial_t \tilde{E}(\zeta_t\, t, u).$$

Thus if

$$\tilde{E}(0,u) \leq \liminf_{t\searrow 0} \partial_t \tilde{E}(\eta_t\, t, u^t), \qquad \tilde{E}(0,u) \geq \limsup_{t\searrow 0} \partial_t \tilde{E}(\zeta_t\, t, u), \tag{6.1}$$

then we may conclude that J is shape differentiable by the squeezing lemma. We obtain

$$\lim_{t\searrow 0} \frac{J(\Omega_t) - J(\Omega)}{t} = \partial_t \tilde{E}(0,u).$$

This result can be seen as a special case of Theorem 4.5. Note that in our example

$$\partial_t \tilde{E}(t,\varphi) = \int_\Omega A'(t)\nabla\varphi\cdot\nabla\varphi + \xi'(t)\varrho(\varphi)\,dx \\ - \int_\Omega \xi'(t) f^t \varphi\,dx + \int_\Omega \xi(t)\, B(t)\nabla f^t \cdot \varphi\,dx.$$

From this identity, the convergence of $u^t \to u$ in $H_0^1(\Omega)$ and the smoothness of $A(t)$, $\xi(t)$ and $B(t)$, we infer that (6.1) are verified.

7 The Averaged Adjoint Approach

Let the Banach spaces E, F and a number $\tau > 0$ be given. Consider a function

$$G : [0,\tau]\times E\times F \to \mathbf{R}, \quad (t,\varphi,\psi)\mapsto G(t,\varphi,\psi)$$

such that $\psi \mapsto G(t,\varphi,\psi)$ is affine for all $(t,\varphi)\in[0,\tau]\times E$. Introduce the *solution set of the state equation*

$$E(t) := \{u\in E|\ d_\psi G(t,u,0;\hat{\psi}) = 0 \text{ for all } \hat{\psi}\in F\}.$$

Introduce the following hypothesis.

Assumption Suppose that $E(t)=\{u^t\}$ is single-valued for all $[0,\tau]$.

(i) For all $t\in[0,\tau]$ and $\tilde{p}\in F$ the mapping

$$[0,1]\to\mathbf{R}:\ s\mapsto G(t, su^t + (1-s)u^0, \tilde{p})$$

is absolutely continuous. This implies that for almost all $s\in[0,1]$ the derivative $d_\varphi G(t, su^t+(1-s)u^0, \tilde{p}; u^t - u^0)$ exists and in particular

$$G(t,u^t,\tilde{p}) - G(t,u^0,\tilde{p}) = \int_0^1 d_\varphi G(t, su^t + (1-s)u^0, \tilde{p}; u^t - u^0)\,ds.$$

(ii) For all $t\in[0,\tau]$, $\varphi\in E$ and $\tilde{p}\in F$

$$s\mapsto d_\varphi G(t, su^t + (1-s)u^0, \tilde{p}; \varphi)$$

is well-defined and belongs to $L_1(0,1)$.

Introduce for $t\in[0,\tau]$, $u^t\in E(t)$ and $u^0\in E(0)$ the following set

$$Y(t,u^t,u^0) := \left\{q\in F|\ \forall\hat{\varphi}\in E:\ \int_0^1 d_\varphi G(t, su^t+(1-s)u^0, q;\hat{\varphi})\,ds = 0\right\},$$

which is called solution set of the *averaged adjoint equation* with respect to t, u^t and u^0. For $t = 0$ the set $Y(0, u^0) := Y(0, u^0, u^0)$ coincides with the solution set of the usual adjoint state equation

$$Y(0, u^0) = \left\{q \in F \mid d_\varphi G(0, u^0, q; \hat{\varphi}) = 0 \quad \text{for all } \hat{\varphi} \in E\right\}.$$

We call any $p \in Y(0, u^0)$ an adjoint state.

Theorem 7.1 *Let linear vector spaces E and F, a real number $\tau > 0$. Suppose that the function*

$$G : [0, \tau] \times E \times F \to \mathbf{R}, \quad (t, \varphi, \psi) \mapsto G(t, \varphi, \psi),$$

is affine in the last argument. Let Assumption (H0) and the following conditions be satisfied.

(H1) *For all $t \in [0, \tau]$ and all $(u, p) \in E(0) \times F$ the derivative $\partial_t G(t, u, p)$ exists.*
(H2) *For all $t \in [0, \tau]$ the set $Y(t, u^t, u^0)$ is nonempty and $Y(0, u^0, u^0)$ is single-valued.*
(H3) *Let $p^0 \in Y(0, u^0)$. For any sequence $(t_n)_{n\in\mathbf{N}}$ of non-negative real numbers converging to zero, there exist a subsequence $(t_{n_k})_{k\in\mathbf{N}}$ and $p^{t_{n_k}} \in Y(t_{n_k}, u^{t_{n_k}}, u^0)$ such that*

$$\lim_{\substack{k\to\infty \\ s\searrow 0}} \partial_t G(s, u^0, p^{t_{n_k}}) = \partial_t G(0, u^0, p^0).$$

Then for any $\psi \in F$:

$$\frac{d}{dt}(G(t, u^t, \psi))|_{t=0} = \partial_t G(0, u^0, p^0).$$

Proof The result was proved in [19].

7.1 Application to the Semi-linear Problem

In this section, we apply Theorem 7.1 to the example (2.1) and (2.2). For convenience, we recall the cost function

$$J(\Omega) = \int_\Omega |u - u_r|^2 \, dx, \tag{7.1}$$

and the weak formulation of (2.1)

$$\int_\Omega \nabla u \cdot \nabla \psi \, dx + \int_\Omega \varrho(u) \, \psi \, dx = \int_\Omega f \psi \, dx \quad \text{for all } \psi \in H_0^1(\Omega). \tag{7.2}$$

Suppose in the following the assumption on the data f, u_r and Ω introduced in the beginning of Sect. 3 is satisfied. Recall that the equation (7.2) on the domain $\Phi_t(\Omega)$ transported back to Ω by $y = \Phi_t(x)$ reads

$$\int_\Omega A(t)\nabla u^t \cdot \nabla\psi\, dx + \int_\Omega \xi(t)\varrho(u^t)\psi\, dx = \int_\Omega \xi(t) f^t \psi\, dx, \quad \text{for all } \psi \in H_0^1(\Omega). \tag{7.3}$$

This equation characterizes the unique minimum of the convex energy (3.5). Recall the definition of the Lagrangian associated to the problem

$$G(t,\varphi,\psi) = \int_\Omega \xi(t)|\varphi - u_r^t|^2\, dx + \int_\Omega A(t)\nabla\varphi\cdot\nabla\psi + \xi(t)\varrho(\varphi)\,\psi\, dx - \int_\Omega \xi(t) f^t\psi\, dx. \tag{7.4}$$

Theorem 7.2 *Let Assumption* $(\mathcal{A})$ *be satisfied. Then* J *defined in* (7.1) *is shape differentiable and its derivative is given by*

$$dJ(\Omega)[\theta] = \partial_t G(0, u^0, p^0),$$

where $p^0 \in Y(0, u^0)$.

Proof Let us verify the conditions (H0)–(H3) for the function G given by (7.4).

(H0) This has already been proven in Sect. 3.
(H1) This is an easy consequence of $\theta \in C_c^2(D, \mathbf{R}^d)$ and Lemma 2.5. The derivative is given by (4.9).
(H2) Note that for all $t \in [0,\tau]$, we have $\in E(t) = \{u^t\}$, where u^t solves (7.3). We have $p^t \in Y(t, u^t, u^0)$ if and only if

$$\int_\Omega A(t)\nabla\psi\cdot\nabla p^t + \xi(t)k(u,u^t)\,\psi\, dx = -\int_\Omega \xi(t)(u^t + u - 2u_r^t)\psi\, dx, \tag{7.5}$$

for all $\psi \in H_0^1(\Omega)$, where $k(u,u^t) := \int_0^1 \varrho'(u_s^t)\, ds$ and $u_s^t := su^t + (1-s)u$. Due to the Lemma of Lax-Milgram the previous equation has a unique solution $p^t \in H_0^1(\Omega)$. Note that the strong formulation of the averaged adjoint on the moved domain, namely $p_t := p^t \circ \Phi_t^{-1}$ on Ω_t satisfies

$$\begin{aligned} -\Delta p_t + k(u\circ\Phi_t^{-1}, u_t)p_t &= -(u_t - u\circ\Phi_t^{-1} - 2u_r) \quad \text{in } \Omega_t \\ p_t &= 0 \quad \text{on } \partial\Omega_t, \end{aligned}$$

where $k(u\circ\Phi_t^{-1}, u^t\circ\Phi_t^{-1}) := \int_0^1 \varrho'(u_s^t\circ\Phi_t^{-1})\, ds = \int_0^1 \varrho'(su_t + (1-s)u\circ\Phi_t^{-1})\, ds$.
(H3) We already know that Assumption $(\mathcal{A})$ implies that $t \mapsto u^t$ is continuous from $[0,\tau]$ into $H_0^1(\Omega)$. But this is actually not necessary as we will show. Suppose

that we do not know that $t \mapsto u^t$ is continuous. Then by inserting $\psi = u^t$ in the state equation (7.3), we obtain after an application of Hölder's inequality $\|u^t\|_{H^1(\Omega)} \le C$ for some constant $C > 0$. For any sequence of non-negative real numbers $(t_n)_{n\in\mathbf{N}}$ converging to zero there exists a subsequence $(t_{n_k})_{n\in\mathbf{N}}$ such that $u^{t_{n_k}} \rightharpoonup z$ as $k \to \infty$. Setting $t = t_{n_k}$ in the state equation and passing to the limit $k \to \infty$ shows $z = u$. Moreover, inserting $\psi = p^t$ into (7.5) as test function and using Hölder's inequality yields for some constant $C > 0$

$$\|p^t\|_{H_0^1(\Omega)} \le C\|u^t + u - 2u_r^t\|_{L_2(\Omega)} \quad \text{for all } t \in [0, \tau].$$

Therefore again for any sequence $(t_n)_{n\in\mathbf{N}}$ there exists a subsequence $(t_{n_k})_{n\in\mathbf{N}}$ such that $y^{t_{n_k}} \rightharpoonup q \quad$ as $k \to \infty$ for some $q \in H_0^1(\Omega)$. Selecting $t = t_{n_k}$ in (7.5), we want to pass to the limit $k \to \infty$ by using Lebesque's dominated convergence theorem. It suffices to show that $w^k(x) := \int_0^1 \varrho'(u_s^{t_{n_k}}(x))\,ds$ is bounded in $L_\infty(\mathbf{R}^d)$ independently of k and that this sequence convergences pointwise almost everywhere in Ω to $\varrho'(u)$. The boundedness of w^k follows from the continuity of u^t on $\overline{\Omega}$ and the continuity of ϱ. The pointwise convergence $w^k(x) \to \varrho(u(x))$ as $k \to \infty$ (possibly a subsequence) follows from the fact that ϱ is continuous and $u^{t_{n_k}}$ converges pointwise to u as $k \to \infty$. Therefore there is a sequence $t_n \searrow 0$ such that we may pass to the limit $n \to \infty$ in (7.5), after inserting $t = t_n$. By uniqueness, we conclude $q = p \in Y(0, u^0)$. Finally note that $(t, \psi) \mapsto \partial_t G(t, u, \psi)$ is weakly continuous.

All conditions (H0)–(H3) are satisfied and we finish the proof. □

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