Shape optimization for free boundary problems

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Abstract

In this paper three different formulations of a Bernoulli type free boundary problem are discussed. By analyzing the shape Hessian in case of matching data it is distinguished between well-posed and ill-posed formulations. A nonlinear Ritz-Galerkin method is applied for discretizing the shape optimization problem. In case of well-posedness existence and convergence of the approximate shapes is proven. In combination with a fast boundary element method efficient first and second order shape optimization algorithms are obtained.

1 Problem formulation

The present paper is dedicated to the solution of a generalized *Bernoulli exterior free boundary problem* which serves as a prototype of many shape optimization problems. Let $T \subset \mathbb{R}^n$ denote a bounded domain with *free* boundary $\partial T = \Gamma$. Inside the domain T we assume the existence of a simply connected subdomain $S \subset T$ with *fixed* boundary $\partial S = \Sigma$. The resulting annular domain $T \setminus \overline{S}$ is denoted by Ω.
The exterior free boundary problem might be formulated as follows: For given data f, g, h, seek the domain Ω and associated function u such that the overdetermined boundary value problem

$$-\Delta u = f \text{ in } \Omega, \qquad -\frac{\partial u}{\partial \mathbf{n}} = g,\ u = 0 \text{ on } \Gamma, \qquad u = h \text{ on } \Sigma, \tag{1.1}$$

is satisfied. Here, $g, h > 0$ and $f \geq 0$ are sufficiently smooth *functions* on $\mathbb{R}^n$ such that u provides enough regularity for a second order shape calculus. We like to stress that the positivity of the Dirichlet data implies that u is positive on Ω and thus it holds in fact $\partial u/\partial \mathbf{n} < 0$.
We are going to consider the following formulations:

(i) If we prescribe the Dirichlet data $u = 0$ at the free boundary problem, then the solution of (1.1) is the minimizer of the Dirichlet energy functional (cf. [4])

$$J_1(\Omega) = \int_\Omega \left\{ \|\nabla u\|^2 - 2fu + g^2 \right\} d\mathbf{x} \to \inf, \tag{1.2}$$

where u satisfies the Dirichlet problem

$$-\Delta u = f \text{ in } \Omega, \qquad u = 0 \text{ on } \Gamma, \qquad u = h \text{ on } \Sigma. \tag{1.3}$$

(ii) For prescribed Dirichlet data $u = 0$ the L^2-least square tracking of the Neumann data g corresponds to the problem

$$J_2(\Omega) = \frac{1}{2} \int_\Gamma \left(g + \frac{\partial u}{\partial \mathbf{n}} \right)^2 d\sigma \to \inf \tag{1.4}$$

with u satisfying (1.3).

(iii) If the Neumann data g is assumed to be prescribed, the L^2-least square tracking of the Dirichlet data $u = 0$ reads as

$$J_3(\Omega) = \frac{1}{2} \int_\Gamma u^2 d\sigma \to \inf, \tag{1.5}$$

subject to the mixed boundary value problem

$$-\Delta u = f \text{ in } \Omega, \qquad -\frac{\partial u}{\partial \mathbf{n}} = g \text{ on } \Gamma, \qquad u = h \text{ on } \Sigma. \tag{1.6}$$

Here, the infimum has to be taken over all sufficiently smooth domains which include the domain S. Two- and three-dimensional solutions of the original Bernoulli free boundary problem, i.e., $f = 0$, $g = const$, $h = 1$, are plotted in Figures 1 and 2.
We do not consider the interesting question of existence of optimal solutions in this paper. Instead, we will tacitly assume the existence of optimal domains, being sufficiently regular to allow for a second order shape calculus. For the existence of solutions to the free boundary problem (1.1) we refer the reader to e.g. [1]. Further notice that shape optimization is a well established tool to solve free boundary value problems like (1.1), see e.g. [3, 4, 5, 7, 9, 10, 11, 12, 13, 14].

2 Sufficient optimality conditions

In [4, 5, 7, 9] we computed the boundary integral representation of the shape gradient and Hessian of the three formulations, especially in case of formulation (ii) and (iii) for arbitrary space dimension $n \in \mathbb{N}$, see [5, 7]. With the shape Hessian at hand we are able to investigate the stability of the global minimizer $\Omega^\star$.
All formulations own a shape Hessian that defines a continuous bilinear form $d^2J_i(\Omega) : H^s(\Gamma) \times H^s(\Gamma) \to \mathbb{R}$ with respect to the *energy space* $H^s(\Gamma)$, that is

$$\big|d^2J_i(\Omega)[dr_1, dr_2]\big| \leq c_S \|dr_1\|_{H^s(\Gamma)} \|dr_2\|_{H^s(\Gamma)}.$$

Precisely, one has $s = 1/2$ for the first and $s = 1$ for the second last formulations. Accordingly, the second order Taylor remainder $R_2\big(J_i(\Omega), dr\big)$ satisfies

$$\big|R_2\big(J_i(\Omega), dr\big)\big| = o\big(\|dr\|_X\big)\|dr\|^2_{H^s(\Gamma)}$$

where $X \supsetneq H^s(\Gamma)$ is the space of differentiation. Therefore, a local minimum is *stable* if the shape Hessian $d^2J_i(\Omega^\star)$ is strictly coercive in its energy space $H^s(\Gamma^\star)$

$$d^2J_i(\Omega^\star)[dr, dr] \geq c_E \|dr\|^2_{H^s(\Gamma^\star)}, \quad c_E > 0.$$

The shape problem under consideration is then *well-posed* and a nonlinear Ritz-Galerkin method produces approximate shapes that converge quasi-optimal with respect to the energy norm, see the next section.
In [4, 5, 7] the following expressions have been proven for the shape Hessian at the optimal domain

$$\begin{aligned}
d^2J_1(\Omega^\star)[dr_1, dr_2] &= \big((\Lambda + \mathcal{A})\mathcal{M}dr_1, \mathcal{M}dr_2\big)_{L^2(\Gamma^\star)},\\
d^2J_2(\Omega^\star)[dr_1, dr_2] &= \big((\Lambda + \mathcal{A})\mathcal{M}dr_1, (\Lambda + \mathcal{A})\mathcal{M}dr_2\big)_{L^2(\Gamma^\star)},\\
d^2J_3(\Omega^\star)[dr_1, dr_2] &= \big(\Lambda^{-1}(\Lambda + \mathcal{A})\mathcal{M}dr_1, \Lambda^{-1}(\Lambda + \mathcal{A})\mathcal{M}dr_2\big)_{L^2(\Gamma^\star)},
\end{aligned}$$

where $\mathcal{M} : L^2(\Gamma^\star) \to L^2(\Gamma^\star)$ is a bijective multiplication operator, $\Lambda : H^{1/2}(\Gamma^\star) \to H^{-1/2}(\Gamma^\star)$ is the Dirichlet-to-Neumann map (associated with the boundary value problem (1.3)), and

$$\mathcal{A} := (n-1)\mathcal{H} + \left[\frac{\partial g}{\partial \mathbf{n}} - f\right] \Big/ g : L^2(\Gamma^\star) \to L^2(\Gamma^\star)$$

($\mathcal{H}$ denotes the mean curvature) is a multiplication operator.
In all cases $\mathcal{A} \geq 0$ is a *sufficient* condition for positiveness of the shape Hessian:

Theorem 2.1 ([4, 5, 7])**.** *Let $\Omega^\star$ be a stationary domain of the shape functional J_i. Then, the shape Hessian is $H^t(\Gamma^\star)$-coercive if $\mathcal{A} \geq 0$. Here, we have $t = s$ if $i = 1, 2$ and $t = s - 1$ if $i = 3$.*

In case of the formulations (i) and (ii) the positiveness is given with respect to the energy space $H^s(\Gamma)$ which implies the well-posedness of these formulations. Whereas in case of the formulation (iii) the positivity holds only in the weaker space $L^2(\Gamma)$, that is

$$d^2 J_3(\Omega^\star)[dr, dr] \geq c_E \|dr\|^2_{L^2(\Gamma^\star)}, \quad c_E > 0,$$

which implies the algebraically *ill-posedness* of the Dirichlet tracking formulation.

3 Shape approximation

The simplest way to discretize the free boundary is to consider an $(n-1)$-dimensional reference manifold $\widehat{\Gamma} \subset \mathbb{R}^n$ and a fixed boundary perturbation field, for example in direction of the outward normal $\widehat{\mathbf{n}}$. Then we are looking for a sufficiently smooth function r that parametrizes the free boundary in accordance with

$$\boldsymbol{\gamma} : \widehat{\Gamma} \to \Gamma, \quad \boldsymbol{\gamma}(\mathbf{x}) = \mathbf{x} + r(\mathbf{x})\widehat{\mathbf{n}}(\mathbf{x}). \tag{3.7}$$

That is, we identify a domain with the scalar function r. A perturbed domain $\Omega_\varepsilon[dr]$ is defined via the variation

$$\boldsymbol{\gamma}_\varepsilon : \widehat{\Gamma} \to \Gamma_\varepsilon, \quad \boldsymbol{\gamma}_\varepsilon(\mathbf{x}) := \boldsymbol{\gamma}(\mathbf{x}) + \varepsilon dr(\mathbf{x})\widehat{\mathbf{n}}(\mathbf{x}), \tag{3.8}$$

where dr is again a sufficiently smooth scalar function. Consequently, both, the shapes and their increments, can be seen as elements of a Banach space X. Moreover, the Sobolev spaces $H^t(\Gamma^\star)$ and $H^t(\widehat{\Gamma})$ are isomorphic for all t within a certain range that depends on the smoothness of $\Gamma^\star$. A quite canonical choice is to take the unit sphere as reference manifold, which corresponds to the restriction to star-shaped domains.
It turns out that we respectively require $X = C^{2,\alpha}(\widehat{\Gamma})$ for the formulations (i) and (iii), whereas $X = C^{3,\alpha}(\widehat{\Gamma})$ is required for the formulation (ii). In all cases $\alpha = 0$ is sufficient for first order optimization algorithms while $\alpha > 0$ needs to be imposed for the Newton method.
In order to solve the minimization problem $J_i(r) \to \inf$, we are seeking for the stationary points $r^\star \in X$ satisfying

$$dJ(r^\star)[dr] = 0 \quad \text{for all } dr \in X. \tag{3.9}$$

In accordance with [8] we shall introduce a Ritz-Galerkin method for the nonlinear equation (3.9). To this end let $\varphi_i : \widehat{\Gamma} \to \mathbb{R}$ denote suitable ansatz functions and consider the ansatz space

$$V_N = \operatorname{span}\{\varphi_1, \varphi_2, \ldots, \varphi_N\} \subset X. \tag{3.10}$$

Especially in case of star-like domains it is convenient to use spherical harmonics in $\mathbb{R}^n$ as ansatz functions.

We now replace (3.9) by its finite dimensional counterpart:

$$\text{seek } r_N^\star \in V_N \text{ such that} \quad dJ(r_N^\star)[dr] = 0 \quad \text{for all } dr \in V_N. \tag{3.11}$$

Note that this is the necessary condition associated with the finite dimensional optimization problem

$$J(r_N) \to \inf, \quad r_N \in V_N. \tag{3.12}$$

Concerning the existence and convergence of approximate shapes we have the following theorem.

Theorem 3.1 ([8]). *Assume that the shape Hessian is strictly $H^s(\Gamma^\star)$-coercive at the stationary domain $r^\star \in X$. Then, there exists a neighbourhood $U(r^\star) \subset X$ such that* (3.12) *admits a unique solution $r_N^\star \in V_N \cap U(r^\star)$ provided that N is large enough. The approximation error stays in the energy norm proportional to the best approximation in V_N, that is*

$$\|r_N^\star - r^\star\|_{H^{1/2}(\widehat{\Gamma})} \lesssim \inf_{r_N \in V_N} \|r_N - r^\star\|_{H^{1/2}(\widehat{\Gamma})}.$$

Of course, from this theorem one can compute the *rate of convergence* by estimating $\inf_{r_N \in V_N} \|r_N - r^\star\|_{H^{1/2}(\widehat{\Gamma})}$.
Different strategies exist to find $r_N \in V_N$ such that (3.11) holds. In general, one makes the ansatz $r_N = \sum_{i=1}^N r_i \varphi_i$ and considers the iterative scheme

$$\mathbf{r}^{(n+1)} = \mathbf{r}^{(n)} - h^{(n)} \mathbf{M}^{(n)} \mathbf{G}^{(n)}, \quad n = 0, 1, 2, \ldots, \tag{3.13}$$

where $h^{(n)}$ is a suitable step width and

$$\mathbf{r}^{(n)} = \big(r_i^{(n)}\big)_{i=1,\ldots,N}, \quad \mathbf{G}^{(n)} := \big(dJ(r_N^{(n)})[\varphi_i]\big)_{i=1,\ldots,N}.$$

First order methods are the gradient method ($\mathbf{M}^{(n)} := \mathbf{I}$) or the quasi Newton method where $\mathbf{M}^{(n)}$ denotes a suitable approximation to the inverse shape Hessian. Choosing

$$\mathbf{M}^{(n)} := \big(d^2 J(r_N^{(n)})[\varphi_i, \varphi_j]\big)^{-1}_{i,j=1,\ldots,N}$$

we arrive at the Newton method, which converges much faster compared to the first order methods, see [9] for example.
The following statement is an immediate consequence of Theorem 3.1.

Corollary 3.2 ([8]). *Under the assumptions of Theorem 3.1 the iterands $r_N^{(n)}$ produced by algorithm* (3.13) *converge to $r_N^\star$ provided that the initial guess $r_N^{(0)}$ is properly chosen.*

4 More flexible boundary representations

If one intends to implement only first order shape optimization algorithms, then one may employ a more general boundary representation than the restrictive approach (3.7), (3.8).
The boundary of a domain Ω can be represented by a bijective positive oriented function

$$\boldsymbol{\gamma} : \widehat{\Gamma} \to \Gamma, \qquad \boldsymbol{\gamma}(\mathbf{x}) = \big[\gamma_1(\mathbf{x}), \ldots, \gamma_n(\mathbf{x})\big]^T, \tag{4.14}$$

such that $\gamma_1, \ldots, \gamma_n \in X$. Consider again the ansatz space V_N from (3.10). To discretize the shape optimization problem we make this time the ansatz

$$\boldsymbol{\gamma}_N = \sum_{k=-N}^{N} \mathbf{a}_k \varphi_k \in V_N^n \tag{4.15}$$

with *vector-valued* coefficients $\mathbf{a}_k \in \mathbb{R}^n$.
On the one hand the ansatz (4.15) does not impose any restriction to the topology of the domain except for its genus (hence $\widehat{\Gamma} = \mathbb{S}^{n-1}$ is an appropriate choice). On the other hand the parametric representation (4.14) of the domain Ω is not unique. In fact, if $\Xi : \widehat{\Gamma} \to \widehat{\Gamma}$ denotes any smooth bijective mapping, then the function $\boldsymbol{\gamma} \circ \Xi$ describes another parametrization of Ω. Consequently, one cannot expect convergence results like that of Theorem 3.1.
To avoid degenerated boundary representations one can apply from time to time a suitable remeshing algorithm. However, even for a large number of degrees of freedom, the surface, and thus the value of the cost functional, is changed considerably by remeshing. Consequently, it might happen that the shape optimization algorithm does not convergence. To our experience it is preferable to regularize the shape functional instead. To this end, one needs to define a suitable mesh functional $M(\Omega)$ which penalizes bad parametrizations. For small $\beta > 0$ one then solves the *regularized* shape problem

$$J(\Omega) + \beta M(\Omega) \to \inf$$

instead of the original problem. We refer the reader to [6] for suitable mesh functionals and further details.

5 Numerical method to compute the state

By using the boundary integral representation of the shape gradient and Hessian one only needs to provide the boundary values of the underlying state and adjoint state function. Thus, if the shape functional is of boundary integral type like for instance (1.4) and (1.5), boundary integral equations are highly attractive since their numerical solution requires only a triangulation of the boundary. That way, large domain deformations become realizable without remeshing as necessary for example when using

finite element methods. Additionally, compared to finite element methods, the complexity is even reduced if we apply modern boundary element methods like e.g. the *wavelet Galerkin scheme* [2].
Nevertheless, also certain shape functionals of domain integral type like e.g. (1.2) can be transformed to boundary integrals. Consider a Newton potential N_f that satisfies $-\Delta N_f = f$ in Ω and make the ansatz $u = N_f + v$. By applying integration by parts we arrive at

$$J_1(\Omega) = \int_\Omega \{g^2 - N_f f\} d\mathbf{x} + \int_\Sigma \frac{\partial(2N_f + v)}{\partial \mathbf{n}} h \, d\sigma_{\mathbf{x}} - \int_{\Gamma \cup \Sigma} N_f \frac{\partial u}{\partial \mathbf{n}} \, d\sigma_{\mathbf{x}}.$$

Hence, in general it suffices to provide the so-called *Dirichlet-to-Neumann map*

$$\mathcal{V} \frac{\partial v}{\partial \mathbf{n}} = \Big(\frac{1}{2} + \mathcal{K}\Big)(h\chi_\Sigma - N_f),$$

involving the single and double layer integral operators $\mathcal{V}$ and $\mathcal{K}$, to compute all ingredients of first and second order shape optimization algorithms, see e.g. [4, 5, 6, 7, 9].

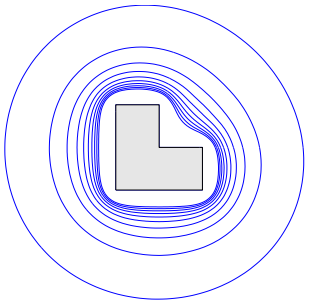

Figure 1: Solutions of the 2D Bernoulli problem with L-shaped boundary Σ.

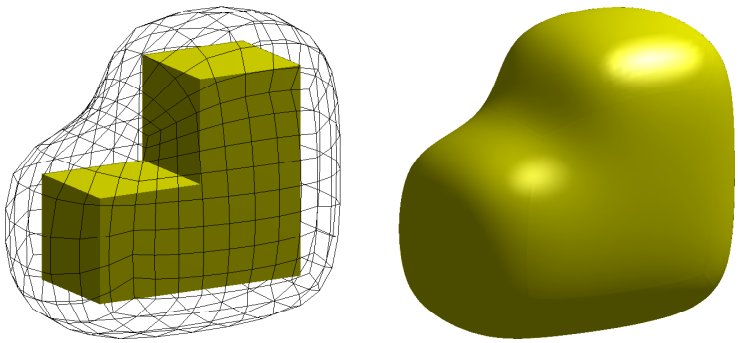

Figure 2: The solution of the 3D Bernoulli problem with L-shaped boundary Σ.

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