Improved Trial Methods for a Class of Generalized Bernoulli Problems

Helmut Harbrecht, Giannoula Mitrou

Institute of Mathematics University of Basel Rheinsprung 21 CH - 4051 Basel Switzerland Preprint No. 2013-22 September, 2013

www.math.unibas.ch

Improved trial methods for a class of generalized Bernoulli problems

Helmut Harbrecht^{1,*}, Giannoula Mitrou²

Mathematisches Institut, Universität Basel, Rheinsprung 21, 4051 Basel, Switzerland

Abstract

The aim of this article is to develop improved trial methods for the solution of a generalized exterior Bernoulli free boundary problem. At the free boundary, we prescribe the Neumann boundary condition and update the free boundary with the help of the remaining Dirichlet boundary condition. Appropriate update rules are obtained by expanding the Dirichlet data at the actual boundary via a Taylor expansion of first and second order. The resulting trial methods converge linearly for both cases, although the trial method based on the second order Taylor expansion is much more robust. Nevertheless, via results of shape sensitivity analysis, we are able to modify the update rules such that their convergence is improved. The feasibility of the proposed trial methods and their performance is demonstrated by numerical results.

Keywords: free boundary problem, trial method, higher order convergence 2000 MSC: 35R35, 35Q99, 65P05, 76B99

1. Introduction

In this article, we consider a generalized version of Bernoulli's exterior free boundary problem which involves Poisson's equation and non-constant boundary data. To mathematically describe the problem under consideration, let $T \subset \mathbb{R}^2$ be 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 ; see Figure 1.1 for a sketch of the geometry.

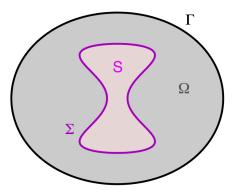


Figure 1.1: The domain Ω and its boundaries Γ and Σ .

^{*}Corresponding author.

Email addresses: helmut.harbrecht@unibas.ch (Helmut Harbrecht), giannoula.mitrou@unibas.ch (Giannoula Mitrou)

¹This author acknowledges the support of the SNF through the project No. 200021_137668.

²This author acknowledges the support of the DFG priority program SPP 1253.

The generalized Bernoulli free boundary problem reads as follows: Seek the domain Ω and the function v which satisfy the overdetermined boundary value problem

$$-\Delta v = f \qquad \text{in } \Omega$$

$$v = g \qquad \text{on } \Sigma$$

$$v = 0, \frac{\partial v}{\partial \mathbf{n}} = h \qquad \text{on } \Gamma.$$
(1.1)

Here, **n** stands for the unit normal vector on Γ and $\partial v/\partial \mathbf{n}$ denotes the normal derivative of v. Moreover, f, g, and h are supposed to be sufficiently smooth functions which satisfy $f \ge 0$, g > 0 and h < 0 such that the solution v is well defined and positive in Ω .

The free boundary problem under consideration can be viewed as the prototype of a large class of stationary free boundary problems involved in many applications such as fluid dynamics, optimal design, electromagnetics and various other engineering fields. We refer to [3, 4, 10] for a review of theoretical results concerning the existence of the solution to a free boundary problem. Results on the geometric form of the boundary Γ can be found in [1] and the references therein.

For the solution of the above free boundary problem, we choose a fixed point type method, the so-called trial method. The trial method is an iterative scheme, described by the following steps:

- 1. Choose an initial guess Γ_0 of the free boundary.
- 2. a) Solve the boundary value problem with Neumann condition on the free boundary Γ_k .
 - b) Update the free boundary Γ_k such that the Dirichlet boundary condition is approximately satisfied on the new boundary Γ_{k+1} .
- 3. Repeat step 2 until the process becomes stationary up to a specified accuracy.

Usually, the update is derived through a Taylor expansion and moves the boundary such that the Dirichlet condition is satisfied. The use of a first order Taylor expansion has been proposed in [10, 20]. In this article, we will even use a second order Taylor expansion which, as numerical results show, is more robust. However, the trial method still convergences only linearly.

In order to obtain higher order convergence, the Neumann boundary condition at the free boundary has been substituted by a Robin boundary condition in [10, 20]. Instead, we intend to improve the convergence of the trial method without changing the boundary condition at the free boundary Γ . This is achieved by modifying the update rule appropriately.

To the several numerical schemes for the solution of free boundary problems belong parametric trial methods as proposed in [2, 10, 19, 20]. The level set method for Bernoulli's problem has been used in [5, 6, 14], enjoying the property of allowing topology changes. In all these papers, however, only the Laplace equation and constant Dirichlet and Neumann data have been considered which corresponds to the original Bernoulli free boundary problem. In [17], for a related time-harmonic inverse acoustic scattering problem, an iterative method based on the idea of the analytic continuation of the field has been used. Shape optimization provides another powerful tool to solve free boundary problems, see e.g. [8, 9, 11, 12] and the references therein.

The remainder of this article is organized as follows. Section 2 is dedicated to the derivation of the trial methods based on first and second order Taylor expansions of the Dirichlet data at the actual boundary. In Section 3, we reformulate the boundary value problem by boundary integral equations and propose their numerical solution by the boundary element method. Some first numerical tests are presented in Subsection 3.4. They give the motivation to get involved with the convergence theory of trial methods in Section 4. It especially enables to appropriately modify the update rule such that the convergence is improved. In addition, the Newton method becomes performable. The practicability of the resulting trial methods is shown by some numerical results in Section 4.5. Finally, in Section 5, the article's conclusion is drawn.

2. Derivation of the update rules

2.1. Background and motivation

Throughout this article, we assume that the domain T is starlike. We can then represent the free boundary Γ by a parametrization $\gamma : [0, 2\pi] \to \mathbb{R}^2$ in polar coordinates, that is

$$\Gamma := \left\{ \boldsymbol{\gamma}(s) = r(s)\mathbf{e}_r(s) : s \in [0, 2\pi] \right\}$$

where $\mathbf{e}_r(s) = (\cos(s), \sin(s))^T$ denotes the unit vector in the radial direction. The radial function r(s) is supposed to be a positive function in $C_{\text{per}}^2([0, 2\pi])$, where

$$C_{\text{per}}^2([0,2\pi]) = \left\{ r \in C^2([0,2\pi]) : r^{(i)}(0) = r^{(i)}(2\pi), \ i = 0, 1, 2 \right\},\$$

such that $dist(\Sigma, \Gamma) > 0$.

The trial method for the solution of the free boundary problem (1.1) requires an update rule. Suppose that the actual boundary is Γ_k . Then, the corresponding state v_k satisfies

$$-\Delta v_k = f \qquad \text{in } \Omega_k$$

$$v_k = g \qquad \text{on } \Sigma$$

$$\frac{\partial v_k}{\partial \mathbf{n}} = h \qquad \text{on } \Gamma_k.$$
(2.1)

The new boundary Γ_{k+1} is now determined by moving the old boundary into the radial direction, which is expressed by the update rule

$$\boldsymbol{\gamma}_{k+1} = \boldsymbol{\gamma}_k + \delta r_k \mathbf{e}_r. \tag{2.2}$$

The update function $\delta r_k \in C^2_{\text{per}}([0, 2\pi])$ is chosen such that the desired homogeneous Dirichlet boundary condition is satisfied at the new boundary Γ_{k+1} , i.e.,

$$\nu_k \circ \boldsymbol{\gamma}_{k+1} \stackrel{!}{=} 0 \quad \text{on } [0, 2\pi]. \tag{2.3}$$

The main tool to find the update function δr_k is Taylor's expansion of the first and second order.

2.2. First order update rule

The first order update rule is obtained by linearizing $v_k \circ (\gamma_k + \delta r \mathbf{e}_r)$ with respect to the update function δr . This yields the equation

$$v_k \circ \boldsymbol{\gamma}_{k+1} \approx v_k \circ \boldsymbol{\gamma}_k + \left(\frac{\partial v_k}{\partial \mathbf{e}_r} \circ \boldsymbol{\gamma}_k\right) \delta r_k.$$
(2.4)

We decompose the derivative of v_k in the direction \mathbf{e}_r into its normal and tangential components:

$$\frac{\partial v_k}{\partial \mathbf{e}_r} = \frac{\partial v_k}{\partial \mathbf{n}} \langle \mathbf{e}_r, \mathbf{n} \rangle + \frac{\partial v_k}{\partial \mathbf{t}} \langle \mathbf{e}_r, \mathbf{t} \rangle \quad \text{on } \Gamma_k.$$
(2.5)

Inserting the Neumann boundary condition $\partial v_k / \partial \mathbf{n} = h$, we arrive at the first order update equation

$$F_1(\delta r_k) := v_k \circ \boldsymbol{\gamma}_k + \left[(h \circ \boldsymbol{\gamma}_k) \langle \mathbf{e}_r, \mathbf{n} \rangle + \left(\frac{\partial v_k}{\partial \mathbf{t}} \circ \boldsymbol{\gamma}_k \right) \langle \mathbf{e}_r, \mathbf{t} \rangle \right] \delta r_k \stackrel{!}{=} 0.$$
(2.6)

This leads to the most common update rule and has, for example, been used in [10, 14, 20]. However, there the update is performed in the normal direction rather than the radial direction which might lead to a degeneration of the domain. Notice finally that the update equation (2.6) is solvable at least in a neighbourhood of Γ^* since there it holds $\partial v^* / \partial \mathbf{e}_r = h \langle \mathbf{e}_r, \mathbf{n} \rangle < 0$ due to h < 0 and $\langle \mathbf{e}_r, \mathbf{n} \rangle > 0$ for starlike domains.

2.3. Second order update rule

The second order update rule is derived from a second order Taylor expansion of $v_k \circ (\gamma_k + \delta r \mathbf{e}_r)$ with respect to δr , that is

$$v_k \circ \boldsymbol{\gamma}_{k+1} \approx v_k \circ \boldsymbol{\gamma}_k + \left(\frac{\partial v_k}{\partial \mathbf{e}_r} \circ \boldsymbol{\gamma}_k\right) \delta r_k + \frac{1}{2} \left(\frac{\partial^2 v_k}{\partial \mathbf{e}_r^2} \circ \boldsymbol{\gamma}_k\right) \delta r_k^2.$$
(2.7)

Because of our regularity assumptions on the boundary Γ_k , we are able to compute the derivatives of the twice continuously differentiable function v_k . Notice that, assuming more regularity of Γ_k , even a higher order Taylor expansion can be exploited here.

The directional derivative $\partial v_k / \partial \mathbf{e}_r$ included in (2.7) is computed by (2.5). Whereas, for the second order directional derivative $\partial^2 v_k / \partial \mathbf{e}_r^2$, we refer to the following lemma.

Lemma 2.1. The second order derivative of v_k in the direction \mathbf{e}_r is given by

$$\frac{\partial^2 v_k}{\partial \mathbf{e}_r^2} = \frac{\partial^2 v_k}{\partial \mathbf{t}^2} \{ \langle \mathbf{e}_r, \mathbf{t} \rangle^2 - \langle \mathbf{e}_r, \mathbf{n} \rangle^2 \} - f \langle \mathbf{e}_r, \mathbf{n} \rangle^2 + 2 \left[\frac{\partial h}{\partial \mathbf{t}} - \kappa \frac{\partial v_k}{\partial \mathbf{t}} \right] \langle \mathbf{e}_r, \mathbf{n} \rangle \langle \mathbf{e}_r, \mathbf{t} \rangle \quad on \ \Gamma_k,$$
(2.8)

where $\kappa = -\langle \boldsymbol{\gamma}_k'', \mathbf{n} \rangle / \| \boldsymbol{\gamma}_k' \|^2$ denotes the curvature of the boundary Γ_k .

Proof. We split the second derivative of v_k in the direction \mathbf{e}_r into its normal and tangential components

$$\frac{\partial^2 v_k}{\partial \mathbf{e}_r^2} = \frac{\partial^2 v_k}{\partial \mathbf{n}^2} \langle \mathbf{e}_r, \mathbf{n} \rangle^2 + 2 \frac{\partial^2 v_k}{\partial \mathbf{n} \partial \mathbf{t}} \langle \mathbf{e}_r, \mathbf{n} \rangle \langle \mathbf{e}_r, \mathbf{t} \rangle + \frac{\partial^2 v_k}{\partial \mathbf{t}^2} \langle \mathbf{e}_r, \mathbf{t} \rangle^2 \quad \text{on } \Gamma_k.$$
(2.9)

The derivative of v_k 's Neumann data with respect to s is given by

$$\frac{\partial}{\partial s} \left(\frac{\partial v_k}{\partial \mathbf{n}} \circ \boldsymbol{\gamma}_k \right) = \| \boldsymbol{\gamma}_k' \| \left(\frac{\partial^2 v_k}{\partial \mathbf{n} \partial \mathbf{t}} \circ \boldsymbol{\gamma}_k \right) + \left\langle \nabla v_k \circ \boldsymbol{\gamma}_k, \frac{\partial \mathbf{n}}{\partial s} \right\rangle.$$

Due to $\partial \mathbf{n}/\partial s = \kappa || \boldsymbol{\gamma}_{k}' || \mathbf{t}$ and the Neumann boundary condition at Γ_{k} , this equation can be rewritten as

$$\frac{\partial^2 v_k}{\partial \mathbf{n} \partial \mathbf{t}} = \frac{\partial h}{\partial \mathbf{t}} - \kappa \frac{\partial v_k}{\partial \mathbf{t}} \quad \text{on } \Gamma_k.$$
(2.10)

The derivatives $\partial^2 v_k / \partial \mathbf{n}^2$ and $\partial^2 v_k / \partial \mathbf{t}^2$ are coupled via the Poisson equation which implies

$$\frac{\partial^2 v_k}{\partial \mathbf{n}^2} = -\frac{\partial^2 v_k}{\partial \mathbf{t}^2} - f \quad \text{on } \Gamma_k.$$
(2.11)

By inserting (2.10) and (2.11) into (2.9), the latter becomes (2.8). This concludes the proof.

Having all the terms of the second order approximation (2.7) of the left hand side of (2.3) at hand, we find the update function δr_k from the numerical solution of the following equation:

$$F_{2}(\delta r_{k}) := F_{1}(\delta r_{k}) + \frac{1}{2} \left\{ \left(\frac{\partial^{2} v_{k}}{\partial \mathbf{t}^{2}} \circ \boldsymbol{\gamma}_{k} \right) \left\{ \langle \mathbf{e}_{r}, \mathbf{t} \rangle^{2} - \langle \mathbf{e}_{r}, \mathbf{n} \rangle^{2} \right\} - (f \circ \boldsymbol{\gamma}_{k}) \langle \mathbf{e}_{r}, \mathbf{n} \rangle^{2} + 2 \left[\left(\frac{\partial h}{\partial \mathbf{t}} - \kappa \frac{\partial v_{k}}{\partial \mathbf{t}} \right) \circ \boldsymbol{\gamma}_{k} \right] \langle \mathbf{e}_{r}, \mathbf{n} \rangle \langle \mathbf{e}_{r}, \mathbf{t} \rangle \right\} \delta r_{k}^{2} \stackrel{!}{=} 0. \quad (2.12)$$

It is especially seen from this representation that the update which is computed from this second order update equation coincides with the update computed by (2.6) except for a higher order term.

2.4. Discretization of the free boundary problem

For the numerical computations, we discretize the radial function r_k^n associated with the boundary Γ_k by a finite Fourier series according to

$$r_k^n(s) = a_0 + \sum_{i=1}^{n-1} \{a_i \cos(is) + b_i \sin(is)\} + a_n \cos(ns).$$
(2.13)

This obviously ensures that r_k^n is always an element of $C_{per}^2([0, 2\pi])$. To determine the update function δr_k^n , represented likewise by a finite Fourier series, we insert the $m \ge 2n$ equidistantly distributed points $s_i = 2\pi i/m$ into the update equations (2.6) and (2.12), respectively:

$$F(\delta r_k^n) \stackrel{!}{=} 0$$
 in all the points s_1, \ldots, s_m .

This is a discrete least-squares problem which can simply be solved by the normal equations in case of the first order update equation (2.6). In case of the second order update equation (2.12) the least-squares problem is nonlinear. Hence, we have to apply the Gauss-Newton method for its solution.

3. Solving the boundary value problem

3.1. Newton potential

Since the solution v_k of the state equation is required only on the boundary Γ_k of the domain Ω_k , the boundary element method is more efficient than other methods. For sake of notational convenience, we drop the index *k* in the rest of the section. Despite Poisson's equation, the boundary element method can be applied by making the ansatz

$$v = u + N_f \tag{3.1}$$

for a suitable Newton potential N_f which satisfies the equation $-\Delta N_f = f$ and a harmonic function u which satisfies the boundary value problem

$$\Delta u = 0 \qquad \text{in } \Omega$$

$$u = g - N_f \qquad \text{on } \Sigma$$

$$\frac{\partial u}{\partial \mathbf{n}} = h - \frac{\partial N_f}{\partial \mathbf{n}} \qquad \text{on } \Gamma.$$
(3.2)

The Newton potential has to be given analytically or computed in a sufficiently large domain $\widehat{\Omega}$. Nevertheless, since this domain can be chosen fairly simple, efficient solution techniques can easily be applied.

3.2. Boundary element method

Our approach to get the system of integral equations is the direct formulation based on Green's fundamental solution. In this case, the solution u of (3.2) is given by Green's representation formula

$$u(\mathbf{x}) = \int_{\Gamma \cup \Sigma} \left\{ G(\mathbf{x}, \mathbf{y}) \frac{\partial u}{\partial \mathbf{n}}(\mathbf{y}) - \frac{\partial G(\mathbf{x}, \mathbf{y})}{\partial \mathbf{n}_{\mathbf{y}}} u(\mathbf{y}) \right\} d\sigma_{\mathbf{y}}, \quad \mathbf{x} \in \Omega.$$
(3.3)

Using the jump properties of the layer potentials, we obtain the direct boundary integral formulation of the problem

$$u(\mathbf{x}) = \int_{\Gamma \cup \Sigma} G(\mathbf{x}, \mathbf{y}) \frac{\partial u}{\partial \mathbf{n}}(\mathbf{y}) \, \mathrm{d}\sigma_{\mathbf{y}} + \frac{1}{2}u(\mathbf{x}) - \int_{\Gamma \cup \Sigma} \frac{\partial G(\mathbf{x}, \mathbf{y})}{\partial \mathbf{n}_{\mathbf{y}}} u(\mathbf{y}) \, \mathrm{d}\sigma_{\mathbf{y}}, \quad \mathbf{x} \in \Gamma \cup \Sigma.$$
(3.4)

Writing the boundaries as $A, B \in \{\Gamma, \Sigma\}$, then (3.4) includes the single layer operator

$$\mathcal{V}: C(A) \to C(B), \quad (\mathcal{V}_{AB}\rho)(\mathbf{x}) = -\frac{1}{2\pi} \int_{A} \log \|\mathbf{x} - \mathbf{y}\| \rho(\mathbf{y}) \, \mathrm{d}\sigma_{\mathbf{y}}$$
(3.5)

and the double layer operator

$$\mathcal{K}: C(A) \to C(B), \quad (\mathcal{K}_{AB}\rho)(\mathbf{x}) = \frac{1}{2\pi} \int_{A} \frac{\langle \mathbf{x} - \mathbf{y}, \mathbf{n}_{\mathbf{y}} \rangle}{\|\mathbf{x} - \mathbf{y}\|^{2}} \rho(\mathbf{y}) \, \mathrm{d}\sigma_{\mathbf{y}}$$
(3.6)

with the densities ρ being the Cauchy data on A. The equation (3.4) in combination with (3.5) and (3.6) indicates the Neumann-to-Dirichlet map, which for problem (3.2) induces the following system of integral equations

$$\begin{bmatrix} \frac{1}{2}I + \mathcal{K}_{\Gamma\Gamma} & -\mathcal{V}_{\Sigma\Gamma} \\ \mathcal{K}_{\Gamma\Sigma} & -\mathcal{V}_{\Sigma\Sigma} \end{bmatrix} \begin{bmatrix} u|_{\Gamma} \\ \frac{\partial u}{\partial \mathbf{n}}|_{\Sigma} \end{bmatrix} = \begin{bmatrix} \mathcal{V}_{\Gamma\Gamma} & -\mathcal{K}_{\Sigma\Gamma} \\ \mathcal{V}_{\Gamma\Sigma} & -\left(\frac{1}{2}I + \mathcal{K}_{\Sigma\Sigma}\right) \end{bmatrix} \begin{bmatrix} \left(h - \frac{\partial N_f}{\partial \mathbf{n}}\right)|_{\Gamma} \\ (g - N_f)|_{\Sigma} \end{bmatrix}.$$
(3.7)

The next step to the solution of the boundary value problem is the numerical approximation of the integral operators included in (3.4) which first requires the parametrization of the integral equations. We use the parametrization of the boundaries as it was described in the beginning of Section 2.1. For the approximation of unknown Cauchy data, we use the collocation method based on trigonometric polynomials. Using the trapezoidal rule for the numerical quadrature and applying the regularization technique along the lines of [13] to deal with the singular integrals, we arrive at an exponentially convergent boundary element method provided that the data and the boundaries and thus the solution are arbitrary smooth.

3.3. Numerical realization of the update rules

We briefly present the equations we solve to determine the updates in case of Poisson's equation. The tangential derivative of u is computed from the identity

$$\frac{\partial u}{\partial \mathbf{t}} \circ \boldsymbol{\gamma} = \left\langle \nabla u \circ \boldsymbol{\gamma}, \frac{\boldsymbol{\gamma}'}{\|\boldsymbol{\gamma}'\|} \right\rangle = \frac{1}{\|\boldsymbol{\gamma}'\|} \frac{\partial (u \circ \boldsymbol{\gamma})}{\partial s}$$

In view of (3.1), the first order update results thus from the solution of

$$F_1(\delta r) = (u + N_f) \circ \boldsymbol{\gamma} + \left[(h \circ \boldsymbol{\gamma}) \langle \mathbf{e}_r, \mathbf{n} \rangle + \left(\frac{1}{\|\boldsymbol{\gamma}'\|} \frac{\partial (u \circ \boldsymbol{\gamma})}{\partial s} + \frac{\partial N_f}{\partial \mathbf{t}} \circ \boldsymbol{\gamma} \right) \langle \mathbf{e}_r, \mathbf{t} \rangle \right] \delta r = 0,$$

cf. (2.6). Likewise, to compute the second order tangential derivative of u, we use

$$\frac{\partial^2 (u \circ \boldsymbol{\gamma})}{\partial s^2} = \|\boldsymbol{\gamma}'\|^2 \left(\frac{\partial^2 u}{\partial \mathbf{t}^2} \circ \boldsymbol{\gamma}\right) + \langle \boldsymbol{\gamma}'', \mathbf{t} \rangle \left(\frac{\partial u}{\partial \mathbf{t}} \circ \boldsymbol{\gamma}\right) + \langle \boldsymbol{\gamma}'', \mathbf{n} \rangle \left(\frac{\partial u}{\partial \mathbf{n}} \circ \boldsymbol{\gamma}\right)$$

This yields the relation

$$\frac{\partial^2 u}{\partial \mathbf{t}^2} \circ \boldsymbol{\gamma} = \frac{1}{\|\boldsymbol{\gamma}'\|^2} \frac{\partial^2 (\boldsymbol{u} \circ \boldsymbol{\gamma})}{\partial s^2} - \frac{\langle \boldsymbol{\gamma}'', \mathbf{t} \rangle}{\|\boldsymbol{\gamma}'\|^3} \frac{\partial (\boldsymbol{u} \circ \boldsymbol{\gamma})}{\partial s} + \kappa \Big(h \circ \boldsymbol{\gamma} - \frac{\partial N_f}{\partial \mathbf{n}} \circ \boldsymbol{\gamma} \Big), \tag{3.8}$$

where we substituted the Neumann data of u according to the desired boundary condition at Γ , cf. (3.2). The combination of (2.12), (3.1), and (3.8) finally yields

$$F_{2}(\delta r) = F_{1}(\delta r) + \frac{1}{2} \left\{ \left[\frac{1}{\|\boldsymbol{\gamma}'\|^{2}} \frac{\partial^{2}(\boldsymbol{u} \circ \boldsymbol{\gamma})}{\partial s^{2}} - \frac{\langle \boldsymbol{\gamma}'', \mathbf{t} \rangle}{\|\boldsymbol{\gamma}'\|^{3}} \frac{\partial(\boldsymbol{u} \circ \boldsymbol{\gamma})}{\partial s} + \kappa \left(h \circ \boldsymbol{\gamma} - \frac{\partial N_{f}}{\partial \mathbf{n}} \circ \boldsymbol{\gamma} \right) + \frac{\partial^{2} N_{f}}{\partial \mathbf{t}^{2}} \circ \boldsymbol{\gamma} \right] \left\{ \langle \mathbf{e}_{r}, \mathbf{t} \rangle^{2} - \langle \mathbf{e}_{r}, \mathbf{n} \rangle^{2} \right\} - (f \circ \boldsymbol{\gamma}) \langle \mathbf{e}_{r}, \mathbf{n} \rangle^{2} + 2 \left[\frac{\partial h}{\partial \mathbf{t}} \circ \boldsymbol{\gamma} - \frac{\kappa}{\|\boldsymbol{\gamma}'\|} \frac{\partial(\boldsymbol{u} \circ \boldsymbol{\gamma})}{\partial s} - \kappa \frac{\partial N_{f}}{\partial \mathbf{t}} \circ \boldsymbol{\gamma} \right] \langle \mathbf{e}_{r}, \mathbf{n} \rangle \langle \mathbf{e}_{r}, \mathbf{t} \rangle \right\} \delta r^{2}.$$

The quantities $\partial(u \circ \gamma)/\partial s$ and $\partial^2(u \circ \gamma)/\partial s^2$ which show up in the above expressions are computed by differentiating the trigonometric representation of the approximation to $u \circ \gamma$.

3.4. Numerical results

In this section, we perform numerical tests in order to compare the trial methods based on the first and the second order update rule. We choose the fixed boundary Σ kite-shaped, parameterized via

$$\gamma_{\Sigma}(s) = \begin{bmatrix} -0.1\cos(s) + 0.065\cos(2s) \\ 0.15\sin(s) \end{bmatrix}$$

As initial guess Γ_0 to the free boundary Γ , a slightly perturbed ellipse is used:

$$\gamma_{\Gamma_0}(s) = \sqrt{0.04 \cos^2(2s) + 0.06 \sin^2(2s)} \begin{bmatrix} \cos(s) \\ \sin(s) \end{bmatrix}.$$

We intend to solve the free boundary problem with respect to the data

$$f(x, y) = 60$$
, $g(x, y) = x^2 + y^2 + 1$, and $h(x, y) = -\lambda(x^2 + y^2 + 1)$,

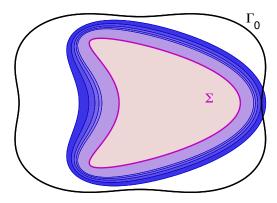


Figure 3.1: Solutions of the generalized Bernoulli free boundary problem in case of a kite-shaped interior boundary.

where λ a positive constant. An appropriate Newton potential can be analytically determined, namely $N_f(x, y) = -15(x^2 + y^2)$. Figure 3.1 shows the boundary Σ and the optimum boundary Γ^* of the free boundary problem for different values of the parameter λ .

In Table 3.1, we present the number of boundary updates which the trial methods requires in order to reach the optimum free boundary Γ^* . The numerical setting was as follows. We used 80 degrees of freedom to represent the unknown boundary Γ_k (i.e., n = 40) and 600 boundary elements per boundary. The trial method was stopped if the update function satisfied $||\delta r|| < 10^{-8}$. As one figures out of the table, the trial method based on the first order update converges only if the parameter λ is small enough (row entitled "1st order update"). Whereas, the trial method based on the second order update converges for all choices of the parameter λ (row entitled "2nd order update").

parameter λ	20	25	30	35	40
1st order update	23	31	-	_	-
1st order update with damping ($\alpha = 0.8$)	23	22	21	20	19
1st order update with damping ($\alpha = 0.5$)	42	41	39	37	36
2nd order update	27	28	29	29	31

Table 3.1: Number of iterations of the trial method.

The following modification helps to enforce convergence in case of the first order update also for large values of λ . Namely, we introduce an appropriate damping parameter $\alpha > 0$ in the update of the radial function: $r_{k+1} = r_k + \alpha \delta r$. Then, as it is seen in Table 3.1, convergence for all values of λ is achieved for the particular choices $\alpha = 0.5$ and $\alpha = 0.8$ (rows entitled "1st order update with damping"). Nevertheless, we emphasize that there is no systematic rule of choosing the damping parameter; see Remark 4.3.

It turns out that both, the trial method based on the first update and the trial method based on the second order update, converge linearly. However, the trial method based on the second order update is much more robust unless we use a suitable damping for the trial method based on the first order update. The last annotation we are going to make is that, for the trial method based on the second order update, we are able to compute with more degrees of freedom for the representation of r_k than for the trial method based on the first order update.

4. Convergence analysis

4.1. Shape sensitivity analysis

We shall investigate the convergence of the trial method. Following the lines of [20], we explore under which conditions we gain convergence and which is the attained rate of the convergence. To that end, some results from shape sensitivity analysis are required.

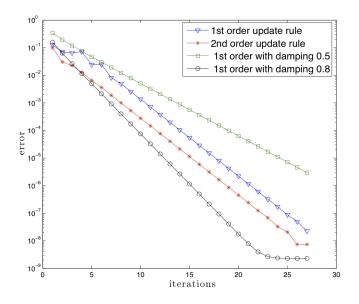


Figure 3.2: Convergence history of the trial method based on the first and second order update equation.

Given a sufficiently smooth domain perturbation field $\mathbf{V} : \Omega \to \mathbb{R}^2$ such that $\mathbf{V}|_{\Sigma} = \mathbf{0}$, we can define the perturbed domain $\Omega_{\varepsilon}[\mathbf{V}]$ by

$$\Omega_{\varepsilon} := \{ (\mathbf{I} + \varepsilon \mathbf{V})(\mathbf{x}) : \mathbf{x} \in \Omega \}.$$

Let *v* and v_{ε} denote the solution of (2.1) with respect to the domains Ω and Ω_{ε} . Then, the local shape derivative $\delta v = \delta v[\mathbf{V}]$ of *v* at Ω in the direction **V** is *formally* (see [15, 18] for a rigorous derivation) obtained by the pointwise limit

$$\delta v(\mathbf{x}) = \lim_{\varepsilon \to 0} \frac{v_{\varepsilon}(\mathbf{x}) - v(\mathbf{x})}{\varepsilon}, \quad \mathbf{x} \in \Omega.$$

The local shape derivative measures the sensitivity of the solution to (2.1) when changing the domain Ω in the direction **V**. According to [7, 18], the local shape derivative can be characterized by a boundary value problem.

Lemma 4.1. Given a sufficiently smooth domain perturbation field $\mathbf{V} : \Omega \to \mathbb{R}^2$ such that $\mathbf{V}|_{\Sigma} = \mathbf{0}$. Then, the local shape derivative $\delta v = \delta v[\mathbf{V}]$ of the boundary value problem (2.1) is given as the solution of the problem

$$\Delta \delta v = 0 \qquad in \ \Omega$$

$$\delta v = 0 \qquad on \ \Sigma$$

$$\frac{\partial \delta v}{\partial \mathbf{n}} = \left[\kappa h + \frac{\partial h}{\partial \mathbf{n}} + f\right] \langle \mathbf{V}, \mathbf{n} \rangle \qquad on \ \Gamma.$$
(4.1)

For more details concerning shape sensitivity analysis, we address the reader to [7, 15, 16, 18].

4.2. Banach's fixed point theorem

The procedure of proving higher order convergence is based on Banach's fixed point theorem. The update rule (2.2) defines a self-mapping

$$\Phi: X \to X, \quad r \mapsto \Phi(r) = r + \delta r(r)$$

in a Banach space X. For the present theory, the space $X = C_{per}^2([0, 2\pi])$ will be appropriate. By construction, the update δr vanishes at the sought free boundary $\Gamma^* = \{ \mathbf{x} \in \mathbb{R}^2 : \mathbf{x} = r^* \mathbf{e}_r \}$. Hence, the radial function r^* which

describes the boundary Γ^{\star} is obviously a fixed point $r^{\star} = \Phi(r^{\star})$ of the mapping Φ . In particular, the trial method corresponds to the fixed point iteration

$$r_{k+1} = r_k + \delta r(r_k), \quad k = 0, 1, 2, \dots$$

According to Banach's fixed point theorem, there exists a unique solution of this fixed point iteration if the mapping Φ is contractive. The convergence rate

$$\lim_{k \to \infty} \frac{\|r_{k+1} - r^{\star}\|_X}{\|r_k - r^{\star}\|_X} = \lim_{k \to \infty} \frac{\|\Phi(r_k) - \Phi(r^{\star})\|_X}{\|r_k - r^{\star}\|_X} = \lim_{k \to \infty} \frac{\|\delta\Phi[r_k - r^{\star}](r^{\star})\|_X}{\|r_k - r^{\star}\|_X}$$

can be estimated by

$$\lim_{k \to \infty} \frac{\|r_{k+1} - r^{\star}\|_{X}}{\|r_{k} - r^{\star}\|_{X}} \le \sup_{\|q\|_{X} = 1} \lim_{\varepsilon \to 0} \frac{\|\Phi(r^{\star} + q) - \Phi(r^{\star})\|_{X}}{\varepsilon} = \sup_{\|q\|_{X} = 1} \|\delta\Phi[q](r^{\star})\|_{X}.$$
(4.2)

As firstly stated in [20], we can thus deduce a sufficient condition for the convergence of the trial method. Namely, if $\sup_{\|q\|_X=1} \|(\delta \Phi[q](r^*)\|_X < 1, \text{ then the trial method converges. If it holds in addition } \inf_{\|q\|_X=1} \|(\delta \Phi[q](r^*)\|_X > 0, \text{ then the trial method converges. } \|q\|_X < 1$ the convergence rate is linear.

Theorem 4.2. Consider the trial method based on the first order update equation (2.6). Then, for a given perturbation $q \in X$, it holds

$$\delta\Phi[q](\mathbf{r}^{\star}) = -\frac{\delta v^{\star}[q] \circ \boldsymbol{\gamma}^{\star}}{(h \circ \boldsymbol{\gamma}^{\star})\langle \mathbf{e}_{\mathbf{r}}, \mathbf{n} \rangle},\tag{4.3}$$

where $\gamma^{\star} = r^{\star} \mathbf{e}_r$ and $\delta v^{\star}[q]$ denotes the local shape derivative (4.3) of v^{\star} into the direction $\mathbf{V} \circ \gamma^{\star} = q \mathbf{e}_r$.

Proof. Define $\gamma_{\varepsilon}^{\star} = (r^{\star} + \varepsilon q)\mathbf{e}_r$ and let v^{\star} and v_{ε}^{\star} denote the solutions to the underlying boundary value problems (2.1) relative to the domains Ω^{\star} and $\Omega_{\varepsilon}^{\star}$, i.e.,

$$-\Delta v^{\star} = f \quad \text{in } \Omega^{\star}, \qquad -\Delta v_{\varepsilon}^{\star} = f \quad \text{in } \Omega_{\varepsilon}^{\star}$$
$$v^{\star} = g \quad \text{on } \Sigma, \qquad v_{\varepsilon}^{\star} = g \quad \text{on } \Sigma$$
$$\frac{\partial v^{\star}}{\partial \mathbf{n}} = h \quad \text{on } \Gamma^{\star}, \qquad \frac{\partial v_{\varepsilon}^{\star}}{\partial \mathbf{n}} = h \quad \text{on } \Gamma_{\varepsilon}^{\star}.$$

Then, in view of the first order update equation (2.6), it holds

$$\delta r(r^{\star}) = -\frac{v^{\star} \circ \gamma^{\star}}{\frac{\partial v^{\star}}{\partial \mathbf{e}_{r}} \circ \gamma^{\star}} = 0 \quad \text{and} \quad \delta r(r^{\star} + \varepsilon q) = -\frac{v^{\star}_{\varepsilon} \circ \gamma^{\star}_{\varepsilon}}{\frac{\partial v^{\star}_{\varepsilon}}{\partial \mathbf{e}_{r}} \circ \gamma^{\star}_{\varepsilon}}.$$

Hence, we obtain

$$\begin{split} \delta\Phi[q](r^{\star}) &= \lim_{\varepsilon \to 0} \frac{\Phi(r^{\star} + \varepsilon q) - \Phi(r^{\star})}{\varepsilon} \\ &= \lim_{\varepsilon \to 0} \frac{r^{\star} + \varepsilon q + \delta r(r^{\star} + \varepsilon q) - r^{\star} - \delta r(r^{\star})}{\varepsilon} \\ &= q - \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \frac{v_{\varepsilon}^{\star} \circ \gamma_{\varepsilon}^{\star}}{\frac{\partial v_{\varepsilon}^{\star}}{\partial e_{\varepsilon}} \circ \gamma_{\varepsilon}^{\star}}. \end{split}$$

On the optimum boundary Γ^{\star} , the following identities are valid:

$$v^{\star} \circ \boldsymbol{\gamma}^{\star} = 0$$
 and $\frac{\partial v^{\star}}{\partial \mathbf{n}} \circ \boldsymbol{\gamma}^{\star} = h \circ \boldsymbol{\gamma}^{\star}.$

So, we conclude

$$\frac{v_{\varepsilon}^{\star} \circ \boldsymbol{\gamma}_{\varepsilon}^{\star}}{\varepsilon} = \frac{v_{\varepsilon}^{\star} \circ \boldsymbol{\gamma}_{\varepsilon}^{\star} - v^{\star} \circ \boldsymbol{\gamma}^{\star}}{\varepsilon} + \frac{(v_{\varepsilon}^{\star} - v^{\star}) \circ \boldsymbol{\gamma}^{\star}}{\varepsilon} \xrightarrow{\varepsilon \to 0} q\left(\frac{\partial v^{\star}}{\partial \mathbf{e}_{r}} \circ \boldsymbol{\gamma}^{\star}\right) + \delta v^{\star}[q] \circ \boldsymbol{\gamma}^{\star}$$

and

$$\frac{\partial v_{\varepsilon}^{\star}}{\partial \mathbf{e}_{r}} \circ \boldsymbol{\gamma}_{\varepsilon}^{\star} \xrightarrow{\varepsilon \to 0} \frac{\partial v^{\star}}{\partial \mathbf{e}_{r}} \circ \boldsymbol{\gamma}^{\star} = (h \circ \boldsymbol{\gamma}^{\star}) \langle \mathbf{e}_{r}, \mathbf{n} \rangle.$$

$$(4.4)$$

Consequently, the derivative of the mapping Φ with respect to q can be simplified according to

$$\delta\Phi[q](r^{\star}) = q - \frac{q(h \circ \gamma^{\star})\langle \mathbf{e}_{r}, \mathbf{n} \rangle}{(h \circ \gamma^{\star})\langle \mathbf{e}_{r}, \mathbf{n} \rangle} - \frac{\delta v^{\star}[q] \circ \gamma^{\star}}{(h \circ \gamma^{\star})\langle \mathbf{e}_{r}, \mathbf{n} \rangle} = -\frac{\delta v^{\star}[q] \circ \gamma^{\star}}{(h \circ \gamma^{\star})\langle \mathbf{e}_{r}, \mathbf{n} \rangle}.$$

From this result, it is obvious that the question whether the trial method based on the first order update equation is (locally) converging or not, i.e., whether the norm $\|(\delta v^*[q] \circ \gamma^*)/((h \circ \gamma^*)\langle \mathbf{e}_r, \mathbf{n} \rangle)\|_X$ is smaller than 1 or not, can be answered by inspecting the local shape derivative. Since it holds in general

$$\left[\kappa h + \frac{\partial h}{\partial \mathbf{n}} + f\right] \neq 0$$
 almost everywhere on Γ^* ,

the Neumann data in (4.1) and thus the local shape derivative $\delta v^*[q]$ is nonzero for all directions $0 \neq q \in X^3$. Therefore, we generally expect only linear convergence of the trial method, as already observed in the numerical experiments of Subsection 3.4.

Remark 4.3. In case of a damping, the self-mapping Φ is modified according to

$$\Phi: X \to X, \quad r \mapsto \Phi(r) = r + \alpha \delta r(r).$$

Therefore, the derivative becomes

$$\delta \Phi[q](r^{\star}) = (1 - \alpha)q - \alpha \frac{\delta v^{\star}[q] \circ \gamma^{\star}}{(h \circ \gamma^{\star})\langle \mathbf{e}_{r}, \mathbf{n} \rangle}$$

From this expression, it is not obvious how to choose the damping parameter α to ensure that $\|\delta \Phi[q](r^{\star})\|_{X} < 1$.

The update $\delta r_2 = \delta r_2(r)$ computed from the second order update equation (2.12) coincides with the update $\delta r_1 = \delta r_1(r)$ computed from the first order update equation (2.6) except for a higher order term, i.e., $\delta r_2(r) = \delta r_1(r) + \varepsilon(r)$ with $\|\varepsilon(r)\|_X = O(\|\delta r_1(r)\|_X^2)$. Hence, all the results about the convergence remain essentially valid also in the case of the trial method based on the second order update equation (2.12).

4.3. Speeding up the convergence

As we have seen before, the computation of the shape derivative $\delta v^*[q]$ enables the evaluation of the convergence rate of the method. Hence, a question of great importance arises. What happens if $\|(\delta v^*[q] \circ \gamma^*)/((h \circ \gamma^*)\langle \mathbf{e}_r, \mathbf{n}\rangle)\|_X \ge$ 1? Can we then enforce convergence of the trial method or is it possible to obtain even superlinear convergence? A superlinearly convergent trial method for Bernoulli's free boundary problem has been proposed in [10], called the implicit Neumann method. Results on a quadratically convergent trial method can be found in [19, 20], where the solution of a Robin boundary value problem was suggested. Unfortunately, this Robin boundary value problem is only well-posed if the free boundary is convex. In contrast, our objective is to avoid the solution of a boundary value problem other than (2.1) since this would require the change of the boundary element method.

As a consequence of the observations in the previous subsection, we shall modify the self-mapping Φ according to

$$\Phi: X \to X, \quad r \mapsto \Phi(r) = r + \alpha(r)\delta r(r).$$
 (4.5)

³Since $\delta v^{\star}[q]$ satisfies the Laplace equation with homogenous boundary condition on Σ , the Dirichlet data $\delta v^{\star}[q] \circ \gamma^{\star}$ can only vanish if it holds $\delta v^{\star}[q] = 0$ in Ω^{\star} .

Notice that r^* is still a fixed point of Φ . We shall now determine the function $\alpha(r) : [0, 2\pi] \to \mathbb{R}$ such that superlinear convergence of the method is ensured. In other words, we seek a function $\alpha(r)$ such that

$$\lim_{k \to \infty} \frac{\|r_{k+1} - r^{\star}\|_{X}}{\|r_{k} - r^{\star}\|_{X}} = \lim_{k \to \infty} \frac{\|\Phi(r_{k}) - \Phi(r^{\star})\|_{X}}{\|r_{k} - r^{\star}\|_{X}} = \lim_{k \to \infty} \frac{\|\delta\Phi[r_{k} - r^{\star}](r^{\star})\|_{X}}{\|r_{k} - r^{\star}\|_{X}} = 0.$$
(4.6)

Following the same procedure as in the proof of Theorem 4.2, the derivative of the mapping Φ with respect to a given direction *q* is computed by

$$\delta\Phi[q](r^{\star}) = \lim_{\varepsilon \to 0} \frac{\Phi(r^{\star} + \varepsilon q) - \Phi(r^{\star})}{\varepsilon} = q - \lim_{\varepsilon \to 0} \frac{\alpha(r^{\star} + \varepsilon q)}{\varepsilon} \frac{v_{\varepsilon}^{\star} \circ \gamma_{\varepsilon}^{\star}}{\frac{\partial v_{\varepsilon}^{\star}}{\partial \mathbf{e}_{r}} \circ \gamma_{\varepsilon}^{\star}}$$

Recall that $v_{\varepsilon}^{\star} \circ \gamma_{\varepsilon}^{\star} \to v^{\star} \circ \gamma^{\star} = 0$ as $\varepsilon \to 0$. Thus, similar as in the proof of Theorem 4.2, we conclude

$$\frac{\alpha(r^{\star} + \varepsilon q)}{\varepsilon} (v_{\varepsilon}^{\star} \circ \gamma_{\varepsilon}^{\star}) = \frac{\alpha(r^{\star} + \varepsilon q) - \alpha(r^{\star})}{\varepsilon} (v_{\varepsilon}^{\star} \circ \gamma_{\varepsilon}^{\star}) + \alpha(r^{\star}) \frac{v_{\varepsilon}^{\star} \circ \gamma_{\varepsilon}^{\star}}{\varepsilon} \xrightarrow{\varepsilon \to 0} \alpha(r^{\star}) \Big[q \Big(\frac{\partial v^{\star}}{\partial \mathbf{e}_{r}} \circ \gamma^{\star} \Big) + \delta v^{\star}[q] \circ \gamma^{\star} \Big].$$

In view of (4.4), we finally arrive at

$$\delta \Phi[q](r^{\star}) = q - \alpha(r^{\star}) \bigg(\frac{\delta v^{\star}[q] \circ \gamma^{\star}}{\frac{\partial v^{\star}}{\partial e_{r}} \circ \gamma^{\star}} + q \bigg).$$

A superlinearly convergent scheme is derived if we define the function $\alpha(r)$ such that (4.6) is satisfied for the direction $q := \lim_{k\to\infty} (r_k - r^*)/||r_k - r^*||_X$ provided that this limit exists. Nevertheless, since r^* is unknown, q would not be accessible even in the case of existence. Hence, we choose just q = 1 which corresponds to the radial direction \mathbf{e}_r . This leads to

$$\alpha(r) = \frac{\frac{\partial v}{\partial \mathbf{e}_r} \circ \boldsymbol{\gamma}}{\delta v[\mathbf{e}_r] \circ \boldsymbol{\gamma} + \frac{\partial v}{\partial \mathbf{e}_r} \circ \boldsymbol{\gamma}}.$$
(4.7)

This expression depends on the actual state v and on its local shape derivative. The local shape derivative $\delta v[\mathbf{e}_r]$ can be evaluated in complete analogy to the solution of the mixed boundary value problem (4.1) by using the Neumann-to-Dirichlet map (3.7) as it was described in Section 3. Hence, one additional solve of the Neumann-to-Dirichlet map (3.7) is necessary per iteration step.

Remark 4.4. The condition

$$\left[\kappa h + \frac{\partial h}{\partial \mathbf{n}} + f\right] \le 0 \quad \text{on } \Gamma^{\star}$$
(4.8)

is very often required in connection with the convergence theory of free boundary problems, see e.g. [8, 9, 21, 22]. Since it holds also $\langle \mathbf{e}_r, \mathbf{n} \rangle > 0$ in case of a starlike domain, the prescribed Neumann data of the local shape derivative $\delta v[\mathbf{e}_r]$ are negative at Γ^* , cf. (4.1). Hence, under the condition (4.8), there holds $\delta v[\mathbf{e}_r] < 0$ in Ω^* and thus $\delta v[\mathbf{e}_r] < 0$ at Γ^* . As a consequence, the denominator of $(\alpha(r^*))(s)$ is negative for all $s \in [0, 2\pi]$. We finally conclude that $\alpha(r)$ is well defined at least in a neighbourhood of r^* if (4.8) holds.

4.4. Newton's method

A quadratically convergent trial method is derived in case of Newton's method. It is obtained by demanding that the update function $\delta r(r)$ becomes zero:

$$\Psi(r) = \delta r(r) \stackrel{!}{=} 0.$$

Linearizing the update function around the actual boundary r_k gives

$$\Psi(r_{k+1}) \approx \Psi(r_k) + \delta \Psi[r_{k+1} - r_k](r_k) \stackrel{!}{=} 0.$$

In complete analogy to the proof of Theorem 4.2, the derivative of the mapping Ψ with respect to a given direction q is given by

$$\delta \Psi[q](r) = \lim_{\varepsilon \to 0} \frac{\Psi(r + \varepsilon q) - \Psi(r)}{\varepsilon} = -\lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left[\frac{v_{\varepsilon} \circ \gamma_{\varepsilon}}{\frac{\partial v_{\varepsilon}}{\partial \mathbf{e}_{r}} \circ \gamma_{\varepsilon}} - \frac{v \circ \gamma}{\frac{\partial v}{\partial \mathbf{e}_{r}} \circ \gamma} \right] = -\left(q + \frac{\delta v[q] \circ \gamma}{\frac{\partial v}{\partial \mathbf{e}_{r}} \circ \gamma}\right).$$

Hence, the Newton update q is determined as the solution of the nonlinear equation

$$\delta \Psi[q](r_k) \stackrel{!}{=} -\Psi(r_k).$$

To solve this nonlinear equation, we perform the fixed-point iteration

$$q_{\ell+1} = \delta r(r_k) - \frac{\delta v[q_\ell] \circ \boldsymbol{\gamma}}{\frac{\partial v}{\partial \mathbf{e}_r} \circ \boldsymbol{\gamma}}, \quad \ell = 0, 1, 2, \dots$$

A good initial guess is given by $q_0 = \delta r(r_k)$ which would be the first iterate when starting with $q_{-1} = 0$. Nevertheless, several of these inner iterations will be performed, each of which requires one solve of the Neumann-to-Dirichlet map (3.7) to calculate the local shape derivative $\delta v[q_\ell]$. To our experience, we need about 10–20 iterations to compute the Newton update sufficiently accurate.

4.5. Numerical results

In the last part of this article, we show practically the improvement in the results by two numerical examples. We consider Poisson's equation (1.1) with

$$f(x, y) = 5$$
, $g(x, y) = 1$, $h(x, y) = -\lambda$.

The fixed boundary Σ is chosen to be peanut-shaped with parametrization

$$\gamma_{\Sigma} : [0, 2\pi] \to \Sigma, \quad s \mapsto \gamma_{\Sigma}(s) = \begin{bmatrix} 0.03 \sin(s)(1.25 + \cos(2s)) \\ 0.045 \cos(s) \end{bmatrix}.$$

The solutions of the free boundary problem are depicted in Figure 4.1.

The numerical setting is as follows. We use 40 degrees of freedom to represent the unknown boundary Γ_k (i.e., n = 20), 600 boundary elements per boundary, and stop the trial method if the update function satisfies $||\delta r|| < 10^{-8}$. The random boundary seen in Figure 4.1 is the initial approximation Γ_0 .

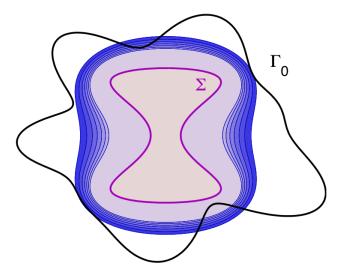


Figure 4.1: The solutions of Bernoulli's free boundary problem for different choices of the parameter λ .

It is seen in Table 4.1 that the trial method based on the first order update equation does never converge for the parameters λ under consideration (row entitled "1st order update"). Whereas, the trial method based on the order

parameter λ	40	45	50	55	60	65	70
1st order update	-	-	-	-	-	-	-
1st order update with damping ($\alpha = 0.7$)	19	20	21	22	23	23	22
improved 1st order update	15	17	19	22	23	28	22
Newton method & improved 1st order update	11	13	15	19	18	22	15
2nd order update	31	31	29	30	28	27	27
improved 2nd order update	14	16	20	16	15	18	19
Newton method & improved second order update	10	18	17	12	11	12	13

Table 4.1: Number of iteration required for convergence.

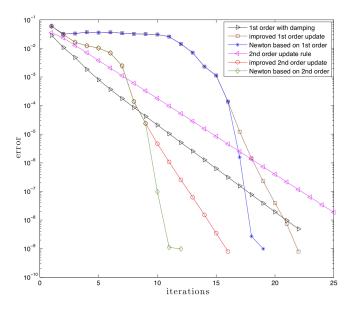


Figure 4.2: Convergence history in case of a peanut-shaped interior boundary and $h \equiv -55$.

second update equation converges always (row entitled "2nd order update"). Notice that a damping of the first order update by $\alpha = 0.7$ enforces convergence of the trial method based on the first order update equation (row entitled "1st order update with damping"). Nevertheless, as long as we add the update δr with the suggested parameter $\alpha(r)$ from (4.7), then we see that the trial method is converging for both cases (rows entitled "improved 1st order update" and "improved 2nd order update"). Indeed, according to Figure 4.2, we obtain a nicely improved (linear) convergence rate after some burn-in where the solution is too far away from the optimum boundary Γ^* . The Newton method does not converge for our initial guess. Hence, we apply one of the improved update rules first until the update function δr is small, that is $||\delta r|| < 10^{-3}$. Then, we start the Newton method. The number of iterations is shown in Table 4.1 in the rows entitled "Newton method & improved 1st order update" and "Newton method & improved 1st order update".

The trial methods we have constructed are also applicable for free boundary problems with several inner boundaries. This is demonstrated by an example where the boundary Σ is composed of the union of four circles as can be seen in Figure 4.3. We consider the original Bernoulli free boundary problem, that is

$$f(x, y) = 0$$
, $g(x, y) = 1$, $h(x, y) = -\lambda$

in (1.1). The extension of the boundary element method introduced in Subsection 3.2 to the new topological config-

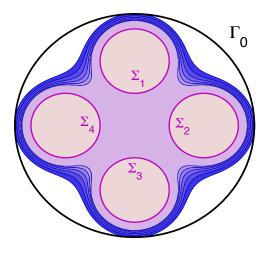


Figure 4.3: Solutions of the free boundary problem in case of several interior boundaries.

parameter λ	10	12	14	16	18	20
1st order update	18	22	27	32	39	48
improved 1st order update	14	18	21	28	35	38
Newton method	7	8	8	9	10	11
2nd order update	18	22	26	32	38	47
improved 2nd order update	12	16	22	28	26	44

Table 4.2: Number of iterations of the trial methods in case of several interior boundaries.

uration is straightforward and left to the reader. On each boundary, we apply 400 boundary elements which leads to 2000 boundary elements in all. The free boundary is discretized by 80 degrees of freedom, that is n = 40 in (2.13). For the initial approximation of the free boundary, we have chosen a circle. The trial method is again stopped if the update function satisfies $||\delta r|| < 10^{-8}$.

In Table 4.2, the number of iterations of the different trial methods are listed. Now, the standard trial method converges for all chosen parameters λ (row entitled "1st order update"). The improved 1st order update converges slightly faster (row entitled "improved 1st order update"). The same is observed for the related trial methods based on the second order equation (rows entitled "2nd order update" and "improved 2nd order update"). The fastest method is again the Newton method which converges immediately for the present initial guess (row entitled "Newton method").

5. Conclusions

We considered the numerical solution of generalized Bernoulli free boundary problems. On the actual domain, we approximated the solution to the boundary value problem which complies the desired Neumann boundary condition at the free boundary. This approximation is computed by a boundary element method which converges exponentially in case of smooth data. We then analyzed and applied trial methods which are based on update rules arising from first and second order Taylor series of the violated Dirichlet boundary condition at the free boundary. It turns out that an update computation based on a second order Taylor expansion of the Dirichlet data at the actual interface leads to a much more stable scheme. Moreover, by computing the local shape derivative to the boundary value problem under consideration, we were able to modify the trial method such that the convergence is improved considerably. In particular, the Newton method yields quadratical convergence rates.

References

- [1] A. ACKER, On the geometric form of Bernoulli configurations, Math. Methods Appl. Sci., 10 (1988), pp. 1–14.
- [2] A. ACKER, How to approximate the solutions of certain free boundary problems for the Laplace equation by using the contraction principle, Z. Angew. Math. Phys. 32 (1981), pp. 22–33.
- [3] H. W. ALT AND L. A. CAFFARELLI, Existence and regularity for a minimum problem with free boundary, J. Reine Angew. Math., 325 (1981), pp. 105–144.
- [4] A. BEURLING, On free-boundary problems for the Laplace equation, Sem. on analytic functions, Inst. Adv. Stud. Princeton, (1957), pp. 248–263.
- [5] F. BOUCHON, S. CLAIN, AND R. TOUZANI, Numerical solution of the free boundary Bernoulli problem using a level set formulation, Comput. Methods Appl. Mech. Engrg., 194 (2005), pp. 3934–3948.
- [6] _____, A perturbation method for the numerical solution of the Bernoulli problem, J. Comput. Math., 26 (2008), pp. 23–36.
- [7] M. C. DELFOUR AND J.-P. ZOLÉSIO, Shapes and geometries, vol. 22 of Advances in Design and Control, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2nd ed., 2011.
- [8] K. EPPLER AND H. HARBRECHT, Efficient treatment of stationary free boundary problems, Appl. Numer. Math., 56 (2006), pp. 1326–1339.
- [9] _____, Tracking Neumann data for stationary free boundary problems, SIAM J. Control Optim., 48 (2009/10), pp. 2901–2916.
- [10] M. FLUCHER AND M. RUMPF, Bernoulli's free-boundary problem, qualitative theory and numerical approximation, J. Reine Angew. Math., 486 (1997), pp. 165–204.
- [11] J. HASLINGER, T. KOZUBEK, K. KUNISCH, AND G. PEICHL, Shape optimization and fictitious domain approach for solving free boundary problems of Bernoulli type, Comput. Optim. Appl., 26 (2003), pp. 231–251.
- [12] K. ITO, K. KUNISCH AND G. PEICHL, Variational approach to shape derivatives for a class of Bernoulli problems, J. Math. Anal. Appl., 314 (2006), pp. 126–149.
- [13] R. KRESS, Linear integral equations, vol. 82 of Applied Mathematical Sciences, Springer-Verlag, New York, 2nd ed., 1999.
- [14] C. M. KUSTER, P. A. GREMAUD, AND R. TOUZANI, Fast numerical methods for Bernoulli free boundary problems, SIAM J. Sci. Comput., 29 (2007), pp. 622–634.
- [15] F. MURAT AND J. SIMON, Etude de probléme d'optimal design, in Proceedings of the 7th IFIP Conference on Optimization Techniques: Modeling and Optimization in the Service of Man, Part 2, London, UK, 1976, Springer-Verlag, pp. 54–62.
- [16] O. PIRONNEAU, Optimal shape design for elliptic systems, Springer series in computational physics, Springer, New York, 1984.
- [17] P. SERRANHO, A hybrid method for inverse obstacle scattering problems, PhD thesis, Georg-August-Universität Göttingen, 2007.
- [18] J. SOKOLOWSKI AND J.-P. ZOLÉSIO, Introduction to shape optimization, vol. 16 of Springer Series in Computational Mathematics, Springer-Verlag, Berlin, 1992. Shape sensitivity analysis.
- [19] T. TIHONEN, Shape optimization and trial methods for free boundary problems, RAIRO Modél. Math. Anal. Numér., 31 (1997), pp. 805–825.
- [20] T. TIHONEN AND J. JÄRVINEN, On fixed point (trial) methods for free boundary problems, in Free boundary problems in continuum mechanics (Novosibirsk, 1991), vol. 106 of Internat. Ser. Numer. Math., Birkhäuser, Basel, 1992, pp. 339–350.
- [21] K. G. VAN DER ZEE, E. H. VAN BRUMMELEN, AND R. DE BORST, Goal-oriented error estimation and adaptivity for free-boundary problems: The domain-map linearization approach, SIAM J. Sci. Comput., 32 (2010), pp. 1064–1092.
- [22] K. G. VAN DER ZEE, E. H. VAN BRUMMELEN, AND R. DE BORST, Goal-oriented error estimation and adaptivity for free-boundary problems: The shape linearization approach, SIAM J. Sci. Comput., 32 (2010), pp. 1093–1118.

LATEST PREPRINTS

No. Author: *Title*

2013-01	H. Harbrecht, M. Peters <i>Comparison of Fast Boundary Element Methods on Parametric Surfaces</i>
2013-02	V. Bosser, A. Surroca <i>Elliptic logarithms, diophantine approximation and the Birch and</i> <i>Swinnerton-Dyer conjecture</i>
2013-03	A. Surroca Ortiz Unpublished Talk: On some conjectures on the Mordell-Weil and the Tate- Shafarevich groups of an abelian variety
2013-04	V. Bosser, A. Surroca Upper bound for the height of S-integral points on elliptic curves
2013-05	Jérémy Blanc, Jean-Philippe Furter, Pierre-Marie Poloni Extension of Automorphisms of Rational Smooth Affine Curves
2013-06	Rupert L. Frank, Enno Lenzmann, Luis Silvestre Uniqueness of Radial Solutions for the Fractional Laplacian
2013-07	Michael Griebel, Helmut Harbrecht On the convergence of the combination technique
2013-08	Gianluca Crippa, Carlotta Donadello, Laura V. Spinolo Initial-Boundary Value Problems for Continuity Equations with BV Coefficients
2013-09	Gianluca Crippa, Carlotta Donadello, Laura V. Spinolo A Note on the Initial-Boundary Value Problem for Continuity Equations with Rough Coefficients
2013-10	Gianluca Crippa Ordinary Differential Equations and Singular Integrals
2013-11	G. Crippa, M. C. Lopes Filho, E. Miot, H. J. Nussenzveig Lopes Flows of Vector Fields with Point Singularities and the Vortex-Wave System
2013-12	L. Graff, J. Fender, H. Harbrecht, M. Zimmermann Key Parameters in High-Dimensional Systems with Uncertainty
2013-13	Jérémy Blanc, Immanuel Stampfli Automorphisms of the Plane Preserving a Curve

LATEST PREPRINTS

No. Author: *Title*

- 2013-14 **Jérémy Blanc, Jung Kyu Canci** Moduli Spaces of Quadratic Rational Maps with a Marked Periodic Point of Small Order
- 2013-15 Marcus J. Grote, Johannes Huber, Drosos Kourounis, Olaf Schenk Inexact Interior-Point Method for Pde-Constrained Nonlinear Optimization
- 2013-16 Helmut Harbrecht, Florian Loos Optimization of Current Carrying Multicables
- 2013-17 **Daniel Alm, Helmut Harbrecht, Ulf Krämer** *The H²-Wavelet Method*
- 2013-18 **Helmut Harbrecht, Michael Peters, Markus Siebenmorgen** Multilevel Accelerated Quadrature for PDEs With Log-Normal Distributed Random Coefficient*
- 2013-19 **Jérémy Blanc, Serge Cantat** Dynamical Degrees of Birational Transformations of Projective Surfaces
- 2013-20 **Jérémy Blanc, Frédéric Mangolte** *Cremona Groups of Real Surfaces*
- 2013-21 Jérémy Blanc, Igor Dolgachev Automorphisms of Cluster Algebras of Rank 2
- 2013-22 Helmut Harbrecht, Giannoula Mitrou Improved Trial Methods for a Class of Generalized Bernoulli Problems