Congreso de Métodos Numéricos en Ingeniería
25-28 junio 2013, Bilbao, España

SHAPE AND TOPOLOGY OPTIMIZATION OF SYSTEMS GOVERNED BY EXTERNAL BERNOULLI FREE BOUNDARY PROBLEMS

Jukka I. Toivanen[1], Jaroslav Haslinger[2] and Raino A. E. Mäkinen[1*]

[1]Department of Mathematical Information Technology,
University of Jyväskylä
PO Box 35 (Agora), 40014 Jyväskylä, Finland
e-mail: {jukka.i.toivanen,raino.a.e.makinen}@jyu.fi

[2]Faculty of Mathematics and Physics, Department of Numerical Mathematics
Charles University Prague
Sokolovska 83, 186 75, Prague 8, Czech Republic
e-mail: hasling@karlin.mff.cuni.cz

Keywords: Bernoulli problem, shape optimization, level set method

Abstract *We consider the shape and topology optimization of systems governed by external Bernoulli-type free boundary problems. Instead of the direct free boundary problem we consider a more complex inverse-like problem where the goal is to find a shape of the inner (non-free) boundary such that the respective free boundary is as close as possible to a given target shape. We use the so-called pseudo-solid domain mapping approach to the solution of governing free boundary problems. Both the classical boundary variation technique and the more versatile level set method are used to define the design domain. The scalar function defining the level sets is parameterized using radial basis functions. The level set problem is thus converted into a parametric optimization problem, which is then solved by a gradient-based method. Numerical examples are included.*

The first and third authors were supported by the grants #257589 and #260076 of the Academy of Finland.
The second author acknowledges the support of the grant P201/12/0671 of GAČR.

1. INTRODUCTION

We consider shape and topology optimization of systems governed by the external Bernoulli-type free boundary problem arising e.g. in the mathematical modelling of free liquid surfaces and electro-chemical machining. Instead of the direct free boundary problem we consider the more complex inverse-like problem where the goal is to design a shape of the inner (non-free) boundary such that the respective free boundary is as close as possible to a given target shape. In this work we combine the so-called pseudo-solid domain mapping approach and shape optimization techniques. The former is used as the solver for the free boundary problem and the latter to optimize the design. Other techniques have been used e.g. in [1] to solve similar type of inverse problems.

The paper is organized as follows. In Section 2 we formulate the state problem. We slightly generalize the free boundary condition compared to earlier papers [2], [3]. In Section 3 we formulate the design optimization problem and describe briefly how to solve it using a level set approach. Finally, in Section 4 numerical examples are given.

2. SETTING OF THE STATE PROBLEM

We start with the definition of the state problem represented by an external Bernoulli-type free boundary problem. Let $\omega \subset \mathbb{R}^2$ be a given open set with a sufficiently regular boundary $\partial\omega$. Let $\gamma : \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}$ be a smooth function satisfying $\gamma \leq \gamma_0 < 0$, for a given constant γ_0. The state problem consists in finding a set $\Omega \supset \overline{\omega}$ and a function $u : \Omega \setminus \overline{\omega} \to \mathbb{R}$ satisfying

$$\begin{cases} \Delta u = 0 & \text{in } \Omega \setminus \overline{\omega} \\ u(x) = 1 & x \in \partial\omega \\ u(x) = 0 \quad \text{and} \quad \dfrac{\partial u}{\partial \mathbf{n}}(x) = \gamma(x, \kappa(x)) & x \in \partial\Omega, \end{cases} \tag{1}$$

where $\kappa(x)$ is the mean curvature of $\partial\Omega$ at a point x. If $\gamma \equiv \gamma_0$, then (1) is the classical Bernoulli free boundary problem.

As the geometry of the free boundary $\partial\Omega$ is an unknown, it must be adjusted during the numerical solution of (1). There are many different ways to do that [4]. Here we use the so-called *pseudo-solid domain mapping approach* (PSA) presented originally in [5] and applied also in [2], [3]. In PSA, the unknown domain Ω is obtained by applying an appropriate load field to the reference configuration ("the pseudo solid") $\widehat{\Omega}$. The load field and the resulting deformation field are then among the unknowns in the re-formulated free boundary problem. The main advantage of the pseudo-solid technique is that no explicit parametrization of the unknown free boundary $\partial\Omega$ is needed. Moreover, in numerical realization we end up in solving a coupled finite element problem that can be done with standard tools.

Let $\widehat{\Omega} \subset \mathbb{R}^2$ be a fixed, simply connected reference domain. Our aim is to construct a mapping $F : \mathbb{R}^2 \to \mathbb{R}^2, \Omega = F(\widehat{\Omega})$ such that Ω solves (1) for a given ω. To construct such F we treat $\widehat{\Omega}$

as an elastic solid that undergoes a small deformation $\mathbf{v}$ caused by an external loading p such that the deformed solid $F(\widehat{\Omega})$ defines such Ω, where $F = \mathrm{id} + \mathbf{v}$.
We introduce the following function spaces:

$$W_\omega = \{\mathbf{w} \in [H^1(\widehat{\Omega})]^2 \mid \mathbf{w} = \mathbf{0} \text{ in } \omega\}$$
$$V_c(\Omega) = \{\varphi \in H^1(\Omega) \mid \varphi = c \text{ in } \omega\}, \quad c \in \mathbb{R}.$$

Above the symbol $H^k(\Omega)$ stands for the Sobolev space of functions which are together with their derivatives up to order k square integrable in Ω, i.e. elements of $L^2(\Omega)$. For any sufficiently small and regular deformation $\mathbf{w}$ we define the domain

$$\Omega_\mathbf{w} = \{\mathbf{x} \in \mathbb{R}^2 \mid \mathbf{x} = \widehat{\mathbf{x}} + \mathbf{w}(\widehat{\mathbf{x}}), \quad \widehat{\mathbf{x}} \in \widehat{\Omega}\}.$$

The pseudo-solid formulation of the free boundary problem (1) then reads as follows: Find $(u, p, \mathbf{v}) \in V_1(\Omega_\mathbf{v}) \times L^2(\partial\widehat{\Omega}) \times W_\omega$ such that

$$\int_{\Omega_\mathbf{v}} \nabla u \cdot \nabla\varphi \, d\mathbf{x} = \int_{\partial\Omega_\mathbf{v}} \gamma\varphi \, ds \quad \forall\varphi \in V_0(\Omega_\mathbf{v}) \tag{2}$$

$$\int_{\partial\Omega_\mathbf{v}} u\psi \, ds = 0 \quad \forall\psi \in L^2(\partial\Omega_\mathbf{v}) \tag{3}$$

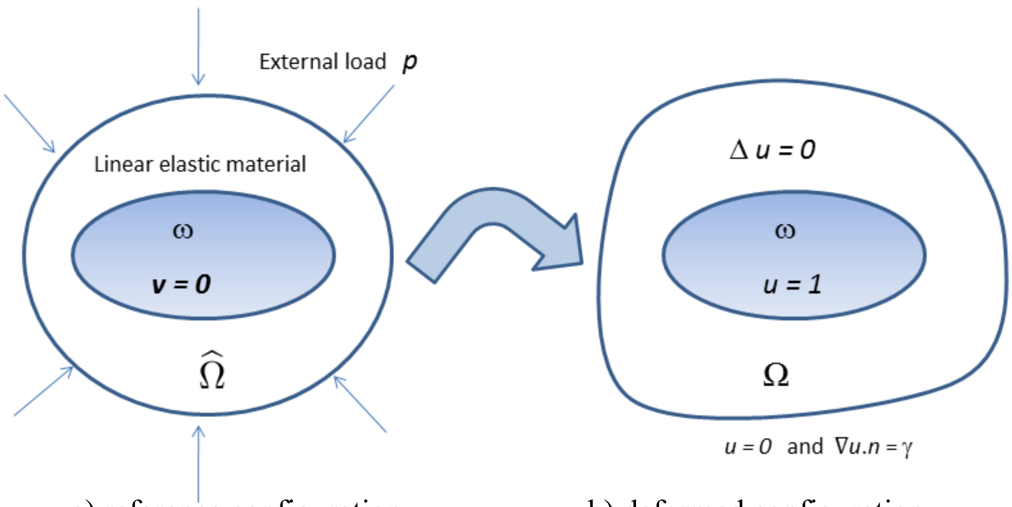
$$\int_{\widehat{\Omega}\setminus\omega} \sigma(\mathbf{v}) : \varepsilon(\mathbf{w}) \, d\mathbf{x} = \int_{\partial\widehat{\Omega}} p\,\mathbf{n} \cdot \mathbf{w} \, ds \quad \forall\mathbf{w} \in W_\omega. \tag{4}$$

Equations (2) and (3) constitute the weak form of the Laplace equation with the mixed boundary conditions in $\Omega_\mathbf{v} \setminus \bar{\omega}$, while equation (4) is the weak form of the linear elasticity problem in $\widehat{\Omega} \setminus \overline{\omega}$. Here $p\mathbf{n}$ is an (unknown) external load and $\varepsilon(\mathbf{v})$, $\sigma(\mathbf{v})$ are the strain and stress tensors, respectively associated with a displacement field $\mathbf{v}$, respectively. As the pseudo-solid has no real physical relevance, the modulus of elasticity and Poisson's ratio in Hooke's law can be chosen to be one and zero, respectively. For the simpler case $\gamma \equiv \gamma_0$, the solvability of (2)–(4) has been analyzed in details in [2]. The solvability of the more general case will be studied in a forthcoming paper. If $(u, p, \mathbf{v})$ is a solution of the coupled system (2)–(4), then the couple $(u_{|\Omega_\mathbf{v}\setminus\overline{\omega}}, \Omega_\mathbf{v})$ solves the original free boundary problem (1).

3. SETTING OF THE SHAPE DESIGN OPTIMIZATION PROBLEM

In the previous section it was assumed that ω is a given, fixed domain. In what follows we shall treat ω as the design that should be chosen to be optimal in some prescribed sense. We restrict to the case when the free boundary $\Gamma(\omega) := \partial\Omega(\omega)$ will be driven by the shape of ω towards a given target boundary Γ_t. Our optimization problem then reads as follows:

$$\begin{cases} \text{Find } \omega^\star \in \mathscr{O} \text{ such that} \\ J(\omega^\star) \le J(\omega) \quad \forall\omega \in \mathscr{O} \end{cases} \tag{5}$$



a) reference configuration b) deformed configuration

Figure 1. Idea of the pseudo-solid approach.

where $\mathcal{O}$ is a set of admissible designs. The cost functional to be considered is $J(\omega) = \mathcal{D}(\Gamma(\omega), \Gamma_t)$, where $\mathcal{D}$ is a function characterizing the distance of $\Gamma(\omega)$ from Γ_t.
Like in papers [2], [3] we assume that $\mathcal{O}$ is chosen in such a way that problem (2)–(4) has a unique solution for any $\omega \in \mathcal{O}$ and that $\Omega(\omega)$ is a *star-like domain* with respect to the origin (see [6]). As $\Gamma(\omega)$ and Γ_t can now be represented in polar coordinates using radius functions g_ω, g_t, the cost function can be defined simply as

$$J(\omega) = \int_0^{2\pi} \left(g_\omega(\theta) - g_t(\theta)\right)^2 \, d\theta.$$

In paper [2], also the design domain ω was assumed to be star-like and was parameterized using B-splines. It was observed that if $\mathcal{O}$ contains only star-like domains, then the target Γ_t may never be matched. Moreover, if the number of the design variables increased, the boundary $\partial\omega$ became more and more oscillating and fractal-like designs indicating possible topological changes of ω was observed in certain cases (see Figure 2).
Indeed, if ω is star-like and the boundary $\partial\omega$ is twice differentiable, then the respective free boundary is of the class C^∞ [6]. Hence if the target free boundary does not belong to C^∞ (as in the case of Figure 2) then it can never be realized for any such ω.
As it is difficult to predict the topology of the optimal $\omega^\star$ a priori, a spline parametrization of $\partial\omega$ is not adequate. Therefore techniques of topology optimization are preferred. The most popular topology optimization techniques have been based on material interpolation schemes [7] or level set methods based on the solution of the Hamilton–Jacobi equation [8]. In what follows we shall use a variant of the level set approach using parameterized level set functions [9].
Let D be a larger domain containing all admissible ω. Let $\psi : D \to \mathbb{R}$, $\psi \in U^{ad}$ be a given

Figure 2. Target Γ_t is a "rounded square" and $\gamma \equiv -1$. Increasing the number of design variables leads to fractal-like design indicating the nonexistence of the minimizer

function and define the set ω by $\omega := \omega(\psi) := \{\mathbf{x} \in D \mid \psi(\mathbf{x}) > 0\}$. Here U^{ad} is a family of admissible level set functions such that $\psi \in U^{ad}$ implies $\omega(\psi) \in \mathscr{O}$. Clearly this parametrization does not fix the topology of $\omega(\psi)$.

Next we re-formulate the state problem in such a way that the explicit tracking of $\partial\omega$ is not needed. Let $0 < \epsilon \ll 1$, $0 < \beta \ll 1$, and $\psi \in U^{ad}$ be given. We introduce the following relaxed state problem which does not contain explicitly any Dirichlet type boundary conditions:

Find $(u, p, \mathbf{v}) \in H^1(\Omega_{\mathbf{v}_\epsilon}) \times L^2(\partial\widehat{\Omega}) \times [H^1(\widehat{\Omega})]^2$ such that[1]

$$\int_{\Omega_{\mathbf{v}}} \nabla u \cdot \nabla\varphi \, d\mathbf{x} - \int_{\partial\Omega_{\mathbf{v}}} \gamma\, \varphi \, ds + \frac{1}{\epsilon}\int_{\Omega_{\mathbf{v}}} H_\beta(\psi)(u-1)\varphi \, d\mathbf{x} = 0 \quad \forall\varphi \in H^1(\Omega_{\mathbf{v}}) \tag{6}$$

$$\int_{\partial\Omega_{\mathbf{v}}} u\lambda \, ds = 0 \quad \forall\lambda \in L^2(\partial\Omega_{\mathbf{v}}) \tag{7}$$

$$\int_{\widehat{\Omega}} \sigma(\mathbf{v}) : \varepsilon(\mathbf{w}) \, d\mathbf{x} - \int_{\partial\widehat{\Omega}} p\, \mathbf{n} \cdot \mathbf{w} \, ds + \frac{1}{\epsilon}\int_{\widehat{\Omega}} H_\beta(\psi)\mathbf{v} \cdot \mathbf{w} \, d\mathbf{x} = 0 \quad \forall\mathbf{w} \in [H^1(\widehat{\Omega})]^2. \tag{8}$$

Here $H_\beta : \mathbb{R} \to [0,1]$ is the C^2 smoothed Heaviside function and $\beta > 0$ is the smoothing parameter. The purpose of the penalty terms in (6) and (8) is to release the constraints $u = 1$ and $\mathbf{v} = \mathbf{0}$ in ω. We can now define the "relaxed" design optimization problem as follows:

$$\begin{cases} \text{Find } \psi^\star_{\epsilon,\beta} \in U^{ad} \text{ such that} \\ \mathscr{J}(\psi^\star_{\epsilon,\beta}) \le \mathscr{J}(\psi) \quad \forall\psi \in U^{ad}, \end{cases} \tag{9}$$

where $\mathscr{J}(\psi) = \mathscr{D}(\Gamma(\omega(\psi)), \Gamma_t)$ and $\Gamma(\omega(\psi))$ is the free boundary corresponding to a level set function ψ.

[1]We supress, for simplicity, the dependency of $(u, p, \mathbf{v})$ on ϵ and β in notations.

4. DISCRETIZATION

To discretize the optimization problem, we parameterize the level set function using the compactly supported C^2-continuous radial basis functions (RBF) [9, 10]. We introduce a set of N^2 basis functions, whose knots $\{x^{(ij)}\}$ are placed on a regular $N \times N$ grid in the interior of the domain D. The RBF associated with a knot $x^{(ij)}$ is then

$$\psi_{ij}(x) = \left(\max\{0, (1 - r_{ij}(x))\}\right)^4 (4r_{ij}(x) + 1),$$

where $r_{ij}(x) = \|x - x^{(ij)}\|/r_s$ and the constant $r_s > 0$ is a given radius of the support of the RBF. The level set function ψ is then approximated by the linear combination $\psi_{\boldsymbol{\alpha}} = \sum_{i,j=1}^{N} \alpha_{ij}\psi_{ij}$. Thus, the design variables of the RBF parameterized optimization problem are the components of the vector $\boldsymbol{\alpha} = (\alpha_{11}, \alpha_{12}, \dots, \alpha_{NN})$.

Like in material interpolation approaches used in topology optimization of stressed structures, the smoothed and penalized state problem (6)–(8) produces “grey regions” where $0 < H_\beta(\psi) < 1$. Such regions should only appear near $\partial\omega$ where u is close to one. To prevent appearance of “nonphysical” grey regions which do not have such interpretation we add the following penalty term to the cost functional:

$$\mathscr{P}_\eta(\psi, u) = \eta \int_\Omega H_{2\beta}(\psi)(u-1)^2\, dx, \quad \eta > 0. \tag{10}$$

This choice, being purely heuristic, seems to work well in practice.

In the final numerical realization, the penalized state problem is discretized using linear triangular elements. The resulting nonlinear system is solved by Newton’s method with analytic Jacobian computed using automatic differentation. The smoothing parameter β is related to $\nabla\psi$ and the local local element size h, and is gradually decreased during the optimization as described in [3].

5. NUMERICAL EXAMPLES

In this section we illustrate the performance of the proposed method in case of a non-constant boundary flux γ. In all examples the target Γ_t is the square of size 4 whose each corner is rounded using a quarter of a circle of radius 1.

The values of the penalty parameters are $\epsilon = 10^{-3}$ and $\eta = 0.1$. We used the gradient based optimizer Donlp2 [11]. The gradient of the cost function was computed using automatic differentiation and adjoint techniques presented in [12], [3].

Example 1 Let the boundary flux be given as $\gamma(x) = -1 + \frac{1}{8}x_2$, i.e. it depends on the second spatial coordinate.

The reference domain $\widehat{\Omega}$ was discretized using 8300 linear triangular elements. The number of RBFs used was 30×30. The initial value of the cost functional and the penalty term was

$\mathscr{J} = 8.245 \times 10^{-1}$, $\mathscr{P}_\eta = 1.822 \times 10^{-3}$, respectively. After 1181 optimization steps (and 4528 cost function evaluations) these values reduced to $\mathscr{J} = 8.320 \times 10^{-5}$, $\mathscr{P}_\eta = 1.098 \times 10^{-4}$.
The obtained approximation of optimal inner domain $\omega^\star$ is represented in Figure 3(left) as the contour line $H_\beta = 0.99$. The contour plot of the corresponding state solution u_h is shown in Figure 3(right).

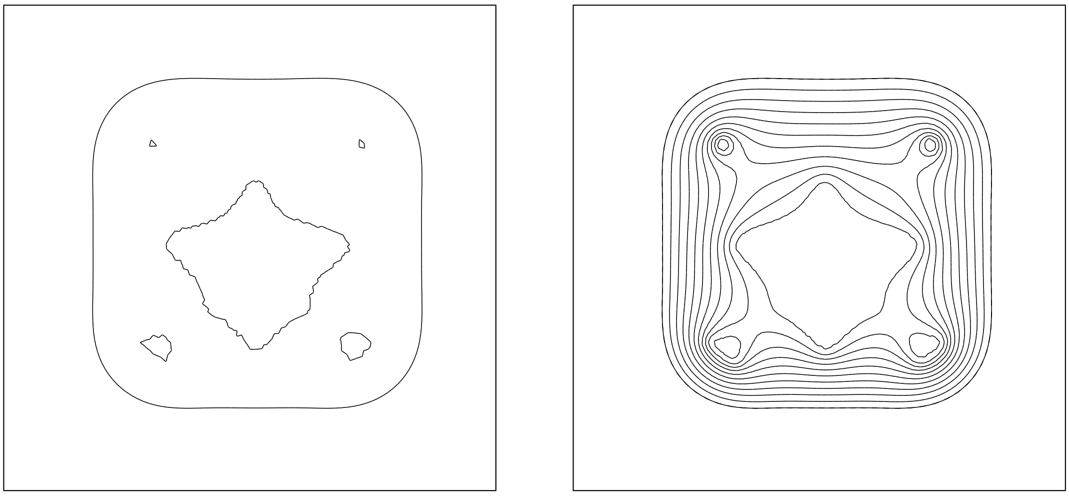


Figure 3. The equipotential contours $H_\beta = 0.99$ (left) and $u_h = 0, 0.1, 0.2, ..., 0.8, 0.9, 0.99$ (right) related to Example 1.

Example 2 In this example $\gamma(x, \kappa) = -1 - \frac{1}{2}\kappa$, i.e. γ depends on the mean curvature of the free boundary.
This time the optimizer needed 776 iterations and 3309 function evaluations. The final values of the cost and the penalty term are $\mathscr{J} = 1.788 \times 10^{-4}$ and $\mathscr{P}_\eta = 1.200 \times 10^{-4}$, respectively.
The obtained approximation of the optimal inner domain $\omega^\star$ is depicted in Figure 4(left) as a contour line $H_\beta = 0.99$. The contour plot of the corresponding state solution u_h is shown in Figure 4(right).

6. CONCLUSIONS

We have considered topological shape optimization problems with the state constraint given by a free boundary problem of Bernoulli type. To solve efficiently the free boundary problems during the optimization, the pseudo-solid domain mapping approach is applied. Its main advantage is that there is no explicit parametrization of the shape of the free boundary using e.g. splines. The novelty of the numerical method proposed in this paper is the combination of the pseudo-solid approach to tackle the free boundary problem with a non-constant boundary flux using a parameterized level set method for shape optimization. It has been found already in [2] that the

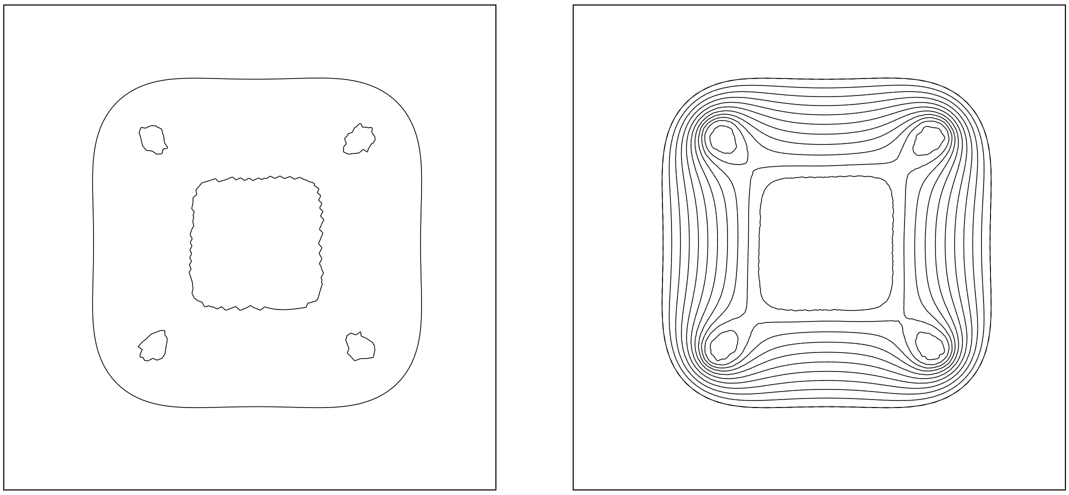


Figure 4. The equipotential contours $H_\beta = 0.99$ (left) and
$u_h = 0, 0.1, 0.2, ..., 0.8, 0.9, 0.99$ (right) related to Example 2.

problem is very badly conditioned as many different choices of ω may lead to nearly identical free boundaries. Therefore the progress of the optimization is often slow. The proposed method can be applied in an analogous way to topology optimization problems governed by other free boundary problems.

REFERENCES

[1] R.H. Nilson and Y.G. Tsuei, Inverted Cauchy problem for the Laplace equation in engineering design, *J. Eng. Math.*, **8** (1974), 329—337.

[2] J.I. Toivanen, J. Haslinger and R.A.E. Mäkinen, Shape optimization of systems governed by Bernoulli free boundary problems, *Comput. Meth. Appl. Mech. Eng.*, **197** (2008), 3803–3815.

[3] J.I. Toivanen, R.A.E. Mäkinen and J. Haslinger, Topology optimization in Bernoulli free boundary problems, *J. Eng. Math.*, (2012), http://dx.doi.org/10.1007/s10665-012-9575-8.

[4] K. Kärkkäinen and T. Tiihonen, Free surfaces: shape sensitivity analysis and numerical methods, *Int. J. Numer. Methods Eng.*, **44**:8 (1999), 1079–1098.

[5] P. Sackinger, P. Schunk and R. Rao, A Newton-Raphson pseudo-solid domain mapping technique for free and moving boundary problems: A finite element implementation, *J. Comput. Phys.*, **125**:1 (1996), 83–103.

[6] M. Flucher and M. Rumpf, Bernoulli's free boundary problem, qualitative theory and numerical approximation, *J. Reine Angew. Math.*, **486** (1997), 165–204.

[7] M.P. Bendsøe and O. Sigmund, Topology Optimization: Theory, Methods and Applications, Springer Verlag, Berlin Heidelberg, 2003.

[8] S. Osher and J.A. Sethian, Fronts propagating with curvature dependent speed: Algorithms based on Hamilton-Jacobi formulations, *J. Comput. Phys.*, **79** (1988), 12–49.

[9] Z. Luo, M.Y. Wang, S. Wang and P. Wei, A level set-based parameterization method for structural shape and topology optimization, *Int. J. Numer. Methods Eng.*, **76** (2008), 1–26.

[10] H. Wendland, Piecewise polynomial, positive definite and compactly supported radial functions of minimal degree, *Adv. Comput. Math.*, **4**:1 (2005), 389–396.

[11] P. Spellucci, An SQP method for general nonlinear programs using only equality constrained subproblems, *Math. Program.*, **82** (1998), 413–448, Software available at `http://www.mathematik.tu-darmstadt.de/fbereiche/numerik/staff/spellucci/DONLP2/`.

[12] J.I. Toivanen and R.A.E. Mäkinen, Implementation of sparse forward mode automatic differentiation with application to electromagnetic shape optimization, *Optim. Meth. Softw.*, **26** (2011), 601–616.