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BOUNDARY INTEGRAL REPRESENTATIONS OF SECOND DERIVATIVES IN SHAPE OPTIMIZATION

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Abstract

For a shape optimization problem second derivatives are investigated, obtained by a special approach for the description of the boundary variation and the use of a potential ansatz for the state. The natural embedding of the problem in a Banach space allows the application of a standard differential calculus in order to get second derivatives by a straight forward "repetition of differentiation". Moreover, by using boundary value characerizations for more regular data, a complete boundary integral representation of the second derivative of the objective is possible. Basing on this, one easily obtains that the second derivative contains only normal components for stationary domains, i.e. for domains, satisfying the first order necessary condition for a free optimum. Moreover, the nature of the second derivative is discussed, which is helpful for the investigation of sufficient optimality conditions.

Keywords: optimal shape design, fundamental solution, boundary integral equation, second-order derivatives, optimality conditions.

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1 Introduction

Shape optimization is quite indispensable in the design and construction of industrial structures. Many such problems that arises in application, particularly in structural mechanics and in the optimal control of distributed parameter systems, can be formulated as the minimization of functionals defined over a class of admissible domains (see [17, 13, 19, 15] and the references therein). Therefore, such problems have been intensively studied in the literature throughout the last 25–30 years and several methods for the description of the domain variation are developed. Especially the velocity field method (Sokolowski, Zolesio [19]) is highly sophisticated and widely used. The method of normal boundary perturbation – the first one from a historical point of view (Hadamard [12]) – and boundary perturbation by smooth fields (Kirsch [14], Potthast [18]) are more heuristic and intuitive.

However, it allows for 2-dimensional simply connected bounded and starshaped domains Ω (without loss of gener.: $\mathbf{0} \in \Omega$) an easy description of the boundary $\Gamma = \partial\Omega$ and of related boundary perturbations by functions $r = r(\phi)$ of the polar angle ϕ (i.e., $\Gamma := \{\gamma(\phi) = \binom{r(\phi)\cos\phi}{r(\phi)\sin\phi} |\ \phi \in [0, 2\pi]\}$, where the smoothness of the boundaries under consideration is according to the smoothness of the "boundary generating" function $r(\cdot)$. Consequently, a Banach space embedding of the shape problem is possible and a standard differential calculus can be used.

This will be applied to the investigation of problems of the following type:

$$(P) \begin{cases} J(\Omega; u_\Omega(\cdot)) &= \int\limits_\Omega j(x, u_\Omega(x))dx \to \inf \\ \text{subject} & \text{to} \\ \Delta u_\Omega &= f(x) \text{ in } \Omega \subset \mathbb{R}^2, \\ u_\Omega|_\Gamma &= g(x) \text{ on } \Gamma = \partial\Omega, \end{cases}$$

where $f(\cdot), g(\cdot)$ and $j(\cdot, \cdot)$ are sufficiently smooth functions and optimization is with respect to $\Gamma \in C^{k,\alpha}$, which is equivalent to (p denotes "periodic")

$$(1)\quad r(\cdot) \in C_p^{k,\alpha}[0, 2\pi] := \{r(\cdot) \in C^{k,\alpha}[0, 2\pi] \,|\, r^{(i)}(0) = r^{(i)}(2\pi),\ i = 0(1)k\}.$$

Moreover, we assume for convenience $B_\delta(\mathbf{0}) \subset \Omega \subset D \subseteq R^2$ (i.e., $r(\phi) \geq \delta,\ \phi \in [0, 2\pi]$), with fixed closed set D.

A potential ansatz is used for the solution of the state equation. This allows, together with the boundary description via polar coordinates, the transformation of all essential parts into an integral representation and an integral equation over the fixed interval $[0, 2\pi]$ respectively, where all informations about the shape is now contained in the kernels of the related integral operators. Furthermore, the first order calculus will be extended to second derivatives, combined with a detailed treatment of several possible representations and some relations between. Moreover, at the end an estimate is discussed, helpful for the investigation of sufficient optimality conditions for such problems. Second shape derivatives for the speed method are treated in [19, 15] and for normal boundary perturbations in [8, 9] and [1]. Nevertheless, it seems to make sense to study something in more detail for the approach, introduced above.

2 Potential solution of the state equation and first derivatives for the shape problem

We only briefly recall some basics from potential theory. The solution u of the state equation of problem (P) can be given by an integral representation with the volume potential part and the double layer potential part of u_Ω, respectively (cf. [11, 10, 16]):

$$
\begin{aligned}
u_\Omega(x) &= V(f;x) + W(\mu;x) \\
&= -\int_\Omega E(x,\xi) f(\xi) d\xi + \int_\Gamma \frac{\partial E(x,\xi)}{\partial n_\xi} \mu(\xi) dS_\xi
\end{aligned}
\tag{2}
$$

where $x \in \Omega$ and $\mu(\cdot)$ satisfies the BIE

$$
\frac{1}{2}\mu(x) - \int_\Gamma \frac{\partial E(x,\xi)}{\partial n_\xi}\mu(\xi) dS_\xi = -g(x) - \int_\Omega E(x,\xi) f(\xi) d\xi, \quad x \in \Gamma.
\tag{3}
$$

The fundamental solution $E(x,\xi)$ in $\mathbb{R}^2$ is $E(x,\xi) = -\frac{1}{2\pi}\ln|x-\xi|$. After a transformation into polar coordinates ($x = \rho\binom{\cos\alpha}{\sin\alpha}$), (2) and (3) becomes

$$
\frac{1}{2}\mu(\alpha) + \frac{1}{2\pi}\int_0^{2\pi} K(\alpha,\phi)\mu(\phi) d\phi = -g(\alpha) + V(f;\alpha), \quad \alpha \in [0, 2\pi],
\tag{4}
$$

$$
u(x) = V(f;x) - \frac{1}{2\pi}\int_0^{2\pi} \bar{K}(x,\phi)\mu(\phi) d\phi, \quad x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \in \Omega,
$$

where

$$
\begin{aligned}
&V(f;x) = V(f;\rho,\alpha) \\
&= \frac{1}{2\pi}\int_0^{2\pi}\int_0^{r(\phi)} \ln\sqrt{\rho^2 + r^2 - 2r\rho\cos(\alpha-\phi)}\, f(r,\phi) r dr d\phi, \\
&\bar{K}(\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \phi) = \frac{(\xi(\phi) - x)\cdot\vec{a}(\phi)}{|x-\xi(\phi)|^2} = \frac{\binom{r(\phi)\cos\phi - x_1}{r(\phi)\sin\phi - x_2}\cdot\binom{r(\phi)\cos\phi + r'(\phi)\sin\phi}{r(\phi)\sin\phi - r'(\phi)\cos\phi}}{(x_1 - r(\phi)\cos\phi)^2 + (x_2 - r(\phi)\sin\phi)^2},
\end{aligned}
$$

or

$$\bar{K}(\rho,\alpha,\phi) = \frac{r^2(\phi) - r(\phi)\rho\cos(\phi-\alpha) - r'(\phi)\rho\sin(\phi-\alpha)}{r^2(\phi) + \rho^2 - 2r(\phi)\rho\cos(\phi-\alpha)}.$$

The kernel function $K(\alpha,\phi)$ (defined analogously to $\bar{K}(\rho,\alpha,\phi)$ with ρ replaced by $r(\phi)$) is continuous on $[0,2\pi]^2$ for $\Gamma \in C^2$, whereas $\bar{K}$ only satisfies $\bar{K}(x,\phi) \leq \frac{c}{|x-\xi(\phi)|}$, that means, for $x \to \Gamma$ the double layer potential becomes strongly singular (limits are Cauchy principal values – implying the well known jump relations), and $g(\alpha) := g(x(\alpha))$, $V(f;\alpha) := V(f;x(\alpha))$.

In all what follows, a reference domain $\Omega \in C^{2,\alpha}$ is given, where the boundary Γ is associated with the describing function $r \in C_p^{2,\alpha}[0,2\pi]$ (see (1)). Moreover, admissible perturbed domains Ω_ε are connected with $r_\varepsilon(\cdot) = r(\cdot) + \varepsilon r_1(\cdot)$ (r_1 is the direction of domain perturbation).

Remark 1. The polar coordinate approach can be viewed as a special kind of a boundary perturbation, defined by a smooth field $\vec{d} \in C^{k,\alpha}(\Gamma)$ on the reference surface (via $\vec{d}(\xi) = r_1(\phi)\vec{e}_r(\phi)$, $\xi = r(\phi)\binom{\cos\phi}{\sin\phi} \in \Gamma$). However, smooth boundary fields are applicable for more general domains, but one has only a "local Banach space embedding" (in a neighbourhood of the reference domain).

First order derivatives of the objective, the state and the density can be obtained similarly to other approaches. For sufficiently smooth data (especially for $\Omega \in C^2$) the derivative $\nabla J[r_1] = \nabla J(\Omega; u(\cdot))[r_1]$ is given by ($\xi = \xi(\phi)$)

$$(5)\qquad \nabla J[r_1] = \int_0^{2\pi} r r_1 j(\xi, g(\xi))(\phi)d\phi + \int_0^{2\pi}\int_0^{r(\alpha)} \frac{\partial j(\cdot,u(\cdot))}{\partial u} du[r_1](\rho,\alpha)\rho d\rho d\alpha.$$

The directional derivative $du[r_1]$ of the state u exists pointwise for all $x \in \Omega$:

$$(6)\qquad du[r_1](x) = dV[r_1](f;x) + W(d\mu[r_1];x) + dW[r_1](\mu;x),$$

where $d\mu[r_1] \in C_p[0,2\pi]$ (especially $d\mu(0) = d\mu(2\pi)$)is the Fréchet-derivative of the density μ and satisfies the following BIE (cf. (4)):

$$(7)\qquad \left(\frac{1}{2}\mathbf{I} + \mathbf{K}\right) d\mu[r_1] = -dg[r_1] + d_\Gamma V[r_1](f;\cdot) - d\mathbf{K}[r_1]\mu.$$

$dV[r_1](f;x)$ and $d_\Gamma V[r_1](f;\cdot)$ are the shape derivatives of the volume potentials, $dW[r_1](\cdot)$ and $d\mathbf{K}[r_1]$ denote integral operators with the shape derivatives of double layer kernels as kernels and $dg[r_1](\alpha) = r_1(\alpha)\frac{\partial g}{\partial \vec{r}}(\alpha)$. The singularity of the kernel $d\bar{K}$ of $dW[r_1]$ increases formally to $d\bar{K}(x,\phi) \leq \frac{c}{|x-\xi(\phi)|^2}$ (special properties guarantee (i), (ii) below), whereas dK (the kernel of $d\mathbf{K}[r_1]$) remains continuous. Due to the noncomparability of perturbed solutions u_ε to u on the whole Ω ("$\frac{u_\varepsilon - u}{\varepsilon}$" makes no sense), du cannot be a Fréchet-derivative with respect to functional spaces, defined on Ω. However, it is Fréchet with respect to appropriate spaces, defined on compact subsets $K \subset \Omega$. In order to ensure the (directional) differentiability of the objective, we additionally need

(i) $du(\cdot) \in L_p(\Omega)$ for (at least) $p < 2$,

(ii) $\displaystyle\int_{\Omega_\varepsilon \cap \Omega} |u_\varepsilon(x) - u(x) - \varepsilon du[r_1](x)| dx = o(\varepsilon)$.

Basing on the explicit character of (5) (by inserting (6)), Fréchet-differentiability of J follows by standard arguments from functional analysis. For more details see [3] and the discussion of second derivatives.

Remark 2. Shape derivatives are usually denoted by $d\cdot[r_1]$ or $\nabla\cdot[r_1]$ in the sequel. Spatial gradients ∇_x and partial derivatives with respect to polar coordinates (especially $\frac{\partial\cdot}{\partial \vec{r}} = \langle \nabla_x \cdot, \vec{e}_r \rangle$) or boundary normals often occur in the formulae and should not be confused with shape derivatives.

Furthermore, it is well known that $du[r_1]$ satisfies the Laplace equation in Ω and has the following boundary values for more regular data $g \in C^{1,\alpha}$

$$
\begin{aligned}
du[r_1](r(\phi),\phi) &= r_1(\phi)\left[\frac{\partial g}{\partial \vec{r}}(r(\phi),\phi) - \frac{\partial u}{\partial \vec{r}}(r(\phi),\phi)\right] \\
&= \langle r_1 \vec{e}_r, \vec{n} \rangle \left[\frac{\partial g}{\partial n} - \frac{\partial u}{\partial n}\right] \quad \text{on } \Gamma = \partial\Omega,
\end{aligned} \tag{8}
$$

where the validity of the last transformation is due to the Dirichlet boundary condition for u.

Therefore, the introduction of an adjoint state p by

$$
\begin{aligned}
-\Delta p &= j_u^0(\cdot,\cdot) \quad \text{in } \Omega \\
p &= 0 \quad \text{on } \Gamma = \partial\Omega,
\end{aligned} \tag{9}
$$

simplifies $\nabla J[r_1]$ to

$$\nabla J[r_1] = \int_\Gamma \langle r_1 \vec{e}_r, \vec{n} \rangle \left[j^0(x) - \frac{\partial p}{\partial n} \left(\frac{\partial g}{\partial n} - \frac{\partial u}{\partial n} \right) \right] dS_\Gamma, \tag{10}$$

where $j^0(x) = j(r(\phi), \phi, g(r(\phi)))$ and the necessary condition for a free minimum reads as

$$j^0(r(\phi), \phi) - \frac{\partial p}{\partial n}(r(\phi), \phi) \left(\frac{\partial g}{\partial n}(r(\phi), \phi) - \frac{\partial u}{\partial n}(r(\phi), \phi) \right) = 0, \quad \phi \in [0, 2\pi].$$

Remark 3. In the case of regular data, p and $du[r_1]$ have the following potential representation ($x = \binom{x_1}{x_2} \in \Omega,\ \alpha \in [0, 2\pi]$):

$$p(x) = \frac{1}{2\pi} \int_\Omega \frac{\partial}{\partial u} j(y, u(y)) \ln |x - y| dy \; - \; \frac{1}{2\pi} \int_0^{2\pi} \bar{K}(x, \phi) \mu_p(\phi) d\phi,$$

$$\frac{1}{2}\mu_p(\alpha) + \frac{1}{2\pi} \int_0^{2\pi} K(\alpha, \phi) \mu_p(\phi) d\phi = \frac{1}{2\pi} \int_\Omega \frac{\partial}{\partial u} j(y, u(y)) \ln |\xi(\alpha) - y| dy, \tag{11}$$

and

$$du[r_1](x) = -\frac{1}{2\pi} \int_0^{2\pi} \bar{K}(x, \phi) \widetilde{d\mu}[r_1](\phi) d\phi, \tag{12}$$

$$\frac{1}{2}\widetilde{d\mu}[r_1](\alpha) + \frac{1}{2\pi} \int_0^{2\pi} K(\alpha, \phi) \widetilde{d\mu}[r_1](\phi) d\phi = -\frac{r_1 r}{\sqrt{r^2 + r'^2}} \left[\frac{\partial g}{\partial n} - \frac{\partial u}{\partial n} \right] (\alpha).$$

The notion $\widetilde{d\mu}[r_1]$ should not be confused with $d\mu[r_1]$.

3 Second derivatives for the shape problem

The computation of second derivatives is "almost straight forward" in the sense of

$$d^2 J(\Omega)[r_1; r_2] = \lim_{\delta \to 0} \frac{\nabla J(\Omega_{\delta r_2})[r_1] - \nabla J(\Omega)[r_1]}{\delta}, \quad \Gamma_{\delta r_2} = \Gamma_\delta = \Gamma + \delta r_2 \vec{e}_r,$$

because the first derivatives contain only domain integrals or integrals over the interval $[0, 2\pi]$ with the perturbation parameter δ in the integrand.

As a starting point we have ($r_\delta(\phi) = r(\phi) + \delta r_2(\phi)$)

$$\begin{aligned}\nabla J(\Omega_\delta)[r_1] &= \int_0^{2\pi} r_\delta(\phi) r_1(\phi) j(r_\delta(\phi), \phi, u_\delta(r_\delta(\phi), \phi))\, d\phi \\ &+ \int_0^{2\pi}\int_0^{r_\delta(\phi)} \frac{\partial j}{\partial u}|_\delta(\rho,\phi) du_\delta[r_1](\rho,\phi)\rho d\rho d\phi.\end{aligned}$$

For $f \in C^1(D),\ g \in C^2(D),\ j \in C^2(D \times R)$ and $r \in C^{2,\alpha}$ this leads to

$$d^2 J(\Omega)[r_1; r_2] = \int_0^{2\pi} I_1^0(\phi; r_1, r_2, r)\, d\phi + \int_0^{2\pi}\int_0^{r(\phi)} I_2^0(\rho, \phi; r_1, r_2)\rho d\rho d\phi, \tag{13}$$

where I_1^0 and I_2^0 are given by

$$\begin{aligned} I_1^0 &= r_1 r_2 j^0 + r r_1 r_2 [\frac{\partial j^0}{\partial \vec{r}}|_0 + \frac{\partial j^0}{\partial u}|_0 \frac{\partial u}{\partial \vec{r}}|_0] + r \frac{\partial j^0}{\partial u}|_0 (r_1 du[r_2] + r_2 du[r_1]), \\ I_2^0 &= \frac{\partial^2 j^0}{\partial u^2}(du[r_2]\cdot du[r_1])(\rho,\phi) + \frac{\partial j^0}{\partial u}\cdot d^2 u[r_2; r_1](\rho, \phi). \end{aligned}$$

The second derivative of the state can be obtained (pointwise for $x \in \Omega$) by

$$\begin{aligned} d^2 u[r_1; r_2](x) &= d^2 V[r_2; r_1](f; x) + W(d^2\mu[r_1; r_2], x)) \\ &+ dW[r_1](d\mu[r_2]; x) + dW[r_2](d\mu[r_1]; x) + d^2 W[r_1; r_2](\mu; x), \end{aligned}$$

where $d^2\mu$ satisfies

$$\begin{aligned} \left(\frac{1}{2}\mathbf{I} + \mathbf{K}\right) d^2\mu[r_1; r_2] &= -r_1 r_2 \frac{\partial^2 g}{\partial \vec{r}^2}|_0 + d_\Gamma^2 V[r_1; r_2](f; \cdot) \\ &- (d\mathbf{K}[r_2] d\mu[r_1] + d\mathbf{K}[r_1] d\mu[r_2]) - d^2\mathbf{K}[r_1; r_2]\mu. \end{aligned}$$

Remark 4. Some singularities in the expressions occur and increase by "repeated shape differentiation". The second shape derivative $d^2V[r_2; r_1]$ of the volume potential contains a part with the same singularity behaviour close to the boundary Γ like first spatial derivatives of a single layer potential. Strong singular boundary (integrand has singularity of order one) and domain integral parts (order two) formally occur in $d_\Gamma^2 V[r_1; r_2]$. However, an equivalent representation with only weak singular (integrable) parts can be obtained by using the well known transformation formula for the gradient of a volume potential (valid for $f \in C^1$)

$$\nabla_x V(f;x) = -\frac{1}{2\pi}\int_{\Omega_0} \ln|x-y|\nabla_y f(y)dy + \frac{1}{2\pi}\int_{\Gamma_0} \ln|x-y|f(y)\cdot\vec{n}_y\, dS_y.$$

Moreover, the singularity of the kernel $\frac{d^2\bar{K}}{dr_1 dr_2}|_0(x,\phi)$ of $d^2W[r_1;r_2]$ increases once again for $x \to \Gamma$, whereas $\frac{d^2K}{dr_1 dr_2}|_0(\alpha,\phi)$ (the kernel of $d^2\mathbf{K}[r_1;r_2]$) is regular like the kernel $\frac{dK}{dr_1}$ (see also [3]). Summarizing up, the BIE and related (higher order) shape derivatives "behave well", but the shape derivatives of the solution representation "make more and more difficulties" (close to Γ), which must be treated carefully.

Remark 5. We do not discuss the structure and the properties of the parts of these representations in more detail (some further informations are contained in [6]), because we assume more regularity with respect to the boundary value field g ($g \in C^{2,\alpha}(D)$) of the state equation and use related shorter representations via the adjoint state p and (explicit) boundary values of $du[r_i]$ and $d^2u[r_1,r_2]$, respectively. By the way, this reduces in addition the regularity assumptions on f to $f \in C^{0,\alpha}(D)$.

4 Boundary values of second derivatives of the state

The characterization of the directional derivative $du[r_1]$ as the solution of a Dirichlet-problem can be directly extended to $d^2u[r_1;r_2]$. Especially, the computation of boundary values can be carried out similarly.

Theorem 1. *For $f \in C^{0,\alpha}(D)$, $r \in C_p^{2,\alpha}[0,2\pi]$ and $g \in C^{2,\alpha}(D)$ the directional derivative $d^2u[r_1,r_2]$ satisfies*

$$(14) \qquad \begin{aligned} \Delta d^2u[r_1;r_2] &= 0 \qquad\qquad \textit{in } \Omega, \quad \textit{and on } \Gamma = \partial\Omega \\ d^2u[r_1;r_2](r(\phi),\phi) &= r_1 r_2\left[\frac{\partial^2 g}{\partial\vec{r}^2} - \frac{\partial^2 u}{\partial\vec{r}^2}\right] - r_2\frac{\partial}{\partial\vec{r}}du[r_1] - r_1\frac{\partial}{\partial\vec{r}}du[r_2]. \end{aligned}$$

Proof. Because of $f \in C^{0,\alpha}(D)$, $g \in C^{1,\alpha}(D)$ it holds $u \in C^{2,\alpha}(\bar{\Omega})$, $du[r_i] \in C^{1,\alpha}(\bar{\Omega})$, $(i = 1,2)$ and $u_\delta \in C^{2,\alpha}(\bar{\Omega}_\delta)$, $du_\delta[r_i] \in C^{1,\alpha}(\bar{\Omega}_\delta)$, respectively. Therefore, the right hand side of the boundary condition is well defined and an element of $C^{0,\alpha}(\Gamma)$. Moreover, we can show

- $\Delta d^2 u[r_1; r_2] = 0$ in Ω,
- $d^2 u[r_1; r_2] \in C^{0,\alpha}(\bar{\Omega})$

independently from the characterization above by using (12) and the results for the first order theory (cf. [4], Appendix B). For the computation of the boundary values we remark that the directional derivatives $du_\delta[r_1]$ satisfy simultaneously to $du[r_1]$

$$du_\delta[r_1](r_\delta(\phi), \phi) = r_1(\phi)\left[\frac{\partial g}{\partial \vec{r}}(r_\delta(\phi), \phi) - \frac{\partial u_\delta}{\partial \vec{r}}(r_\delta(\phi), \phi)\right] \quad \text{on } \Gamma_\delta = \partial\Omega_\delta.$$

Moreover, we use the sets

$$M_2^+ = \{\phi \in [0, 2\pi] \mid r_2(\phi) > 0\},\ M_2^- = \{\dots r_2(\phi) < 0\},$$
$$M_2^0 = \{\dots r_2(\phi) = 0\}.$$

We obtain for $\phi \in M_2^+ (\Rightarrow r(\phi)\vec{e}_r(\phi) \in \Omega_\delta)$

$$\begin{aligned}
&\frac{(du_\delta(r(\phi)) - du(r(\phi))}{\delta} \\
&= \frac{du_\delta(r(\phi)) - du_\delta(r_\delta(\phi))}{\delta} + \frac{du_\delta(r_\delta(\phi)) - du(r(\phi)}{\delta} \\
&= -r_2(\phi)\frac{\partial du_\delta}{\partial \vec{r}}|_{r+\theta r_2} + \frac{r_1(\phi)}{\delta}\left[\frac{\partial g(r_\delta)}{\partial \vec{r}} - \frac{\partial u_\delta(r_\delta)}{\partial \vec{r}} - \frac{\partial g(r)}{\partial \vec{r}} + \frac{\partial u(r)}{\partial \vec{r}}\right],
\end{aligned}$$

by using the boundary values for the first derivatives. The second part becomes

$$r_1 r_2 \frac{\partial^2 g}{\partial \vec{r}^2}|_{r+\theta r_2} - \frac{r_1(\phi)}{\delta}\left[\frac{\partial u_\delta(r_\delta)}{\partial \vec{r}} - \frac{\partial u_\delta(r)}{\partial \vec{r}} + \frac{\partial u_\delta(r)}{\partial \vec{r}} - \frac{\partial u(r)}{\partial \vec{r}}\right]$$
$$= r_1 r_2 \frac{\partial^2 g}{\partial \vec{r}^2}|_{r+\theta r_2} - r_1 r_2 \frac{\partial^2 u_\delta}{\partial \vec{r}^2}|_{r+\theta r_2} - r_1 \frac{\partial}{\partial \vec{r}} \frac{u_\delta(r) - u(r)}{\delta},$$

and a careful discussion of the limit by the regularity of states and first derivatives gives (14). The transformations are similar for M_2^- and on M_2^0 the perturbed and the reference boundary as well as all related quantities coincide. Hence, (14) holds by definition. ■

Remark 6. In comparison to the computation of boundary values of du, a third term occur for $d^2 u$. Moreover, a complete representation of these boundary values by only normal components (like for the first derivatives, see (8)) is not possible. However, from

$$du[r_1] - r_1 \left[\frac{\partial g}{\partial \vec{r}} - \frac{\partial u}{\partial \vec{r}}\right] = 0, \quad \text{on } \Gamma,$$

we obtain

$$r_2 \frac{\partial}{\partial \vec{r}} \left\{ du[r_1] - r_1 \left[\frac{\partial g}{\partial \vec{r}} - \frac{\partial u}{\partial \vec{r}}\right]\right\}$$
$$= \langle r_2 \vec{e}_r, n\rangle \frac{\partial}{\partial n} \left\{ du[r_1] - r_1 \left[\frac{\partial g}{\partial \vec{r}} - \frac{\partial u}{\partial \vec{r}}\right]\right\}.$$

Consequently, the boundary values of d^2u can be equivalently expressed as

$$d^2u[r_1, r_2]|_\Gamma = \frac{r^2 r_1 r_2}{r^2 + r'^2} \frac{\partial^2}{\partial n^2}(g-u) - \frac{r r_2}{\sqrt{r^2 + r'^2}} \frac{\partial du[r_1]}{\partial n} - r_1 \frac{\partial du[r_2]}{\partial \vec{r}}. \tag{15}$$

Remark 7. For the more general case of boundary perturbations defined by smooth fields $\vec{d}_1$ and $\vec{d}_2$ (cf. Remark 1), the boundary values of d^2u become

$$d^2u[\vec{d}_1; \vec{d}_2]|_\Gamma = \langle \nabla_x^2 (g-u) \cdot \vec{d}_2, \vec{d}_1\rangle - \langle \nabla_x du[\vec{d}_1], \vec{d}_2\rangle - \langle \nabla_x du[\vec{d}_2], \vec{d}_1\rangle.$$

5 Boundary representation of second shape derivatives

At first we want to simplify as much as possible the expression for $d^2J(\Omega)[r_1, r_2] = \nabla^2 J(r)[r_1; r_2]$. From (13) we arrive at

Corollary 1. *Under the regularity assumptions of Theorem* 1 *on the data and the domain, the second shape derivative of the objective is given by*

$$\begin{aligned} & d^2J(\Omega)[r_1; r_2] \\ &= \int_0^{2\pi} \int_0^{r(\phi)} \frac{\partial^2 j^0}{\partial u^2} (du[r_1] \cdot du[r_2])(\rho, \phi)\, \rho d\rho d\phi + \int_0^{2\pi} d\phi \Big\{ r_1 r_2 j(r, g) \\ &+ r_1 r_2 r \left[\frac{\partial j(r,g)}{\partial \vec{r}} + 2 \frac{\partial j(r,g)}{\partial u} \frac{\partial g(r)}{\partial \vec{r}} - \frac{\partial j(r,g)}{\partial u} \frac{\partial u(r)}{\partial \vec{r}}\right] \\ &- \frac{\partial p}{\partial n} \sqrt{r^2 + r'^2} \left[r_1 r_2 (\frac{\partial^2 g}{\partial \vec{r}^2} - \frac{\partial^2 u}{\partial \vec{r}^2}) - r_1 \frac{\partial du[r_2]}{\partial \vec{r}} - r_2 \frac{\partial du[r_1]}{\partial \vec{r}} \right] \Big\}. \end{aligned} \tag{16}$$

Proof. The use of boundary values for du and d^2u (see (8) and (14)), together with the transformation of the last domain integral part of (13) – compare the definition of I_2^0 – similar to the gradient ∇J (cf. (10)), leads immediately to (16). Starting from (12), the existence of d^2J can be guaranteed by showing estimates for d^2u, similar to (i), (ii) (cf. Section 2). ■

A complete "boundary integral" representation of the second derivative can be obtained from (10) by differentiating ∇J (on Ω_δ) once again. From

$$\begin{aligned} &\nabla J(\Omega_\delta)[r_1] \\ (17)\qquad &= \int_{\Gamma_\delta} \langle r_1 \vec{e}_r, \vec{n}_\delta\rangle \left[j^\delta(\xi_\delta) - \langle \nabla_x p_\delta, \nabla_x\left(g(\xi_\delta) - u_\delta(\xi_\delta)\right)\right] dS_{\Gamma_\delta}, \end{aligned}$$

(in $j^\delta(\xi_\delta) = j(\xi_\delta,\, g(\xi_\delta))$ the boundary values are inserted, cf. (5)), we get

Theorem 2. *The second shape derivative of the objective can be equivalently expressed by*

$$\begin{aligned} &\nabla^2 J(\Omega)[r_1; r_2] \\ (18)\qquad &= \int_0^{2\pi} r_1 r_2 \left\{[j^0 - \nabla_x p \cdot \nabla_x(g-u)] + r\frac{\partial}{\partial \vec{r}}[j^0 - \nabla_x p \cdot \nabla_x(g-u)]\right\} \\ &+ r r_1 \left\{\frac{\partial p}{\partial n}\frac{\partial}{\partial n} du[r_2] - \frac{\partial}{\partial n} dp[r_2] \frac{\partial}{\partial n}(g-u)\right\} d\phi. \end{aligned}$$

Proof. The notion $\frac{\partial}{\partial \vec{r}}[j^0 - \nabla_x p \cdot \nabla_x(g-u)]$ has to be understood in the following sense: The expression $[\ldots](x) = j(x, (g(x)) - \ldots = [\ldots](r,\phi)$ defines a smooth function on $\bar{\Omega}$, which can be written in polar coordinates, too. Now $\frac{\partial \ldots}{\partial \vec{r}}$ is meant as $\langle \nabla_x[\ldots], \vec{e}_r\rangle$, whereas $\frac{\partial j(r,\phi,g)}{\partial \vec{r}}$ indicates the partial derivative with respect to the first argument. Furthermore, the reformulation (17) of (10), basing on

$$(19)\quad \nabla_x p|_\Gamma = \frac{\partial p}{\partial n}\cdot \vec{n}, \text{ and } \nabla_x (g-u)|_\Gamma = \frac{\partial (g-u)}{\partial n}\cdot \vec{n} \quad (p|_\Gamma = g-u|_\Gamma = 0),$$

makes sense, because all quantities (after rewriting the boundary integral in a parametrized version) have an extension outside of Γ_δ in order to perform the differentiation with respect to the shape. We obtain

$$\begin{aligned}
& d^2J(\Omega)[r_1;r_2] \\
&= \int_0^{2\pi} r_1 r_2 [j^0(\phi) - \langle \nabla_x p, \nabla_x (g-u)\rangle] \\
&+ \ r r_1 r_2 \left[\frac{\partial j}{\partial \vec{r}} + \frac{\partial j}{\partial u}\frac{\partial g}{\partial \vec{r}} - \langle \nabla_x p, \nabla_x (\frac{\partial g}{\partial \vec{r}} - \frac{\partial u}{\partial \vec{r}})\rangle - \langle \nabla_x \frac{\partial p}{\partial \vec{r}}, \nabla_x (g-u)\rangle\right]|_\Gamma \\
&+ \ r r_1 \{\langle \nabla_x p, \nabla_x du[r_2]\rangle - \langle \nabla_x dp[r_2], \nabla_x (g-u)\rangle\}\, d\phi
\end{aligned}$$

and (18) follows by using (19) once again. Furthermore, the shape derivative $dp[r_2]$ of the adjoint state is given as the solution of

$$\begin{aligned}
-\Delta dp &= \frac{\partial^2 j}{\partial u^2} du[r_2] \quad \text{in } \Omega \\
dp &= -r_2 \frac{\partial p}{\partial \vec{r}} = -\langle r_2 \vec{e}_r, n\rangle \frac{\partial p}{\partial n} \quad \text{on } \Gamma.
\end{aligned} \tag{20}$$

Finally we remark that all transformations above are valid due to $p \in C^{2,\alpha}(\bar{\Omega})$, $dp[r_2] \in C^{1,\alpha}(\bar{\Omega})$, which is according to the regularity of the data we have ($f \in C^{0,\alpha}$, $r \in C^{2,\alpha}$, $g \in C^{2,\alpha}$ and $j \in C^2$). ■

As an easy but interesting consequence we get

Corollary 2. *If the necessary condition for a free minimum ($[j^0 - \nabla_x p \cdot \nabla_x (g-u_0)]|_{\Gamma_0} = 0$) is satisfied for some Ω_0, the second derivative simplifies to*

$$\begin{aligned}
& \nabla^2 J(\Omega_0)[r_1;r_2] \\
&= \int_0^{2\pi} r_0 r_1 r_2 \langle \vec{e}_r, \vec{n}\rangle \frac{\partial}{\partial n}[j^0 - \nabla_x p \cdot \nabla_x (g-u_0)] \\
&+ \ r_0 r_1 \left\{\frac{\partial p}{\partial n}\frac{\partial}{\partial n} du_0[r_2] - \frac{\partial}{\partial n} dp[r_2] \frac{\partial}{\partial n}(g-u_0)\right\} d\phi \\
&= \int_{\Gamma_0} r_1 r_2 \langle \vec{e}_r, \vec{n}\rangle^2 \frac{\partial}{\partial n}[j^0 - \nabla_x p \cdot \nabla_x (g-u_0)] \\
&+ \ \langle r_1 \vec{e}_r, \vec{n}\rangle \left\{\frac{\partial p}{\partial n}\frac{\partial}{\partial n} du_0[r_2] - \frac{\partial}{\partial n} dp[r_2] \frac{\partial}{\partial n}(g-u_0)\right\} dS_\Gamma,
\end{aligned} \tag{21}$$

i.e. the second derivative for "stationary domains" has a complete boundary integral representation, containing only normal components.

Remark 8. The equivalence of (18) and (16) can be seen in more detail by applying the second Green's formula on the domain integral part of (16). Making use of (20) we have

$$\begin{aligned}
&\int_0^{2\pi}\int_0^{r(\phi)} \frac{\partial^2 j^0}{\partial u^2}(du[r_1]\cdot du[r_2])(\rho,\phi) \,+\, 0\,\rho d\rho d\phi \\
&= -\int_\Omega \Delta dp[r_2]\cdot du[r_1] + \Delta du[r_1]\cdot dp[r_2]\, dx \\
&= -\int_\Gamma du[r_1]\frac{\partial dp[r_2]}{\partial n} - dp[r_2]\frac{\partial du[r_1]}{\partial n}\, dS_\Gamma \\
&= \int_\Gamma -\langle r_1\vec{e}_r,\vec{n}\rangle\left[\frac{\partial g}{\partial n}-\frac{\partial u}{\partial n}\right]\frac{\partial dp[r_2]}{\partial n} - \langle r_2\vec{e}_r,\vec{n}\rangle\frac{\partial p}{\partial n}\frac{\partial du[r_1]}{\partial n}\, dS_\Gamma,
\end{aligned}$$

and it becomes clear that this integral is hidden behind the last expressions of (18).

The last part is devoted to a property of the second derivative, interesting especially for the study of optimality conditions.

Lemma 1. *For the shape derivative $\nabla^2 J(\Omega)[r_1, r_2]$ holds the estimate*

$$|\nabla^2 J(\Omega)[r_1;r_2]| \le c_0\, \|r_1\|_{H^{\frac{1}{2}}}\cdot\|r_2\|_{H^{\frac{1}{2}}}\,,\ c_0 = c_0(\Omega), \tag{22}$$

but no similar estimate with respect to a weaker space is possible in general.

Proof. From (16) we have 3 different parts of d^2J. At first there is the volume integral

$$I_1(\Omega)[r_1;r_2] = \int_0^{2\pi}\int_0^{r(\phi)} \frac{\partial^2 j^0}{\partial u^2}\, du[r_1]\, du[r_2]\, \rho d\rho d\phi,$$

the second "crucial part" is

$$I_2(\Omega)[r_1;r_2] = \int_0^{2\pi}\left(\sqrt{r^2+r'^2}\frac{\partial p}{\partial n}\right)\left[r_1\frac{\partial}{\partial\vec{r}}du[r_2] + r_2\frac{\partial}{\partial\vec{r}}du[r_1]\right]\, d\phi,$$

or similarly (from the boundary representation)

$$I_2^m(\Omega)[r_1;r_2] = \int_0^{2\pi}\left(2r\frac{\partial p}{\partial n}\right) r_1\frac{\partial}{\partial n}du[r_2]\, d\phi,$$

whereas the others are "L_2-terms" and therefore (more or less) uninteresting

$$|I_o(\Omega)[r_1;r_2]\,| = |\int_0^{2\pi} f_o(\phi)\cdot r_1 r_2\, d\phi\,| \le c_f \|r_1\|_{L_2}\|r_2\|_{L_2}.$$

By using the structure of $du[r_i]$ (cf. (12)), I_1 allows also a L_2-estimate

$$\begin{aligned} |I_1(\Omega)[r_1;r_2]\,| &\le c\,\|W(\widetilde{d\mu}[r_1];\cdot)\|_{L_2(\Omega)}\,\|W(\widetilde{d\mu}[r_2];\cdot)\|_{L_2(\Omega)} \\ &\le c_0\,\|r_1\|_{L_2}\|r_2\|_{L_2}. \end{aligned}$$

The estimates are valid due to properties of double layer potentials $W(\cdot;\cdot)$ as well as to properties of the BIE, more precisely, we have $W: L_2(\Gamma)\mapsto H^{\frac{1}{2}}(\Omega)$ and $(i=1,2)$

$$\left(\frac{1}{2}\mathbf{I}+\mathbf{K}\right)^{-1}:\ L_2(\Gamma)\mapsto L_2(\Gamma),$$

or

$$\|du[r_i]\|_{H^{\frac{1}{2}}(\Omega)} \le c\,\|\widetilde{d\mu_i}\|_{L_2} \le \hat{c}\,\|r_i\|_{L_2}.$$

However, for the remaining part only

$$|I_2^m(\Omega)[r_1;r_2]| \le c_0\cdot\|r_1\|_{H^{\frac{1}{2}}}\|\frac{\partial du[r_2]}{\partial n}\|_{H^{-\frac{1}{2}}} \le \tilde{c_0}\|r_1\|_{H^{\frac{1}{2}}}\|r_2\|_{H^{\frac{1}{2}}},$$

is possible, where we used first of all the Dirichlet-to-Neumann-map D

$$D: H^{\frac{1}{2}}(\Gamma)\mapsto H^{-\frac{1}{2}}(\Gamma),$$

or

$$\|\frac{\partial du[r_2]}{\partial n}\|_{H^{-\frac{1}{2}}} \le \tilde{c}\,\|du[r_2]\|_{H^{\frac{1}{2}}},$$

and in addition for the boundary values of $du[r_2]$

$$\|\langle r_2\vec{e}_r,\vec{n}\rangle\left[\frac{\partial g}{\partial n}-\frac{\partial u}{\partial n}\right]\|_{H^{\frac{1}{2}}} \le \|r_2\|_{H^{\frac{1}{2}}}\cdot\|\langle\vec{e}_r,\vec{n}\rangle\left[\frac{\partial g}{\partial n}-\frac{\partial u}{\partial n}\right]\|_{C^1}.$$ ■

Remark 9. The notions $\|r_i\|_{H^{\frac{1}{2}}}$ and $\|r_i\|_{L_2}$ are used in the sense of $H^{\frac{1}{2}}(\Gamma)$ and $L_2(\Gamma)$, respectively, but this is obviously equivalent to $H^{\frac{1}{2}}[0,2\pi]$ ($L_2[0,2\pi]$). An example for the $H^{\frac{1}{2}}$-behaviour of d^2J can be found in [6]. Clearly, second shape derivatives of domain integral functionals allow L_2-estimates (see [7] or [5]).

Remark 10. The results can be extended to objectives of the type $J(\Omega) = \int\limits_{\Omega} j(x, u_\Omega(x), \nabla_x u_\Omega(x))dx$.

Remark 11. The knowledge about first and second derivatives in shape optimization is widely used for numerical algorithms and for the study of necessary optimality conditions (cf. Corollary 2). Nevertheless, due to some difficulties arising from theoretical as well as from technical point of view, the study of sufficient conditions seems to be not very well developed at the moment. However, combining the presented investigations with some ideas from [7], at least for a restricted class of problems related remainder estimates can be carried out in detail in a forthcoming paper.

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