Optimal Control of Parameter-Dependent Convection-Diffusion Problems around Rigid Bodies

Timo Tonn, Karsten Urban und Stefan Volkwein

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Fakultät für Mathematik und Wirtschaftswissenschaften
UNIVERSITÄT ULM

OPTIMAL CONTROL OF PARAMETER-DEPENDENT CONVECTION-DIFFUSION PROBLEMS AROUND RIGID BODIES

TIMO TONN, KARSTEN URBAN, AND STEFAN VOLKWEIN

Abstract. This paper is concerned with optimal control problems of partial differential equations. In particular, parameterized convection-diffusion problems are considered, where the parameter appears in the coefficients of the partial differential equation. Moreover, the presence of one or more rigid bodies is assumed inside the domain. Both the theory (existence, differentiability, optimality criteria) is investigated and the numerical solution (projected gradient scheme) of such problems is carried out. Finally, it is shown that optimizing the efficiency of a rotating propeller fits into the presented framework and results of corresponding numerical experiments are given.

1. Introduction

This research has been motivated by an industrial optimization problem, namely the optimization of the hydromechanics of the Voith Schneider Propeller (VSP)[1], a ship propulsion and steering system. As we show in Section 6 this optimization problem involving moving domains can be reduced to an optimization problem with a partial differential equation (pde) having parameter-dependent non-constant coefficients. Moreover, the blades of the propeller are rigid bodies that are present in the flow domain. In the full VSP problem [5], the pde models a turbulent incompressible flow, i.e., typically the time-dependent Navier-Stokes equations are used. Here, we restrict ourselves to stationary, linear convection-diffusion problems as a first step.

The particular interest in this application also leads to a specific form of the cost functional. One important target is of course to optimize the efficiency of the propeller. The efficiency is the ratio of the generated thrust and the required energy, which in turns reduces to the ratio of normal and tangential components of the force on the boundary of the blades. Hence, the cost functional is not of the classical type but involves surface integrals. To the best of our knowledge, not much seems to be known in the literature for such optimal control problems.

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[1]Voith Turbo Marine, Heidenheim, Germany, http://www.voithturbo.de/marine

Casas [3] considered the optimal control in coefficients of elliptic equations (even with inequality constraints) for the cost functional

$$J(\alpha) = \frac{1}{2}\int_\Omega (u_\alpha - u_\circ)^2\,\mathrm{d}\mathbf{x} + \frac{\kappa}{2}\int_\Omega \alpha^2\,\mathrm{d}\mathbf{x},$$

where $\alpha : \Omega \to \mathbb{R}$ is a suitable control coefficient and u_α is the solution of an elliptic Dirichlet problem with coefficient α. Finally, $u_\circ$ is a nominal state. In [8, 12] parabolic problems are addressed, even in general Hilbert spaces, but both results and techniques are quite particular for parabolic problems. In [1, 7], a variational inequality with controls in the coefficients is considered.

Even though the motivation for this research stems from an industrial application, we find several aspects also interesting from a pure academic point of view. The particular form of the cost functional has already been mentioned. The second issue is the lack of regularity due to the presence of the obstacles (i.e., the rigid bodies). In fact, this framework usually prohibits optimal regularity. Hence, we have to take into account that the state may not be in H^2. These two facts require a new mathematical investigation both for the existence of an optimal solution and corresponding first-order necessary optimality conditions. We also study the influence of these effects to the performance of the numerical scheme by corresponding numerical experiments.

This paper is organized as follows. In Section 2, we formulate the optimal control problem under consideration and collect all required facts and notation. Section 3 is devoted to the theoretical investigation, in particular we show existence of optimal solutions. In Section 4, we present first-order necessary conditions utilizing the Lagrangian approach and in Section 5, a projected gradient method is introduced. It is shown in Section 6 that the problem of determining a hydrodynamic control for optimizing the efficiency of the VSP can be reduced to the problem under consideration. Corresponding numerical results are presented in Section 7.

2. Problem formulation

In this section, we fix the notation for the optimal control problem under consideration and collect preliminary facts.

2.1. **Preliminaries and notation.**

We consider a parameter-dependent convection-diffusion problem on an open domain $\Omega \subset \mathbb{R}^2$. In Ω, one or more rigid bodies are present that can be seen as obstacles. The position of these obstacles is fixed and is assumed to be represented by a closed subset B. We write $B \Subset \Omega$. Then, we define $\Omega_B := \Omega \setminus B$ which is an open, but not convex set in $\mathbb{R}^2$. We are interested in weak solutions of a partial differential equation on Ω_B. Therefore, we introduce the Hilbert space $V := H^1(\Omega_B)$ endowed with the H^1-inner product

$$\langle u, v\rangle_V = \int_{\Omega_B} \Big(\nabla u(\mathbf{x})\cdot\nabla v(\mathbf{x}) + u(\mathbf{x})\,v(\mathbf{x})\Big)\,\mathrm{d}\mathbf{x}, \quad u, v \in V,$$

and its induced norm $\|u\|_V = \sqrt{\langle u, u\rangle_V}$ for $u \in V$.

Let us denote the outer boundary by $\Gamma := \partial\Omega$ and we consider a decomposition of Γ into a part $\Gamma_\mathrm{D} \subset \Gamma$, where we will enforce Dirichlet boundary conditions, as well as a part $\Gamma_\mathrm{N} \subset \Gamma$, where Neumann conditions are imposed. Moreover, the set $\Gamma_\mathrm{D} \cap \Gamma_\mathrm{N}$ has zero Lebesgue measure. For the derivation of the variational formulation, we define the two subspaces

$$V_{\mathrm{D}} := \{v \in V : v = 0 \text{ on } \Gamma_{\mathrm{D}}\} \quad \text{and} \quad V_0 := \{v \in V_{\mathrm{D}} : v = 0 \text{ on } \partial B\},$$

both endowed with the topology in V.

2.2. **The state equation.** We consider a convection-diffusion problem of the following form

$$-\nabla \cdot \big(A(\mathbf{x},\mu)\nabla u(\mathbf{x})\big) + b(\mathbf{x},\mu)\cdot\nabla u(\mathbf{x}) = f(\mathbf{x}), \qquad \text{f.a.a. } \mathbf{x} \in \Omega_B, \tag{2.1a}$$

$$u(\mathbf{x}) = 0, \qquad \text{f.a.a. } \mathbf{x} \in \partial B, \tag{2.1b}$$

$$u(\mathbf{x}) = 0, \qquad \text{f.a.a. } \mathbf{x} \in \Gamma_{\mathrm{D}}, \tag{2.1c}$$

$$n(\mathbf{x}) \cdot \big(A(\mathbf{x},\mu)\nabla u(\mathbf{x})\big) = g(\mathbf{x}), \qquad \text{f.a.a. } \mathbf{x} \in \Gamma_{\mathrm{N}}. \tag{2.1d}$$

Here, $\mu \in D_{\mathrm{ad}} \subset \mathbb{R}^N =: D$ is a parameter and D_{ad} serves as the set of admissible parameters. Moreover, $A : \overline{\Omega}_B \times D_{\mathrm{ad}} \to \mathbb{R}^{2\times 2}$, $b : \Omega_B \times D_{\mathrm{ad}} \to \mathbb{R}^2$, $f : \Omega_B \to \mathbb{R}$, $g : \Gamma_N \to \mathbb{R}$ are given data functions and $n = n(\mathbf{x})$ stands for the outward normal at $\mathbf{x} \in \Gamma$. Finally, we write 'f.a.a.' for 'for almost all'. This means that we consider a state equation, where the parameter μ appears in the coefficients of the partial differential equation.

We call u a weak solution to (2.1) if $u \in V_0$ holds and if u satisfies

$$a(u,\varphi;\mu) = \langle f,\varphi\rangle_{L_2(\Omega_B)} + \langle g,\varphi\rangle_{L_2(\Gamma_{\mathrm{N}})} \quad \text{for all } \varphi \in V_0, \tag{2.2}$$

where for $\mu \in D$ the parameter-dependent and bounded bilinear form $a(\cdot\,,\cdot\,;\mu) : V \times V \to \mathbb{R}$ is defined as

$$a(\varphi,\psi;\mu) = \int_{\Omega_B} \Big(\big(A(\mathbf{x},\mu)\nabla\varphi(\mathbf{x})\big)\cdot\nabla\psi(\mathbf{x}) + \big(b(\mathbf{x},\mu)\cdot\nabla\varphi(\mathbf{x})\big)\psi(\mathbf{x})\Big)\,\mathrm{d}\mathbf{x},$$

for $\varphi, \psi \in V$. We start by investigating the well-posedness of (2.1).

Proposition 2.1. *Suppose that $A \in L_\infty(\Omega_B \times D; \mathbb{R}^{2\times 2})$ satisfying $A(\mathbf{x},\mu) = A(\mathbf{x},\mu)^T$ f.a.a. $\mathbf{x} \in \Omega_B$ and all $\mu \in D_{\mathrm{ad}}$. Moreover, assume that for given $\mu \in D_{\mathrm{ad}}$ there exists a constant $c_\mu > 0$ such that*

$$a(\varphi,\varphi;\mu) \geq c_\mu \|\varphi\|_V^2 \quad \textit{for all } \varphi \in V_0. \tag{2.3}$$

Then, (2.1) *possesses a unique weak solution $u \in V_0$ satisfying*

$$\|u\|_V^2 \leq \eta_\mu \left(\|f\|_{L_2(\Omega_B)}^2 + \|g\|_{L_2(\Gamma_{\mathrm{N}})}^2\right) \tag{2.4}$$

with a constant $\eta_\mu > 0$ depending on μ.

Proof. Existence of a unique solution $u \in V_0$ follows from the Lax-Milgram theorem, see e.g. [4, p. 297]. From the trace theorem (e.g. [4, p. 258]) it follows that there exists a constant $\gamma_\mu > 0$ such that

$$\|u\|_{L_2(\Gamma_{\mathrm{N}})} \leq \gamma_\mu \|u\|_V \quad \text{for } u \in V_0. \tag{2.5}$$

Taking $\varphi = u \in V_0$ in (2.2), utilizing (2.3), (2.5) and Young's inequality twice we arrive at

$$\begin{aligned} c_\mu \|u\|_V^2 \le a(u,u;\mu) &= \int_{\Omega_B} f(\mathbf{x})\, u(\mathbf{x})\,\mathrm{d}\mathbf{x} + \int_{\Gamma_\mathrm{N}} g(\mathbf{x})\, u(\mathbf{x})\,\mathrm{d}\mathbf{x} \\ &\le \frac{1}{c_\mu}\|f\|^2_{L_2(\Omega_B)} + \frac{c_\mu}{4}\|u\|^2_{L_2(\Omega_B)} + \gamma_\mu \|g\|_{L_2(\Gamma_\mathrm{N})}\|u\|_V \\ &\le \frac{1}{c_\mu}\|f\|^2_{L_2(\Omega_B)} + \frac{\gamma_\mu^2}{c_\mu}\|g\|^2_{L_2(\Gamma_\mathrm{N})} + \frac{c_\mu}{2}\|u\|_V^2 \end{aligned}$$

which proves (2.4) with $\eta_\mu = \frac{2}{c_\mu^2}\max\{1,\gamma_\mu^2\} > 0$. $\square$

It will be convenient to collect all our assumptions as follows.

Assumption 1. *We assume the following conditions:*

1) *For the data we have $f \in L_2(\Omega_B)$ and $g \in L_2(\Gamma_\mathrm{N})$.*
2) *The admissible set $D_\mathrm{ad} \subset D$ of parameters is nonempty, bounded, closed and convex.*
3) *We have $A \in C(\bar\Omega_B \times D_\mathrm{ad};\mathbb{R}^{2\times 2})$ and $b \in C(\Omega_B \times D_\mathrm{ad};\mathbb{R}^2)$. Moreover, we assume that $A(\mathbf{x},\mu) = A(\mathbf{x},\mu)^T$ f.a.a. $\mathbf{x} \in \Omega_B$ and all $\mu \in D_\mathrm{ad}$.*
4) *There exist a constant $c > 0$ independent of μ such that*
$$a(\varphi,\varphi;\mu) \ge c\,\|\varphi\|_V^2 \quad \textit{for all } \varphi \in V_\mathrm{D} \textit{ and } \mu \in D_\mathrm{ad}.$$
5) *There exists a constant $\eta > 0$ independent of μ satisfying*
$$\|u\|_V^2 \le \eta\left(\|f\|^2_{L_2(\Omega_B)} + \|g\|^2_{L_2(\Gamma_\mathrm{N})}\right) \quad \textit{for all } \mu \in D_\mathrm{ad}.$$

Remark 2.2.
1) Existence of a unique solution can also be ensured by using Fredholm theory [4, p. 640-644]. If there does not exist a unique solution $v \neq 0$ of the homogeneous problem
$$\begin{aligned} -\nabla\cdot\big(A(\mathbf{x},\mu)\nabla v(\mathbf{x})\big) + b(\mathbf{x},\mu)\cdot\nabla v(\mathbf{x}) &= 0, &&\text{f.a.a. } \mathbf{x} \in \Omega_B, \\ v(\mathbf{x}) &= 0, &&\text{f.a.a. } \mathbf{x} \in \partial B, \\ v(\mathbf{x}) &= 0, &&\text{f.a.a. } \mathbf{x} \in \Gamma_\mathrm{D}, \\ n(\mathbf{x})\cdot\big(A(\mathbf{x},\mu)\nabla v(\mathbf{x})\big) &= 0, &&\text{f.a.a. } \mathbf{x} \in \Gamma_\mathrm{N}, \end{aligned}$$
then (2.1) possesses a unique weak solution $u \in V_0$.
2) Compared to (2.3) the constant c in Assumption 1, part 4) does not depend on μ.
3) Following the lines of the proof of Proposition 2.1 shows the existence of a constant $\eta > 0$ as in Assumption 1, part 5) independent of μ provided Assumption 1, part 4) holds and the trace constant γ_μ in (2.5) does not depend on μ. $\Diamond$

2.3. **The optimal control problem.** In order to formulate the optimal control problem under consideration, we set

$$X := V_0 \times \mathbb{R}^N, \quad X_\mathrm{ad} := V_0 \times D_\mathrm{ad} \subset X,$$

where the Hilbert space X is endowed with the common product topology. Let $J : X_\mathrm{ad} \to \mathbb{R}_0^+$ be given as

$$J(u,\mu) := \frac{1}{2}\left(\int_{\partial B}\big|F\big(n(\mathbf{x})\cdot(A(\mathbf{x},\mu)\nabla u(\mathbf{x}))\big)\big|^2\,\mathrm{d}\mathbf{x} + \kappa\,|\mu-\mu^\circ|_2^2\right), \tag{2.6}$$

where $F : H^{-1/2}(\partial B) \to L_2(\partial B)$ is a continuously Fréchet-differentiable mapping, $|\cdot|_2$ denotes the Euclidean norm in $\mathbb{R}^N$, $\kappa \geq 0$ is a regularization parameter and μ° is a given nominal vector in D.

Remark 2.3. From $u \in V$ we obtain $\frac{\partial u}{\partial n} \in H^{-1/2}(\partial B)$. Thus, the function F can be interpreted as a smoothing operator which will be useful for the analysis and the numerical realization of the norm of $\frac{\partial u}{\partial n}$ on ∂B. The role of F will also be investigated by our numerical experiments. $\Diamond$

Then, our optimization problem reads

$$(\mathbf{P}_\mu) \qquad \min J(u,\mu) \quad \text{subject to (s.t.)} \quad (u,\mu) \in V_0 \times D_{\mathrm{ad}} = X_{\mathrm{ad}} \text{ satisfies (2.2).}$$

It will be convenient to reformulate this problem in an abstract setting. In order to do so, let us introduce the nonlinear operator $e : X_{\mathrm{ad}} \to V_{\mathrm{D}}'$ by

$$\begin{aligned}\langle e(u,\mu),\varphi\rangle_{V_{\mathrm{D}}',V_{\mathrm{D}}} &= a(u,\varphi;\mu) - \langle n\cdot(A(\cdot,\mu)\nabla u),\varphi\rangle_{H^{-1/2}(\partial B),H^{1/2}(\partial B)}\\ &\quad - \langle f,\varphi\rangle_{L_2(\Omega_B)} - \langle g,\varphi\rangle_{L_2(\Gamma_{\mathrm{N}})} \quad \text{for all } \varphi\in V_{\mathrm{D}}\end{aligned}$$

and for $(u,\mu) \in X_{\mathrm{ad}}$. With this definition at hand, we can express $(\mathbf{P}_\mu)$ equivalently as the following abstract constrained optimal control problem

$$(\mathbf{P}_\mu) \qquad \min J(u,\mu) \quad \text{s.t.} \quad (u,\mu) \in X_{\mathrm{ad}} \text{ and } e(u,\mu) = 0 \text{ in } V_{\mathrm{D}}',$$

which can be seen as follows.

Lemma 2.4. *For $(u,\mu) \in X_{\mathrm{ad}}$, the operator equation $e(u,\mu) = 0$ in V_{D}' is equivalent to*

$$\begin{aligned}a(u,\varphi;\mu) &= \int_\Omega \Big(\big(A(\mathbf{x},\mu)\nabla u(\mathbf{x})\big)\cdot\nabla\varphi(\mathbf{x}) + \big(b(\mathbf{x},\mu)\cdot\nabla u(\mathbf{x})\big)\varphi(\mathbf{x})\Big)\,\mathrm{d}\mathbf{x}\\ &= \langle n\cdot(A(\cdot\,,\mu)\nabla u,\varphi\rangle_{H^{-1/2}(\partial B),H^{1/2}(\partial B)} + \langle f,\varphi\rangle_{L_2(\Omega_B)}\\ &\quad + \langle g,\varphi\rangle_{L_2(\Gamma_{\mathrm{N}})} \qquad \textit{for all } \varphi\in V_{\mathrm{D}}.\end{aligned} \tag{2.7}$$

Proof. Choosing test functions $\varphi \in H_0^1(\Omega_B) \subset V_0 \subset V_{\mathrm{D}}$ we infer from (2.7) and integration by parts that

$$\big\langle -\nabla\cdot\big(A(\cdot\,,\mu)\nabla u\big) + b(\cdot\,,\mu)\cdot\nabla u,\varphi\big\rangle_{H^{-1}(\Omega_B),H_0^1(\Omega_B)} = \langle f,\varphi\rangle_{L_2(\Omega_B)}.$$

In other words, we have

$$-\nabla\cdot\big(A(\cdot\,,\mu)\nabla u\big) + b(\cdot\,,\mu)\cdot\nabla u = f \quad \text{in } H^{-1}(\Omega_B). \tag{2.8a}$$

Combining (2.7) and (2.8a) we obtain

$$\langle n\cdot(A(\cdot\,,\mu)\nabla u,\varphi\rangle_{H^{-1/2}(\Gamma_{\mathrm{N}}),H^{1/2}(\Gamma_{\mathrm{N}})} = \langle g,\varphi\rangle_{L_2(\Gamma_{\mathrm{N}})} \quad \text{for all } \varphi\in V_{\mathrm{D}},$$

which gives

$$n\cdot\big(A(\cdot\,,\mu)\nabla u\big) = g \quad \text{in } H^{-1/2}(\Gamma_{\mathrm{N}}). \tag{2.8b}$$

Finally, $u \in V_0$ implies

$$u = 0 \quad \text{in } H^{1/2}(\Gamma_{\mathrm{D}}\cup\partial B). \tag{2.8c}$$

It follows from (2.8) that u is a weak solution to the state equation (2.1). $\square$

3. Existence of optimal solutions

In this section, we present sufficient conditions ensuring the existence of at least one optimal solution to our optimization problem ($\mathbf{P}_\mu$). Under Assumption 1 there exists a unique solution $u_\mu \in V_0$ to (2.2) for any $\mu \in D_{\text{ad}}$. In particular, we have $e(u_\mu, \mu) = 0$ in V_{D}'. Therefore, we can also introduce the reduced cost functional $J^{\text{red}} : D_{\text{ad}} \to \mathbb{R}_0^+$ by

$$J^{\text{red}}(\mu) := J(u_\mu, \mu) \quad \text{for } \mu \in D_{\text{ad}}. \tag{3.1}$$

Then, ($\mathbf{P}_\mu$) can be equivalently expressed as

$$\min J^{\text{red}}(\mu) \quad \text{s.t.} \quad \mu \in D_{\text{ad}}. \tag{$\mathbf{P}_\mu^{\text{red}}$}$$

In contrast to ($\mathbf{P}_\mu$), problem ($\mathbf{P}_\mu^{\text{red}}$) has no explicit equality constraints, since they are included in the reduced cost functional. In our numerical solution algorithm we apply a projected gradient method to ($\mathbf{P}_\mu^{\text{red}}$).

Theorem 3.1. *Let Assumption* 1 *hold. Suppose that the mapping*

$$v \mapsto \int_{\partial B} \big|F(v(\mathbf{x}))\big|^2 \,\mathrm{d}\mathbf{x} \quad \textit{for } v \in H^{-1/2}(\partial B) \tag{3.2}$$

is weakly lower semi-continuous. Then ($\mathbf{P}_\mu$) *has at least one optimal solution* $x^* = (u^*, \mu^*) \in X_{\text{ad}}$.

Proof. By Assumption 1, part 2), the admissible set D_{ad} is nonempty. Given $\mu \in D_{\text{ad}}$, Assumption 1, parts 3)–5), ensure existence of a unique solution $u = u_\mu \in V_0$ to (2.2). Hence,

$$\mathcal{F}(\mathbf{P}_\mu) = \big\{(u, \mu) \in X_{\text{ad}} \,\big|\, e(u, \mu) = 0 \text{ in } V_{\text{D}}'\big\} \neq \emptyset. \tag{3.3}$$

Let $\{(u^n, \mu^n)\}_{n\in\mathbb{N}}$ be a minimizing sequence in $\mathcal{F}(\mathbf{P}_\mu)$ satisfying

$$\lim_{n\to\infty} J(u^n, \mu^n) = \inf \big\{J(u, \mu) \,\big|\, (u, \mu) \in \mathcal{F}(\mathbf{P}_\mu)\big\} \geq 0. \tag{3.4}$$

Due to Assumption 1, part 2), the sequence $\{\mu^n\}_{n\in\mathbb{N}}$ is bounded. Since D_{ad} is supposed to be closed and convex, there is an element $\mu^* \in D_{\text{ad}}$ and a subsequence $\{\mu^{n_k}\}_{k\in\mathbb{N}}$ such that

$$\mu^{n_k} \to \mu^* \text{ as } k \to \infty. \tag{3.5}$$

Note that u^n solves (2.2) for the corresponding parameter $\mu = \mu^n$, i.e., $u^n = u_{\mu^n}$. From Assumption 1, part 5), it follows that the sequence $\{u^n\}_{n\in\mathbb{N}}$ is uniformly bounded in V_0. Thus, there is an element $u^* \in V_0$ and a subsequence $\{u^{n_k}\}_{k\in\mathbb{N}}$ such that

$$u^{n_k} \rightharpoonup u^* \text{ in } V_0 \text{ as } k \to \infty. \tag{3.6}$$

From (3.6) we infer that

$$\lim_{k\to\infty} \int_{\Omega_B} \big(\nabla u^{n_k} - \nabla u^*\big) \cdot \chi \,\mathrm{d}\mathbf{x} = 0 \quad \text{for all } \chi \in L_2(\Omega_B)^2 := L_2(\Omega_B) \times L_2(\Omega_B). \tag{3.7}$$

Hence, the sequence $\{\nabla u^{n_k}\}_{k\in\mathbb{N}}$ is uniformly bounded in $L_2(\Omega_B)^2$. Thus, there exists a constant $C > 0$ such that

$$\|\nabla u^{n_k}\|_{L_2(\Omega_B)^2} \leq C \quad \text{for all } k \in \mathbb{N}. \tag{3.8}$$

It is easily seen that

$$
\begin{aligned}
&A(\cdot\,,\mu^{n_k})\nabla u^{n_k} - A(\cdot\,,\mu^*)\nabla u^* \\
&\qquad = \big(A(\cdot\,,\mu^{n_k}) - A(\cdot\,,\mu^*)\big)\nabla u^{n_k} + A(\cdot\,,\mu^*)\big(\nabla u^{n_k} - \nabla u^*\big),
\end{aligned}
\tag{3.9}
$$

and we recall that by Assumption 1, part 3), the mapping $\mu \mapsto A(\cdot\,,\mu)$ is continuous in Ω_B. For the first term, (3.5) and (3.8) imply for all $\varphi \in V$

$$
\begin{aligned}
&\int_{\Omega_B} \Big(\big(A(\cdot\,,\mu^{n_k}) - A(\cdot\,,\mu^*)\big)\nabla u^{n_k}\Big)\cdot\nabla\varphi \,\mathrm{d}\mathbf{x} \\
&\qquad \le \|A(\cdot\,,\mu^{n_k}) - A(\cdot\,,\mu^*)\|_{L_\infty(\Omega_B)}\|\nabla u^{n_k}\|_{L_2(\Omega_B)^2}\|\nabla\varphi\|_{L_2(\Omega_B)^2} \overset{k\to\infty}{\longrightarrow} 0.
\end{aligned}
\tag{3.10}
$$

From $A(\cdot\,,\mu^*) \in C(\bar{\Omega}_B;\mathbb{R}^{2\times 2})$ we infer that $A(\cdot\,,\mu^*)\nabla\varphi \in L_2(\Omega_B;\mathbb{R}^2)$ for $\varphi \in V$. Consequently, (3.7) and the symmetry of A imply that

$$
\begin{aligned}
&\int_{\Omega_B} A(\cdot\,,\mu^*)\big(\nabla u^{n_k} - \nabla u^*\big)\cdot\nabla\varphi\,\mathrm{d}\mathbf{x} \\
&\qquad = \int_{\Omega_B} \big(\nabla u^{n_k} - \nabla u^*\big)\cdot\big(A(\cdot\,,\mu^*)\nabla\varphi\big)\,\mathrm{d}\mathbf{x} \overset{k\to\infty}{\longrightarrow} 0 \quad \text{for all } \varphi \in V_{\mathrm{D}}.
\end{aligned}
\tag{3.11}
$$

Combining (3.9), (3.10) and (3.11), we find

$$
\lim_{k\to\infty}\int_{\Omega_B} \big(A(\cdot\,,\mu^{n_k})\nabla u^{n_k} - A(\cdot\,,\mu^*)\nabla u^*\big)\cdot\nabla\varphi\,\mathrm{d}\mathbf{x} = 0 \quad \text{for all } \varphi \in V_{\mathrm{D}}.
\tag{3.12}
$$

In a completely analogous way, we get

$$
\lim_{k\to\infty}\int_{\Omega_B} \big(b(\cdot\,,\mu^{n_k})\cdot\nabla u^{n_k} - b(\cdot\,,\mu^*)\cdot\nabla u^*\big)\,\varphi\,\mathrm{d}\mathbf{x} = 0 \quad \text{for all } \varphi \in V_{\mathrm{D}},
\tag{3.13}
$$

and

$$
\lim_{k\to\infty}\Big\langle n\cdot\big(A(\cdot\,,\mu^{n_k})\nabla u^{n_k} - A(\cdot\,,\mu^*)\nabla u^*\big),\phi\Big\rangle_{H^{-1/2}(\partial B),H^{1/2}(\partial B)} = 0
\tag{3.14}
$$

for all $\phi \in H^{1/2}(\partial B)$. From (3.12)-(3.14) and $(u^{n_k},\mu^{n_k}) \in \mathcal{F}(\mathbf{P}_\mu)$ for all $k \in \mathbb{N}$ we infer that

$$
0 = \lim_{k\to\infty} e(u^{n_k},\mu^{n_k}) = e(u^*,\mu^*) \quad \text{in } V_{\mathrm{D}}'.
$$

Due to (3.2) the cost functional is weakly lower semi-continuous so that we conclude from (3.4) and (3.14)

$$
J(u^*,\mu^*) \le \lim_{k\to\infty} J(u^{n_k},\mu^{n_k}) = \inf\big\{J(u,\mu)\,\big|\,(u,\mu)\in\mathcal{F}(\mathbf{P}_\mu)\big\} \le J(u^*,\mu^*)
$$

so that (u^*,μ^*) is a solution to $(\mathbf{P}_\mu)$. □

4. First-order necessary optimality conditions

Problem $(\mathbf{P}_\mu)$ is a non-convex programming problem so that different local minima might occur. A numerical method will produce a local minimum close to its starting value. Hence, we do not restrict our investigations to global solutions of $(\mathbf{P}_\mu)$. We will assume that a fixed reference solution $x^* = (u^*,\mu^*) \in \mathcal{F}(\mathbf{P}_\mu)$ is given satisfying certain optimality conditions (ensuring local optimality of the solution). In this section, we study first-order necessary optimality conditions for $(\mathbf{P}_\mu)$.

4.1. **Differentiability properties.** We begin by proving that both the cost functional J and the constraint function e are Fréchet-differentiable. For that purpose, differentiability properties of the coefficient functions A and b are required that are stronger then the continuity conditions in Assumption 1, part 3). The following assumptions are definitely satisfied in the applications we have in mind.

Assumption 2. *We assume:*

1) *The functions* $\mu \mapsto A(\mathbf{x},\mu)$, $\mathbf{x} \in \bar{\Omega}_B$, *and* $\mu \mapsto b(\mathbf{x},\mu)$, $\mathbf{x} \in \Omega_B$, *are continuously differentiable and their partial derivatives* $A_\mu(\cdot\,,\mu)$, $b_\mu(\cdot\,,\mu)$ *with respect to* μ *are bounded for all* $\mu \in D_{\mathrm{ad}}$.
2) *The function* F *is continuously Fréchet-differentiable from* $H^{-1/2}(\partial B)$ *to* $L_2(\partial B)$.

Lemma 4.1. *Let Assumptions* 1 and 2 *be satisfied. Then, for every* $(u,\mu) \in X_{\mathrm{ad}}$, *the cost functional* J *is Fréchet-differentiable.*

Proof. The partial directional derivative $J_\mu(u,\mu)$ of J at $(u,\mu) \in X_{\mathrm{ad}}$ in any direction $\mu_\delta \in D$ is given by

$$\begin{aligned} J_\mu(u,\mu)\,\mu_\delta &= \int_{\partial B} F'(v)\big(n\cdot((A_\mu(\cdot\,,\mu)\mu_\delta)\nabla u)\big)F(v)\,\mathrm{d}\mathbf{x} + \kappa\left(\mu-\mu^\circ\right)^T\mu_\delta \\ &= \big\langle F'(v)\big(n\cdot((A_\mu(\cdot\,,\mu)\mu_\delta)\nabla u)\big), F(v)\big\rangle_{L_2(\partial B)} + \kappa\left(\mu-\mu^\circ\right)^T\mu_\delta \\ &= \big\langle n\cdot((A_\mu(\cdot\,,\mu)\mu_\delta)\nabla u), F'(v)^\star F(v)\big\rangle_{H^{-1/2}(\partial B),H^{1/2}(\partial B)} \\ &\quad + \kappa\left(\mu-\mu^\circ\right)^T\mu_\delta, \end{aligned} \tag{4.1}$$

where we set $v := n\cdot(A(\cdot\,,\mu)\nabla u) \in H^{-1/2}(\partial B)$, $F'(v) : H^{-1/2}(\partial B) \to L_2(\partial B)$ denotes the Fréchet-derivative of F at v, and $F'(v)^\star : L_2(\partial B) \to H^{1/2}(\partial B)$ is the adjoint of $F'(v)$ satisfying

$$\langle F'(v)w,\psi\rangle_{L_2(\partial B)} = \langle w, F'(v)^\star\psi\rangle_{H^{-1/2}(\partial B),H^{1/2}(\partial B)} \tag{4.2}$$

for all $(w,\psi) \in H^{-1/2}(\partial B)\times L_2(\partial B)$. Let $v_\delta := n\cdot(A(\cdot\,,\mu+\mu_\delta)\nabla u) \in H^{-1/2}(\partial B)$. To prove that $J_\mu(u,\mu)$ is the partial Fréchet-derivative of J with respect to μ, we estimate

$$\begin{aligned} &\big|J(u,\mu+\mu_\delta) - J(u,\mu) - J_\mu(u,\mu)\mu_\delta\big| \\ &\quad\le \frac{1}{2}\Big|\big\|F(v_\delta)\big\|^2_{L_2(\partial B)} - \big\|F(v)\big\|^2_{L_2(\partial B)} \\ &\qquad\quad - 2\big\langle F'(v)\big(n\cdot((A_\mu(\cdot\,,\mu)\mu_\delta)\nabla u)\big), F(v)\big\rangle_{L_2(\partial B)}\Big| \\ &\qquad + \frac{\kappa}{2}\left||\mu+\mu_\delta-\mu^\circ|_2^2 - |\mu-\mu^\circ|_2^2 - 2\left(\mu-\mu^\circ\right)^T\mu_\delta\right|. \end{aligned} \tag{4.3}$$

By Assumption 2, the mapping $\mu \mapsto A(\cdot\,,\mu)$ is continuously differentiable and $\phi \mapsto F(\phi)$ is continuously Fréchet-differentiable. Thus,

$$\begin{aligned} &\Big|\big\|F(v_\delta)\big\|^2_{L_2(\partial B)} - \big\|F(v)\big\|^2_{L_2(\partial B)} \\ &\quad - 2\big\langle F'(v)\big(n\cdot((A_\mu(\cdot\,,\mu)\mu_\delta)\nabla u)\big), F(v)\big\rangle_{L_2(\partial B)}\Big| = o\big(|\mu_\delta|_2\big) \text{ for } |\mu_\delta|_2 \to 0. \end{aligned} \tag{4.4}$$

Combining (4.3) and (4.4) we arrive at

$$\big|J(u,\mu+\mu_\delta) - J(u,\mu) - J_\mu(u,\mu)\mu_\delta\big| \le o\big(|\mu_\delta|_2\big) + \frac{\kappa}{2}\,|\mu_\delta|_2^2 = o\big(|\mu_\delta|_2\big)$$

for $|\mu_\delta|_2 \to 0$. Hence, $J_\mu(u,\mu)$ is the partial Fréchet-derivative of J at $(u,\mu) \in X_{\rm ad}$ with respect to μ.

The directional derivative $J_u(u,\mu)$ of J at $(u,\mu) \in X_{\rm ad}$ with respect to u is given by

$$J_u(u,\mu)u_\delta = \int_{\partial B} \big(F'(v)v_\delta\big)F(v)\,\mathrm{d}\mathbf{x} \quad \text{for } u_\delta \in V_0,$$

with $v := n \cdot (A(\cdot\,,u)\nabla u)$ and $v_\delta := n \cdot (A(\cdot\,,u)\nabla u_\delta)$. From Assumption 2 we infer that the mapping $G : H^{-1/2}(\partial B) \to L_1(\partial B)$ with $\phi \mapsto G(\phi) = \frac{1}{2}\,|F(\phi)|^2$ is Fréchet-differentiable and its derivative is given by $G'(\phi)\phi_\delta = (F'(\phi)\phi_\delta)F(\phi)$ in any direction $\phi_\delta \in H^{-1/2}(\partial B)$. To prove that this directional derivative is already the Fréchet-derivative, we estimate

$$\begin{aligned}
&\big|J(u+u_\delta,\mu) - J(u,\mu) - J_u(u,\mu)u_\delta\big| = \left|\int_{\partial B} G(v+v_\delta) - G(v) - G'(v)v_\delta\,\mathrm{d}\mathbf{x}\right| \\
&\le \big\|G(v+v_\delta) - G(v) - G'(v)v_\delta\big\|_{L_1(\partial B)} = o\big(\|v_\delta\|_{H^{-1/2}(\partial B)}\big) \\
&= o\big(\|n\cdot\nabla u_\delta\|_{H^{-1/2}(\partial B)}\big).
\end{aligned}$$

If $\|u_\delta\|_{V_0} \to 0$ holds, then it follows that $\|n\cdot\nabla u_\delta\|_{H^{-1/2}(\partial B)} \to 0$. This gives the claims. □

Next we investigate the differentiability of the constraint operator e.

Lemma 4.2. *The operator $e : X_{\rm ad} \to V_{\rm D}'$ is Fréchet-differentiable.*

Proof. The directional derivative $e_\mu(u,\mu)$ of e at $(u,\mu) \in X_{\rm ad}$ in an arbitrary direction $\mu_\delta \in D$ is given by

$$\begin{aligned}
\langle e_\mu(u,\mu)\mu_\delta, \varphi\rangle_{V_{\rm D}',V_{\rm D}} = &\int_{\Omega_B} \Big(\big(A_\mu(\cdot\,,\mu)\mu_\delta\big)\nabla u\Big)\cdot\nabla\varphi + \Big(\big(b_\mu(\cdot\,,\mu)\mu_\delta\big)\cdot\nabla u\Big)\varphi\,\mathrm{d}\mathbf{x} \\
&- \Big\langle n\cdot\big(\big(A_\mu(\cdot\,,\mu)\mu_\delta\big)\nabla u\big), \varphi\Big\rangle_{H^{-1/2}(\partial B),H^{1/2}(\partial B)}
\end{aligned}$$

for $\varphi \in V_{\rm D}$. Since A and b are differentiable, we have

$$\begin{aligned}
\|A(\cdot\,,\mu+\mu_\delta) - A(\cdot\,,\mu) - A_\mu(\cdot\,,\mu)\mu_\delta\|_{L_\infty(\Omega_B)} &= o\big(|\mu_\delta|_2\big), \\
\|b(\cdot\,,\mu+\mu_\delta) - b(\cdot\,,\mu) - b_\mu(\cdot\,,\mu)\mu_\delta\|_{L_\infty(\Omega_B)} &= o\big(|\mu_\delta|_2\big)
\end{aligned}$$

for $|\mu_\delta|_2 \to 0$. Hence, we estimate

$$
\begin{aligned}
&\big\| e(u,\mu+\mu_\delta) - e(u,\mu) - e_\mu(u,\mu)\mu_\delta \big\|_{V'_{\mathrm{D}}} \\
&= \sup_{\|\varphi\|_V=1} \big| \langle e(u,\mu+\mu_\delta) - e(u,\mu) - e_\mu(u,\mu)\mu_\delta, \varphi\rangle_{V'_{\mathrm{D}},V_{\mathrm{D}}} \big| \\
&= \sup_{\|\varphi\|_V=1} \bigg\{ \int_{\Omega_B} \Big[\Big(\big[A(\cdot\,,\mu+\mu_\delta) - A(\cdot\,,\mu) - A_\mu(\cdot\,,\mu)\mu_\delta\big]\nabla u\Big)\cdot\nabla\varphi \\
&\qquad\qquad + \Big(\big[b(\cdot\,,\mu+\mu_\delta) - b(\cdot\,,\mu) - b_\mu(\cdot\,,\mu)\mu_\delta\big]\nabla u\Big)\varphi\Big]\,\mathrm{d}\mathbf{x} \\
&\qquad\qquad - \Big\langle n\cdot\big[A(\cdot\,,\mu+\mu_\delta) - A(\cdot\,,\mu) \\
&\qquad\qquad\qquad - A_\mu(\cdot\,,\mu)\mu_\delta\big]\nabla u, \varphi\Big\rangle_{H^{-1/2}(\partial B),H^{1/2}(\partial B)} \bigg\} \\
&\le \|A(\cdot\,,\mu+\mu_\delta) - A(\cdot\,,\mu) - A_\mu(\cdot\,,\mu)\mu_\delta\|_{L_\infty(\Omega_B)}\|u\|_V \\
&\quad + \|b(\cdot\,,\mu+\mu_\delta) - b(\cdot\,,\mu) - b_\mu(\cdot\,,\mu)\mu_\delta\|_{L_\infty(\Omega_B)}\|u\|_V \\
&\quad + \|A(\cdot\,,\mu+\mu_\delta) - A(\cdot\,,\mu) - A_\mu(\cdot\,,\mu)\mu_\delta\|_{L_\infty(\Gamma_{\mathrm{D}})}\big\|\tfrac{\partial u}{\partial n}\big\|_{H^{-1/2}(\partial B)} \\
&= o\big(|\mu_\delta|_2\big),
\end{aligned}
$$

so that $e_\mu(u,\mu)$ is the partial Fréchet-derivative of e at (u,μ) with respect to μ. The directional derivative $e_u(u,\mu)$ of e at (u,μ) with respect to u in any direction $u_\delta \in V_0$ reads

$$
\begin{aligned}
\langle e_u(u,\mu)u_\delta, \varphi\rangle_{V'_{\mathrm{D}},V_{\mathrm{D}}} = &\int_{\Omega_B} \Big[\big(A(\cdot\,,\mu)\nabla u_\delta\big)\cdot\nabla\varphi + \big(b(\cdot\,,\mu)\cdot\nabla u_\delta\big)\,\varphi\Big]\,\mathrm{d}\mathbf{x} \\
&- \Big\langle n\cdot\big(A(\cdot\,,\mu)\nabla u_\delta\big),\varphi\Big\rangle_{H^{-1/2}(\partial B),H^{1/2}(\partial B)}
\end{aligned}
$$

for all $\varphi \in V_{\mathrm{D}}$. Since $u \mapsto e(u,\mu)$ is linear and bounded for any $\mu \in D_{\mathrm{ad}}$, the directional derivative $e_u(u,\mu)$ is the partial Fréchet-derivative of e at (u,μ) with respect to u. □

Finally, we investigate the differentiability of the bilinear form $a(\cdot,\cdot;\mu)$ with respect to the parameter $\mu \in D_{\mathrm{ad}}$, since such derivatives may occur in optimization schemes, where μ is the parameter. To this end, consider the mapping

$$R : D_{\mathrm{ad}} \to V_0, \qquad R(\mu) := u(\mu) \in V_0 \text{ for } \mu \in D_{\mathrm{ad}},$$

where $u(\mu)$ denotes the unique solution of (3.6). Then, we have

Theorem 4.3. *Let Assumption 2 hold. The mapping R is C^1. Moreover, for any $\mu \in D_{\mathrm{ad}}$ and every $\mu_\delta \in D_{\mathrm{ad}}$ the function $z := R'(\mu)\mu_\delta \in V_0$ is the unique solution of the following boundary value problem*

$$a(z,v;\mu) = -\frac{\partial}{\partial\mu}a(u(\mu),v;\mu_\delta) \quad \textit{for all } \varphi \in V_0.$$

Proof. The proof is very much similar to the proof of [3, Theorem 1]. Consider the mapping $H : D \times V \to V'$ defined by

$$\langle H(\mu,u),\varphi\rangle_{V',V} = a(u,\varphi;\mu) - \langle f,\varphi\rangle_{L_2(\Omega_B)} - \langle g,\varphi\rangle_{L_2(\Gamma_{\mathrm{N}})} \quad \text{for all } \varphi \in V_0,$$

which is of class C^1 in view of Assumption 2. Moreover $H(\mu,u(\mu)) = 0$ in V' and the partial derivative $H_u(\mu,u) = a(u,\cdot;\mu)$ is isomorphism from V to V' for every fixed $\mu \in D_{\mathrm{ad}}$. Then, the implicit function theorem [11, p. 366] implies that R is of class C^1 and that

$$H_u(\mu, u(\mu))z = -H_\mu(\mu, u(\mu))(\mu_\delta).$$

Finally, it follows immediately from the definition of H that

$$\begin{aligned}
\langle H_u(\mu, u(\mu))z, \varphi\rangle_{V',V} &= a(z, \varphi; \mu) && \text{for all } \varphi \in V_0,\\
\langle H_\mu(\mu, u(\mu))\mu_\delta, \varphi\rangle_{V',V} &= \frac{\partial}{\partial\mu} a(u(\mu), \varphi; \mu_\delta) && \text{for all } \varphi \in V_0,
\end{aligned}$$

which proves the claim. □

4.2. **Regular point condition.** To ensure the existence of Lagrange multipliers, a constraint qualification has to be satisfied at a local solution $x^* = (u^*, \mu^*) \in X_{\mathrm{ad}}$. We make use of the following regular point condition.

Definition 4.4. *A point $x^\circ \in \mathcal{F}(\mathbf{P}_\mu)$ is said to be a* regular point for $(\mathbf{P}_\mu)$ *provided the linearization $\nabla e(x^\circ) = (e_u, e_\mu)(x^\circ) : X \to V_{\mathrm{D}}'$ of the operator e is onto.*

Lemma 4.5. *Let Assumption* 1 *be satisfied. Then, for every $x^\circ \in \mathcal{F}(\mathbf{P}_\mu)$ the operator $e_u(x^*)$ is bijective.*

Proof. It follows from the proof of Lemma 4.2 that the operator $e_u(x^*)$ is bijective if for every $P \in V_{\mathrm{D}}'$ there exists a unique $u_\delta \in V_0$ satisfying $u_\delta = 0$ in $H^{1/2}(\Gamma_{\mathrm{D}} \cup \partial B)$ and

$$\begin{aligned}
&\int_{\Omega_B} \Big[\big(A(\cdot\,,\mu)\nabla u_\delta\big)\cdot\nabla\varphi + \big(b(\cdot\,,\mu)\cdot\nabla u_\delta\big)\Big]\varphi\,\mathrm{d}\mathbf{x}\\
&\quad - \big\langle n\cdot\big(A(\cdot\,,\mu)\nabla u_\delta\big), \varphi\big\rangle_{H^{-1/2}(\partial B), H^{1/2}(\partial B)} = \langle P, \varphi\rangle_{V_{\mathrm{D}}', V_{\mathrm{D}}} \text{ for all } \varphi \in V_{\mathrm{D}}.
\end{aligned} \tag{4.5}$$

Choosing $\varphi \in H^{-1}(\Omega_B) \subset V_{\mathrm{D}}$ we infer from (4.5) that u_δ is the weak solution of

$$-\nabla\cdot\big(A(\cdot\,,\mu)\nabla u_\delta\big) + b(\cdot\,,\mu)\cdot\nabla u_\delta = P \quad \text{in } V_{\mathrm{D}}' \subset H^{-1}(\Omega_B). \tag{4.6a}$$

Combining (4.5), (4.6a) and using integration by parts we obtain

$$\big\langle n\cdot\big(A(\cdot\,,\mu)\nabla u_\delta\big), \varphi\big\rangle_{H^{-1/2}(\Gamma_{\mathrm{N}}), H^{1/2}(\Gamma_{\mathrm{N}})} = 0 \quad \text{for all } \varphi \in V_{\mathrm{D}}.$$

Thus,

$$n\cdot\big(A(\cdot\,,\mu)\nabla u_\delta\big) = 0 \quad \text{in } H^{-1/2}(\Gamma_{\mathrm{N}}). \tag{4.6b}$$

From the Lax-Milgram theorem [4, p. 297] and Assumption 1, part 4), it follows that there exists a unique solution $u_\delta \in V_0$ to (4.6). This gives the claim. □

Remark 4.6. We infer from Lemma 4.5 that for every $x^\circ \in \mathcal{F}(\mathbf{P}_\mu)$ the linear operator $\nabla e(x^\circ) : X \to V_{\mathrm{D}}'$ is surjective provided Assumption 1 holds. Definition 4.4 implies that any feasible point is regular for $(\mathbf{P}_\mu)$. ◊

4.3. **Optimality condition.** Let $x^* = (u^*, \mu^*)$ be a local optimal solution to $(\mathbf{P}_\mu)$. To characterize x^* via optimality conditions we introduce the Lagrange functional $L : X \times V_\mathrm{D} \to \mathbb{R}$ for $x = (u, \mu) \in X_\mathrm{ad}$ and $p \in V_\mathrm{D}$ by

$$\begin{aligned}
L(x,p) &:= J(x) + \langle e(u,\mu), p\rangle_{V_\mathrm{D}', V_\mathrm{D}} \\
&= \frac{1}{2}\bigg(\int_{\partial B} \big| F\big(n\cdot(A(\cdot\,,\mu)\nabla u)\big)\big|^2 \,\mathrm{d}\mathbf{x} + \kappa\,|\mu-\mu^\circ|_2^2 \bigg) \\
&\quad + \int_{\Omega_B} \Big[A(\cdot\,,\mu)\nabla u\cdot\nabla p + \big(b(\cdot\,,\mu)\cdot\nabla u - f\big)p\Big]\,\mathrm{d}\mathbf{x} - \int_{\Gamma_\mathrm{N}} g\,p\,\mathrm{d}\mathbf{x} \\
&\quad - \big\langle n\cdot\big(A(u,\mu)\nabla u\big), p\big\rangle_{H^{-1/2}(\partial B), H^{1/2}(\partial B)}.
\end{aligned}$$

Let Assumptions 1 and 2 hold. Due to Lemmas 4.1 and 4.2, the Lagrange functional is Fréchet-differentiable. Moreover, Remark 4.6 and [9] imply that there exists a unique Lagrange multiplier $p^* \in V_\mathrm{D}$ satisfying with x^* the *first-order necessary optimality conditions*

$$L_\mu(x^*,p^*)(\mu-\mu^*) \geq 0 \qquad \text{for all } \mu \in D_\mathrm{ad}, \tag{4.7a}$$

$$L_u(x^*,p^*)u = 0 \qquad \text{for all } u \in V_0, \tag{4.7b}$$

$$L_p(x^*,p^*)p = 0 \qquad \text{for all } p \in V_\mathrm{D}. \tag{4.7c}$$

Notice that (4.7c) implies $e(x^*) = 0$ in V_D. Thus, x^* satisfies the state equation (2.1), see also Lemma 2.4. Next we investigate (4.7b). For any direction $u \in V_0$ we find

$$\begin{aligned}
L_u(x^*,p^*)u = &\int_{\partial B} \Big(F'(v^*)\Big(n\cdot\big(A(\cdot\,,\mu^*)\nabla u\big)\Big)\Big) F(v^*)\,\mathrm{d}\mathbf{x} \\
&- \big\langle n\cdot\big(A(\cdot\,,\mu^*)\nabla u\big), p^*\big\rangle_{H^{-1/2}(\partial B), H^{1/2}(\partial B)} \\
&+ \int_{\Omega_B} \big(A(\cdot\,,\mu^*)\nabla u\big)\cdot\nabla p^* + \big(b(\cdot\,,\mu^*)\cdot\nabla u\big)\,p^*\,\mathrm{d}\mathbf{x}
\end{aligned}\tag{4.8}$$

with $v^* = n\cdot(A(\cdot\,,\mu^*)\nabla u^*)$. Choosing $u \in H_0^1(\Omega_B) \subset V_0 \subset V_\mathrm{D}$, using integration by parts and (4.7b) we find

$$\big\langle -\nabla\cdot\big(A(\cdot\,,\mu^*)^T\nabla p^* + b(\cdot\,,\mu^*)p^*\big), u\big\rangle_{H^{-1}(\Omega_B), H_0^1(\Omega_B)} = 0 \quad \text{for all } u \in H_0^1(\Omega_B).$$

Thus, $p^* \in V_\mathrm{D}$ satisfies the differential equation

$$-\nabla\cdot\big(A(\cdot\,,\mu^*)^T\nabla p^* + b(\cdot\,,\mu^*)p^*\big) = 0 \quad \text{in } V_\mathrm{D}' \subset H^{-1}(\Omega_B). \tag{4.9}$$

Combining (4.7b), (4.8), (4.9) and using $u = 0$ in $H^{1/2}(\Gamma_\mathrm{D}\cup\partial B)$, we have

$$\begin{aligned}
0 = &\int_{\partial B} \Big(F'(v^*)\Big(n\cdot\big(A(\cdot\,,\mu^*)\nabla u\big)\Big)\Big) F(v^*)\,\mathrm{d}\mathbf{x} \\
&- \big\langle n\cdot\big(A(\cdot\,,\mu^*)\nabla u\big), p^*\big\rangle_{H^{-1/2}(\partial B), H^{1/2}(\partial B)} \\
&+ \big\langle n\cdot\big(A(\cdot\,,\mu^*)^T\nabla p^* + b(\cdot\,,\mu^*)p^*\big), u\big\rangle_{H^{-1/2}(\Gamma_\mathrm{N}), H^{1/2}(\Gamma_\mathrm{N})}
\end{aligned}\tag{4.10}$$

for all $u \in V_0$. We choose $u \in V_0$ satisfying $n\cdot(A(\cdot\,,\mu^*)\nabla u) = 0$ in $H^{-1/2}(\partial B)$. Then, it follows from (4.10) that

$$\big\langle n\cdot\big(A(\cdot\,,\mu^*)^T\nabla p^* + b(\cdot\,,\mu^*)p^*\big), u\big\rangle_{H^{-1/2}(\Gamma_\mathrm{N}), H^{1/2}(\Gamma_\mathrm{N})} = 0.$$

Consequently, p^* satisfies

$$n\cdot\big(A(\cdot\,,\mu^*)^T\nabla p^* + b(\cdot\,,\mu^*)p^*\big) = 0 \quad \text{in } H^{-1/2}(\Gamma_\mathrm{N}). \tag{4.11}$$

Recall that

$$\begin{aligned}
&\int_{\partial B} \Big(F'(v^*)\Big(n \cdot \big(A(\cdot\,,\mu^*)\nabla u\big)\Big)\Big) F(v^*)\,\mathrm{d}\mathbf{x} \\
&\quad = \Big(F'(v^*)\Big(n \cdot \big(A(\cdot\,,\mu^*)\nabla u\big)\Big), F(v^*)\Big)_{L_2(\Omega_B)} \\
&\quad = \big\langle n \cdot \big(A(\cdot\,,\mu^*)\nabla u\big), F'(v^*)^\star\, F(v^*)\big\rangle_{H^{-1/2}(\partial B), H^{1/2}(\partial B)},
\end{aligned}$$

so that (4.10) and (4.11) give

$$\big\langle n \cdot \big(A(\cdot\,,\mu^*)\nabla u\big), F'(v^*)^\star\, F(v^*) - p^*\big\rangle_{H^{-1/2}(\partial B), H^{1/2}(\partial B)} = 0.$$

Therefore,

$$p^* = F'(v^*)^\star\, F(v^*) \quad \text{in } H^{1/2}(\partial B). \tag{4.12}$$

From (4.9), (4.11), (4.12), and $p^* \in V_{\mathrm{D}}$ we derive the following theorem.

Theorem 4.7. *Assume that a fixed reference solution $x^* = (u^*, \mu^*) \in X_{\mathrm{ad}}$ to $(\mathbf{P}_\mu)$ is given. Let Assumptions* 1 *and* 2 *hold. Then there exists a unique Lagrange multiplier p^* satisfying the* adjoint system

$$-\nabla \cdot \big(A(\cdot\,,\mu^*)^T \nabla p^* + b(\cdot\,,\mu^*) p^*\big) = 0 \qquad \textit{in } \Omega_B, \tag{4.13a}$$

$$n \cdot \big(A(\cdot\,,\mu^*)^T \nabla p^* + b(\cdot\,,\mu^*) p^*\big) = 0 \qquad \textit{on } \Gamma_{\mathrm{N}}, \tag{4.13b}$$

$$p^* = F'(v^*)^\star\, F(v^*) \qquad \textit{on } \partial B, \tag{4.13c}$$

$$p^* = 0 \qquad \textit{on } \Gamma_{\mathrm{D}}. \tag{4.13d}$$

□

Next we turn to the variational inequality (4.7a), which is equivalent with

$$\begin{aligned}
&L_\mu(x^*, p^*)(\mu - \mu^*) \\
&= \Big\langle n \cdot \Big(\big(A_\mu(\cdot\,,\mu^*)(\mu - \mu^*)\big)\nabla u^*\Big), F'(v^*)^\star\, F(v^*)\Big\rangle_{H^{-1/2}(\partial B), H^{1/2}(\partial B)} \\
&\quad + \kappa\,(\mu^* - \mu^\circ)^T (\mu - \mu^*) \\
&\quad + \int_{\Omega_B} \Big(\big(A_\mu(\cdot\,,\mu^*)(\mu - \mu^*)\big)\nabla u^*\Big) \cdot \nabla p^*\,\mathrm{d}\mathbf{x} \\
&\quad + \int_{\Omega_B} \Big(\big(b_\mu(\cdot\,,\mu^*)(\mu - \mu^*)\big) \cdot \nabla u^*\Big)\, p^*\,\mathrm{d}\mathbf{x} \\
&\quad - \Big\langle n \cdot \Big(\big(A_\mu(\cdot\,,\mu^*)(\mu - \mu^*)\big)\nabla u^*\Big), p^*\Big\rangle_{H^{-1/2}(\partial B), H^{1/2}(\partial B)} \geq 0
\end{aligned} \tag{4.14}$$

for all $\mu \in D_{\mathrm{ad}}$, where $v^* = n \cdot (A(\cdot\,,\mu^*)\nabla u^*) \in H^{-1/2}(\partial B)$. Since $A(\mathbf{x}, \mu^*)$ belongs to $\mathbb{R}^{2\times 2}$ for all $\mathbf{x} \in \bar{\Omega}_B$, we infer that $A_\mu(\mathbf{x}, \mu^*)$ is a tensor in $\mathbb{R}^{2\times 2\times N}$. In particular, $A_\mu(\mathbf{x}, \mu^*)(\mu - \mu^*) \in \mathbb{R}^{2\times 2}$ holds for all $\mathbf{x} \in \bar{\Omega}_B$ and

$$\big(A_\mu(\mathbf{x}, \mu^*)(\mu - \mu^*)\big)_{ij} = \sum_{k=1}^{N} \big(A_\mu(\mathbf{x}, \mu^*)\big)_{ijk}\,(\mu_k - \mu_k^*),$$

where μ_k and μ_k^* denote the k-th component of the vectors μ and μ^*, respectively. Therefore,

$$
\begin{aligned}
&\Big(\big(A_\mu(\cdot\,,\mu^*)(\mu-\mu^*)\big)\nabla u^*\Big)\cdot\nabla p^* \\
&\quad=\sum_{i=1}^{2}\frac{\partial p^*}{\partial x_i}\left(\sum_{j=1}^{2}\left(\sum_{k=1}^{N}\left(A_\mu(\mathbf{x},\mu^*)\right)_{ijk}(\mu_k-\mu_k^*)\right)\frac{\partial u^*}{\partial x_j}\right)\\
&\quad=\sum_{k=1}^{N}(\mu_k-\mu_k^*)\left(\sum_{i=1}^{2}\frac{\partial p^*}{\partial x_i}\sum_{j=1}^{2}\Big(\left(A_\mu(\mathbf{x},\mu^*)\right)_{ijk}\Big)\frac{\partial u^*}{\partial x_j}\right)\\
&\quad=\sum_{k=1}^{N}(\mu_k-\mu_k^*)\left(\sum_{i=1}^{2}\frac{\partial p^*}{\partial x_i}\sum_{j=1}^{2}\big(A_k\big)_{ij}\frac{\partial u^*}{\partial x_j}\right)\\
&\quad=\sum_{k=1}^{N}(\mu_k-\mu_k^*)\Big(\big(A_k\nabla u^*\big)\cdot\nabla p^*\Big),
\end{aligned}
\tag{4.15}
$$

where for $1\le k\le N$ we introduce the matrices

$$A_k=\Big(\big(A_k\big)_{ij}\Big)\in\mathbb{R}^{2\times 2}\quad\text{with}\quad \big(A_k\big)_{ij}=\left(A_\mu(\mathbf{x},\mu^*)\right)_{ijk}\ \text{ for } 1\le i,j\le 2.$$

Analogously, $b_\mu(\mathbf{x},\mu^*)$ is a matrix in $\mathbb{R}^{2\times N}$ f.a.a. $\mathbf{x}\in\Omega_B$ and

$$\Big(\big(b_\mu(\cdot\,,\mu^*)(\mu-\mu^*)\big)\cdot\nabla u^*\Big)\,p^*=\sum_{k=1}^{N}(\mu_k-\mu_k^*)\Big(\big(b_k\cdot\nabla u^*\big)p^*\Big),\tag{4.16}$$

where for $1\le k\le N$ we introduce the vectors

$$b_k=\big(\big(b_k\big)_i\big)\in\mathbb{R}^2\quad\text{with}\quad\big(b_k\big)_i=\left(b_\mu(\mathbf{x},\mu^*)\right)_{ik}\ \text{ for } 1\le i\le 2.$$

Combining (4.14)–(4.16) and (4.13c) we obtain the following result

Theorem 4.8. *Assume that a fixed reference solution $x^*=(u^*,\mu^*)\in X_{\mathrm{ad}}$ to $(\mathbf{P}_\mu)$ is given. Let Assumptions* 1 *and* 2 *hold and let p^* denote the unique Lagrange multiplier satisfying* (4.13). *Then, the* variational inequality

$$\sum_{k=1}^{N}(\mu_k-\mu_k^*)\cdot\left(\kappa\left(\mu_k^*-\mu_k^\circ\right)+\int_{\Omega_B}\big(A_k\nabla u^*\big)\cdot\nabla p^*+\big(b_k\cdot\nabla u^*\big)p^*\,\mathrm{d}\mathbf{x}\right)\ge 0$$

holds for all $\mu\in D_{\mathrm{ad}}$. □

4.4. **The reduced gradient.** In Section 3 we have introduced the reduced cost functional $J^{\mathrm{red}}:D_{\mathrm{ad}}\to[0,\infty)$ by

$$J^{\mathrm{red}}(\mu)=J(u_\mu,\mu)\quad\text{for }\mu\in D_{\mathrm{ad}},$$

where $u_\mu\in V_0$ satisfies $e(u_\mu,\mu)=0$ in V_{D}'.

Let Assumptions 1 and 2 hold. From Lemmas 4.1 and 4.2 it follows that J^{red} is differentiable and its derivative $\nabla J^{\mathrm{red}}(\mu)\in\mathbb{R}^N$ at a given $\mu\in D_{\mathrm{ad}}$ satisfies

$$\nabla J^{\mathrm{red}}(\mu)^T\mu_\delta=\langle J_u(u_\mu,\mu),u_\mu'\mu_\delta\rangle_{V_0',V_0}+J_\mu(u_\mu,\mu)\mu_\delta\tag{4.17}$$

for any direction $\mu_\delta\in D$. From $e(u_\mu,\mu)=0$ and Lemma 4.2 we conclude that

$$e_u(u_\mu,\mu)u_\mu'\mu_\delta+e_\mu(u_\mu,\mu)\mu_\delta=0\in V_{\mathrm{D}}'\tag{4.18}$$

for any direction $\mu_\delta \in D$. Note that (u_μ, μ) belongs to $\mathcal{F}(\mathbf{P}_\mu)$. Then, Lemma 4.5 implies that $e_u(u_\mu, \mu)^{-1} : V_{\mathrm{D}}' \to V_0$ is a linear and bounded operator so that we infer from (4.18)

$$u_\mu' \mu_\delta = -e_u(u_\mu, \mu)^{-1}\big(e_\mu(u_\mu, \mu)\mu_\delta\big) \in V_0. \tag{4.19}$$

Inserting (4.19) into (4.17) we find

$$\begin{aligned}
\nabla J^{\mathrm{red}}(\mu)^T \mu_\delta &= -\big\langle J_u(u_\mu, \mu), e_u(u_\mu, \mu)^{-1}\big(e_\mu(u_\mu, \mu)\mu_\delta\big)\big\rangle_{V_0', V_0} + J_\mu(u_\mu, \mu)^T \mu_\delta \\
&= J_\mu(u_\mu, \mu)^T \mu_\delta - \big\langle e_\mu(u_\mu, \mu)\mu_\delta, e_u(u_\mu, \mu)^{-1}\big(J_u(u_\mu, \mu)\big)\big\rangle_{V_0', V_0} \\
&= \Big(J_\mu(u_\mu, \mu) - e_\mu(u_\mu, \mu)^\star \, e_u(u_\mu, \mu)^{-\star}\big(J_u(u_\mu, \mu)\big)\Big)^T \mu_\delta,
\end{aligned}$$

where

$$e_u(u_\mu, \mu)^{-\star} : V_0' \to V_{\mathrm{D}} \quad \text{and} \quad e_\mu(u_\mu, \mu)^\star : V_{\mathrm{D}} \to D$$

are the adjoint operators of $e_u(u_\mu, \mu)^{-1}$ and $e_\mu(u_\mu, \mu)$, respectively. Setting

$$\lambda = -e_u(u_\mu, \mu)^{-\star}\big(J_u(u_\mu, \mu)\big) \in V_{\mathrm{D}},$$

the reduced gradient is represented by

$$\nabla J^{\mathrm{red}}(\mu) = J_\mu(u_\mu, \mu) + e_\mu(u_\mu, \mu)^\star \, \lambda \in \mathbb{R}^N. \tag{4.20}$$

Notice that $L_\mu(u_\mu, \mu, \lambda) = \nabla J^{\mathrm{red}}(\mu)$ holds. In particular, we obtain

$$\begin{aligned}
\big(\nabla J^{\mathrm{red}}(\mu)\big)_k &= \big(L_\mu(u_\mu, \mu, p)\big)_k \\
&= \kappa\left(\mu_k - \mu_k^\circ\right) + \int_{\Omega_B} \big(A_k \nabla u_\mu\big) \cdot \nabla p + \big(b_k \cdot \nabla u_\mu\big) p \, \mathrm{d}\mathbf{x}
\end{aligned}$$

for $k = 1, \ldots, N$, where p solves the adjoint system and u is the solution to the state equation for the parameter μ.

5. A Numerical optimization method

We solve the minimization problem $(\mathbf{P}_\mu^{\mathrm{red}})$ (see beginning of Section 3) numerically by applying a gradient projection method; see, e.g., in [6, 10]. The admissible parameter space is an N-dimensional cube given by

$$D_{\mathrm{ad}} \quad := \quad \bigtimes_{i=1}^{N} J_i, \qquad J_i := [\underline{\mu}_i, \overline{\mu}_i],$$

with

$$\underline{\mu}_i \le \mu_i \le \overline{\mu}_i, \quad i = 1, \ldots, N.$$

By $\mathcal{P} : \mathbb{R}^N \to D_{\mathrm{ad}}$ we denote the common projection defined by

$$\big(\mathcal{P}(\mu)\big)_i = \begin{cases} \underline{\mu}_i & \text{if } \mu_i < \underline{\mu}_i, \\ \mu_i & \text{if } \underline{\mu}_{i-1} \le \mu_i \le \overline{\mu}_i, \\ \overline{\mu}_i & \text{if } \mu_i > \overline{\mu}_i \end{cases}$$

for $\mu = (\mu_1, \ldots, \mu_N) \in D$ and $i = 1, \ldots, N$. The gradient projection method is presented in Algorithm 1. If ∇J^{red} is Lipschitz continuous, then every accumulation point $\mu^* \in D_{\mathrm{ad}}$ of the sequence $\{\mu^k\}_{k \in \mathbb{N}}$ generated by Algorithm 1 is a stationary point, i.e., $\nabla J^{\mathrm{red}}(\mu^*) = 0$; see [6, p. 95], for instance.

Algorithm 1 (Gradient projection method)

Choose a starting value $\mu^{(0)} \in D_{\mathrm{ad}}$, the stopping tolerances $0 < \varepsilon_{\mathrm{rel}} \leq \varepsilon_{\mathrm{abs}}$, a maximal number $k_{\max}$ of iterations, the scalars $\varrho > 0$, $\beta \in (0,1)$ and $c \in (0,1)$ (e.g., $c = 10^{-4}$); set $k = 0$.
repeat
  Compute the cost $J^{\mathrm{red}}(\mu^{(k)})$ and its gradient $\nabla J^{\mathrm{red}}(\mu^{(k)})$.
  if $|\nabla J^{\mathrm{red}}(\mu^{(k)})|_2 < \varepsilon_{\mathrm{abs}}$ **or** $|\nabla J^{\mathrm{red}}(\mu^{(k)})|_2 < \varepsilon_{\mathrm{rel}}\, |\nabla J^{\mathrm{red}}(\mu^{(0)})|_2$ **then**
    Return $\mu^{(k)}$ and stop.
  else {Projection step}
    Set $d^{(k)} = -\nabla J^{\mathrm{red}}(\mu^{(k)})$.
    Find the least integer m such that

$$J^{\mathrm{red}}(\mu_k(\beta^m)) - J^{\mathrm{red}}(\mu^{(k)}) \leq \frac{-c}{\beta^m} \,\|\mu_k(\beta^m) - \mu^{(k)}\|_2$$

    with $\mu_k(\beta^m) := \mathcal{P}(\mu^{(k)} + \beta^m\, d^{(k)})$.
    Set $\mu^{(k+1)} = \mu_k(\beta^m)$ and $k = k + 1$.
  end if
until $k = k_{\max}$.

6. An Application: A rotor with moving blades

In this section, we describe the already mentioned example that has been motivated by the Voith Schneider Propeller (VSP)[2], a ship propulsion and steering system, see e.g. [2, 13]. On the VSP, a rotor casing which ends flush with the ship's bottom is fitted with a number of axially parallel blades and rotates about a vertical axis. To generate thrust, each of the propeller blades performs an oscillating motion about its own axis (similar to the motion of the tail fin of a fish). This is superimposed by a uniform rotary motion. We use this as a model here.

6.1. **Problem formulation.** We consider the case of five blades that are fixed on a rotating disc (the rotor) which are rotated with an angle ϕ. At each rotation angle ϕ (the *phase angle*) of the rotor, each blade B_i, $i \in \{1, \dots, 5\}$, is oriented around an angle $\nu_i \in J_i$ with respect to the tangential of the circle. The geometry is shown in Figure 6.1. Note the particular subdivision of the domain, where we have labeled the blades in the reference situation (c.p. Section 6.2) as well as the outer part of the domain (Ω_E) to which we will refer in the sequel.

In the true model, the angles ν_i are not completely free, but linked by a mechanical control (see Figure 6.1) in the following sense. Given a so-called *blade steering curve*

$$\alpha \in C^2_{2\pi} = \left\{ \tilde{\alpha} \in C^2([0, 2\pi]) \,\middle|\, \tilde{\alpha} \text{ is } 2\pi \text{ periodic} \right\},$$

the angles are given by $\nu_i(\phi) := \alpha\big(\phi + 2\pi(i-1)/N_B\big)$ for $i = 1, \dots, N_B$ (the number of blades, i.e., here $N_B = 5$). The ultimate goal is to determine a blade steering curve that gives rise to optimal efficiency, [5, 13]. This requires of course an instationary model. Here, we consider a simplified stationary model, i.e., instead of varying the *blade steering curve* itself, in each blade we consider an independent variation from a fixed *blade steering curve*, i.e. $\nu_i(\phi) := \alpha\big(\phi + 2\pi(i-1)/N_B\big) + \tilde{\nu}_i$

[2]Voith Turbo Marine, Heidenheim, Germany, http://www.voithturbo.de/marine

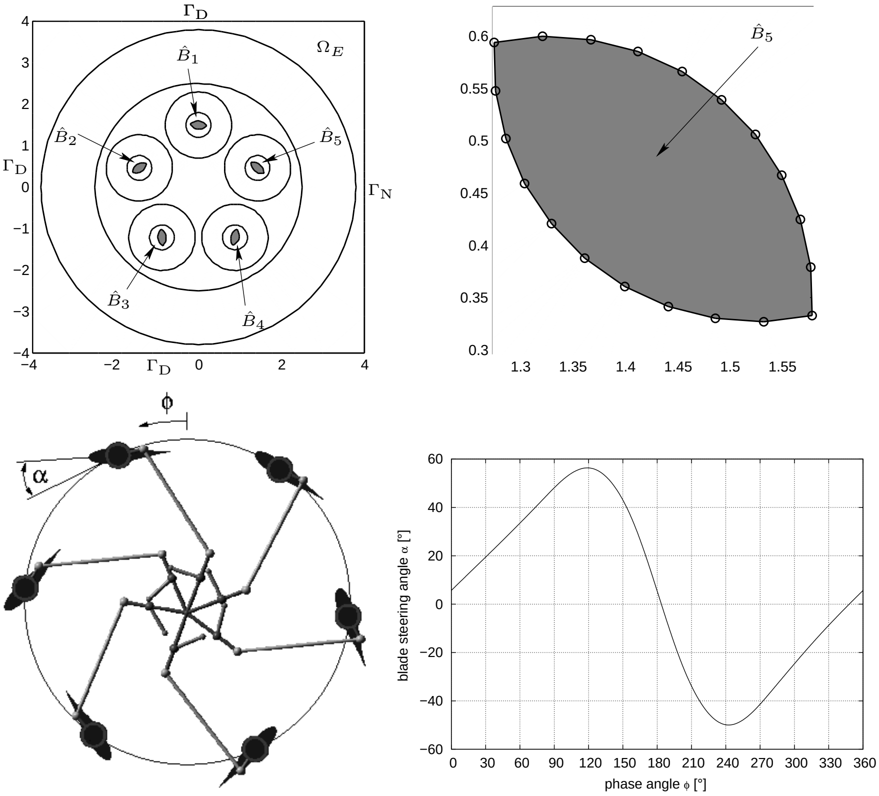

FIGURE 6.1. Top: Initial configuration for our numerical tests (left); Magnification of an arbitrary blade (right). Bottom: Blade angle ϕ and steering angle α for a VSP with 6 blades (left); Blade steering curve (right).

for $i = 1, \dots, N_B$, for a variable phase angle ϕ. For technical reasons, the range of these variations $(\tilde{\nu}_i)_{i=1,\dots,5}$ is typically restricted to

$$\tilde{\nu}_i \in J_i = \left[-\frac{\pi}{12}, \frac{\pi}{12} \right] = \big[-15°, 15° \big] \quad \text{for } i \in \{1, \dots, 5\}.$$

Moreover, since the whole model is periodic, it is sufficient to consider $\phi \in I = [-\pi/5, \pi/5]$ in the case of five blades. Hence, we have the parameter vector

$$(\tilde{\nu}_1, \dots, \tilde{\nu}_5, \phi) \in D_{\mathrm{ad}} := \big(J_1 \times \dots \times J_5\big) \times \left[-\frac{\pi}{5}, \frac{\pi}{5} \right] =: \bigtimes_{i=1}^{6} J_i \subset \mathbb{R}^6$$

describing the location of the five blades. It will be convenient to denote $\tilde{\nu}_6 := \phi$ so that we have a parameter vector

$$\mu = (\tilde{\nu}_1, \dots, \tilde{\nu}_{N_B+1})^T \in D_{\mathrm{ad}} \subset \mathbb{R}^{N_B+1},$$

i.e., $N = N_B + 1$ in the context of Sections 2–4. The blades in their original position (determined by the given α) are denoted by $B_{i,0}$, $i = 1, \dots, N_B$, and the moved ones by $B_{i,\mu}$. By

$$B_\mu := \bigcup_{i=1}^{N_B} B_{i,\mu} \subset \Omega,$$

we denote the part of Ω containing the rigid bodies for a parameter vector μ and we set $\Omega_\mu = \Omega \setminus B_\mu$. Suppose that for any $\mathbf{x} \in \Omega_\mu$ the matrix $\underline{\underline{\alpha}}(\mathbf{x})$ is bounded, $\underline{\underline{\alpha}} \in C^1_{\text{loc}}(\bar{\Omega}_\mu; \mathbb{R}^{2\times 2})$ and symmetric, i.e. $\underline{\underline{\alpha}}(\mathbf{x}) = \underline{\underline{\alpha}}(\mathbf{x})^T$ for all $\mathbf{x} \in \Omega_\mu$. Furthermore, let $\underline{\beta} \in C^1_{\text{loc}}(\bar{\Omega}_\mu; \mathbb{R}^2)$ be a given bounded convection field. Then, we consider the convection-diffusion problem for u

$$-\nabla \cdot (\underline{\underline{\alpha}}(\mathbf{x})\nabla u(\mathbf{x})) + \underline{\beta}(\mathbf{x}) \cdot \nabla u(\mathbf{x}) = f(\mathbf{x}) \qquad \text{f.a.a. } \mathbf{x} \in \Omega_\mu, \tag{6.1a}$$

$$u(\mathbf{x}) = 0 \qquad \text{f.a.a. } \mathbf{x} \in \partial B_\mu, \tag{6.1b}$$

$$u(\mathbf{x}) = 0 \qquad \text{f.a.a. } \mathbf{x} \in \Gamma_{\mathrm{D}}, \tag{6.1c}$$

$$n(\mathbf{x}) \cdot (\underline{\underline{\alpha}}(\mathbf{x})\nabla u(\mathbf{x})) = g(\mathbf{x}) \qquad \text{f.a.a. } \mathbf{x} \in \Gamma_{\mathrm{N}}, \tag{6.1d}$$

where Γ_{N} is the Neumann part of the outer boundary, Γ_{D} the Dirichlet part of $\partial\Omega$, $f : \Omega_\mu \to \mathbb{R}$ denotes a fixed inhomogeneity, $g : \Gamma_{\mathrm{N}} \to \mathbb{R}$ is a given boundary data, and $n = n(\mathbf{x})$ denotes the outward normal vector. For the right-hand side f, we assume

$$f\big|_{\Omega_\mu \setminus \Omega_E} \equiv 0, \tag{6.2}$$

which means that f vanishes outside of Ω_E (c.p. Figure 6.1). Note, that (6.2) allows also non-homogeneous Dirichlet boundary conditions in (6.1c). In fact, posing $u = \tilde{g}$ on Γ_{D} instead of (6.1c) requires to solve (6.1a) with the exterior force $\tilde{f} := f + \nabla \cdot (\underline{\underline{\alpha}}(\cdot)\nabla u_{\tilde{g}}) - \underline{\beta}(\cdot) \cdot \nabla u_{\tilde{g}}$, where $u_{\tilde{g}}$ is a homogenizer that should vanish outside of Ω_E, i.e., $u_{\tilde{g}}|_{\Gamma_{\mathrm{D}}} = \tilde{g}$ and $u_{\tilde{g}}|_{\Omega\setminus\Omega_E} \equiv 0$, to meet (6.2) for $\tilde{f}$.

In order to state the weak formulation of (6.1), we have to define parameter-dependend trial and test spaces as follows

$$\begin{aligned} V_\mu &:= H^1(\Omega_{B_\mu}) \\ V_{\mathrm{D};\mu} &:= \{v \in V_\mu : \, v = 0 \text{ on } \Gamma_{\mathrm{D}}\}, \\ V_{0;\mu} &:= \{v \in V_{\mathrm{D};\mu} : v = 0 \text{ on } \partial B_\mu\}, \end{aligned}$$

Then, for chosen $\mu \in \mathbb{R}^{N_B+1}$, the function $u \in V_{0;\mu}$ is called a *weak solution to* (6.1) provided

$$\int_{\Omega_\mu} \big(\underline{\underline{\alpha}}\nabla u\big) \cdot \nabla\varphi + \big(\underline{\beta} \cdot \nabla u\big)\varphi \, \mathrm{d}\mathbf{x} = \int_{\Omega_E} f\,\varphi \, \mathrm{d}\mathbf{x} + \int_{\Gamma_N} g\,\varphi \, \mathrm{d}\mathbf{x} \quad \text{for } \varphi \in V_{0;\mu}. \tag{6.3}$$

Introducing for $\mu \in \mathbb{R}^{N_B+1}$ the parametrized bilinear and bounded form $a(\cdot\,,\cdot\,;\mu) : V_\mu \times V_\mu \to \mathbb{R}$ as

$$a(\varphi, \psi; \mu) = \int_{\Omega_\mu} \big(\underline{\underline{\alpha}}\nabla\varphi\big) \cdot \nabla\psi + \big(\underline{\beta} \cdot \nabla\varphi\big)\psi \, \mathrm{d}\mathbf{x} \quad \text{for } \varphi \in V_\mu,$$

we can write (6.3) compactly as

$$a(u, \varphi; \mu) = \langle f, \varphi\rangle_{L_2(\Omega_E)} + \langle g, \varphi\rangle_{L_2(\Gamma_N)} \quad \text{for all } \varphi \in V_{0;\mu}. \tag{6.4}$$

Obviously, this problem does not fit immediately into the framework of parameterized convection-diffusion problems as presented above since here the domain Ω_μ depends on the parameter. However, using a standard approach, namely transforming this parameter-dependend domain to a fixed reference domain, will lead us to the above form. In fact, the change of variables causes the presence of parameter-dependend coefficient functions. Hence, we will now describe the reduction to a reference situation.

6.2. **Reduction to a reference situation.** As already said, it is natural to transform the problem to a reference situation with a fixed domain. In the example problem of the Voith-Schneider propeller, the parameter μ describes a rotation. Therefore, the desired transformation is not too difficult, if we subdivide the domain as shown in the left part of Figure 6.1.

The reference situation is given in terms of the initial position of the blades, i.e., $\hat{\mu} \equiv 0$,

$$\hat{B} := B_{\hat{\mu}} = \bigcup_{i=1}^{N_B} B_{i,\hat{\mu}}$$

and the reference domain by $\hat{\Omega} := \Omega \setminus \hat{B}$. Then, we set

$$\hat{V} := V_{\hat{\mu}}, \quad \hat{V}_{\mathrm{D}} := V_{\mathrm{D};\hat{\mu}}, \quad \hat{V}_0 = V_{0;\hat{\mu}},$$

and proceed by transforming the variational problem (6.3) to a reference domain $\hat{\Omega}$. Then, we shall see that a weak solution $\hat{u} \in \hat{V}_0$ satisfies

$$\begin{aligned} &\int_{\hat{\Omega}} \Big(\big(T^{(1)}(\hat{\mathbf{x}}, \mu)\nabla\hat{u}(\hat{\mathbf{x}})\big) \cdot \nabla\hat{\varphi}(\hat{\mathbf{x}}) + \big(T^{(2)}(\hat{\mathbf{x}}, \mu) \cdot \nabla\hat{u}(\hat{\mathbf{x}})\big)\hat{\varphi}(\hat{\mathbf{x}}) \Big)\, \mathrm{d}\hat{\mathbf{x}} \\ &\qquad = \int_{\Omega_E} f(\hat{\mathbf{x}})\, \hat{\varphi}(\hat{\mathbf{x}})\, \mathrm{d}\hat{\mathbf{x}} + \int_{\Gamma_{\mathrm{N}}} g(\hat{\mathbf{x}})\, \hat{\varphi}(\hat{\mathbf{x}})\, \mathrm{d}\hat{\mathbf{x}} \quad \text{for all } \hat{\varphi} \in \hat{V}_0, \end{aligned} \tag{6.5}$$

where $T^{(1)} : \hat{\Omega} \times D_{\mathrm{ad}} \to \mathbb{R}^{2\times 2}$ and $T^{(2)} : \hat{\Omega} \times D_{\mathrm{ad}} \to \mathbb{R}^2$ denote the appropriate, continuous transformations depending on the coefficient functions $\underline{\underline{\alpha}}$ and $\underline{\beta}$, respectively. If

$$\tau : \Omega_\mu \times D_{\mathrm{ad}} \to \hat{\Omega}, \tag{6.6}$$

represents the transformation $\mathbf{x} \in \Omega_\mu \mapsto \hat{\mathbf{x}} = \tau(\mathbf{x}, \mu) \in \hat{\Omega}$, then $\hat{u}(\hat{\mathbf{x}}) = u(\tau(\mathbf{x}, \mu))$ solves (6.5) provided u solves (6.3). Note, that in our case $\tau|_{\Omega_E} \equiv \mathrm{Id}$, i.e. the transformation is the identity in Ω_E, and therefore, the integrals over Ω_E and Γ_{N} in (6.3) remain unchanged in (6.5). Moreover, due to (6.2), f in (6.5) remains independent on the parameter μ in entire $\hat{\Omega}$. Hence, we have reduced this problem to (2.1) with $A \equiv T^{(1)}$, $b \equiv T^{(2)}$ and Ω_B replaced by the reference domain $\hat{\Omega}$.

7. Numerical Experiments

In this final section, we report on the results of several numerical experiments that we have performed. They were all done using FEMLAB version 2.3 in conjunction with MATLAB 6.5. We consider the VSP optimization problem described in the previous section. We always start with the reference configuration that is shown in the Figure 6.1 (left part) as initial value for the optimization. Furthermore, it visualizes the particular division of $\hat{\Omega}$ into sub-domains that is needed to define the transformation τ (see (6.6)) appropriately. For more details refer to [13].

In the right part of Figure 6.1, one arbitrary blade is visualized in order to show that the discretization is chosen in such a way that each edge has the same length. This fact simplifies the implementation of a convolution along the boundary of the blade, which is our choice for the smoothing operator F (c.p. (2.6)). To be more precise, let $\hat{v} = \hat{n} \cdot \big(T^{(1)}(\cdot,\mu)\nabla\hat{u}\big)$, then on blade $\hat{B}_i$ we have

$$\int_{\partial\hat{B}_i} |F(\hat{v}(\hat{\mathbf{x}}))|^2 \,\mathrm{d}\hat{\mathbf{x}} = \int_0^{N_E} |F(\hat{v}(\hat{\mathbf{x}}(s)))|^2 \left|\frac{\partial}{\partial s}\hat{\mathbf{x}}(s)\right|_2 \mathrm{d}s,$$

where N_E is the number of edges, $\hat{\mathbf{x}}(s)$ is an appropriate parameterization of $\partial\hat{B}_i$ and we set

$$F(\hat{v}(\hat{\mathbf{x}}(s))) := \int_{-1}^{1} k(t)\hat{v}(\hat{\mathbf{x}}(s-t))\,\mathrm{d}t.$$

For the kernel we consider two cases, namely the characteristic function $k = \chi_{[-1,1]}$ and the delta dirac function $k = \delta_0$, which obviously results in $F \equiv \mathrm{Id}$. Note, that $k = \chi_{[-1,1]}$ is covered by our analysis concerning the regularity properties of the mapping F, whereas $k = \delta_0$ is not. Recall that by (4.12), the choice of F is crucial for the Dirichlet boundary conditions for the adjoint system on $\partial\hat{B}$. Thus, Figure 7.1 visualizes the functions $\hat{v}(\hat{\mathbf{x}}(s))$ and $p(\hat{\mathbf{x}}(s))$ (c.p. (4.12)) on an arbitrary blade.

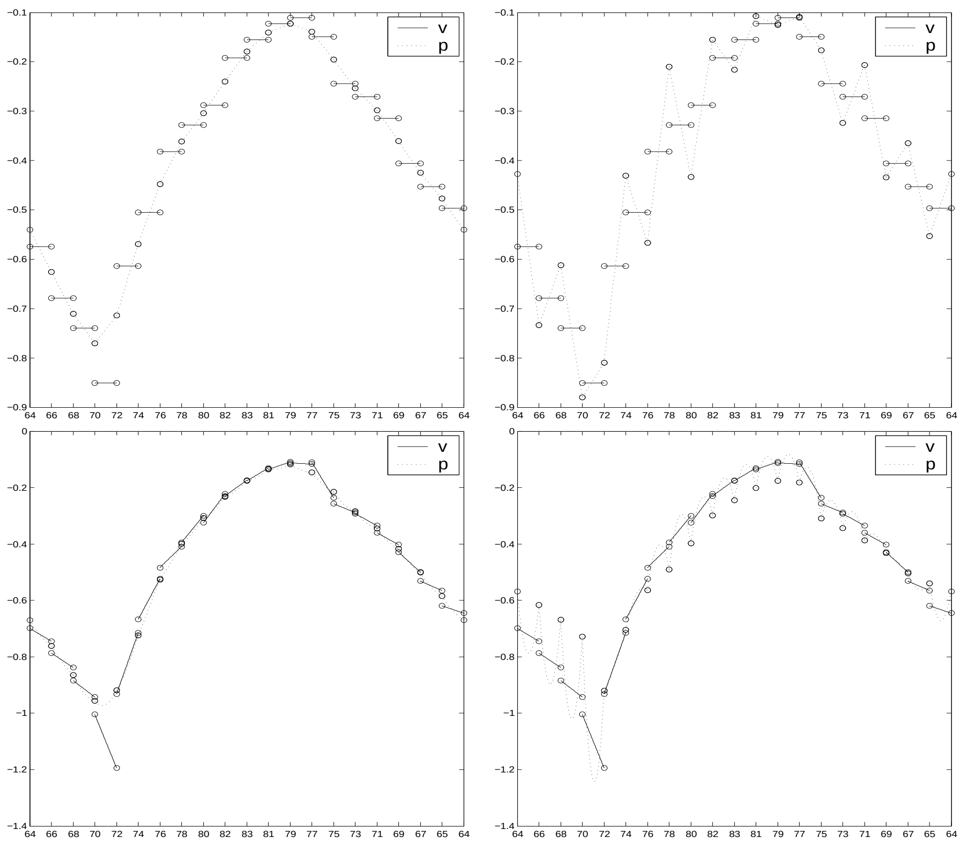

FIGURE 7.1. $\hat{v} = \hat{n} \cdot \big(T^{(1)}(\cdot,\mu)\nabla\hat{u}\big)$ and p on an arbitrary blade using linear (top) and quadratic elements (bottom) and kernels $k = \chi_{[-1,1]}$ (left) and $k = \delta_0$ (right).

7.1. **Standard gradient method.** Before we consider the gradient projection method described above, we want to validate our implementation. This is done by allowing steering angles of the propellers in the interval $[-90°, 90°]$, which means that no constraints are posed, as in this case no projection is expected.

We start visualizing the optimized configuration for a constant (left part of Figure 7.2) and a non-constant (right part of Figure 7.2) velocity field. The results are quite natural since each blade is aligned within the velocity field.

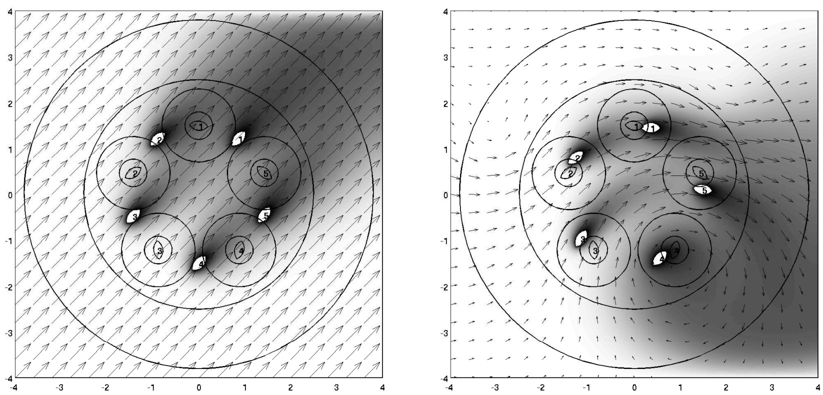

FIGURE 7.2. Optimized configuration for constant (left) and non-constant (right) velocity field and variations from steering curve in $[-90°, 90°]$. In black lines also the start configuration for the optimization method is shown.

For a quantitative analysis, we first consider three different mesh sizes $h = 0.2, 0.1, 0.05$ for the finite element mesh. In Figure 7.3, we show that the convergence history for the reduced cost functional (left) as well as the reduced gradient (right), where we have used the value of the final iteration as 'exact' optimal value of the reduced cost functional. Besides the very last stage of the algorithm (where the final approximation is already basically reached), we obtain the expected asymptotic behavior.

Next, in Figure 7.4 we consider different orders of the finite elements, namely linear and quadratic elements, as well as two different choices of the smoothing function F as described above. We can clearly see the better asymptotic rate of convergence for quadratic elements (Lag=2) as compared to linear elements (Lag=1). Furthermore, we observe basically the same behavior for $k = \chi_{[-1,1]}$, which is covered by our analysis, and for $k = \delta_0$, which is not justified. We interpret this as a quite promising result.

7.2. **Gradient projection method.** In order to investigate the influence of the projection within the scheme, we restrict the steering angles to $[-15°, 15°]$ and run the same tests as for the 'standard' gradient method described above. Again, we start by visualizing the optimized configuration in Figure 7.5. In this case not all the blades are aligned completely within the velocity field. This is obviously due to the restriction within the steering angles.

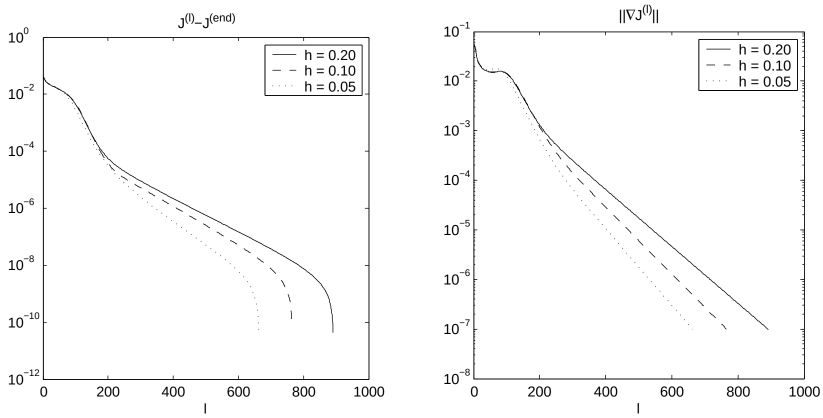

FIGURE 7.3. Convergence history for the gradient method (no projection) for linear elements and mesh sizes $h = 0.2, 0.1, 0.05$.

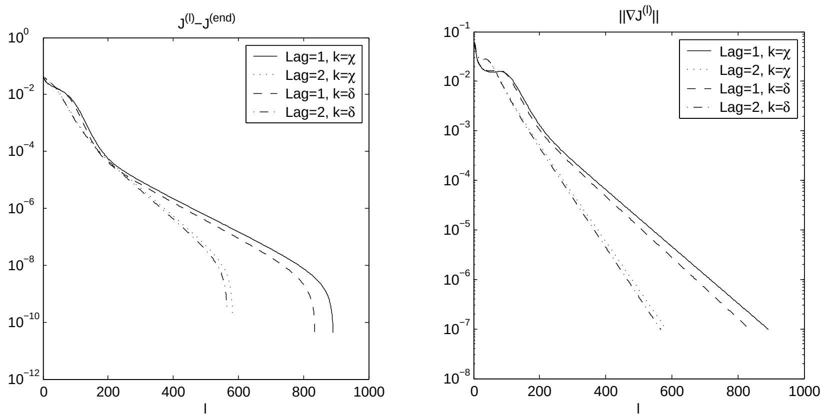

FIGURE 7.4. Convergence history for the gradient method (no projection) for mesh size $h = 0.2$, linear and quadratic elements, as well as smoothing kernels $k = \chi_{[-1,2]}$ and $k = \delta_0$.

Next, we again consider the three different mesh sizes ($h = 0.2, 0.1, 0.05$) for the finite element mesh. In Figure 7.6, we show the convergence history for the reduced cost functional (left) as well as the norm of the projected reduced gradient (right). One can clearly see whenever the next component of the reduced gradient is projected within the scheme. This corresponds to a change of the slope in the right part of the figure.

Finally, in Figure 7.7, we consider again different orders of the finite elements as well as the two different smoothing kernels. Also this case of a projection we can clearly observe the better rate of convergence for quadratic elements (Lag=2) as compared to linear elements (Lag=1). Furthermore, we basically find the same behavior for $k = \chi_{[-1,1]}$ and $k = \delta_0$, as well.

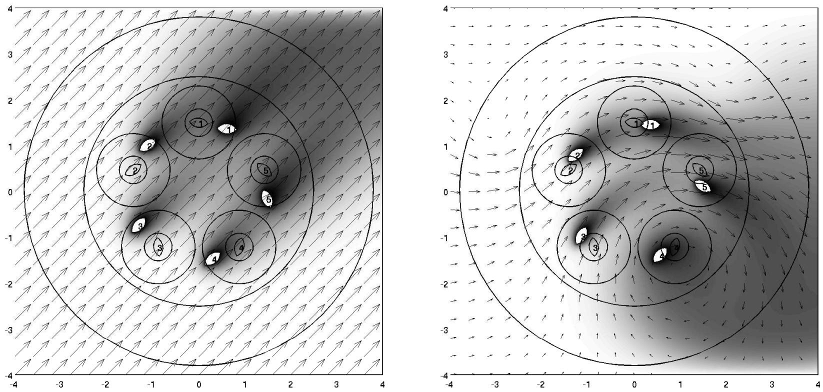

FIGURE 7.5. Optimized configuration for a constant (left) and a non-constant (right) velocity field and variations from steering curve in $[-15°, 15°]$. In black lines also the start configuration for the optimization method is shown.

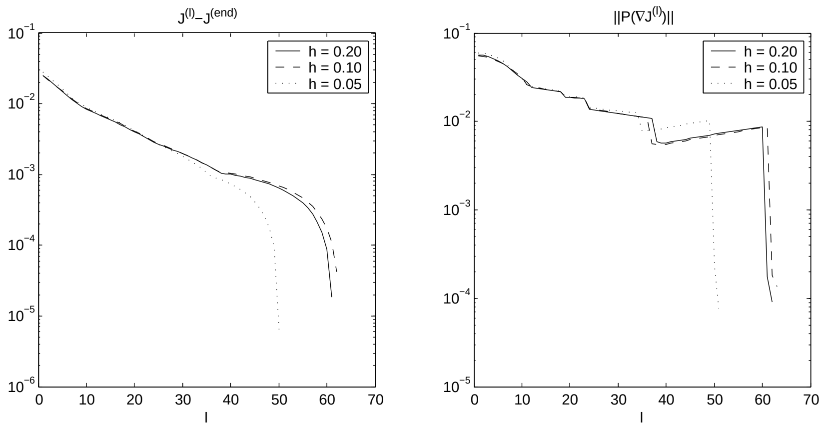

FIGURE 7.6. Convergence history for the projected gradient method for linear elements and mesh sizes $h = 0.2, 0.1, 0.05$.

8. Conclusions and Outlook

We have investigated an optimal control problem for parameterized convection-diffusion equations with a non-classical cost functional and possible lack of regularity in the state. For the latter, from the analytic point of view it has turned out to be essential to introduce a smoothing operator F. We have analyzed existence of solutions, first-order necessary optimality conditions and differentiability of the (reduced) cost functional. For the optimization method itself we utilize the gradient projection method.

For a possible application we choose a simplified model of the VSP. In our numerical experiments, we observe the expected (asymptotic) behavior of a gradient method in all cases. Furthermore, the choice of the smoothing operator $F \equiv \text{Id}$ does not

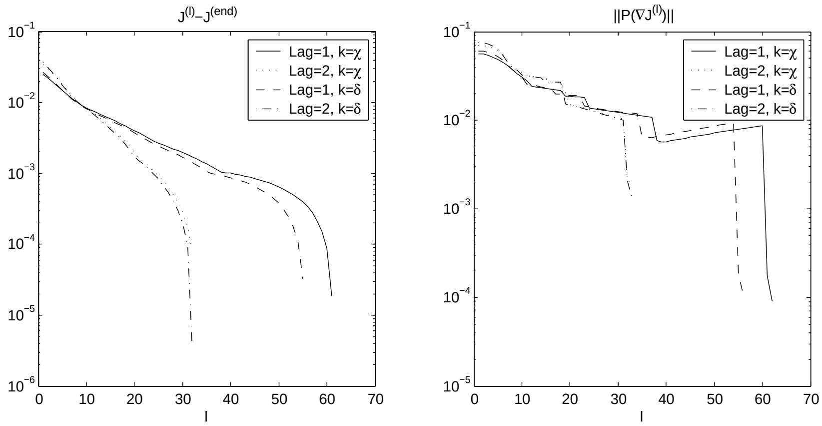

FIGURE 7.7. Convergence history for the projected gradient method for mesh size $h = 0.2$, linear and quadratic elements, as well as convolution kernels $k = \chi_{[-1,1]}$ and $k = \delta_0$.

seem to have a negative influence on the method, although this case is not covered by our analysis.

These quite promising results motivate us to continue the investigation of this problem. One possible direction is to consider the full VSP problem using incompressible flows. Another direction is the application of reduced-basis methods for a rapid computation of the reduced cost functional and the reduced gradient. In terms of this, optimization methods different from the gradient projection method, e.g., a quasi-Newton method, can be investigated and compared.

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Timo Tonn, University of Ulm, Institute for Numerical Mathematics, Helmholtzstrasse 18, D-89069 Ulm, Germany

E-mail address: `timo.tonn@uni-ulm.de`

Karsten Urban, University of Ulm, Institute for Numerical Mathematics, Helmholtzstrasse 18, D-89069 Ulm, Germany

E-mail address: `karsten.urban@uni-ulm.de`

Stefan Volkwein, University of Graz, Institute for Mathematics and Scientific Computing, Heinrichstrasse 36, A-8010 Graz, Austria

E-mail address: `stefan.volkwein@uni-graz.at`