On Hadamard shape gradient representations in linear elasticity

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Abstract

The paper discusses the derivation of Hadamard representations of shape gradients in linear elasticity. In particular, we present a derivation not using a variational Lagrange principle. That is, we use the adjoint equation as an auxiliary construction for the derivation of the reduced shape gradient in the Hadamard sense.

Key words: shape calculus, hadamard representation, linear elasticity, adjoint equation
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1 Introduction

In shape optimization, the so-called Hadamard representation of shape gradients play an essential role. In particular, it avoids the explicit dependence from either local or material shape derivatives of the state by introducing an adjoint state appropriately. Besides other features, it is a convenient "starting point" for computing second derivatives, since the resulting expressions for the shape Hessian do not contain second shape derivatives of the state. Basically, a standard procedure for deriving the "reduced gradient representation" is well known for "classical" control problems. In particular, integration by parts play an essential role for these transformations, very similar to those for the derivation of the weak formulation for the original state equation. However, further "pre-and postprocessing steps" (in particular, some integration by parts on the boundary) are performed within such transformations in shape optimization problems, which cannot be seen as derivation steps for a weak formulation. Of course, this outline may sound rather technical. Nevertheless, the derivation is strict if beeing sucessful. Therefore, the main aim of the note is to demonstrate the method for some particular shape problems in elasticity.

The two basic shape problems under consideration are introduced in section 2. Furthermore, the expressions are provided in this section, resulting from a formal shape calculus. The transformation to the Hadamard representation is investigated in very detail in section 3. Finally, we comment on the usefulness of the resulting representations as well as on the relationship to the so-called variational Lagrange principle, developed by Lions [10] for "classical control problems" and investigated first by Céa [3] and later intensively by Delfour and Zolesio [5] for shape problems.

2 The basic shape problems and formal shape calculus

2.1 Setting the state equation: The model equations of linear elasticity

First, we recall the model equation of linear elasticity. We refer to [4,7,11] for the mathematical investigation, see also [8] for the numerical solution of related shape optimization problems. Let $\Omega \subset \mathbb{R}^n$ ($n = 2$ or 3) be a bounded open set, occupied by an isotropic material with linear stress-strain relation (Hooke's law C). In particular (for homogeneous material),

$$C\xi = 2\mu\xi + \lambda\Big(\mathsf{Tr}\,\xi\Big)\mathbf{I}, \quad \forall \xi = \xi^T \in \mathbb{R}^{n,n}, \quad \mu, \lambda \;-\; \text{Lamé moduli.}$$

The boundary $\partial\Omega = \bar{\Omega} \cap \Omega^c$ of the domain consists of two disjoint parts, the fixed "Dirichlet-boundary" (zero displacements) Σ and the "Neumann-boundary" (application of surface loads) Γ, respectively, i.e.,

$$\partial\Omega = \Sigma \cup \Gamma, \quad \Sigma \cap \Gamma = \emptyset.$$

We denote by $f,\, g : \mathbb{R}^n \to \mathbb{R}^n$ the vector function of volume forces and surface loads, respectively, where the domain of definition for both fields are subject to shape optimization requirements. At least, they have to be prescribed on a sufficiently large hold all D. Then the displacement vector field $u = u(\Omega) : \bar{\Omega} \to \mathbb{R}^n$ satisfies the following boundary value problem

$$\begin{aligned} -\operatorname{div}\Big(Ce(u)\Big) &= f, \quad \text{in } \; \Omega, \\ u &= 0 \quad \text{on } \; \Sigma, \\ Ce(u)\cdot\mathbf{n} &= g \quad \text{on } \; \Gamma. \end{aligned} \tag{1}$$

Here, the strain and stress tensors are defined as usual

$$e(u) := \frac{1}{2}\Big(\nabla u + \nabla^T u\Big), \quad \tau = Ce(u).$$

The weak formulation of the BVP (1) reads as follows

$$\int_\Omega Ce(u) : e(\psi)\, dx = \int_\Omega f \cdot \psi\, dx + \int_\Gamma g \cdot \psi\, d\sigma, \quad \forall \psi \in H^1_\Sigma(\Omega; \mathbb{R}^n), \tag{2}$$

where the test space and the notation $A : B$ are defined as

$$H^1_\Sigma(\Omega; \mathbb{R}^n) := \{\psi \in H^1(\Omega; \mathbb{R}^n) \,:\, \psi|_\Sigma = 0\},$$
$$A : B = \sum_{i,j=1}^{n} a_{ij} b_{ij}, \quad A,\, B \in \mathbb{R}^{n,n}.$$

In principle, a weak solution $u \in H^1_\Sigma(\Omega; \mathbb{R}^n)$ for problem (2) already exists for the requirements $\Omega \in C^{0,1}$, $f \in H^{-1}(\Omega; \mathbb{R}^n)$, $g \in L_2(\Gamma; \mathbb{R}^n)$. However, since we will investigate differentiability with respect to the shape, further regularity will be assumed for the data, see the next subsection.

2.2 Shape problem formulation and formal shape gradient representation

Basically, we consider two different objectives and a geometrical situation, shown in Fig. 1. In particular, we choose the inner boundary as the Dirichlet boundary and the outer boundary is subject to the application of certain loads. The geometry is not convenient for any practical problem, but simplifies assumption for shape differentiability, since the Dirichlet and Neumann boundaries are strictly seperated. Note that both boundaries are subject to shape optimization. As objectives, we consider as prototype examples both

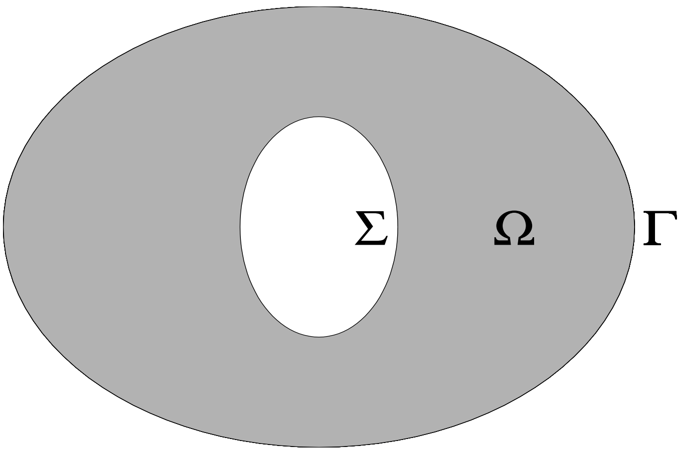

Fig. 1. The domain Ω and its boundaries Γ and Σ.

the internal energy and a tracking type objective (the desired displacement field $u_0 : D \to \mathbb{R}^n$ is defined a-priori on a hold all D, $\alpha \in (1, \infty)$), i.e.,

$$J_1(\Omega; u) = \int_\Omega Ce(u) : e(u) dx,$$
$$J_2(\Omega; u) = \left\{ \int_\Omega k(x)|u - u_0|^\alpha dx \right\}^{1/\alpha}.$$

That is, we consider the following two shape optimization problems

$$J_1(\Omega, u) \to \min, \quad \text{subject to } (2), \qquad (P1), \tag{3}$$

$$J_2(\Omega, u) \to \min, \quad \text{subject to } (2), \qquad (P2). \tag{4}$$

Assumptions on the domains and on the data. Since the main aim of the present note is on the derivation of the Hadamard representation in principle, we do not discuss the precise assumptions in detail for providing the existence of a first order shape derivative. Moreover, further regularity is required for some transformations. Having this in mind, we state the following assumptions.

We consider classes of regular domains $\Omega\,(\Gamma,\,\Sigma) \in C^{2,\gamma}$, $\gamma \in (0,1]$, contained in a hold all D and of the principal structure, depicted in Fig. 1. We assume $f \in C^{0,\gamma}(\bar{D})$, $g \in C^{1,\gamma}(\bar{D})$, for the volume forces and the boundary loads, respectively. $\alpha \geq 2$ is a constant and for the weight field k we assume $k(\cdot) \in C(\bar{D})$. For the description of the shape variations, we consider perturbation fields $V \in C^{2,\alpha}(\bar{D}; \mathbb{R}^n))$ and the perturbation of identity method, $\Omega_t = \Omega + tV$, [14]. However, the speed method ([15]) can be investigated as well, since first order derivatives are equivalent.

For convenience, we briefly recall the notions of material and local shape derivatives.

Definition 1 *(Sokolowski and Zolesio [15]) The element $\dot{u}[\Omega; V] \in W^{s,p}(\Omega)$ is the strong (weak) material derivative of $u(\Omega) \in W^{s,p}(\Omega)$ in the direction V, if there exists the strong (weak) limit (in the sense of $W^{s,p}(\Omega)$)*

$$\dot{u}[\Omega; V] = \frac{du^t[V]}{dt}|_{t=0} = \lim_{t \to 0} \frac{u^t - u}{t} \in W^{s,p}(\Omega),$$

where the "transported solutions" u^t, $u^t(X) = u_t(T_t(X))$, $X \in \Omega$, are defined as

$$u^t = u(\Omega_t) \circ T_t \in W^{s,p}(\Omega), \text{ for all } t \in [0, \delta].$$

Similarily, the strong (weak) material derivative is defined on the boundary, $\dot{u}[\Gamma; V] \in W^{s,p}(\Gamma)$ for an element $u(\Gamma) \in W^{s,p}(\Gamma)$.

The notion of the local or shape derivative du (also denoted by u') of u can be introduced by considering the limit $(u_t(x) := u(\Omega_t)(x))$

$$du(x) = \frac{\partial u_t(x)[V]}{\partial t}|_{t=0} = \lim_{t \to 0} \frac{u_t(x) - u(x)}{t}, \quad x \in \Omega. \tag{5}$$

Remark 2 *The difference quotient* $\frac{u_t(x)-u(x)}{t}$ *exists for* $x \in \Omega \cap \Omega_t$. *By the regularity of the mappings* T_t, *there exists a* $t(x, V)$ *such that* $x \in \Omega \cap \Omega_t$, $0 \leq t < t(x, V)$, for any $x \in \Omega$, $V \in C(0, \tau; C^k(\mathbb{R}^n; \mathbb{R}^n))$, $k \geq 1$. *However, a useful functional analytic setting exists for these limit only on compact subsets* $K \subset\subset \Omega$ *(cf. Simon [14]). Note that* (5) *do not have a useful meaning for* $x \in \partial\Omega$ *- except of certain subsets beeing fixed.*

Definition 3 *If the limit in (5) exists on* $K \subset\subset \Omega$ *in the strong (weak) sense of* $W^{s,p}(K)$, *it is called the strong (weak)local* $W(s,p)(K)$ *derivative of* $u(\Omega)$ *in direction* V. *We have* $du \in W^{s,p}_{loc}(\Omega)$ *strongly (weakly), if the limit exists for arbitrary* $K' \subset\subset \Omega$.

Remark 4 *There is the following obvious relation between material and local derivative*

$$\dot{u}[\Omega; V] = \frac{du^t[V]}{dt}|_{t=0} = \frac{\partial u_t(x)[V]}{\partial t}|_{t=0} + \langle \nabla u, V \rangle = du[\Omega; V] + \langle \nabla u, V \rangle. \quad (6)$$

In particular, this provides the definition of boundary values for du, since (5) *has no meaning on* Γ *or* Σ, *respectively.*

As already mentioned, shape differentiability, in particular the chain rule, is shown by means of material derivatives. Nevertheless, a (formal) derivation of equivalent shape gradient representations is possible by using local shape derivatives as well, see, e.g., [6]. For our cases under consideration, we obtain

$$\begin{aligned} dJ_1(\Omega; u)[V] = & \, 2 \int_\Omega Ce(u) : e(du[V]) dx \\ & + \int_{\partial\Omega} \langle V, \mathbf{n} \rangle Ce(u) : e(u) d\sigma, \end{aligned} \quad (7)$$

$$\begin{aligned} dJ_2(\Omega; u)[V] = & \, C_0(u) \left\{ \int_\Omega k(x) |u - u_0|^{\alpha-2} \langle u - u_0, du[V] \rangle dx \right. \\ & \left. + \frac{1}{\alpha} \int_{\partial\Omega} \langle V, \mathbf{n} \rangle k(x) |u - u_0|^\alpha d\sigma \right\}, \end{aligned} \quad (8)$$

where the quantity $C_0 = C_0(u)$ is defined as follows

$$C_0(u) = \left\{ \int_\Omega k(x) |u - u_0|^\alpha dx \right\}^{\frac{1}{\alpha} - 1}.$$

The local shape derivative $du = du[V]$ is given as the solution to the following BVP.

$$
\begin{aligned}
\operatorname{div}\Big(Ce(du)\Big) &= 0, \quad \text{in } \Omega, \\
du &= -\nabla^T u \cdot V, \quad \text{on } \Sigma, \\
Ce(du)\cdot \mathbf{n} &= \nabla^T g \cdot V - D\Big(Ce(u)\Big)[V]\cdot \mathbf{n} - Ce(u)\cdot dn[V] \quad \text{on } \Gamma.
\end{aligned} \tag{9}
$$

By the expression $D\Big(Ce(u)\Big)[V]$ we mean (pointwise) the spatial directional derivative of the tensor $Ce(u)$ in direction V at $x \in \Gamma$. For the particular case of a second order tensor (field) $A = (a_{ij})$, we obtain again a second order tensor, i.e.,

$$
D\Big(A\Big)[V] = (d_{ij}), \quad \text{where } d_{ij} := \langle \nabla a_{ij}, V\rangle, \quad \forall\, i,j = 1(1)n.
$$

Moreover, the structure of the boundary condition on Γ can be seen clearly by comparing the reference solution u_0 on Ω with the perturbed solution u_ε on Ω_ε by using the perturbation of identity concept, that is

$$
\Omega_\varepsilon = \Omega + \varepsilon V, \ \Rightarrow\ \Gamma_\varepsilon = \Gamma + \varepsilon V, \quad \text{in detail: } \Gamma_\varepsilon \ni x_\varepsilon = x_0 + \varepsilon V(x_0),\ x_0 \in \Gamma.
$$

Then, we may compute as follows (we assume first $x_\varepsilon \in \Omega$)

$$
\begin{aligned}
Ce(u_\varepsilon)(x_\varepsilon)\cdot \mathbf{n}_\varepsilon(x_\varepsilon) - g(x_\varepsilon) &= Ce(u_0)(x_0)\cdot \mathbf{n}_0(x_0) - g(x_0) = 0, \ \Rightarrow \\
g(x_\varepsilon) - g(x_0) &= \quad Ce(u_\varepsilon)(x_\varepsilon)\cdot \mathbf{n}_\varepsilon(x_\varepsilon) - Ce(u_0)(x_\varepsilon)\cdot \mathbf{n}_\varepsilon(x_\varepsilon) \\
&\quad + Ce(u_0)(x_\varepsilon)\cdot \mathbf{n}_\varepsilon(x_\varepsilon) - Ce(u_0)(x_\varepsilon)\cdot \mathbf{n}_0(x_0) \\
&\quad + Ce(u_0)(x_\varepsilon)\cdot \mathbf{n}_0(x_0) - Ce(u_0)(x_0)\cdot \mathbf{n}_0(x_0), \\
\Rightarrow \qquad \frac{g(x_\varepsilon) - g(x_0)}{\varepsilon} &= \quad Ce\left(\frac{u_\varepsilon - u_0}{\varepsilon}\right)(x_\varepsilon)\cdot \mathbf{n}_\varepsilon(x_\varepsilon) \\
&\quad + Ce(u_0)(x_\varepsilon)\cdot \frac{\mathbf{n}_\varepsilon(x_\varepsilon) - \mathbf{n}_0(x_0)}{\varepsilon} \\
&\quad + C\frac{e\Big(u_0(x_\varepsilon)\Big) - e\Big(u_0(x_0)\Big)}{\varepsilon}\cdot \mathbf{n}_0(x_0).
\end{aligned}
$$

Passing to the limit (while assuming enough regularity) gives the boundary condition for du (note that $dn[V] := \lim_{\varepsilon\to 0}\frac{\mathbf{n}_\varepsilon(x_\varepsilon)-\mathbf{n}_0(x_0)}{\varepsilon}$ denotes the shape derivative of the normal field). The procedure is similar for $x_0 \in \Omega_\varepsilon,\ \varepsilon > 0$.

3 Derivation of Hadamard representations

3.1 Transformation of the boundary conditions for local derivatives

As already mentioned in the previous subsection, all data are sufficiently regular for the subsequent transformations. The transformations on the Dirichlet boundary are completely analoguos to the case of scalar equations. Namely, from $u_i|_\Sigma \equiv 0$, we immediately find

$$\nabla_\Gamma u_i|_\Sigma = 0 \;\Rightarrow\; \nabla u_i|_\Sigma = \frac{\partial u_i}{\partial \mathbf{n}} \cdot \mathbf{n}.$$

Consequently, we have on Σ

$$\nabla^T u \cdot V = \Big(\langle \nabla u_i, V\rangle\Big)_{i=1}^n = \langle V, \mathbf{n}\rangle \nabla^T u \cdot \mathbf{n}, \Rightarrow$$

$$du[V]|_\Sigma = -\langle V, \mathbf{n}\rangle \nabla^T u \cdot \mathbf{n} = -\langle V, \mathbf{n}\rangle \frac{\partial u}{\partial \mathbf{n}}. \tag{10}$$

For the transformation on the Neumann boundary, we remark first that

$$\nabla_\Gamma \{Ce(u) \cdot \mathbf{n} - g\} \equiv \mathbf{0}, \quad \text{on } \Gamma,$$

holds (vector-valued) by the same reasoning like above. Hence, the following identities are satisfied for any admissible V

$$\begin{aligned} (\nabla_\Gamma)^T \{Ce(u) \cdot \mathbf{n} - g\} \cdot V &= 0, \quad \Rightarrow \\ \nabla^T \{Ce(u) \cdot \mathbf{n} - g\} \cdot V_\Gamma &= 0, \end{aligned} \tag{11}$$

where $V_\Gamma = V - \langle V, \mathbf{n}\rangle \cdot \mathbf{n}$ denotes the tangential component of the shape perturbation field V.

Next, we want to derive a useful expression for the (directional) shape derivative of the normal field $dn[V]$. The following relation is well known, see [15]

$$dn[V] = -\nabla V \cdot \mathbf{n} + \langle \nabla V \cdot \mathbf{n}, \mathbf{n}\rangle \mathbf{n}.$$

According to the investigations in [13], we may compute further

$$\begin{aligned} \nabla\Big\{\langle V, \mathbf{n}\rangle\Big\} &= \nabla V \cdot \mathbf{n} + \nabla \mathbf{n} \cdot V \Rightarrow \\ \nabla_\Gamma\Big\{\langle V, \mathbf{n}\rangle\Big\} &= \nabla V \cdot \mathbf{n} - \langle \nabla V \cdot \mathbf{n}, \mathbf{n}\rangle \mathbf{n} \\ &\quad + \nabla \mathbf{n} \cdot V - \langle \nabla \mathbf{n} \cdot V, \mathbf{n}\rangle \mathbf{n} \end{aligned}$$

Remark 5 *The notation $\nabla \mathbf{n}$ is meant in the sense $\nabla \mathbf{n} = \nabla \mathcal{N}|_\Gamma$ for a unitary extension of the normal field. Usually, a common construction is by the gradient of the oriented distance funtion. Another possibility is the description of the boundary $\partial\Omega$ by a zero level set of a smooth function ϕ, i.e.,*

$$\Gamma \subset \partial\Omega := \{x \,:\, \phi(x) = 0\} \;\rightarrow \mathcal{N}(x) := \nabla\phi(x)/|\nabla\phi(x)|.$$

Since we have (in the latter case; $\mathbf{I} = \delta_{ij}$*)*

$$\nabla \mathcal{N} = \frac{\nabla^2 \phi}{|\nabla \phi|} \Big[\mathbf{I} - \mathcal{N} \cdot \mathcal{N}^T \Big],$$

and (also a consequence of the formula above)

$$\langle \mathcal{N}(x), \mathcal{N}(x) \rangle \equiv 1 \ \Rightarrow \nabla \mathcal{N} \cdot \mathcal{N} \equiv 0,$$

we may conclude for arbitrary vector fields V

$$\nabla \mathbf{n} \cdot V = \nabla \mathbf{n} \cdot V_\Gamma = \frac{\nabla^2 \phi}{|\nabla \phi|} \cdot V_\Gamma \,.$$

Finally, we find the relation

$$dn[V] = -\nabla_\Gamma \Big\{ \langle V, \mathbf{n} \rangle \Big\} + \Big(\nabla \mathbf{n} \cdot V \Big)_\Gamma = -\nabla_\Gamma \Big\{ \langle V, \mathbf{n} \rangle \Big\} + \Big(\nabla \mathbf{n} \cdot V_\Gamma \Big)_\Gamma, \qquad (12)$$

valid for any admissible shape perturbation field V.

By using (11) and (12), we may transform the Neumann boundary condition for $du[V]$ on Γ as follows

$$\begin{aligned} Ce(du) \cdot \mathbf{n} = & \nabla^T g \cdot V - D\Big(Ce(u)\Big)[V] \cdot \mathbf{n} - Ce(u) \cdot (\nabla \mathbf{n} \cdot V)_\Gamma + Ce(u) \cdot \nabla_\Gamma \Big\{ \langle V, \mathbf{n} \rangle \Big\} \\ = & \nabla^T g \cdot V - \nabla^T g \cdot V_\Gamma + Ce(u) \cdot \nabla_\Gamma \Big\{ \langle V, \mathbf{n} \rangle \Big\} \\ & - D\Big(Ce(u)\Big)[V] \cdot \mathbf{n} - Ce(u) \cdot (\nabla \mathbf{n} \cdot V)_\Gamma + \nabla^T \left\{ Ce(u) \cdot \mathbf{n} \right\} \cdot V_\Gamma . \end{aligned}$$

By explicit calculations, we find

$$\nabla^T \Big(A \cdot b \Big) = \nabla^T \left[(\sum_{j=1}^n a_{ij} b_j)_{i=1}^n \right] = \left(\partial \left[\sum_{j=1}^n a_{ij} b_j \right] / \partial x_k \right)_{i,k=1}^n = \left(\sum_{j=1}^n \frac{\partial a_{ij}}{\partial x_k} b_j \right) + A \cdot \nabla^T b,$$

$$\text{and} \qquad \left(\sum_{j=1}^n \frac{\partial a_{ij}}{\partial x_k} b_j \right) \cdot c = D(A)[c] \cdot b,$$

for any Matrix A and vector fields b, c. Thus, we obtain for the Neumann-BC

$$Ce(du) \cdot \mathbf{n} = \langle V, \mathbf{n} \rangle \left\{ \nabla^T g \cdot \mathbf{n} - D\Big(Ce(u)\Big)[\mathbf{n}] \cdot \mathbf{n} \right\} + Ce(u) \cdot \nabla_\Gamma \Big\{ \langle V, \mathbf{n} \rangle \Big\}.$$

By introducing the tangential component of the stress $\tau = \Big(\tau_i^T \Big)_{i=1}^3 = Ce(u)$,

$$\tau_\Gamma := \tau - \Big[\tau \cdot \mathbf{n} \Big] \cdot \mathbf{n}^T, \ \text{ i.e., } \ \tau_\Gamma = \left(\Big[\tau_i \Big]_\Gamma^T \right)_{i=1}^3, \ \tau_i = (\tau_{i1}, \ldots, \tau_{i3})^T, \qquad (13)$$

we may transform the last part as follows

$$Ce(u) \cdot \nabla_\Gamma \Big\{ \langle V, \mathbf{n} \rangle \Big\} = \operatorname{div}_\Gamma \Big\{ \langle V, \mathbf{n} \rangle \tau_\Gamma \Big\} - \langle V, \mathbf{n} \rangle \operatorname{div}_\Gamma \Big\{ \tau_\Gamma \Big\}.$$

Finally, the local shape derivative $du[V]$ satisfies (equivalently to (9))

$$\begin{aligned} \operatorname{div}\Big(Ce(du)\Big) &= 0 && \text{in } \Omega, \\ du &= -\langle V, \mathbf{n} \rangle \nabla^T u \cdot \mathbf{n} && \text{on } \Sigma, \\ Ce(du) \cdot \mathbf{n} &= \langle V, \mathbf{n} \rangle \Big\{ \nabla^T g \cdot \mathbf{n} - D\Big(Ce(u)\Big)[\mathbf{n}] \cdot \mathbf{n} \Big\} \\ &\quad - \langle V, \mathbf{n} \rangle \operatorname{div}_\Gamma \Big\{ Ce(u)_\Gamma \Big\} + \operatorname{div}_\Gamma \Big\{ \langle V, \mathbf{n} \rangle Ce(u)_\Gamma \Big\} && \text{on } \Gamma. \end{aligned} \tag{14}$$

3.2 Transformation of shape derivatives for the objectives

Next, we want to derive the Hadamard representations for both objectives. Applying integration by parts in (7) and using (14), we find

$$\begin{aligned} \int_\Omega Ce(u) : e(du)\, dx &= -\int_\Omega \operatorname{div}\Big(Ce(du)\Big) \cdot u\, dx + \int_{\partial\Omega} \Big[Ce(du) \cdot \mathbf{n}\Big] \cdot u\, d\sigma \\ &= \int_\Gamma \Big[Ce(du) \cdot \mathbf{n}\Big] \cdot u\, d\sigma. \end{aligned}$$

Therefore, we obtain

$$\begin{aligned} dJ_1(\Omega; u)[V] &= \int_{\Sigma \cup \Gamma} \langle V, \mathbf{n} \rangle Ce(u) : e(u) d\sigma + 2 \int_\Gamma \operatorname{div}_\Gamma \Big\{ \langle V, \mathbf{n} \rangle Ce(u)_\Gamma \Big\} \cdot u\, d\sigma \\ &\quad + 2 \int_\Gamma \langle V, \mathbf{n} \rangle \Big\{ \nabla^T g \cdot \mathbf{n} - D\Big(Ce(u)\Big)[\mathbf{n}] \cdot \mathbf{n} - \operatorname{div}_\Gamma \Big\{ Ce(u)_\Gamma \Big\} \Big\} \cdot u\, d\sigma. \end{aligned}$$

For the transformation of (8), we introduce the adjoint state p as the solution of

$$\begin{aligned} -\operatorname{div}\Big(Ce(p)\Big) &= C_0(u) k(x) |u - u_0|^{\alpha - 2} \cdot (u - u_0) && \text{in } \Omega, \\ p &= 0 && \text{on } \Sigma, \\ Ce(p) \cdot \mathbf{n} &= 0 && \text{on } \Gamma. \end{aligned} \tag{15}$$

Therefore, we rewrite the domain integral part for dJ_2 as follows

$$\begin{aligned}\int_\Omega -\operatorname{div}\left(Ce(p)\right)\cdot du[V]\,dx &= \int_\Omega Ce(p) : e(du)\,dx - \int_{\partial\Omega}\left[Ce(p)\cdot\mathbf{n}\right]\cdot du\,d\sigma\\ &= \int_{\partial\Omega}\left[Ce(du)\cdot\mathbf{n}\right]\cdot p\,d\sigma - \int_{\partial\Omega}\left[Ce(p)\cdot\mathbf{n}\right]\cdot du\,d\sigma\\ &= \int_{\Gamma}\left[Ce(du)\cdot\mathbf{n}\right]\cdot p\,d\sigma - \int_{\Sigma}\left[Ce(p)\cdot\mathbf{n}\right]\cdot du\,d\sigma\end{aligned}$$

Consequently, we find the identity

$$\begin{aligned}C_0(u)\int_\Omega k(x)|u-u_0|^{\alpha-2}\langle u-u_0, du[V]\rangle dx &= \int_\Sigma \langle V,\mathbf{n}\rangle\left[Ce(p)\cdot\mathbf{n}\right]\cdot\left[\nabla^T u\cdot\mathbf{n}\right]d\sigma\\ &+\int_\Gamma\langle V,\mathbf{n}\rangle\left\{\nabla^T g\cdot\mathbf{n} - D\big(Ce(u)\big)[\mathbf{n}]\cdot\mathbf{n} - \operatorname{div}_\Gamma\left\{Ce(u)_\Gamma\right\}\right\}\cdot p\,d\sigma\\ &+\int_\Gamma \operatorname{div}_\Gamma\left\{\langle V,\mathbf{n}\rangle Ce(u)_\Gamma\right\}\cdot p\,d\sigma.\end{aligned}$$

Since it holds

$$\int_\Gamma \operatorname{div}_\Gamma\left\{u_i v_n\left[\tau_i\right]_\Gamma\right\}d\sigma = 0 = \int_\Gamma u_i\operatorname{div}_\Gamma\left\{v_n\left[\tau_i\right]_\Gamma\right\} + v_n\langle\left[\tau_i\right]_\Gamma, \nabla_\Gamma u_i\rangle d\sigma,$$

we find

$$\int_\Gamma \operatorname{div}_\Gamma\left\{\langle V,\mathbf{n}\rangle Ce(u)_\Gamma\right\}\cdot u\,d\sigma = -\int_\Gamma\langle V,\mathbf{n}\rangle Ce(u)_\Gamma : [\nabla^T u]_\Gamma\,d\sigma$$

and, analoguosly

$$\int_\Gamma \operatorname{div}_\Gamma\left\{\langle V,\mathbf{n}\rangle Ce(u)_\Gamma\right\}\cdot p\,d\sigma = -\int_\Gamma\langle V,\mathbf{n}\rangle Ce(u)_\Gamma : [\nabla^T p]_\Gamma\,d\sigma.$$

Summarizing up, we finally obtain the following two representations for the shape gradients

$$\begin{aligned}dJ_1(\Omega;u)[V] &= \int_{\partial\Omega}\langle V,\mathbf{n}\rangle Ce(u) : e(u)d\sigma - 2\int_\Gamma\langle V,\mathbf{n}\rangle Ce(u)_\Gamma : [\nabla^T u]_\Gamma\,d\sigma\\ &+2\int_\Gamma\langle V,\mathbf{n}\rangle\left\{\nabla^T g\cdot\mathbf{n} - D\big(Ce(u)\big)[\mathbf{n}]\cdot\mathbf{n} - \operatorname{div}_\Gamma\left\{Ce(u)_\Gamma\right\}\right\}\cdot u\,d\sigma,\end{aligned}\tag{16}$$

$$\begin{aligned}dJ_2(\Omega;u)[V] &= \frac{C_0(u)}{\alpha}\int_{\partial\Omega}\langle V,\mathbf{n}\rangle k(x)|u-u_0|^\alpha d\sigma + \int_\Sigma\langle V,\mathbf{n}\rangle\left[Ce(p)\cdot\mathbf{n}\right]\cdot\left[\nabla^T u\cdot\mathbf{n}\right]d\sigma\\ &+\int_\Gamma\langle V,\mathbf{n}\rangle\left\{\nabla^T g\cdot\mathbf{n} - D\big(Ce(u)\big)[\mathbf{n}]\cdot\mathbf{n} - \operatorname{div}_\Gamma\left\{Ce(u)_\Gamma\right\}\right\}\cdot p\,d\sigma\\ &-\int_\Gamma\langle V,\mathbf{n}\rangle Ce(u)_\Gamma : [\nabla^T p]_\Gamma\,d\sigma.\end{aligned}\tag{17}$$

Investigating these representations in more detail, we particularily have

$$Ce(u)_\Gamma := Ce(u) - \left[Ce(u)\cdot\mathbf{n}\right]\mathbf{n}^T = Ce(u) - g\mathbf{n}^T.$$

However, this is a symmetric operator **only** in the tangent space T_Γ, i.e., it holds

$$\langle Ce(u)_\Gamma \cdot a, b\rangle = \langle a, Ce(u)_\Gamma \cdot b\rangle, \quad \forall \langle a, \mathbf{n}\rangle = \langle b, \mathbf{n}\rangle = 0.$$

on the one hand, but on the other hand it holds in general

$$\langle Ce(u)_\Gamma \cdot a, b\rangle \neq \langle a, Ce(u)_\Gamma \cdot b\rangle, \quad \text{if } \langle a, \mathbf{n}\rangle \neq 0 \text{ and/or } \langle b, \mathbf{n}\rangle \neq 0.$$

Consequently, one has $Ce(u)_\Gamma : [\nabla^T p]_\Gamma \neq Ce(u) : e(p)$ in general on Γ (despite of $Ce(p) \cdot \mathbf{n}|_\Gamma = 0$). Nevertheless, it holds

$$\begin{aligned} Ce(u)_\Gamma : [\nabla^T u]_\Gamma &= \Big[Ce(u) - g\mathbf{n}^T\Big] : \Big[\nabla^T u - \nabla^T u \cdot \mathbf{n}\mathbf{n}^T\Big] \\ &= Ce(u) : e(u) - \Big[Ce(u) \cdot \mathbf{n}\Big] \cdot \Big[\nabla^T u \cdot \mathbf{n}\Big]. \end{aligned}$$

That is, we find the identity

$$Ce(u) : e(u) - Ce(u)_\Gamma : [\nabla^T u]_\Gamma = g \cdot \frac{\partial u}{\partial \mathbf{n}}. \tag{18}$$

Remark 6 *The formulae* (16) *and* (17) *above can be already seen as Hadamard representations, since an explicite form of the distribution $G = G|_{\partial\Omega}$ is found. However, they are "preliminary" from a "practical point of view" because it remains difficult to compute the expression*

$$D\Big(Ce(u)\Big)[\mathbf{n}] \cdot \mathbf{n} + \mathrm{div}_\Gamma \Big\{Ce(u)_\Gamma\Big\}.$$

In the (easier) case of Poisson equation, the similar expressions are ($\mathcal{H}$ denotes mean curvature)

$$\frac{\partial^2 u}{\partial \mathbf{n}^2} + \mathrm{div}_\Gamma \Big\{\nabla_\Gamma u\Big\} = \Big\{\Delta u\Big\}|_\Gamma - (n-1)\mathcal{H}\frac{\partial u}{\partial \mathbf{n}} == -f - (n-1)\mathcal{H}g.$$

Thus, they can be expressed in terms of the data of the problem.

This issue is discussed in more detail in the next subsection.

3.3 Equivalent expressions for both objectives

For the internal energy, the following equivalence is well known and is a direct consequence of the weak formulation (2).

$$J_1(\Omega; u) = \int_\Omega Ce(u) : e(u) dx = \int_\Omega f \cdot u \, dx + \int_\Gamma g \cdot u \, d\sigma. \tag{19}$$

By differentiating the second representation, we (formally) obtain

$$
\begin{aligned}
dJ_1(\Omega;u)[V] &= \int_\Omega f\cdot du[V]\,dx + \int_\Gamma g\cdot du[V]\,d\sigma + \int_\Gamma \langle V,\mathbf{n}\rangle f\cdot u\,d\sigma \\
&\quad + \int_\Gamma \langle \nabla\big[g\cdot u], V\rangle + (g\cdot u)\,\mathrm{div}_\Gamma V\,d\sigma \\
&= \int_\Omega f\cdot du[V]\,dx + \int_\Gamma g\cdot du[V]\,d\sigma + \int_\Gamma \langle V,\mathbf{n}\rangle f\cdot u\,d\sigma \\
&\quad + \int_\Gamma \langle V,\mathbf{n}\rangle\Big[\frac{\partial[g\cdot u]}{\partial\mathbf{n}} + (g\cdot u)(n-1)\mathcal{H}\Big]\,d\sigma,
\end{aligned}
$$

where the latter expression is due to standard transformations. By taking (1) and (14) into account, we find

$$
\begin{aligned}
\int_\Omega f\cdot du[V]\,dx &= \int_\Omega Ce(u):e(du[V])dx - \int_{\partial\Omega} Ce(u)\cdot\mathbf{n}\cdot du[V]\,d\sigma \\
&= \int_{\partial\Omega} \langle u, Ce(du[V])\cdot\mathbf{n}\rangle d\sigma - \int_{\partial\Omega} Ce(u)\cdot\mathbf{n}\cdot du[V]\,d\sigma.
\end{aligned}
$$

Consequently, it holds

$$
\begin{aligned}
\int_\Omega f\cdot du\,dx + \int_\Gamma g\cdot du\,d\sigma &= \int_\Sigma \langle V,\mathbf{n}\rangle Ce(u)\cdot\mathbf{n}\cdot\Big[\nabla^T u\cdot\mathbf{n}\Big]\,d\sigma + \int_\Gamma u\cdot Ce(du)\cdot\mathbf{n}\,d\sigma \\
&= \int_\Sigma \langle V,\mathbf{n}\rangle Ce(u):e(u)\,d\sigma + \int_\Gamma u\cdot \mathrm{div}_\Gamma\Big\{\langle V,\mathbf{n}\rangle\cdot\Big\{Ce(u)_\Gamma\Big\}\Big\}\,d\sigma \\
&\quad + \int_\Gamma \langle V,\mathbf{n}\rangle\Big\{u\nabla^T g\cdot\mathbf{n} - D\Big(Ce(u)\Big)[\mathbf{n}]\cdot\mathbf{n} - \mathrm{div}_\Gamma\Big\{Ce(u)_\Gamma\Big\}\Big\}\,d\sigma,
\end{aligned}
$$

where we have used the boundary condition $u = 0$ on Σ, hence

$$
Ce(u)\cdot\mathbf{n}\cdot\Big[\nabla^T u\cdot\mathbf{n}\Big]|_\Sigma = Ce(u):\Big[\nabla^T u\cdot\mathbf{n}\mathbf{n}^T\Big]|_\Sigma = Ce(u):e(u)|_\Sigma.
$$

Thus, we find for the overall shape Gradient

$$
\begin{aligned}
dJ_1(\Omega;u)[V] &= \int_\Gamma \langle V,\mathbf{n}\rangle\Big[\frac{\partial[g\cdot u]}{\partial\mathbf{n}} + (g\cdot u)(n-1)\mathcal{H} + f\cdot u\Big]\,d\sigma \\
&\quad + \int_\Sigma \langle V,\mathbf{n}\rangle Ce(u):e(u)\,d\sigma - \int_\Gamma \langle V,\mathbf{n}\rangle\cdot\Big\{Ce(u)_\Gamma\Big\}:\nabla^T u_\Gamma\,d\sigma \\
&\quad + \int_\Gamma \langle V,\mathbf{n}\rangle\Big\{u\nabla^T g\cdot\mathbf{n} - D\Big(Ce(u)\Big)[\mathbf{n}]\cdot\mathbf{n} - \mathrm{div}_\Gamma\Big\{Ce(u)_\Gamma\Big\}\Big\}\,d\sigma.
\end{aligned}
$$

After some rearrangement, we obtain

$$
\begin{aligned}
dJ_1(\Omega;u)[V] = & \int_{\partial\Omega} \langle V,\mathbf{n}\rangle Ce(u) : e(u)\,d\sigma + \int_\Gamma \langle V,\mathbf{n}\rangle \cdot 2g\frac{\partial u}{\partial \mathbf{n}} d\sigma \\
& + \int_\Gamma \langle V,\mathbf{n}\rangle u \cdot \left\{ \frac{\partial g}{\partial \mathbf{n}} + f + (n-1)\mathcal{H}g \right\} d\sigma \qquad (20) \\
& + \int_\Gamma \langle V,\mathbf{n}\rangle u \cdot \left\{ \frac{\partial g}{\partial \mathbf{n}} - D\Big(Ce(u)\Big)[\mathbf{n}]\cdot\mathbf{n} - \mathrm{div}_\Gamma \left\{Ce(u)_\Gamma\right\} \right\} d\sigma,
\end{aligned}
$$

where we made use of relation (18).

The comparison of the two formulae (16) and (20) motivates the following Lemma.

Lemma 7 *Let the data and the boundary Γ sufficiently regular, that the following expressions are well defined (at least as traces in $L_2(\Gamma)$). Then it holds the identity*

$$
D\Big(Ce(u)\Big)[\mathbf{n}]\cdot\mathbf{n} + \mathrm{div}_\Gamma \left\{Ce(u)_\Gamma\right\} = -f - (n-1)\mathcal{H}g, \qquad (21)
$$

along the Neumann-boundary Γ.

PROOF. Assuming the PDE in (1) is valid up to the boundary, we have (e.g., in the sense of traces, $\Gamma \subset \bar{\Omega}$)

$$
\mathrm{div}\left(Ce(u)\right)\Big|_\Gamma = \mathrm{div}\,\tau\Big|_\Gamma = \mathrm{div}\left(\tau_i^T\right)_{i=1}^3 = (\mathrm{div}\,\tau_i)_{i=1}^3 = -f\Big|_\Gamma,
$$

where we used the notation from (13). For any smooth vector field $\mathbf{a} : \bar{\Omega} \to \mathbb{R}^3$, we have the decomposition

$$
\begin{aligned}
\mathrm{div}\,\mathbf{a} &= \mathrm{div}_\Gamma\,\mathbf{a} + \frac{\partial \mathbf{a_n}}{\partial \mathbf{n}}, \quad \mathbf{a_n} := \langle \mathbf{a},\mathbf{n}\rangle, \ \frac{\partial \mathbf{a_n}}{\partial \mathbf{n}} := \langle \nabla\mathbf{a}\cdot\mathbf{n},\mathbf{n}\rangle, \\
&= \mathrm{div}_\Gamma\,\mathbf{a}_\Gamma + (n-1)\mathcal{H}\mathbf{a_n} + \frac{\partial \mathbf{a_n}}{\partial \mathbf{n}}.
\end{aligned}
$$

Hence, we may apply this formula for all components of the stress tensor

$$
\mathrm{div}\left(Ce(u)\right) = \mathrm{div}_\Gamma\,\tau_\Gamma + (n-1)\mathcal{H}\left(\tau_{i\mathbf{n}}\right)_{i=1}^3 + \left(\langle\nabla\tau_i\cdot\mathbf{n},\mathbf{n}\rangle\right)_{i=1}^3.
$$

By explicit calculations, we find from the BC on Γ in (1)

$$
(\tau_{i\mathbf{n}})_{i=1}^3 = Ce(u)\cdot\mathbf{n} = g,
$$

and similarily,

$$
\left(\langle\nabla\tau_i\cdot\mathbf{n},\mathbf{n}\rangle\right)_{i=1}^3 = \left(\frac{\partial\tau_{ij}}{\partial\mathbf{n}}\right)_{i,j=1}^3 \cdot\mathbf{n} = D\Big(Ce(u)\Big)[\mathbf{n}]\cdot\mathbf{n}
$$

Consequently, we verify the validity of (21) on Γ.

Corollary 8 *Under the assumptions of Lemma 7, we have for any vector field* $h \in L_2(\Gamma)$

$$\int_\Gamma \langle V, \mathbf{n}\rangle h \left\{ -D\big(Ce(u)\big)[\mathbf{n}] \cdot \mathbf{n} - \operatorname{div}_\Gamma \left\{ Ce(u)_\Gamma \right\} \right\} d\sigma = \int_\Gamma \langle V, \mathbf{n}\rangle h \left\{ f + (n-1)\mathcal{H}g \right\} d\sigma.$$

Hence, we have the following shape gradient representations, equivalent to equations 16 and 17, respectively.

$$\begin{aligned} dJ_1(\Omega; u)[V] = & \int_{\partial\Omega} \langle V, \mathbf{n}\rangle Ce(u) : e(u)\, d\sigma + \int_\Gamma \langle V, \mathbf{n}\rangle \cdot 2g \frac{\partial u}{\partial \mathbf{n}} d\sigma \\ & + 2 \int_\Gamma \langle V, \mathbf{n}\rangle u \cdot \left\{ \frac{\partial g}{\partial \mathbf{n}} + f + (n-1)\mathcal{H}g \right\} d\sigma, \end{aligned} \tag{22}$$

$$\begin{aligned} dJ_2(\Omega; u)[V] = & \frac{C_0(u)}{\alpha} \int_{\partial\Omega} \langle V, \mathbf{n}\rangle k(x) |u - u_0|^\alpha d\sigma + \int_\Sigma \langle V, \mathbf{n}\rangle \Big[Ce(p) \cdot \mathbf{n} \Big] \cdot \Big[\nabla^T u \cdot \mathbf{n} \Big]\, d\sigma \\ & + \int_\Gamma \langle V, \mathbf{n}\rangle \left\{ \nabla^T g \cdot \mathbf{n} + f + (n-1)\mathcal{H}g \right\} \cdot p\, d\sigma \\ & - \int_\Gamma \langle V, \mathbf{n}\rangle Ce(u)_\Gamma : [\nabla^T p]_\Gamma\, d\sigma. \end{aligned} \tag{23}$$

Concluding remarks. (i) If contact points (lines) appears in the problem. i.e., if

$$\mathcal{K} := \partial\Sigma \cap \partial\Gamma \neq \emptyset,$$

the abovementioned transformations remain valid provided that the regularity of u and p imply the existences of (meaningful) traces on $\mathcal{K}$, since then

$$u|_\Sigma \equiv 0 \Rightarrow u|_{\mathcal{K}} = 0,$$

and similarily for p.
(ii) Obviously, the results coincide with shape derivative representations, obtained e.g., in [1]. However, the computations, presented in this note may remain useful for investigating e.g., second derivatives.

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