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Vorwort

Das Tätigkeitsfeld des Fraunhofer-Instituts für Techno- und Wirtschaftsmathematik ITWM umfasst anwendungsnahe Grundlagenforschung, angewandte Forschung sowie Beratung und kundenspezifische Lösungen auf allen Gebieten, die für Techno- und Wirtschaftsmathematik bedeutsam sind.

In der Reihe »Berichte des Fraunhofer ITWM« soll die Arbeit des Instituts kontinuierlich einer interessierten Öffentlichkeit in Industrie, Wirtschaft und Wissenschaft vorgestellt werden. Durch die enge Verzahnung mit dem Fachbereich Mathematik der Universität Kaiserslautern sowie durch zahlreiche Kooperationen mit internationalen Institutionen und Hochschulen in den Bereichen Ausbildung und Forschung ist ein großes Potenzial für Forschungsberichte vorhanden. In die Berichtreihe werden sowohl hervorragende Diplom- und Projektarbeiten und Dissertationen als auch Forschungsberichte der Institutsmitarbeiter und Institutsgäste zu aktuellen Fragen der Techno- und Wirtschaftsmathematik aufgenommen.

Darüber hinaus bietet die Reihe ein Forum für die Berichterstattung über die zahlreichen Kooperationsprojekte des Instituts mit Partnern aus Industrie und Wirtschaft.

Berichterstattung heißt hier Dokumentation des Transfers aktueller Ergebnisse aus mathematischer Forschungs- und Entwicklungsarbeit in industrielle Anwendungen und Softwareprodukte – und umgekehrt, denn Probleme der Praxis generieren neue interessante mathematische Fragestellungen.

Prof. Dr. Dieter Prätzel-Wolters
Institutsleiter

Kaiserslautern, im Juni 2001

ON ADJOINT-BASED OPTIMIZATION OF A FREE SURFACE STOKES FLOW

SABINE REPKE, NICOLE MARHEINEKE, AND RENÉ PINNAU

Abstract. This work deals with the optimal control of a free surface Stokes flow which responds to an applied outer pressure. Typical applications are fiber spinning or thin film manufacturing. We present and discuss two adjoint-based optimization approaches that differ in the treatment of the free boundary as either state or control variable. In both cases the free boundary is modeled as the graph of a function. The PDE-constrained optimization problems are numerically solved by the BFGS method, where the gradient of the reduced cost function is expressed in terms of adjoint variables. Numerical results for both strategies are finally compared with respect to accuracy and efficiency.

Keywords. Film casting process; thin films; free surface Stokes flow; optimal control; Lagrange formalism

AMS-Classification. 49-xx, 35Q93, 76D55, 49Q10

1. Introduction

Free boundary value problems and their optimal control play a crucial role in many applications, e.g. in solidification, technical textile, or thin film manufacturing processes [1, 7, 19]. In film casting processes [2, 4, 14, 15, 16] a molten polymer is pressed through a nozzle, stretched, and cooled down by surrounding air flows to form a thin long film which is finally winded up by a spindle. The uniform thickness of the manufactured film is an important criterion for the quality of the resulting products. Hence, quality assessment requires the optimal control of the free surfaces.

Motivated by this process, for which asymptotic 2d-membrane models were derived and numerical simulations performed in [2, 4, 16], our goal is the adjoint-based optimization of a free surface flow. For simplicity, we restrict our considerations to a stationary isothermal Stokes flow whose shape responds to an ambient aerodynamic pressure acting on the free surfaces, see figure 2.1. Free boundaries make the optimization complex and costly, in particular the formulation of the necessary optimality conditions and the efficient numerical handling. Thus previous control approaches longing for a uniform thickness profile of the film close to the spindle [15] treated the boundaries as fixed, yielding a suboptimal optimization approach. In this paper, in contrast, we deal with the optimization of the full free surface and present two adjoint-based optimization approaches. They differ in the treatment of the free boundaries as either state or control variables, where the boundary is described by the graph of a function. This graph approach was already successfully applied to optimize a free boundary in a two-phase Stefan problem with outer wall temperature [7] and/or near-wall Lorentz forces [8] as control. A less restrictive approach for the Stefan problem, where the free boundary has been modeled by a level set function, was studied in [1].

Certainly, the resulting two PDE-constrained optimization problems differ in complexity. Considering the graph of the free surface as state variable yields a free boundary value Stokes flow as forward problem whose adjoints are given by Stokes flow on a fixed domain with an additional ordinary differential equation for the adjoint graph. Alternatively, we reformulate the free boundary value problem as a minimization problem where the kinematic boundary condition is incorporated in the cost function. Then, the graph of the free surface acts as a control variable and the forward problem simplifies to Stokes flow on a given domain. This approach is an approximation of the optimal control of a free surface flow, but the numerical handling is much easier due to fixed flow

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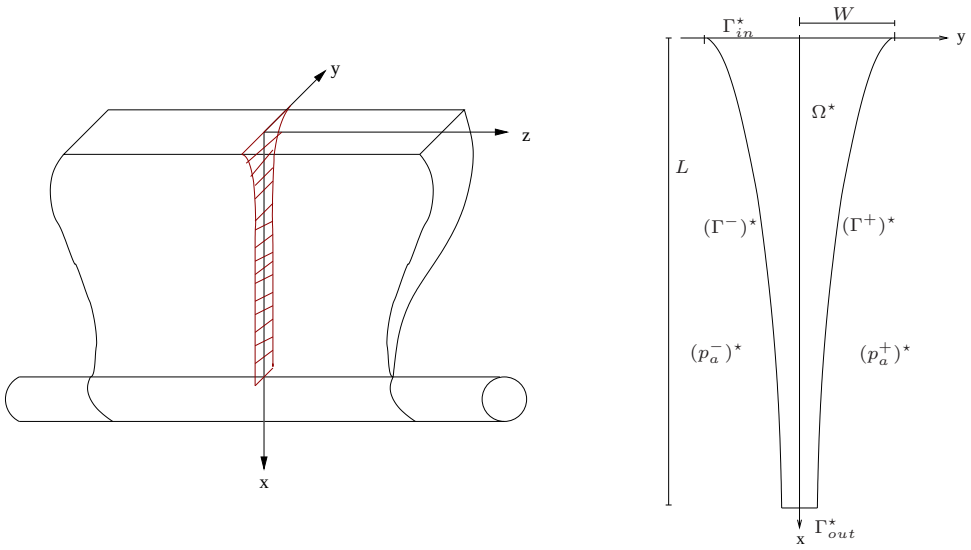


Fig. 2.1: Left: Schematic sketch of a spun film. The cross area yields the simplified flow domain for our considerations. Right: The simplified film domain with its geometrical quantities.

domains. The idea of shifting the additional boundary condition for the free boundary into the cost function was e.g. carried out for the optimization of a welding process in [19].

This paper is structured as follows. Starting with a mathematical model in section 2, we describe the thin film by a stationary incompressible two-dimensional Stokes flow whose free boundaries are represented by graphs. The shape design via an outer aerodynamic pressure is formulated in terms of two PDE-constrained optimization problems in section 3. Thereby, we distinguish between the free surface as state variable and as control variable. Using the Lagrangian formalism we derive the necessary optimality conditions. In section 4 we present the numerical treatment which is based on the BFGS method [9, 11]. Special attention is paid particularly to the numerical approaches for forward and backward problems in the optimization of the free boundary Stokes flow. Numerical results for both optimization problems are presented and discussed in section 5. Particularly, we compare the two optimization strategies with respect to accuracy and efficiency. Finally, a summary and outlook conclude the paper.

2. Model

In film casting processes molten polymer is pressed through a long narrow nozzle to form thin endless films. These are stretched and cooled down by surrounding air flows to be finally winded up by a spindle. In view of the complexity of the desired optimization we restrict ourselves to a simplified stationary scenario in this paper. Neglecting temperature dependencies a spun film of certain length is studied whose shape responds to an outer aerodynamic pressure acting on the free surfaces. We consider a slender highly viscous incompressible film that leaves vertically the spinning nozzle and falls straight down. Assuming the velocity profile at the inlet to be uniform with magnitude v_{in} and homogeneous in direction of the z-axis, allows the study of the film in terms of a stationary incompressible Stokes flow for velocity and pressure in a 2d domain $\Omega^\star \subset \mathbb{R}^2$ with boundary $\partial\Omega^\star = \Gamma^\star_{in} \cup \Gamma^\star_{out} \cup (\Gamma^+)^\star \cup (\Gamma^-)^\star$ as visualized in figure 2.1. Let W denote the nozzle's half width and L the length of the considered flow domain. The shape of the *a priori* unknown surfaces $(\Gamma^\pm)^\star$ is formed by the acting outer pressure $(p_a^\pm)^\star$ that is assumed to change over the film length.

Note that throughout this work we denote quantities for the right flow boundary with an index $^+$ and for the left boundary with $^-$ and summarize them with the abbreviation $^\pm$. To keep the

expressions short we also summarize equations being valid on both boundaries with their respective quantities in the $^{\pm}$-notation.

Making the free surface Stokes flow dimensionless with help of the film length L and magnitude of the inflow velocity v_{in} and introducing the typical pressure $\mu v_{in}/L$ with kinematic flow viscosity μ, we obtain the following system of model equations

$$\nabla \cdot \mathbf{v} = 0, \qquad \nabla \cdot \mathbf{T} = \mathbf{0} \qquad \text{in } \Omega(\psi^{\pm}), \tag{2.1a}$$

$$\mathbf{v} - \mathbf{v}_{in} = \mathbf{0} \qquad \text{on } \Gamma_{in}, \tag{2.1b}$$

$$\mathbf{T} \cdot \mathbf{n} = \mathbf{0} \qquad \text{on } \Gamma_{out}, \tag{2.1c}$$

$$(\mathbf{T} + p_a^{\pm}\mathbf{I}) \cdot \mathbf{n} = \mathbf{0} \qquad \text{on } \Gamma^{\pm}, \tag{2.1d}$$

$$\mathbf{v} \cdot \mathbf{n} = \mathbf{0} \qquad \text{on } \Gamma^{\pm}, \tag{2.1e}$$

with the dimensionless flow geometry-associated quantities Ω, Γ_{in}, Γ_{out}, $\Gamma^{\pm}$ and unit outer normal vector $\mathbf{n}$. Here, $\mathbf{v} = (v_1, v_2)^{\mathrm{T}}$ and p denote the unknown fluid velocity and pressure, $\mathbf{T} = -p\mathbf{I} + (\nabla\mathbf{v} + \nabla\mathbf{v}^{\mathrm{T}})$ is the symmetric Newtonian stress tensor and $\mathbf{I}$ the unit tensor. Since the flow geometry is an unknown of the problem, the incompressible Stokes equations for mass and momentum conservation are equipped not only with Dirichlet conditions with inflow $\mathbf{v}_{in}$ on Γ_{in}, stress-free conditions on the outlet Γ_{out}, dynamic conditions balancing the outer aerodynamic pressure $p_a^{\pm}$ acting on $\Gamma^{\pm}$, but also with an additional kinematic condition (2.1e) on $\Gamma^{\pm}$. We assume that the right and left flow boundaries $\Gamma^{\pm}$ can be represented by graphs $\psi^{\pm} : \mathrm{I} = (0,1) \to \mathbb{R}$, respectively. In view of film casting this assumption on the shape is certainly applicable, not much restrictive and a common approach see e.g. [2, 15, 16]. Then the flow domain is given by

$$\Omega(\psi^{\pm}) = \{(x,y) \in \mathbb{R}^2 : \, x \in \mathrm{I}, \; y \in [\psi^{-}(x), \psi^{+}(x)], \;\; \text{with } \psi^{\pm}(0) = \pm w\}, \quad w = W/L,$$

with the boundaries $\Gamma^{\pm}$ and their respective unit outer normal vectors $\mathbf{n}^{\pm}$

$$\Gamma^{\pm} = \left\{ \left(x, \psi^{\pm}(x)\right) : x \in \mathrm{I} \right\}, \qquad \mathbf{n}^{\pm} = \frac{1}{\sqrt{1 + (\psi_x^{\pm})^2}} (\mp\psi_x^{\pm}, \pm 1)^{\mathrm{T}}, \tag{2.2}$$

where $\psi_x^{\pm}$ denotes the derivative of the graphs. We define $\Psi^{\pm} : \mathrm{I} \to \mathbb{R}^2$, $\Psi^{\pm}(x) = (x, \psi^{\pm}(x))$.

3. Optimization

Our goal is the optimal control of the flow boundaries $\Gamma^{\pm}$ using an applied outer aerodynamic pressure $p_a^{\pm}$ as control variable. The introduction of the graph functions $\psi^{\pm}$ ensures direct access to the free boundaries (2.2) in terms of optimization variables, analogously to [7, 8]. Consequently, the desired boundaries $\Gamma_d^{\pm}$ are also described by graphs $\psi_d^{\pm}$. In this section we study two adjoint-based approaches for the free surface Stokes flow, that differ in the treatment of the graphs as either state or control variables. We state the two different minimization problems and, with help of the Lagrangian formalism, we derive the respective first-order necessary optimality conditions.

3.1. PDE-constrained minimization problems.

In an optimal control problem, the optimal state $\bar{y}$ and its associated optimal control $\bar{u}$ are determined as minimizers of a suitable cost function $J(y,u)$, measuring the error between the actual and the desired system responses. The general form of such a minimization problem reads

$$\min_{(y,u) \in \mathcal{Y} \times \mathcal{U}} J(y,u), \tag{3.1a}$$

$$\text{subject to } e(y,u) = 0, \tag{3.1b}$$

where y and u are state and control variables, respectively. The space of the state $\mathcal{Y}$ and of the admissible controls $\mathcal{U}$ are assumed to be equipped with a Hilbert space structure. Besides the equality constraint $e(y,u) = 0$ represents the equations of state.

Graphs as state variable. Treating the graphs as state variable [13], the state variable consists of fluid velocity $\mathbf{v}$, pressure p and graphs $\psi^\pm$, whereas the control is the ambient pressure $p_a^\pm$. To keep the expressions short we define $y_1 := (\mathbf{v}, p, \psi^\pm)$ and $u_1 := p_a^\pm$. Then our first minimization problem reads

$$\left.\begin{aligned} \min J_1\left(\psi^\pm, p_a^\pm\right) := \frac{\alpha^\pm}{2}\int_0^1 \left(\psi^\pm - \psi_d^\pm\right)^2 \,\mathrm{d}x + \frac{\beta^\pm}{2}\int_0^1 \left(\partial_x\left(\psi^\pm - \psi_d^\pm\right)\right)^2 \,\mathrm{d}x \\ + \frac{\gamma^\pm}{2}\int_0^1 \left(p_a^\pm\right)^2 \mathrm{d}x \\ \text{subject to } e_1(y_1, u_1) = 0, \text{ given by (2.1)}, \end{aligned}\right\} \qquad \text{(P1)}$$

where the parameters $\alpha^\pm, \beta^\pm, \gamma^\pm \geq 0$ weight the objective and control costs. For the control space we have $\mathcal{U}_1 = \mathcal{L}^2(\mathrm{I})$. The cost function J_1 measures the deviation of the free boundaries from the desired ones. A penalty term thereby forces sufficient regularity of the graphs $\psi^\pm$, in particular we assume $\psi^\pm \in \mathcal{H}^1(\mathrm{I})$. Note, that here and throughout the paper, in the definitions of the cost functions, the $\pm$-abbreviation for an summand actually stands for two summands, one with the upper signs and one with the lower signs.

Graphs as control variable. Characteristic for free surface problems is the additional kinematic boundary condition for the free surface. Analogously to Volkov et al. [18, 19], we incorporate it now in the cost function such that the graphs become extra control variables in addition to the ambient pressure. This involves a Stokes system on a fixed domain as equality constraint. With the state variable $y_2 := (\mathbf{v}, p)$ and the control $u_2 := (\psi^\pm, p_a^\pm,)$ our second PDE-constrained minimization problem reads

$$\left.\begin{aligned} \min J_2\left(\mathbf{v}, \psi^\pm, p_a^\pm\right) := \frac{\alpha^\pm}{2}\int_0^1 \left(\psi^\pm - \psi_d^\pm\right)^2 \,\mathrm{d}x + \frac{\beta^\pm}{2}\int_0^1 \left(\partial_x\left(\psi^\pm - \psi_d^\pm\right)\right)^2 \,\mathrm{d}x \\ + \frac{\gamma^\pm}{2}\int_0^1 \left(p_a^\pm\right)^2 \mathrm{d}x + \frac{\delta^\pm}{2}\int_0^1 \left((\mathbf{v}\circ\Psi^\pm)\cdot\begin{pmatrix}\mp\psi_x^\pm\\ \pm 1\end{pmatrix}\right)^2 \frac{1}{\sqrt{1+\left(\psi_x^\pm\right)^2}}\,\mathrm{d}x \\ \text{subject to } e_2(y_2, u_2) = 0, \text{ given by (2.1a)-(2.1d) on } \Omega(\psi^\pm) \text{ for fixed } \psi^\pm, \end{aligned}\right\} \qquad \text{(P2)}$$

with weights $\alpha^\pm, \beta^\pm, \gamma^\pm, \delta^\pm \geq 0$. Let $\mathcal{H}^1_{0,0}(\mathrm{I}) := \{\phi \in \mathcal{H}^1(\mathrm{I}) : \phi(0) = 0\}$, then the control space is $\mathcal{U}_2 = \{\pm w + \mathcal{H}^1_{0,0}(\mathrm{I})\} \times \mathcal{L}^2(\mathrm{I})$. The last term in J_2, representing (2.1e), results from the parameterization (2.2), i.e.

$$\int_{\Gamma^\pm} (\mathbf{v}\cdot\mathbf{n})^2 \,\mathrm{d}S = \int_0^1 \left((\mathbf{v}\circ\Psi^\pm)\cdot\begin{pmatrix}\mp\psi_x^\pm\\ \pm 1\end{pmatrix}\frac{1}{\sqrt{1+\left(\psi_x^\pm\right)^2}}\right)^2 \sqrt{1+(\psi_x^\pm)^2}\,\mathrm{d}x.$$

3.2. **Lagrange formalism.** Before applying the Lagrange techniques to our optimal control problems (P1) and (P2), we briefly recall the Lagrange formalism [6, 17] for the general PDE-constrained optimization problem (3.1). Assume that the equality constraint $e : \mathcal{Y}\times\mathcal{U} \to \mathcal{Z}$ with suitable space $\mathcal{Z}$ and the cost function $J : \mathcal{Y}\times\mathcal{U} \to \mathbb{R}$ are continuously Fréchet differentiable. The Lagrange function $L : \mathcal{Y}\times\mathcal{U}\times\mathcal{Z}^* \to \mathbb{R}$, associated to (3.1), is defined by

$$L(y, u, \hat{y}) = J(y, u) + \langle \hat{y}, e(y, u)\rangle_{\mathcal{Z}^*,\mathcal{Z}}$$

with Lagrange multiplier $\hat{y} \in \mathcal{Z}^*$ and appropriate duality pairing $\langle .,.\rangle_{\mathcal{Z}^*,\mathcal{Z}}$. According to the Lagrange multiplier theorem, the variations of the Lagrangian with respect to its arguments vanish at a critical point $(\bar{y}, \bar{u}, \bar{\hat{y}})$, which yields the first order optimality system, or Karush-Kuhn-Tucker (KKT) system,

$$\partial_y L(\bar{y}, \bar{u}, \bar{\hat{y}})[\tilde{y}] = 0, \qquad \partial_{\hat{y}} L(\bar{y}, \bar{u}, \bar{\hat{y}})[\tilde{\hat{y}}] = 0, \qquad \partial_u L(\bar{y}, \bar{u}, \bar{\hat{y}})[\tilde{u}] = 0,$$

for all feasible directions $\tilde{y}, \tilde{\hat{y}}, \tilde{u}$. In particular, the variation wrt. the state variables gives the adjoint equations, wrt. the Lagrange multiplier the equality constraint, and wrt. the control the optimality condition, i.e. the gradient of the reduced cost function $\tilde{J}(u) = J(y(u), u)$. This presupposes that

each control u admits a unique solution y. In the following we formally apply the Lagrange approach to (P1) and (P2). For a detailed derivation of the optimality conditions we refer to [12].

Lagrange approach for (P1). The adjoint equations for (P1) are

$$\nabla \cdot \hat{\mathbf{v}} = 0, \qquad \nabla \cdot \hat{\mathbf{T}} = \mathbf{0} \quad \text{in } \Omega(\psi^\pm), \tag{3.2a}$$
$$\hat{\mathbf{v}} = \mathbf{0} \quad \text{on } \Gamma_{in}, \tag{3.2b}$$
$$\hat{\mathbf{T}} \cdot \mathbf{n} = \mathbf{0} \quad \text{on } \Gamma_{out}, \tag{3.2c}$$
$$\hat{\mathbf{T}} \cdot \mathbf{n} = \hat{\psi}^\pm \mathbf{n} \quad \text{on } \Gamma^\pm, \tag{3.2d}$$
$$\frac{1}{v_1 \circ \Psi^\pm}\Big(\alpha^\pm\left(\psi^\pm - \psi_d^\pm\right) - \beta^\pm \partial_{xx}\left(\psi^\pm - \psi_d^\pm\right) \mp \partial_x p_a^\pm \left(\hat{v}_1 \circ \Psi^\pm\right) \mp \Big(\partial_1 \hat{\mathbf{v}} \circ \Psi^\pm \cdot \left(\mathbf{T} \circ \Psi^\pm + p_a^\pm \mathbf{I}\right)\Big)_1\Big) = \hat{\psi}_x^\pm \quad x \in \mathrm{I}, \tag{3.2e}$$
$$\frac{1}{v_1 \circ \Psi^\pm}\Big(\Big(\hat{\mathbf{v}} \circ \Psi^\pm \cdot \left(\mathbf{T} \circ \Psi^\pm + p_a^\pm \mathbf{I}\right)\Big)_1 \pm \beta^\pm \partial_x\left(\psi^\pm - \psi_d^\pm\right)\Big) = \hat{\psi}^\pm \quad x = 1, \tag{3.2f}$$

It is a Stokes system (3.2a)-(3.2d) for the adjoint fluid velocity $\hat{\mathbf{v}} = (\hat{v}_1, \hat{v}_2)^{\mathrm{T}}$ and pressure $\hat{p}$ with adjoint stress tensor $\hat{\mathbf{T}} = -\hat{p}\mathbf{I} + \left(\nabla\hat{\mathbf{v}} + \nabla\hat{\mathbf{v}}^{\mathrm{T}}\right)$ on the *a priori* known domain that is given by the solutions $\psi^\pm$ of (2.1). The system is coupled to a reverse value problem of an ordinary differential equation (ODE) of first order (3.2e)-(3.2f) for the adjoint graph functions $\hat{\psi}^\pm$ which enter in the dynamic boundary conditions on $\Gamma^\pm$ (3.2d). Note that $\mathbf{v}, p, \psi^\pm$ are the solutions of (2.1). Due to the set-up of the problem the velocity component in x-direction satisfies $v_1 \neq 0$, cf. figure 2.1. Be aware that the subscript $_1$ at a vector denotes its first component and ∂_i abbreviates the partial derivative with respect to the ith component, $i = 1, 2$.

The gradient of the reduced cost function is

$$\nabla \tilde{J}_1\left(p_a^\pm\right) = \gamma^\pm p_a^\pm - \mathbf{n}^\pm \cdot \left(\hat{\mathbf{v}} \circ \Psi^\pm\right)\sqrt{1 + (\psi_x^\pm)^2}, \quad x \in \mathrm{I}.$$

Lagrange approach for (P2). The adjoint equations for (P2) are

$$\nabla \cdot \hat{\mathbf{v}} = 0, \qquad \nabla \cdot \hat{\mathbf{T}} = \mathbf{0} \quad \text{in } \Omega(\psi^\pm),$$
$$\hat{\mathbf{v}} = \mathbf{0} \quad \text{on } \Gamma_{in},$$
$$\hat{\mathbf{T}} \cdot \mathbf{n} = \mathbf{0} \quad \text{on } \Gamma_{out},$$
$$\hat{\mathbf{T}} \cdot \mathbf{n} = \delta^\pm \mathbf{n}\left(\mathbf{v} \cdot \mathbf{n}\right) \quad \text{on } \Gamma^\pm.$$

Again, we have a Stokes system for the adjoint velocity $\hat{\mathbf{v}}$ and pressure $\hat{p}$ on the same domain as its forward problem, i.e. $\psi^\pm$ is given.

Since $\partial_{\psi^\pm} \tilde{J}_2 \in \mathcal{H}^{-1}(\mathrm{I})$

$$\left\langle \partial_{\psi^\pm} \tilde{J}_2, \tilde{\psi}^\pm \right\rangle_{\mathcal{H}^{-1}(\mathrm{I}), \mathcal{H}^1(\mathrm{I})} = \int_0^1 \left(\tilde{\psi}_x^\pm a^\pm + \tilde{\psi}^\pm b^\pm\right) \mathrm{d}x \pm \tilde{\psi}^\pm p_a^\pm \left(\hat{v}_1 \circ \Psi^\pm\right)\big|_{x=1},$$

with

$$a^\pm = \beta^\pm \partial_x\left(\psi^\pm - \psi_d^\pm\right) - \frac{\delta^\pm}{2}\left(\left(\mathbf{v} \circ \Psi^\pm\right) \cdot \mathbf{n}\right)^2 \frac{\psi_x^\pm}{\sqrt{1 + (\psi_x^\pm)^2}} \mp \delta^\pm \left(v_1 \circ \Psi^\pm\right)\left(\left(\mathbf{v} \circ \Psi^\pm\right) \cdot \mathbf{n}\right),$$
$$b^\pm = \alpha^\pm\left(\psi^\pm - \psi_d^\pm\right) \pm \delta^\pm \left(\left(\mathbf{v} \circ \Psi^\pm\right) \cdot \mathbf{n}\right)\left(-\psi_x^\pm \partial_2 v_1 \circ \Psi^\pm + \partial_2 v_2 \circ \Psi^\pm\right)$$
$$\mp \partial_x p_a^\pm \left(\hat{v}_1 \circ \Psi^\pm\right) \mp \left(\partial_1 \hat{\mathbf{v}} \circ \Psi^\pm \cdot \left(\mathbf{T} \circ \Psi^\pm + p_a^\pm \mathbf{I}\right)\right)_1,$$

Algorithm 1 BGFS Method to Solve a Minimization Problem

Input: initial control $u^{(0)}$
Output: optimized control $\bar{u}$ and corresponding optimal state $\bar{y}$
Solve forward and backward problem (use $u^{(0)}$ to compute $y^{(0)}, \hat{y}^{(0)}$)
Evaluate $\nabla\tilde{J}(u^{(0)})$
$k \leftarrow 0$
Set restart parameter r
$B \leftarrow \mathbf{I}$
while $\left\|\nabla\tilde{J}(u^{(k)})\right\| / \|\nabla\tilde{J}(u^{(0)})\| > tol$ **do**
  Compute search direction: $d^{(k)} \leftarrow -B^{-1}\nabla\tilde{J}(u^{(k)})$
  if $d^{(k)}$ is not a search direction or $k \bmod r = 0$ **then**
    $B \leftarrow \mathbf{I}$
    $d^{(k)} \leftarrow -\nabla\tilde{J}(u^{(k)})$
  end if
  Compute step length $\sigma^{(k)}$ fulfilling Armijo rule (4.1)
  Update the control: $u^{(k+1)} \leftarrow u^{(k)} + \sigma^{(k)} d^{(k)}$
  Solve forward and backward problem (use $u^{(k+1)}$ to compute $y^{(k+1)}, \hat{y}^{(k+1)}$)
  Evaluate $\nabla\tilde{J}(u^{(k+1)})$
  Update Hessian B: set $s \leftarrow \sigma^{(k)} d^{(k)}$, $z \leftarrow \nabla\tilde{J}(u^{(k+1)}) - \nabla\tilde{J}(u^{(k)})$
    $B \leftarrow B + \frac{zz^{\mathrm{T}}}{z^{\mathrm{T}}s} - \frac{(Bs)(Bs)^{\mathrm{T}}}{s^{\mathrm{T}}Bs}$
  $k \leftarrow k + 1$
end while
$\bar{u} \leftarrow u^{(k)}$, $\bar{y} \leftarrow y^{(k)}$

we determine the Riesz representative of the gradient $g^{\pm} \in \mathcal{H}^1(\mathrm{I})$ as the weak solution of

$$\begin{aligned} -\eta^{\pm}\partial_{xx} g^{\pm} + g^{\pm} &= -\partial_x a^{\pm} + b^{\pm} && \text{for } x \in \mathrm{I}, \\ g^{\pm} &= 0 && \text{for } x = 0, \\ \partial_x g^{\pm} &= \frac{a^{\pm} \pm p_a^{\pm}\,(\hat{v}_1 \circ \Psi^{\pm})}{\eta^{\pm}} && \text{for } x = 1. \end{aligned}$$

for an appropriately chosen smoothing parameter $\eta^{\pm} > 0$. Then the gradient of the reduced cost function is

$$\nabla\tilde{J}_2\left(\psi^{\pm}, p_a^{\pm}\right) = \begin{pmatrix} g^{\pm} \\ \gamma^{\pm} p_a^{\pm} - \mathbf{n}^{\pm} \cdot (\hat{\mathbf{v}} \circ \Psi^{\pm}) \sqrt{1 + (\psi_x^{\pm})^2} \end{pmatrix}, \quad x \in \mathrm{I}.$$

Note $\left\|\nabla\tilde{J}_2\right\|_{\mathcal{U}_2}^2 := \left\|g^{\pm}\right\|_{\mathcal{L}^2(\mathrm{I})}^2 + \eta^{\pm}\left\|g_x^{\pm}\right\|_{\mathcal{L}^2(\mathrm{I})}^2 + \left\|\partial_{p_a^{\pm}}\tilde{J}_2\right\|_{\mathcal{L}^2(\mathrm{I})}^2$.

4. Numerical approach

Both optimization problems, (P1) and (P2), are numerically solved using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method [9, 11] that is briefly presented in the following. The gradients of the reduced cost functions are expressed in terms of the respective adjoint variables. For generality we suppress the indices specifying the single problems. Moreover, we pay special attention to the free surface problem of (P1) whose numerical treatment we discuss in detail.

4.1. **BFGS method.** To find a minimizer $\bar{u}$ of the reduced cost function $\tilde{J}$ we apply the BFGS method. It is a Quasi-Newton method where the Hessian is approximated with help of gradient information, see algorithm 1 and [9, 11]. In each iteration k of the optimization procedure a search direction $d^{(k)} = -B^{-1}\nabla\tilde{J}(u^{(k)})$ is determined by help of an approximated Hessian B. Then the control is computed as

$$u^{(k+1)} = u^{(k)} + \sigma^{(k)} d^{(k)},$$

Algorithm 2 Algorithm for the Forward System (2.1)

Input: $p_a^{\pm}$
Output: $\mathbf{v}, p, \psi^{\pm}$
$i \leftarrow 0$
Initial boundary $\psi^{\pm(0)} \leftarrow \pm w$
FEM-Solve for system (2.1a)-(2.1d): use $\psi^{\pm(0)}$ to compute $\mathbf{v}^{(0)}, p^{(0)}$
while $\left\|\mathbf{v}^{(i)} \cdot \mathbf{n}^{(i)}\right\|_{\mathcal{L}^2(\Gamma^{\pm})} > tol_1$ **do**
  $i \leftarrow i + 1$
  ODE-Solve: compute $\psi^{\pm(i)}$ via (4.3)
  FEM-Solve for system (2.1a)-(2.1d): use $\psi^{\pm(i)}$ to compute $\mathbf{v}^{(i)}, p^{(i)}$
  while $\left\|\mathbf{v}^{(i)} \cdot \mathbf{n}^{(i)}\right\|_{\mathcal{L}^2(\Gamma^{\pm})} > \left\|\mathbf{v}^{(i-1)} \cdot \mathbf{n}^{(i-1)}\right\|_{\mathcal{L}^2(\Gamma^{\pm})}$ **do**
    $\psi^{\pm(i)} \leftarrow (\psi^{\pm(i)} + \psi^{\pm(i-1)})/2$
    FEM-Solve for system (2.1a)-(2.1d): use $\psi^{\pm(i)}$ to compute $\mathbf{v}^{(i)}, p^{(i)}$
  end while
end while
$\mathbf{v} \leftarrow \mathbf{v}^{(i)}$, $p \leftarrow p^{(i)}$, $\psi^{\pm} \leftarrow \psi^{\pm(i)}$

with appropriately chosen step length $\sigma^{(k)} > 0$. The step length needs to ensure a substantial reduction of the objective function $\tilde{J}$. Applying Armijo's rule we choose $\sigma^{(k)} = \kappa^m$, where $\kappa \in (0,1)$ and $m \geq 0$ is the smallest nonnegative integer such that $\sigma^{(k)}$ guarantees sufficient decrease of $\tilde{J}$, i.e.

$$\tilde{J}(u^{(k)} + \sigma^{(k)} d^{(k)}) \leq \tilde{J}(u^{(k)}) + \epsilon \sigma^{(k)} \langle \nabla \tilde{J}(u^{(k)}), d^{(k)} \rangle, \tag{4.1}$$

with some constant $\epsilon \in (0,1)$. The approximation of the Hessian B is updated by

$$B = B + \frac{zz^{\mathrm{T}}}{z^{\mathrm{T}}s} - \frac{(Bs)(Bs)^{\mathrm{T}}}{s^{\mathrm{T}}Bs},$$

with $s := \sigma^{(k)} d^{(k)}$ and $z := \nabla \tilde{J}(u^{(k+1)}) - \nabla \tilde{J}(u^{(k)})$. Due to reasons of convergence a restart functionality is incorporated in algorithm 1.

4.2. **Algorithms for the free boundary problem (P1).** The main challenge of the numerical handling of problem (P1) is the *a priori* unknown flow domain $\Omega(\psi^{\pm})$ of the forward problem. The adjoint system of problem (P1) consists of a Stokes system coupled to a first order ODE for the adjoint graphs. We suggest to use, for both problems, a numerical approach based on fixed point iterations, since we couple existing software routines.

Forward problem. To find, for a given ambient pressure $p_a^{\pm}$, the graph functions $\psi^{\pm}$ as well as velocity and pressure fields $\mathbf{v}$, p we perform the computation of (2.1) via a fixed point iteration consisting of two parts. As a result of the graph approach, we are able to reformulate the kinematic boundary condition (2.1e) in terms of a first oder ODE

$$\psi_x^{\pm}(x) = \frac{v_2}{v_1}(x, \psi^{\pm}(x)) \quad \text{for } x \in \mathrm{I}, \quad \psi^{\pm}(0) = \pm w. \tag{4.2}$$

The initial condition follows from the geometrical set-up. On the domain given by $\psi^{\pm}$ we determine the flow quantities $\mathbf{v}, p$ from the remaining system. We go on with the iteration i until the $\mathcal{L}^2$-error of the kinematic boundary condition is smaller than a tolerance. Note that for the numerical evaluation of (4.2), we use the quantities of the last fixed point iteration step, i.e. $\mathbf{v}^{(i-1)}$ on $\psi^{\pm(i-1)}$, to approximate the new graph $\psi^{\pm(i)}$. Explicit integration yields

$$\psi^{\pm(i)}(x) = \pm w + \int_0^x \frac{v_2^{(i-1)}}{v_1^{(i-1)}}(\tilde{x}, \psi^{\pm(i-1)}(\tilde{x}))\, \mathrm{d}\tilde{x}. \tag{4.3}$$

Due to this simplification we might apply a relaxation, determining the new graph as linear combination of the old one and the one of (4.3), see algorithm 2. The iteration is initialized with $\psi^{\pm(0)} \equiv \pm w$.

Algorithm 3 Algorithm for the Adjoint System (3.2)

Input: $p_a^\pm$ and solutions of the forward problem for $p_a^\pm$: $\mathbf{v}, p, \psi^\pm$
Output: $\hat{\mathbf{v}}$, $\hat{p}$, $\hat{\psi}^\pm$
$i \leftarrow 0$
Initial adjoint graph function $\hat{\psi}^{\pm(0)}(x) \leftarrow 0$
FEM-Solve for equations (3.2a)-(3.2d): use $\hat{\psi}^{\pm(0)}$ to compute $\hat{\mathbf{v}}^{(0)}, \hat{p}^{(0)}$
Evaluate $\ell^{\pm(0)}$ (4.4)
while $\|\ell^{\pm(i)} - \hat{\psi}_x^{\pm(i)}\|_{\mathcal{L}^2(\mathrm{I})} > tol_2$ **do**
  $i \leftarrow i+1$
  ODE-Solve: compute $\hat{\psi}^{\pm(i)}$ via (4.5)
  FEM-Solve for equations (3.2a)-(3.2d): use $\hat{\psi}^{\pm(i)}$ to compute $\hat{\mathbf{v}}^{(i)}, \hat{p}^{(i)}$
  Evaluate $\ell^{\pm(i)}$
end while
$\hat{\mathbf{v}} \leftarrow \hat{\mathbf{v}}^{(i)}$, $\hat{p} \leftarrow \hat{p}^{(i)}$, $\hat{\psi}^\pm \leftarrow \hat{\psi}^{\pm(i)}$

Adjoint problem. For the adjoint system the domain is known. However, we also deal with a coupled system consisting of Stokes equations and a first order ODE for the graphs $\hat{\psi}^\pm$. Analogously to algorithm 2, we apply a fixed point method and solve (3.2e)-(3.2f) and (3.2a)-(3.2d) iterative-wise. In this case the explicit integration of the ODE is no simplification, since the left hand side $\ell^\pm$ of the ODE does not depend on $\hat{\psi}^\pm$,

$$\ell^{\pm(i)} := \frac{\alpha^\pm\left(\psi^\pm - \psi_d^\pm\right) - \beta^\pm\partial_{xx}\left(\psi^\pm - \psi_d^\pm\right) \mp (\partial_x p_a^\pm)\hat{v}_1^{(i)} \circ \Psi^\pm \mp \left(\partial_1\hat{\mathbf{v}}^{(i)} \cdot (\mathbf{T} + p_a^\pm\mathbf{I}) \circ \Psi^\pm\right)_1}{v_1 \circ \Psi^\pm}. \tag{4.4}$$

Thus, the adjoint graph function in the ith iteration is

$$\hat{\psi}^{\pm(i)}(x) = \left.\frac{\left(\hat{\mathbf{v}}^{(i-1)} \cdot (\mathbf{T} + p_a^\pm\mathbf{I}) \circ \Psi^\pm\right)_1 \pm \beta^\pm\partial_x(\psi^\pm - \psi_d^\pm)}{v_1 \circ \Psi^\pm}\right|_{x=1} - \int_x^1 \ell^{\pm(i-1)}(x)\,\mathrm{d}x. \tag{4.5}$$

As termination criterion of the iteration we use the validity of the ODE, i.e. the $\mathcal{L}^2$-error between graph derivative and left hand side has to satisfy $\|\ell^{\pm(i)} - \hat{\psi}_x^{\pm(i)}\|_{\mathcal{L}^2(\mathrm{I})} \leq tol_2$. A detailed description is given in algorithm 3.

Remark 1. *Within the optimization procedure we accelerate the forward solve (algorithm 2) by using the solution $\psi^\pm$ of the previous forward solve as an initial guess for the boundary graph. Analogously we accelerate the backward solve (algorithm 3) by choosing the solution $\hat{\psi}^\pm$ of the previous backward solve as an initial guess.*

Remark 2. *For both optimization problems, the BFGS approach including the stated algorithms for solving the forward and adjoint systems and the computation of the gradients have been implemented in the software* `Freefem++`*, a free software for numerically solving PDEs by the Finite Element Method (FEM). Automatic mesh generation, mesh adaption, mesh movement, several triangular finite elements, as well as a large variety of solvers are already included* [5]*. The flow domain $\Omega(\psi^\pm)$ is discretized into a Delaunay mesh of triangles by* `Freefem++`*. For the basis function for the pressure/adjoint pressure and velocity/adjoint velocity we choose* **P1** *and* **P1-bubble** *finite elements, cf.* [3, 5] *for technical details.*

5. Numerical results and discussion

In this section we discuss the numerical results for both optimization problems (P1) and (P2), focusing on the accuracy and efficiency of the strategies and studying the impact of the weighting

*Software by Laboratoire Jaques-Louis Lions, Université Pierre et Marie Curie, Paris, France. Authors: F. Hecht, O. Pironneau, A. Le Hyaric, and K. Ohtsuka. `www.freefem.org/ff++`

maximal discretization width $h_{\max}$	$\|\bar{p}_a\|_{\mathcal{L}^2(\mathrm{I})}$	$\|\bar{\psi}\|_{\mathcal{L}^2(\mathrm{I})}$	# of Armijo steps ($\varnothing$)	# of BFGS iterations
(P1):				
0.05	2.629	0.4312	1.3	7
0.025	2.568	0.4314	1.2	6
0.0125	2.566	0.4314	1.3	5
0.00625	2.568	0.4315	1.0	5
(P2):				
0.05	5.68	0.434	1.2	11
0.025	5.62	0.435	1.2	10
0.0125	5.58	0.435	1.2	10
0.00625	5.56	0.435	1.2	10

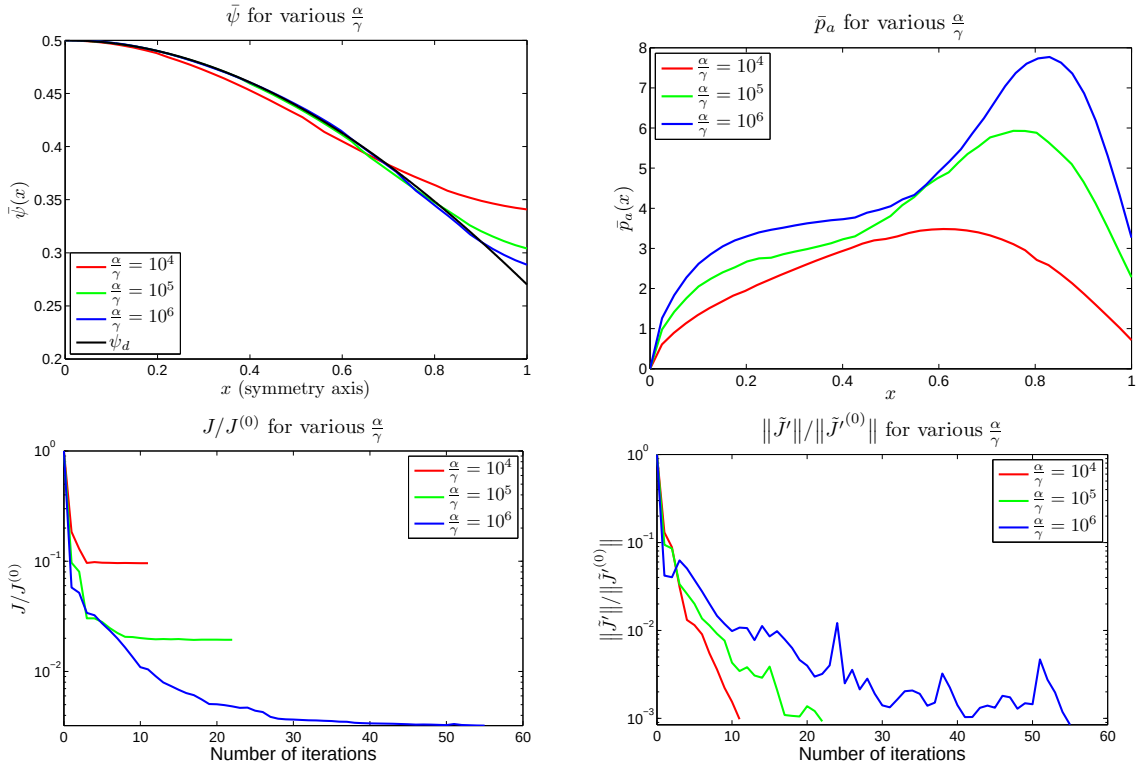
Table 5.1: Grid study: (P1) top and (P2) bottom. Dependence of optimal solutions, mean number of Armijo steps and number of BFGS iterations on the grid spacing.

parameters in the cost functions. We investigate different desired graphs $\psi_d^{\pm}$ and varying parameters $\alpha^{\pm}, \beta^{\pm}, \gamma^{\pm}, \delta^{\pm}$ and furthermore perform a study of the discretization.

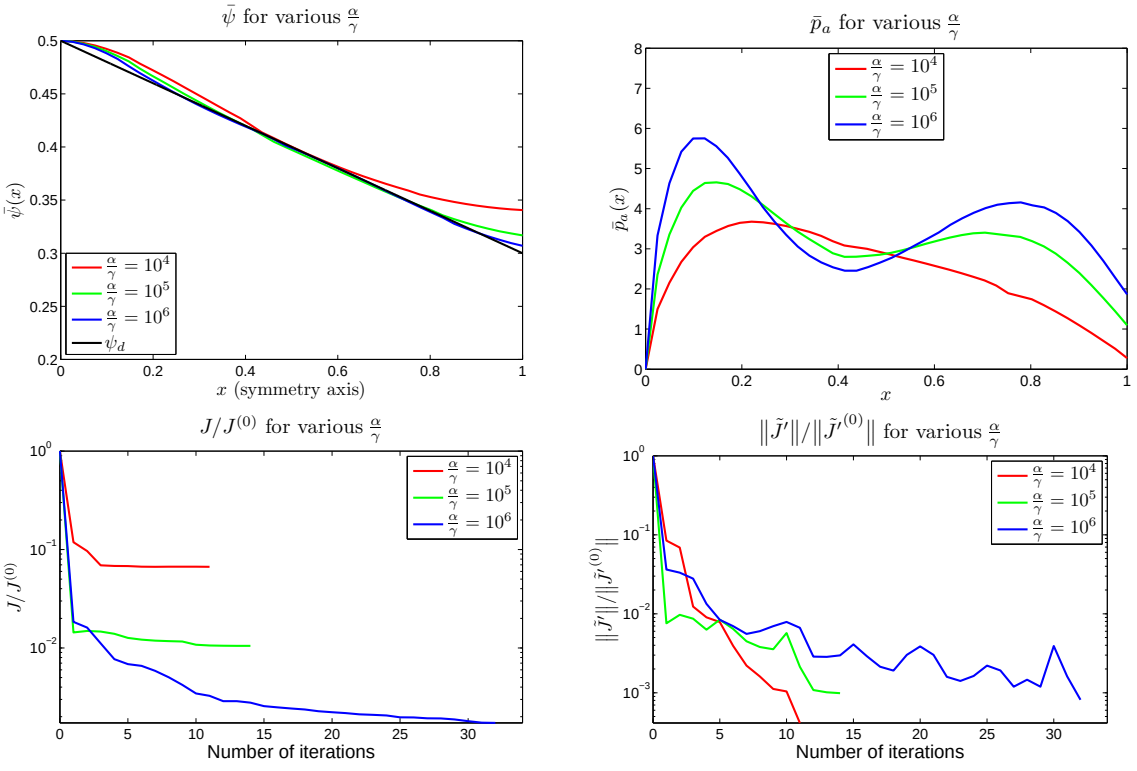
Hence, all numerical simulations presented in this paper are performed for fixed processing conditions $w = 0.5$ and $\mathbf{v}_{in} = (1,0)^{\mathrm{T}}$. The desired boundaries are considered to be symmetrically shaped, i.e. $\psi_d^+ = -\psi_d^- =: \psi_d$ which results in axis-symmetric optimization problems, cf. figure 2.1. Thus, we deal with the representative half problems and omit the $\pm$-notation. In accordance to the maximal discretization length $h_{\max}$ for the flow domain, we set the tolerances to be $tol_1 = h_{\max}$ and $tol_2 = h_{\max}^3$ in algorithms 2 and 3 for (P1). The computation of the $\mathcal{H}^1$-gradient g for (P2) involves a smoothing parameter η. It turns out to be reasonable to choose η in the same order of magnitude as α. In the BFGS method (algorithm 1) we use $r = 5$ as restart parameter and $\epsilon = 10^{-4}$ for the step length computation (4.1), cf. [9, 11].

Both optimization strategies turn out to be independent of the chosen discretization, as desired. For this purpose we investigate the optimal solutions $(\bar{\psi}, \bar{p}_a)$, the number of BFGS iterations and the mean number of interior Armijo steps with respect to various grid spacing for different settings. Table 5.1 exemplarily summarizes the results for $h_{\max} = 0.1/2^i$, $i = 1, ..., 4$, considering the desired boundary $\psi_d(x) = 0.5 \cos x$. The termination tolerance in the BFGS algorithm is $tol = 10^{-2}$ and the weighting parameters in the cost functions are $(\alpha, \beta) = (1000, 0)$ as well as $\gamma = 0.1$ and $(\gamma, \delta) = (0.01, 200)$ in (P1) and (P2), respectively. In the following we use $h_{\max} = 0.025$.

Obviously, the different choice of γ yields different pressure values in (P1) and (P2), cf. table 5.1. To provide the comparability of the two strategies with regard to accuracy and computational effort we consider the same weights (α, β, γ). The penalty parameter δ of (P2) is chosen in such a way that the kinematic boundary condition is satisfied within the same tolerances as in algorithm 2, i.e. $\|\bar{\mathbf{v}} \cdot \mathbf{n}\| \leq tol_1$. Due to the differing gradients this requires different termination tolerances in the BFGS algorithm, in particular we have here $tol = 10^{-3}$ for (P1) and $tol = 10^{-2}$ for (P2). Figures 5.2 and 5.3 show the optimization results for two desired boundaries, a cosine-shaped $\psi_d(x) = 0.5 \cos x$ and a linear-shaped graph $\psi_d(x) = 0.5 - 0.2x$. In particular, the optimal graph $\bar{\psi}$, the associated outer pressure $\bar{p}_a$, the evolution of the relative cost functions and of the gradients are visualized for varying regularizations $\gamma \in \{10^{-1}, 10^{-2}, 10^{-3}\}$ and $(\alpha, \beta) = (10^3, 10^{-1})$ fixed. Here, $\delta \in (100, 200)$ ensures a comparable approximation quality of the kinematic boundary condition in both approaches. We see qualitatively similar results for (P1) and (P2). But for (P2) the deviation of the optimized graph from the desired one is larger and the ambient pressure smaller than for (P1). However, we observe that the computed solution of (P1) also satisfies (P2) within the chosen tolerances. Inserting instead the solution of (P2) as initial guess, the BFGS method for (P1) converges to its optimal results that are visualized.

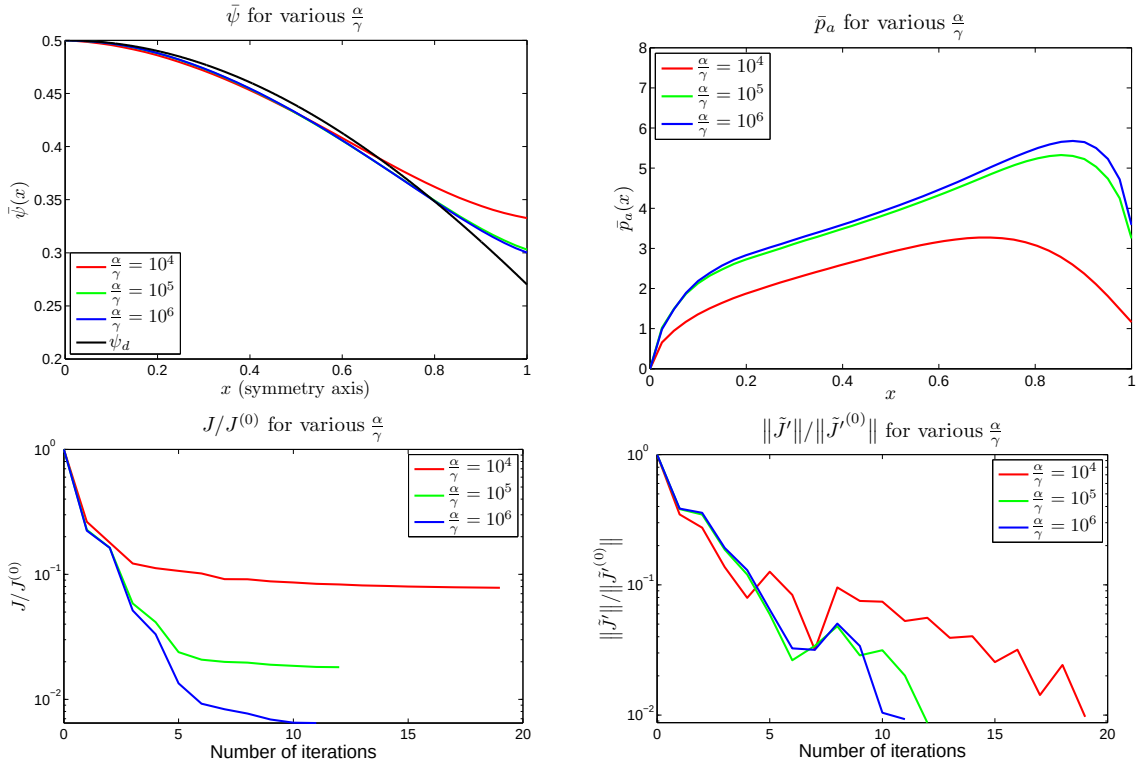


(a) Cosine-shaped desired boundary $\psi_d = 0.5\cos x$

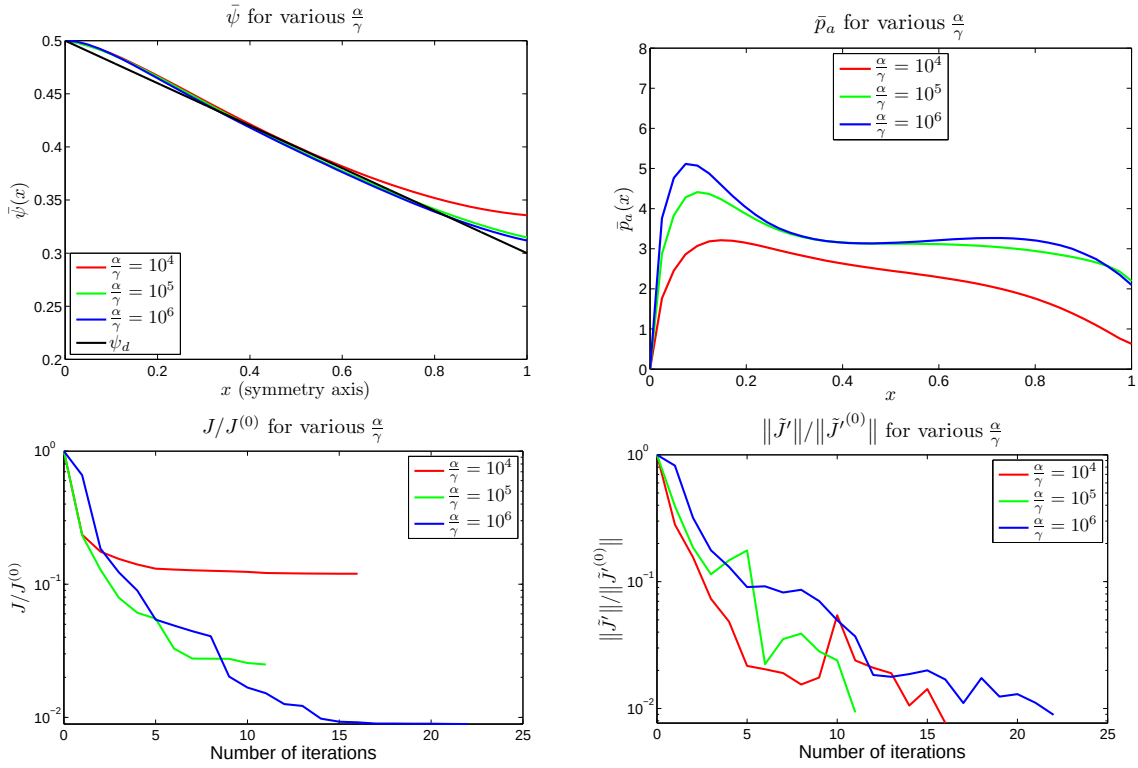


(b) Linear-shaped desired boundary $\psi_d = 0.5 - 0.2x$

Fig. 5.2: Optimization results for (P1) with (a) cosine-shaped ψ_d, (b) linear-shaped ψ_d: $\bar\psi$ (top left), $\bar p_a$ (top right), evolution of the relative cost function (bottom left) and of the relative gradients (bottom right) for varying regularizations $\alpha/\gamma \in \{10^4, 10^5, 10^6\}$ plotted in (red, green, blue).



(a) Cosine-shaped desired boundary $\psi_d = 0.5 \cos x$



(b) Linear-shaped desired boundary $\psi_d = 0.5 - 0.2x$

Fig. 5.3: Optimization results for (P2) with (a) cosine-shaped ψ_d, (b) linear-shaped ψ_d: $\bar{\psi}$ (top left), $\bar{p}_a$ (top right), evolution of the relative cost function (bottom left) and of the relative gradients (bottom right) for varying regularizations $\alpha/\gamma \in \{10^4, 10^5, 10^6\}$ plotted in (red, green, blue).

Setting α/γ	# of BFGS iterations	# of Armijo steps (∅)	# FWD Stokes solves (∅)	# BWD Stokes solves (∅)	CPU-time
(P1):					
10^4	12	3.5	9.3	4.1	272.3
10^5	14	3.1	8.3	6.3	329.8
10^6	32	1.1	4.5	5.0	483.2
(P2):					
10^4	16	2.0	2.0	1.0	64.6
10^5	11	3.6	3.6	1.0	78.9
10^6	22	2.0	2.0	1.0	115.4

Table 5.2: Comparison wrt. efficiency: (P1) top and (P2) bottom. Total number of BFGS iterations, mean number of Armijo steps, forward and backward Stokes solves needed per BFGS iteration, and CPU-time for different regularizations.

Hence, (P2) is more robust to variations of the control p_a. This is not surprising since the kinematic boundary condition is incorporated and satisfied in terms of a penalty term in the cost function J_2. The peaks in the evolution of the relative gradients arise from the restarts within the BFGS algorithm.

The computational costs for both optimization approaches arise mainly from moving and adapting the mesh. In `Freefem++` the moving and (re-)meshing routine takes approximately thrice as long as a FEM-solve of the Stokes equations, the effort for evaluating ODEs is in comparison irrelevant. Remeshing is generally required in every Armijo step of a BFGS iteration, which involves the solving of the forward problem to evaluate the new cost function and update the control. Whereas the forward solve for the free boundary value problem in (P1) implies several remeshing procedures due to the fixed point iteration used in algorithm 2, it is just one for (P2). In table 5.2 the number of BFGS iterations, the mean number of Armijo steps, forward and backward Stokes solves needed per BFGS iteration are listed for the exemplary setting of the figures 5.2b and 5.3b. The CPU-time is clearly correlated to the product of BFGS iterations and forward Stokes solves, as expected. Moreover, the number of BFGS iterations rise for decreasing regularization in the cost function (smaller γ). The strategy of treating the graph as control variable yields a speed-up of factor 4 in CPU-time which makes it obviously much more efficient.

6. Conclusion

In this paper we have presented and discussed two strategies for the adjoint-based optimization of a free surface Stokes flow via an outer pressure. They differ in the treatment of the free boundary represented by graphs as either state or control variable (i.e. state- and control-approach). The numerical investigations show that the control-approach is much more efficient since it avoids the time-consuming and costly remeshing within the fixed point iteration that is needed to solve the free boundary value problem as forward problem in the state-approach. This yields an evident speed-up of the optimization. However, it also turns out that the control-approach is less sensitive to variations of the outer pressure which is not surprising since the free boundary is just incorporated in the cost function as penalty term.

In view of the application further research should address time-dependent problems. In particular, more sophisticated flow equations like the Navier-Stokes equations with surface tension, temperature dependency and body forces play an important role for film casting processes. Furthermore the optimization of a free surface which cannot be described by a graph stays an interesting topic of research [1, 10].

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