Boundary control of a chemotaxis system

Von der Fakultät für Mathematik der
Universität Duisburg-Essen
zur Erlangung des akademischen Grades eines
Dr. rer. nat.

genehmigte Dissertation

von
Dipl.-Math. Hendrik Feldhordt
aus
Essen

Datum der Einreichung: 11.04.2017

Gutachter: Prof. Dr. Arnd Rösch
Prof. Dr. Christian Meyer

Tag der mündlichen Prüfung: 11.07.2017

Abstract

Chemotaxis describes the directed movement of cells along the gradient of a chemical substance. Mathematically, this can be described by a quasilinear parabolic system of partial differential equations. In the work at hand we analyze an optimal control problem for the chemotaxis equations where the control is located at the boundary. Using the concept of maximal parabolic regularity, we show that for controls $g \in L_r(0,T;L_p(\Gamma))$, where $r \geq 2$ and $p > N$ such that $\frac{2}{r} + \frac{N}{p} < 1$, the state system has a unique solution $(u,v) \in \left[L_r(0,T;W_p^1(\Omega)) \cap W_r^1(0,T;W_p^{-1}(\Omega))\right]^2$. Under the additional assumption that $r > 2p$, the adjoint system, which is needed to derive optimality conditions, has the same regularity. After that, we show that the control problem possesses an optimal solution. We derive necessary optimality conditions of first order for the control problem, which serve as a basis for many numerical methods for finding a solution, as well as sufficient optimality conditions of second order for the control problem. These second order conditions allow us to prove quadratic convergence of an SQP method. This is illustrated in a numerical example.

Zusammenfassung

Chemotaxis beschreibt die gerichtete Bewegung von Zellen entlang des Konzentrationsgradienten eines Lock- oder Schreckstoffs. Mathematisch lässt sich dieses Phänomen durch ein quasilineares System parabolischer Differentialgleichungen beschreiben. In dieser Arbeit betrachten wir ein Optimalsteuerproblem für diese Gleichungen mit Steuerung am Rand des Gebiets. Mit Hilfe des Konzepts der maximalen parabolischen Regularität zeigen wir, dass das Zustandssystem für Steuerungen $g \in L_r(0,T;L_p(\Gamma))$ mit $r \geq 2$ und $p > N$ so, dass $\frac{2}{r} + \frac{N}{p} < 1$ gilt, eindeutig lösbar ist und seine Lösungen im Raum $\left[L_r(0,T;W_p^1(\Omega)) \cap W_r^1(0,T;W_p^{-1}(\Omega))\right]^2$ liegen. Unter der zusätzlichen Bedingung $r > 2p$ besitzt auch das adjungierte System, welches wir für die Formulierung von Optimalitätsbedingungen brauchen, eine eindeutige Lösung im gleichen Raum. Danach zeigen wir, dass auch das Steuerproblem selbst eine Lösung besitzt. Wir leiten sowohl notwendige Optimalitätsbedingungen her, die als Basis für viele numerische Verfahren dienen, als auch hinreichende Bedingungen zweiter Ordnung. Letztere erlauben uns zu zeigen, dass ein SQP-Verfahren für das Steuerproblem quadratisch konvergiert. Dies veranschaulichen wir anhand eines Beispiels.

Danksagung

Diese Dissertation ist in meiner Zeit als wissenschaftlicher Mitarbeiter an der Universität Duisburg-Essen entstanden. Zuerst möchte ich mich bei meinem Betreuer Prof. Dr. Arnd Rösch für seinen Rat, seine Betreuung und die hervorragenden Arbeitsbedingungen bedanken. Mein Dank gilt auch Prof. Dr. Chrisitan Meyer für die Begutachtung meiner Arbeit und vor allem für die sehr hilfreichen Gespräche und Denkanstöße in den letzten Jahren.
Vielen Dank auch an meine Kolleginnen und Kollegen für eine schöne Zeit und gute Atmosphäre, für den Zusammenhalt während und außerhalb der Arbeit.
Vor allem möchte ich auch meiner Familie, meinen Eltern und meinem Bruder Philip für ihr Vertrauen und ihre Unterstützung danken. Ohne sie wäre diese Arbeit nicht möglich gewesen.

Für Knut

Contents

Chapter 1

Introduction

The purpose of the work at hand is to give a detailed analysis of an optimal control problem involving chemotaxis equations with the control acting at the boundary. It contains a proof of existence and uniqueness of solutions to the chemotaxis system with inhomogeneous Neumann boundary values as well as first and second order optimality conditions. In the last two chapters, we will prove quadratic convergence of an SQP method and illustrate the results in a numerical example.

1.1 Chemotaxis

Chemotaxis is a biological phenomenon of self organization and pattern forming of cell populations caused by chemical substances. It describes the directed movement of cells along the concentration gradient of an attractant (positive chemotaxis) or repellent (negative chemotaxis). Many processes in biology are governed by this phenomenon. For example, it plays an important role in the process of embryonic growth, in the growth and spreading of tumor cells or the movement of immune cells towards inflamed tissues. The mathematical analysis of equations modeling chemotaxis has been a field of extensive research over the last decades. Based on the model by Patlak, Keller and Segel (cf. [47], [40]), a lot of work has been done in order to understand the behaviour of solutions to different variants of the model, in particular different choices of the sensitivity function (cf. e.g. [14] [21], [39]). For the minimal model, i.e. choosing $f(u) = u$, global existence has been shown for $N = 1$, for $N > 1$

blow ups of solutions in finite time are known to occur depending on the initial values. Beyond that, there are several approaches of how to produce models which are physically more realistic, for example by including volume filling effects (cf. [32], [46]). [36] is motivated by understanding the mathematical qualities of the blow ups. Most of these models contain the minimal model as a limit case. For more details we refer to [49] and the overview papers [33], [35] as well as the references therein.

So let us introduce the system we will be looking at and give a short explanation: For a cell population u and an attracting substance v, the process of chemotaxis can be described by the quasilinear parabolic system

$$\begin{aligned} u_t &= \Delta u - \nabla \cdot \{f(u)\nabla v\} \\ v_t &= \Delta v - v + u \end{aligned} \quad \text{in } \Omega \times (0,T),$$
$$\begin{aligned} \partial_n u - f(u)\partial_n v &= 0 \\ \partial_n v &= g \end{aligned} \quad \text{on } \Gamma \times (0,T), \qquad \begin{aligned} u(0) &= u_0 \\ v(0) &= v_0 \end{aligned} \quad \text{in } \Omega. \tag{1.1}$$

The second equation is linear and rather simple: The attractant diffuses ("Δv") and disperses ("$-v$") over time, and since it can serve as a means of communication amongst the cells, these cells are able to produce the attracting substance ("$+u$"). Additionally, in order to control the process we want to be able to "inject" quantities of the attractant at the boundary ("$\partial_n v = g$"). Note that since ∂_n denotes the outward normal, injecting means negative values of g. The cells in turn diffuse as well, or rather move around in a random-walk-like fashion ("Δu"). If they sense a concentration gradient of the attractant however, they move towards higher concentrations ("$-\nabla \cdot \{f(u)\nabla v\}$"). This process is mediated by some sensitivity function f depending on the density of cells u. For them we assume no-flux boundary conditions ("$\partial_n u - f(u)\partial_n v = 0$").

1.2 Optimal control with PDE constraints

The mathematical theory of optimal control has become a field of growing importance and has been evolving rapidly over the last decades, combining the theories of partial (or ordinary) differential equations, optimization and numerics. Due to the technological advances, both the number of applications where optimal control is helpful as well as the resources that can be used to tackle these problems are increasing constantly. As a starting point, partial differential equations describe a vast amount of different processes and phenomena in nature and technological applications, in our case the behaviour of bacteria over a certain period of time.

Apart from understanding such a process itself, in the optimal control problem we are interested in the following question: Given we can take influence on one or more parameters in the system, what do we have to do to make the state (i.e. the solution to the system) behave in a desired way? A very simple example would be the question of how a radiator should be regulated in order to keep a certain temperature in a room using as little energy as possible. This can be formulated as an optimization problem: We want to minimize the difference $\frac{1}{2}\|u - u_Q\|^2$ between a desired state u_Q and the actual state u given that u is the solution to the state equation at hand.

For us this means: Assuming we can "inject" the attracting substance from the boundary into the domain we are looking at, how do we have to do this to get the cells to arrange in a certain way at the end of the time interval we are looking at (approximating u_Ω) or during the whole process (approximating u_Q)? Assuming further that we want to use as little of the substance as possible, the objective of the control problem may look like this:

$$J(u, v; g) = \frac{\alpha_1}{2}\|u(T) - u_\Omega\|^2_{L_2(\Omega)} + \frac{\alpha_2}{2}\|u - u_Q\|^2_{L_2(Q)} + \frac{\lambda}{2}\|g\|^2_{L_2(\Sigma)}. \tag{1.2}$$

Another assumption which is reasonable from a mathematical as well as from a physical point of view is to introduce control constraints, that is the amount of the attractant which we can insert into the system is bounded by a minimum amount, naturally it would be reasonable to set this to zero, and a maximum amount,

$$g \in G_{ad} := \{g \in L_r(0, T; L_p(\Gamma)) : g_a \leq g \leq g_b \text{ a.e. in } \Gamma \times (0, T)\}. \tag{1.3}$$

For the distributed control problem, some results can be found in the literature (cf. e.g. [19], [53]). Also, the question of parameter identification which is closely related to optimal control has been studied [17]. To the author's knowledge however there has been no thorough analysis of such a system with boundary control. Since we rely on the theory of maximal parabolic regularity in order to formulate and solve the differential equations, the methods applied in this work are fairly general and would for example allow for mixed boundary conditions or additional terms involving measures.

Of course, in order to make the considerations in optimal control theory applicable to real world problems, efficient methods are needed to be able to obtain solutions numerically. Among others, the SQP (Sequential Quadratic Programming) method, a Newton-like algorithm that solves a sequence of linear quadratic subproblems, has proven to be an good choice.

1.3 Structure of the thesis

This work is structured as follows: In the **second chapter**, we will specify notation and give the analytical background needed in the course of the thesis. In particular, the concept of maximal parabolic regularity is introduced and the central results and methods we need are presented.
In the **third chapter**, we are going to present the results on existence, uniqueness and regularity of solutions to the particular partial differential equations that occur throughout this work. This way, the difficulties arising from the pdes and the key arguments of the optimal control problem are separated a bit and it is easier to focus on each of these fields one by one.
In **chapter four**, we will introduce the control-to-state operator $\mathcal{G}$ mapping the control g onto the solution (u, v) of the system (1.1). By substituting the state (u, v) in the objective (1.2), we can reduce the optimal control problem and just minimize with respect to the control g. This simplifies the further analysis of the problem. Also, the adjoint equation, which will be part of the first order optimality system, is introduced.
Chapter five guarantees the solvability of (1.1)-(1.3), that is we prove that there exists an optimal solution to the problem (which, due to the nonlinear constraints, does not need to be unique). The arguments needed here are rather standard.
In **chapter six**, necessary optimality conditions of first order are derived and the KKT system is presented. Typically, this is the basis for most numerical methods to compute an optimal solution, the simplest for example being the gradient method.
In **chapter seven**, necessary — and more importantly sufficient optimality

conditions of second order are derived. Although there is no simple way to check these conditions numerically, if they hold they guarantee convergence of fast and efficient numerical methods such as the SQP algorithm.
Chapters eight and **nine** are devoted to proving convergence of such an SQP method and illustrating its behaviour in a numerical example.

1.4 General assumptions

In the course of this work, we will put several restrictions on the functions and coefficients describing the control problem. These will be introduced and explained whenever they are needed. For convenience and to get a better overview, before we get started let us gather that information here. We will always assume:

- $N \geq 2$, $\Omega \subset \mathbb{R}^N$ open, bounded an strongly Lipschitz, $T > 0$;
- $p > N$ and $r > 2p$ such that $\frac{2}{r} + \frac{N}{p} < 1$. From chapter 7 onwards, we will additionally need that $p > 2N$;
- $u_0 \in \mathcal{D}_{r,p}$, $v_0 \in W_p^1(\Omega)$, $u_Q \in L_r(L_p(Q))$, $u_\Omega \in \mathcal{D}_{r,p}$;
- $f : \mathbb{R}^+ \to \mathbb{R}$ twice continuously differentiable and such that

$$\left.\begin{array}{r}
f(x) \leq c_f,\ f'(x) \leq c_{f'}\ f''(x) \leq c_{f''} \text{ for all } x \in \mathbb{R}^+ \\
\left.\begin{array}{rl}
|f(x) - f(y)| \leq & L|x-y|, \\
|f'(x) - f'(y)| \leq & L_{f'}|x-y|, \\
|f''(x) - f''(y)| \leq & L_{f''}|x-y|
\end{array}\right\} \text{ for all } x, y \in \mathbb{R}^+;
\end{array}\right\}$$

- $\alpha_1 > 0$, $\alpha_2 > 0$, $\lambda > 0$;
- $g_a, g_b \in L_r(L_p(\Gamma))$ such that $g_a(x,t) \leq g_b(x,t)$ for a.e. $(x,t) \in \Sigma$.

Chapter 2

Linear parabolic problems

Throughout this work, we will assume Ω to be an open and bounded subset of $\mathbb{R}^N$, $N \geq 2$ with Lipschitz boundary (often also called a strong Lipschitz domain, cf. [30], Def. 1.2.1.1). Most of the results remain true for less regular domains and the case $N = 1$ can be carried out with slight modifications as well, for the sake of clarity however we are not going to go into detail. For $T > 0$ and the time interval $[0, T]$, we denote by $Q := \Omega \times (0, T)$ the parabolic cylinder and by $\Sigma := \Gamma \times (0, T)$ its boundary.

2.1 Function spaces

To get started, we will go through the function spaces over Ω that will be used in the following. For more information, we refer for example to [18]. First of all, with $C(\bar{\Omega})$ ($\bar{\cdot}$ denoting the closure) we denote the Banach space of all continuous functions $u : \bar{\Omega} \to \mathbb{R}$ equipped with the norm

$$\|u\|_{C(\bar{\Omega})} := \max_{x \in \bar{\Omega}} |u(x)|.$$

For $1 \leq p < \infty$, the space of all real-valued functions defined on Ω, whose p-th powers are integrable with respect to the Lebesgue measure, endowed with the norm

$$\|u\|_{L_p(\Omega)} := \left(\int_\Omega |u(x)|^p \, dx \right)^{\frac{1}{p}}$$

is a Banach space and denoted by $L_p(\Omega)$. For $p=\infty$, we obtain the Banach space of all essentially bounded functions $u:\Omega\to\mathbb{R}$, where

$$\|u\|_{L_\infty(\Omega)} := \operatorname{ess\,sup}_{x\in\Omega} |u(x)|.$$

For $1<p<\infty$, the dual space to $L_p(\Omega)$ can be identified with $L_{p'}(\Omega)$, where $1<p'<\infty$ is the Hölder conjugate of p defined by $\frac{1}{p}+\frac{1}{p'}=1$. For $u\in L_p(\Omega)$, $v\in L_{p'}(\Omega)$, the dual pairing is defined as

$$\langle u,v\rangle_{L_p,L_{p'}} := \int\limits_\Omega u(x)v(x)\;dx.$$

For $p=p'=2$, this duality product becomes the scalar product of the Hilbert space $L_2(\Omega)$. For $k\in\mathbb{N}$, $1\le p<\infty$, the Sobolev space $W_p^k(\Omega)$ of all functions $u\in L_p(\Omega)$, whose weak derivatives up to power k are in $L_p(\Omega)$, becomes a Banach space with the help of the norm

$$\|u\|_{W_p^k(\Omega)} := \left(\sum_{|\alpha|\le k} \|D^\alpha u\|_{L_p}^p\right)^{\frac{1}{p}}$$

($\alpha\in\mathbb{N}^N$ is a multiindex). The dual space to $W_p^k(\Omega)$ is denoted by

$$W_{p'}^{-k}(\Omega) := \left(W_p^k(\Omega)\right)^*,$$

$\frac{1}{p}+\frac{1}{p'}=1$ (note that this is not the same as the dual space to $W_{p,0}^k(\Omega)$ which is commonly denoted by $W_{p'}^{-k}(\Omega)$ as well). For $u\in W_p^k(\Omega)$, $\phi\in W_{p'}^{-k}(\Omega)$, the naturally induced duality pairing is given by

$$\langle\phi,u\rangle_{W_p^{-k},W_{p'}^k} := \phi(u).$$

Once again, in the case $p=p'=2$ $H^k(\Omega):=W_2^k(\Omega)$ becomes a Hilbert space. On several occasions, we will need some kind of intermediate spaces between the classical Sobolev spaces. In the context of maximal parabolic regularity it is most convenient to use spaces of Bessel potentials $H_p^s(\Omega)$, $s\ge 0$, defined by the restriction to Ω of

$$H_p^s(\mathbb{R}^n) := \left\{u\in L_p(\mathbb{R}^n):\ \|u\|_{H_p^s(\mathbb{R}^n)} := \|\mathcal{F}^{-1}\left((1+|\cdot|^2)^{\frac{s}{2}}\mathcal{F}u\right)\|_{L_p(\mathbb{R}^n)}<\infty\right\},$$

where $\mathcal{F}$ denotes the Fourier transform equipped with the norm

$$\|u\|_{H_p^s(\Omega)} := \inf_{v\in H_p^s(\mathbb{R}^n),v|_\Omega=u} \|v\|_{H_p^s(\mathbb{R}^n)},$$

(cf. [56] 2.3.3, 4.2.1). As before, for $s < 0$ the spaces $H_p^s(\Omega)$ are defined by duality. For $s = k \in \mathbb{N}$, $W_p^k(\Omega)$ and $H_p^k(\Omega)$ can actually be identified with each other. For general $s \in \mathbb{R}$, Sobolev spaces and Bessel potential spaces are connected as well: We have

$$[W_p^{-1}(\Omega), W_p^1(\Omega)]_\theta = H_p^s(\Omega),$$

where $[\cdot,\cdot]_\theta$ is the complex interpolation functor and $s = -1 + 2\theta$, $0 < \theta < 1$. For nonsmooth domains like the ones we are looking at, this result can be found in [25]. In particular, it holds that

$$[W_p^{-1}(\Omega), W_p^1(\Omega)]_{\frac{1}{2}} = L_p(\Omega).$$

In the course of this thesis we will also need real interpolation spaces between $W_p^{-1}(\Omega)$ and $W_p^1(\Omega)$, which would lead to Besov spaces $B_{p,q}^s(\Omega)$. For our purposes however, it is enough to point out that there is a continuous embedding

$$(W_p^{-1}(\Omega), W_p^1(\Omega))_{1-\frac{1}{r},r} \hookrightarrow [W_p^{-1}(\Omega), W_p^1(\Omega)]_\theta = H_p^{-1+2\theta}(\Omega) = H_p^{1-\frac{2}{r}-\varepsilon}(\Omega)$$

for $\theta \in (0, 1-\frac{1}{r})$ and $0 < \varepsilon < 2-\frac{2}{r}$ (cf. [34], Lemma 3.17). For more details on interpolation we refer to [1], [11] and [56]. The following embedding properties can be found for example in [56], 4.6.1: For $0 \le t \le s < \infty$, $1 < p \le q < \infty$ it holds that

$$\begin{aligned} H_p^s(\Omega) &\hookrightarrow H_q^t(\Omega) \quad \text{for } s - \frac{N}{p} \ge t - \frac{N}{q}, \\ H_p^s(\Omega) &\hookrightarrow C(\bar{\Omega}) \quad \text{for } s > \frac{N}{p}. \end{aligned} \tag{2.1}$$

Due to duality arguments, the first embedding indeed more generally holds for every $-\infty < s, t < \infty$.

Finally, since functions in $L_p(\Omega)$ are only defined almost everywhere in its domain, looking at boundary value problems we have to specify what exactly we mean by the value of such a function on the boundary Γ. This question is answered by the

Theorem 2.1 (Trace Theorem)**.** *Let $2 \le p < \infty$ and $s > \frac{1}{p}$. There is a linear continuous mapping $\gamma : H_p^s(\Omega) \to L_p(\Gamma)$ such that for all $u \in C(\bar{\Omega}) \subset H_p^s(\Omega)$ we have*

$$(\gamma u)(x) = u(x) \quad \textit{for all } x \in \Gamma,$$

hence there is a constant $c > 0$ *such that*

$$\|\gamma u\|_{L_p(\Gamma)} \leq c\|u\|_{H_p^s(\Omega)}$$

for all $u \in H_p^s(\Omega)$.

This result can be found for example in [1], 7.43, 7.45 formulated in the Besov space $B_{p,p}^s(\Omega)$. It holds however that $H_p^s(\Omega) \hookrightarrow B_{p,p}^s(\Omega)$, $p \geq 2$, so that the above formulation works as well. γ is called the *trace operator* and γu the *trace of* u. We will particularly make use of the adjoint operator of γ, which is linear and continuous as well: For $1 < q < \infty$ such that $\frac{1}{p} + \frac{1}{q} = 1$ and hence $s > \frac{1}{p} = 1 - \frac{1}{q}$, we have $\gamma^* : L_q(\Gamma) \to H_q^{-s}(\Omega)$ and

$$\|\gamma^* g\|_{H_q^{-s}(\Omega)} \leq c\|g\|_{L_q(\Gamma)} \quad \text{for all } g \in L_q(\Gamma). \tag{2.2}$$

2.2 The Bochner integral

In order to deal with the time dependence, we are going to need a notion of an integral for functions mapping into Banach spaces, in particular into those spaces which contain the space dependence. This leads to the concept of the Bochner integral. For functions mapping from an interval $[a, b] \subset \mathbb{R}$ ($-\infty < a < b < \infty$) into a Banach space X, in the standard way the Banach space $C([a, b]; X)$ of continuous functions $u : [a, b] \to X$ equipped with the maximum norm

$$\|u\|_{C([a,b];X)} := \max_{t\in[a,b]} \|u(t)\|_X$$

is defined. Similarly, we have the space $L_r(a, b; X)$, $1 \leq r \leq \infty$ of Bochner measurable functions $u : [a, b] \to \mathbb{R}$ with finite norm

$$\|u\|_{L_r(a,b;X)} := \begin{cases} \left(\int\limits_a^b \|u(t)\|_X^r dt\right)^{\frac{1}{r}}, & 1 \leq r < \infty, \\ \operatorname{ess\,sup}_{t\in[a,b]} \|u(t)\|_X, & r = \infty. \end{cases}$$

For u' defined in a X-valued distributional sense, we furthermore define the space $W_r^1(a, b; X)$ of all $u \in L_r(a, b; X)$ having a distributional derivative $u' \in L_r(a, b; X)$ and

$$\|u\|_{W_r^1(a,b;X)} := \left(\|u\|_{L_r(a,b;X)}^r + \|u'\|_{L_r(a,b;X)}^r\right)^{\frac{1}{r}}.$$

For more detailed information we refer to [59], [61]. When no confusion is possible, throughout this thesis we will not mention the domains explicitly and just write $L_r(L_p(\Omega))$ or even $L_r(L_p)$ instead of $L(a,b;L_p(\Omega))$. One result is of particular importance when comparing the state system with the adjoint system (cf. [59], Satz 3.11):

Lemma 2.2 (Integration by parts formula)**.** *Assume* $u, p \in L_2(H^1(\Omega)) \cap H^1(H^{-1}(\Omega))$ *(commonly known as* $W(0,T)$*). It holds that*

$$\int_0^T \langle u'(t), p(t)\rangle_{H^{-1},H^1}\ dt + \int_0^T \langle p'(t), u(t)\rangle_{H^{-1},H^1}\ dt = \langle u(T), p(T)\rangle_{L_2(\Omega)} - \langle u(0), p(0)\rangle_{L_2(\Omega)}.$$

2.3 Maximal parabolic regularity

In the theory of partial differential equations, apart from existence and uniqueness of a solution it is an important question to determine what can be said about its regularity depending on the given data. In the case of elliptic equations with a differential operator of second order

$$Au = f$$

for example, assuming we have a right hand side $f \in L_2(\Omega)$ we cannot expect the solution to be more regular than $H^2(\Omega)$. Naturally, the question arises under which conditions on the differential operator, the domain and the underlying spaces we can expect to achieve this optimal regularity result. The same question can be asked in the case of parabolic equations

$$u_t + Au = f.$$

If for example we have $f \in L_2(Q)$, this implies $u_t, Au \in L_2(Q)$, so the best we can hope for is that the solution u possesses a weak derivative in time with values in $L_2(\Omega)$, in other words $u \in H^1(L_2(\Omega))$, and is twice weakly differentiable in space, $u \in L_2(H^2(\Omega))$. In the last decades, a lot of work has been done on finding criteria under which we can expect a solution to have this optimal regularity (cf. e.g. the monographies [6], [42], [51]). Let us already point out a difficulty that can be seen in the example above: The above setting is suited for boundary values which are either homogeneous and included in the domain of definition of the operator A or possess some order of differentiability (precise results can be found in [50]). In our case, with less regular nonhomogeneous boundary values, due to Theorem 2.1 it will hence be better to look at the equation in some dual space like $H^{-1}(\Omega)$.

2.3.1 The abstract setting

We are now going to introduce some general terminology and results known about maximal parabolic regularity. Concerning notation we are going to follow the lines of [6]: Given two Banach spaces E_0 and E_1, where E_1 is densely embedded in E_0, a linear continuous operator $A : E_1 \to E_0$ (i.e. $A \in \mathcal{L}(E_1, E_0)$), an initial value $u_0 \in E_0$ and a function $f \in L_1(a, b; E_0)$ we look at the linear Cauchy problem

$$u_t + Au = f, \qquad u(0) = u_0. \tag{2.3}$$

A function u is called *generalized solution* or *W^1_r-solution to the Cauchy problem* ($r \geq 1$) if

$$u \in L_r(0, T; E_1) \cap W^1_r(0, T; E_0) \text{ and } (\partial + A)u = f,\ u(0) = u_0,$$

where ∂ is the distributional derivative with respect to t. Due to the following result, such a solution is actually continuous in time with image in some interpolation space:

Lemma 2.3 ([6], III 4.10.2)**.** *There is a continuous embedding*

$$L_r(a, b; E_1) \cap W^1_r(a, b; E_0) \hookrightarrow C([a, b]; (E_0, E_1)_{1-\frac{1}{r},r}).$$

Of course we would like to be able to recover such a generalized solution from data having as little regularity as possible. The optimal situation can be described in the following way:

Definition 2.4. *Let $1 < r < \infty$. Let E_0, E_1 be Banach spaces such that $E_1 \hookrightarrow E_0$ densely and let $E := (E_0, E_1)_{1-\frac{1}{r},r}$ be the real interpolation space.*

An operator $A \in \mathcal{L}(E_1, E_0)$ *possesses the property of maximal parabolic* L_r*-regularity with respect to* (E_1, E_0) *if the map*

$$L_r(a,b;E_1) \cap W_r^1(a,b;E_0) \to L_r(a,b;E_0) \times E, \quad u \mapsto ((\partial + A)u, u(0))$$

is a bounded isomorphism.

Note that in particular, this means there is a constant $c > 0$ such that

$$\|u\|_{L_r(E_1)} + \|u\|_{W_r^1(E_0)} \le c\left(\|u_0\|_E + \|f\|_{L_r(E_0)}\right). \tag{2.4}$$

The property of maximal parabolic regularity comes with a few very useful consequences which can for example be found in [6], [16], [34]:

Theorem 2.5. *(i) If there is an* $r \in (1,\infty)$ *such that* A *satisfies maximal parabolic* L_r*-regularity, then the same is true for every* $r \in (1,\infty)$.

(ii) If A *satisfies maximal parabolic regularity on some interval* (a,b)*, then it does so on every (bounded) interval. The constant in* (2.4) *does not depend on the length of the interval.*

(iii) The operator $-A$ *generates an analytic semigroup* $\{S(t)\}_{t\ge 0}$ *on* E_0.

The second result (which follows eg. from [6], III 4.10.1) is of particular importance for the way we are going to carry out the proof of existence and uniqueness of a solution to the state system: It allows us to first restrict ourselves to small time intervals, which helps us to obtain the contraction property we need for Banach's fixed point theorem. After that, we just extend the solution to the whole interval.

2.3.2 Maximal regularity in $W_p^{-1}(\Omega)$

In the introduction of this section, we already implied that the underlying spaces need to be chosen with care. In our case, there are mainly two aspects we need to think about: For one thing we will need the solutions to be continuous in space. Due to (2.1) this calls for the condition $p > N$ since in that case we have $W_p^1 \hookrightarrow C(\bar{\Omega})$. Unfortunately, that means we will not be able to work in a Hilbert space setting. Secondly, we intend to impose boundary conditions $g \in L_r(L_p(\Gamma)$. This rules out $L_p(\Omega)$ as the underlying space anyway, even more so because as a consequence, the cross-diffusion term $-\nabla \cdot \{f(u)\nabla v\}$ will not have enough regularity. It turns out that setting

$$E_0 := W_p^{-1}(\Omega), \qquad\qquad E_1 := W_p^1(\Omega)$$

for $p > N$ is a reasonable choice. We will generally refer to the space of maximal parabolic regularity we obtain by

$$\mathbb{W}_{r,p} := L_r(W_p^1(\Omega)) \cap W_r^1(W_p^{-1}(\Omega)), \tag{2.5}$$

for the interpolation space E from above we will write

$$\mathcal{D}_{r,p} := (W_p^{-1}(\Omega), W_p^1(\Omega))_{1-\frac{1}{r},r} \left(\hookrightarrow H_p^{1-\frac{2}{r}-\varepsilon}(\Omega)\right). \tag{2.6}$$

When it comes to establishing the optimality system, it will be important to be precise and actually work with $\mathcal{D}_{r,p}$ instead of $H_p^{1-\frac{2}{r}-\varepsilon}(\Omega)$: The final value $u(T)$ of the state will be in $\mathcal{D}_{r,p}$ and that is exactly the regularity we need for the initial value of the adjoint state.

Now in order to apply the results of the previous subsection to our state system, we need to make sure that the W_p^{-1}-realization of the negative Laplacian has the property of maximal parabolic regularity. For this we define:

Definition 2.6. *Set $A : W_p^1(\Omega) \to W_p^{-1}(\Omega)$, $A + 1 : W_p^1(\Omega) \to W_p^{-1}(\Omega)$*

$$\langle Au, \phi\rangle_{W_p^{-1},W_{p'}^1} := \int_\Omega \nabla u(x) \cdot \nabla\phi(x)\ dx,$$

$$\langle (A+1)u, \phi\rangle_{W_p^{-1},W_{p'}^1} := \int_\Omega \nabla u(x) \cdot \nabla\phi(x) dx + \int_\Omega u(x)\phi(x)\ dx$$

for all $u \in W_p^1(\Omega)$, $\phi \in W_{p'}^1(\Omega)$.

With this definition, we can make use of the following very important result which is shown in [31], Thm 5.6 and [10] Thm 11.5 and builds the basis of our analysis:

Theorem 2.7. *The operators A and $A + 1$ defined above have the property of maximal parabolic regularity with respect to the spaces $E_0 = W_p^{-1}(\Omega)$ and $E_1 = W_p^1(\Omega)$.*

Finally, let us give a precise definition of how the cross diffusion term on the right hand side of the state equation is to be understood:

Definition 2.8. *For $\zeta \in L_\infty(\Omega)$, $\psi \in W^1_p(\Omega)$ define the linear and bounded functional $-\nabla \cdot \{\zeta \nabla \psi\} \in W^{-1}_p(\Omega)$ via*

$$-\nabla \cdot \{\zeta \nabla \psi\}(\cdot) : \phi \mapsto \int_\Omega \zeta \nabla \psi \nabla \phi \; dx \qquad \text{for all } \phi \in W^1_{p'}(\Omega).$$

We will often use that this functional is bounded in the following way: There is a constant $c > 0$ such that

$$\begin{aligned} \| -\nabla \{\zeta \nabla \psi\}\|_{W^{-1}_p} \leq & \sup_{\substack{\phi \in W^1_{p'} \\ \|\phi\|_{W^1_{p'}}=1}} \int_\Omega |\zeta \nabla \psi \nabla \phi| \; dx \\ \leq & c \sup_{\substack{\phi \in W^1_{p'} \\ \|\phi\|_{W^1_{p'}}=1}} \|\zeta \nabla \psi\|_{L_p} \|\nabla \phi\|_{L_{p'}} \leq c \|\zeta\|_{L_\infty} \|\nabla \psi\|_{W^1_p}. \end{aligned} \tag{2.7}$$

2.4 Mild solutions

The concept of maximal regularity is a very powerful tool to solve parabolic equations, it does however have its limitations. For example, if we want to take precise influence on the order of integrability in time r, it turns out that semigroup estimates provide very helpful additional results. Fortunately, due to Theorem 2.5 we can make use of these as well. Since $-A$ generates an analytic semigroup $\{S_A(t)\}_{t \geq 0}$ in $W^{-1}_p(\Omega)$, for a right hand side $f \in L_1(0, T; W^{-1}_p(\Omega))$ and an initial value $u_0 \in W^{-1}_p(\Omega)$ we can define a *mild solution* $u \in C([0, T]; W^{-1}_p(\Omega))$ to the Cauchy Problem (2.3) as a solution to the integral equation

$$u(t) = S_A(t) u_0 + \int_0^t S_A(t-s) f(s) ds.$$

Given u is sufficiently regular, this solution coincides with the generalized solution (cf. [6], Prop. III 1.3.1). We actually know the following thing (cf. [6], Thm. III 1.5.2):

Lemma 2.9. *Assume the operator A satisfies maximal parabolic regularity with respect to spaces E_0, E_1 and let $\{S(t)\}_{t\geq 0}$ be the analytic semigroup generated by $-A$. The mappings*

$$R_A : u_0 \mapsto S(\cdot)u_0, \qquad K_A : f \mapsto \int_0^{\cdot} S(\cdot - s)f(s)ds$$

are linear and continuous from $E = (E_0, E_1)_{1-\frac{1}{r}}$, to $L_r(E_1) \cap W_r^1(E_0)$ and $L_r(E_0)$ to $L_r(E_1) \cap W_r^1(E_0)$ respectively.

The key to the following results is the fact that the operator A from Definition 2.6 is in fact a positive operator (cf. [31], Lemma 5.7). This implies that we can define fractional powers A^α, which are again closed, densely defined operators (cf. [20] section 2.14, [48]) and whose domains $D(A^\alpha)$ equipped with the graph norm provide very useful intermediate spaces. In the standard case of operators with range in $L_p(\Omega)$ and domains with smooth boundary, these spaces have been characterized in [54]. For operators with range in $W_p^{-1}(\Omega)$ we refer to [25] and [56], 1.15.3: We have

$$D(A^{\alpha(1-\theta)+\beta\theta}) = [D(A^\alpha), D(A^\beta)]_\theta$$

for $0 \leq \alpha < \beta < \infty$ and hence

$$D(A^\theta) = [H_p^{-1}(\Omega), H_p^1(\Omega)]_\theta = H_p^{-1+2\theta}(\Omega) \tag{2.8}$$

for $0 < \theta < 1$. This can be combined with standard semigroup estimates:

Lemma 2.10 ([48] Thm. 2.6.13)**.** *Assume A is a positive operator on E_0 and $\{S(t)\}_{t\geq 0}$ the analytic semigroup generated by $-A$. For $\alpha > 0$ we have*

(i) $A^\alpha S(t)u = S(t)A^\alpha u$ for every $u \in D(A^\alpha)$,

(ii) $\|A^\alpha S(t)u\|_{E_0} \leq c_\alpha t^{-\alpha} e^{-\delta t}\|u\|_{E_0}$ for every $u \in E_0$ and some $c_\alpha > 0$.

Lemma 2.11. *Let A be a positive operator on $W_p^{-1}(\Omega)$ and $\{S(t)\}_{t\geq 0}$ the analytic semigroup generated by $-A$. Let $-1 \leq \beta \leq \alpha \leq 1$ and $1 < q \leq p \leq \infty$. Then*

$$\|S(t)u\|_{H_p^\alpha} \leq ct^{-\theta}\|u\|_{H_q^\beta}$$

for some $c > 0$, $\theta = \frac{\alpha-\beta}{2} + \frac{N}{2}(\frac{1}{q} - \frac{1}{p})$ and every $u \in H_q^\beta(\Omega)$.

Proof. Let $\nu = \frac{1}{2}(1+\alpha)$. Then for $0 < \sigma < \nu$ we can estimate

$$\begin{aligned}\|S(t)u\|_{H_p^\alpha(\Omega)} \le c\|A^\nu S(t)u\|_{H_p^{-1}(\Omega)} \le & c\|A^{\nu-\sigma}S(t)A^\sigma u\|_{H_p^{-1}(\Omega)} \\ \le & ct^{-(\nu-\sigma)}\|A^\sigma u\|_{H_p^{-1}(\Omega)} \\ \le & ct^{-(\nu-\sigma)}\|u\|_{H_p^{-1+2\sigma}(\Omega)} \\ \le & ct^{-(\nu-\sigma)}\|u\|_{H_q^\beta(\Omega)},\end{aligned}$$

where we used (2.8), the lemma above and the embedding $H_p^\beta(\Omega) \hookrightarrow H_p^{-1+2\sigma}(\Omega)$ for $\beta - \frac{N}{q} = -1 + 2\sigma + \frac{N}{p}$, so $\sigma = \frac{1}{2} + \frac{\beta}{2} + \frac{N}{2}(\frac{1}{p} - \frac{1}{q})$. Setting $\theta = \nu - \sigma$ yields the assertion. □

The idea now is the following: Given for example $u \in L_r(W_p^1(\Omega))$, $r > 2$, we would have

$$\|\int_0^t S(t-s)u(s)\ ds\|_{W_p^1(\Omega)} \le c\int_0^t (t-s)^{-\frac{1}{2}}\|u(s)\|_{L_p(\Omega)}\ ds.$$

The right hand side can be viewed as a convolution, so that with the help of Young's inequality for convolutions (A.4), with $\frac{1}{r} + \frac{1}{r'} = 1$ (and hence $r' < 2$) we get

$$\begin{aligned}\|\int_0^\cdot S(\cdot - s)u(s)ds\|_{L_\infty(W_p^1(\Omega))} \le & c\left(\int_0^T t^{-\frac{r'}{2}}dt\right)^{\frac{1}{r'}}\|u\|_{L_r(L_p(\Omega))} \\ \le & c(T)\|u\|_{L_r(L_p(\Omega))}.\end{aligned}$$

In some sense, estimates of this type allow us to "trade" regularity in space for regularity in time. This will be a very useful tool in the next chapter.

Chapter 3

The chemotaxis equations

Since the systems of differential equations that appear in this thesis are interesting in their own right, before we start looking at the optimal control problem we are first going to collect results on existence, uniqueness and regularity of solutions to these systems. This way, to some extend we can focus on the features of the control problem and the pdes separately. As said before, we will always assume that for $N \geq 2$, $\Omega \subset \mathbb{R}^N$ is a bounded domain with Lipschitz boundary and $T > 0$. For $N = 1$, the arguments remain valid with slight modifications.

3.1 The state equation

Let us first give a short explanation on how the system is to be understood. As mentioned in the introduction, the chemotaxis model we are looking at is described by

$$\begin{aligned} u_t =& \Delta u - \nabla \cdot \{f(u)\nabla v\} \\ v_t =& \Delta v - v + u \end{aligned} \quad \text{in } \Omega \times (0,T),$$

$$\begin{aligned} \partial_n u + f(u)\partial_n v =& 0 \\ \partial_n v =& g \end{aligned} \quad \text{on } \Gamma \times (0,T), \qquad \begin{aligned} u(0) =& u_0 \\ v(0) =& v_0 \end{aligned} \quad \text{in } \Omega.$$

Since we want to prescribe boundary values $g \in L_r(L_p(\Gamma))$, we clearly cannot expect classical solutions and will hence look at a variational formulation of the problem. Assuming sufficient smoothness, we can multiply both equations with test functions, integrate over Ω and apply the integration by parts formula to get

$$\int_\Omega u_t(t)\varphi\, dx + \int_\Omega \nabla u(t)\nabla\varphi\, dx = \int_\Omega f(u(t))\nabla v(t)\nabla\varphi\, dx$$

$$\int_\Omega v_t(t)\psi\, dx + \int_\Omega \nabla v(t)\nabla\psi\, dx + \int_\Omega v(t)\psi\, dx = \int_\Omega u(t)\psi\, dx + \int_\Gamma g(t)\gamma\psi\, ds$$

for almost every $t \in [0,T]$. In a Hilbert space setting, so assuming the test functions would be in $H^1(\Omega)$, the right hand sides could be interpreted as functionals $F_i(\varphi)$ in $H^{-1}(\Omega)$. For what is to come, it is convenient to replace the boundary integral in the second equation by taking the adjoint of the trace operator $\gamma : H^1(\Omega) \to L_2(\Gamma)$, that is $\gamma^* : L_2(\Gamma) \to H^{-1}(\Omega)$, to get

$$\int_\Gamma g(t)\gamma\psi\, ds = \langle \gamma^* g(t), \psi\rangle_{H^{-1},H^1}\,.$$

This way, from now on we will interpret the Neumann boundary condition as a right hand side $\gamma^* g(t)$ and the operator $-\nabla\cdot\{f(u(t))\nabla v(t)\}$ in the sense of Definition 2.8 . Unfortunately, we cannot work in a Hilbert space setting, since we will need to make use of the embedding $W^1_p(\Omega) \hookrightarrow C(\bar\Omega)$ which requires the condition $p > N$, however the arguments can be carried over directly to $W^{-1}_p - W^1_{p'}$ duality products. We will now go into detail and show existence and uniqueness of a solution to the state system as well as a uniform bound for the solution.

Theorem 3.1. *Assume $r \geq 2$, $p > N$ such that $\frac{2}{r} + \frac{N}{p} < 1$. Let $f \in C(\mathbb{R}^+)$ be bounded by a constant $c_f > 0$ and (globally) Lipschitz continuous with a Lipschitz constant $L_f > 0$. Let $u_0, v_0 \in \mathcal{D}_{r,p} = (W^{-1}_p(\Omega), W^1_p(\Omega))_{1-\frac{1}{r},r}$ and $g \in L_r(L_p(\Gamma))$. The system*

$$u_t = \Delta u - \nabla\cdot\{f(u)\nabla v\} \quad \text{in } \Omega\times(0,T), \qquad u(0) = u_0 \text{ in } \Omega, \tag{3.1}$$

$$v_t = \Delta v - v + u + \gamma^* g \quad \text{in } \Omega\times(0,T), \qquad v(0) = v_0 \text{ in } \Omega \tag{3.2}$$

has a unique solution $(u,v) \in \mathbb{W}^2_{r,p} = \left[L_r(W^1_p) \cap W^1_r(W^{-1}_p)\right]^2$ such that

$$\|u\|_{\mathbb{W}_{r,p}} + \|v\|_{\mathbb{W}_{r,p}} \leq c\left(\|u_0\|_{\mathcal{D}_{r,p}} + \|v_0\|_{\mathcal{D}_{r,p}} + \|g\|_{L_r(L_p(\Gamma))}\right) \tag{3.3}$$

for some $c > 0$.

Proof. Let us first take a look at the linear equation (3.2). For $u \in L_r(W_p^{-1})$ fixed, due to Theorem 2.7 and (2.2) there is a unique solution $v = v(u) \in \mathbb{W}_{r,p}$ such that

$$\begin{aligned} \|v\|_{\mathbb{W}_{r,p}} \leq & c\left(\|v_0\|_{\mathcal{D}_{r,p}} + \|\gamma^* g\|_{L_r(W_p^{-1}(\Omega))} + \|u\|_{L_r(W_p^{-1})}\right) \\ \leq & c\left(\|v_0\|_{\mathcal{D}_{r,p}} + \|g\|_{L_r(L_p(\Gamma))} + \|u\|_{L_r(W_p^{-1})}\right) \end{aligned} \tag{3.4}$$

for some $c > 0$. Also, given $u_1, u_2 \in L_r(W_p^{-1})$ and corresponding solutions $v_1 = v(u_1)$, $v_2 = v(u_2) \in \mathbb{W}_{r,p}$, there is a constant $L > 0$ such that

$$\|v_1 - v_2\|_{\mathbb{W}_{r,p}} \leq L\|u_1 - u_2\|_{L_r(W_p^{-1})}. \tag{3.5}$$

Due to Theorem 2.5 (ii), these estimates continue to hold with the same constants if we restrict ourselves to smaller time intervals. Having established this, we can replace (3.2) by a map $u \mapsto v(u)$ and hence reduce the system (3.1)-(3.2) to the problem of solving the nonlinear equation

$$u_t - \Delta u = -\nabla \cdot \{f(u)\nabla v(u)\} \text{ in } Q, \qquad u(0) = u_0 \text{ in } \Omega.$$

The proof of existence and uniqueness of a solution to this equation is best divided in three steps: First, we show that there is a $T_{max} > 0$ and a solution $(u^{T_{max}}, v^{T_{max}})$ on the time interval $[0, T_{max})$, and that either $T_{max} = \infty$ or $\|u(T_{max})\|_{L_\infty(\Omega)} = \infty$. In a second step, we show that the solution stays bounded, meaning there is a solution on every time interval $[0, T]$, $T > 0$, and lastly we show uniqueness of the solution on $[0, T]$.

(i) *Existence on* $[0, T_{max})$*:* As a starting point, for some $T_1 > 0$ we want to apply Banach's fixed point theorem to the map $\tilde{u} \mapsto u(\tilde{u})$ defined by

$$u_t - \Delta u = -\nabla \cdot \{f(\tilde{u})\nabla v(\tilde{u})\} \text{ in } Q, \qquad u(0) = u_0 \text{ in } \Omega \tag{3.6}$$

in $\mathbb{W}_{r,p}^{T_1}$, the restriction of $\mathbb{W}_{r,p}$ to the time interval $[0, T_1]$. In order to simplify notation we will drop the superscript T_1 as long as no confusion is likely. Once we established the existence of a solution on $[0, T_1]$, we can apply the same argument on some interval $[T_1, T_2]$, $T_2 > T_1$ with initial value $u(T_1)$ and so on. As long as u stays bounded, the interval lengths do not tend to zero.

So let us choose $M_1 > 0$, $T_1 > 0$ both to be fixed later. Now choose some arbitrary but fixed $\tilde{u} \in \mathbb{W}_{r,p}$, $\|\tilde{u}\|_{\mathbb{W}_{r,p}} \leq M_1$ on $[0, T_1]$. From (3.4) we get

$$\|v\|_{\mathbb{W}_{r,p}} \leq c \left(\|v_0\|_{\mathcal{D}_{r,p}} + \|g\|_{L_r(L_p(\Gamma))} + \|\tilde{u}\|_{L_r(W_p^{-1})} \right)$$

for some $c > 0$. Due to this and since $f(\tilde{u}) \in C(\bar{Q})$, the right hand side of (3.6) is known and in $L_r(W_p^{-1})$. Once again, we have a linear equation satisfying maximal parabolic regularity, so that by (2.7) there is a unique solution $u \in \mathbb{W}_{r,p}$ such that

$$\begin{aligned} \|u\|_{\mathbb{W}_{r,p}} \leq& c \left(\|u_0\|_{\mathcal{D}_{r,p}} + \|f(\tilde{u}) \nabla v(\tilde{u})\|_{L_r(L_p)} \right) \\ \leq& c \left(\|u_0\|_{\mathcal{D}_{r,p}} + c_f \|v(\tilde{u})\|_{L_r(W_p^1)} \right) \\ \leq& c\|u_0\|_{\mathcal{D}_{r,p}} + c(f) \left(\|v_0\|_{\mathcal{D}_{r,p}} + \|g\|_{L_r(L_p(\Gamma))} + \|\tilde{u}\|_{L_r(W_p^{-1})} \right) \end{aligned} \tag{3.7}$$

for $c, c(f) > 0$. Note that due to Theorem 2.5, the constant does not depend on the time interval. Extracting the maximum of $\tilde{u}$ with respect to time and using the embedding $\mathbb{W}_{r,p} \hookrightarrow C([0, T_1]; W_p^{-1})$, we get

$$\|\tilde{u}\|_{L_r(W_p^{-1})} \leq c T_1^{\frac{1}{r}} \|\tilde{u}\|_{C([0,T]; W_p^{-1})} \leq c T_1^{\frac{1}{r}} \|\tilde{u}\|_{\mathbb{W}_{r,p}} \tag{3.8}$$

and hence

$$\|u\|_{\mathbb{W}_{r,p}} \leq c \left(\|u_0\|_{\mathcal{D}_{r,p}} + \|v_0\|_{\mathcal{D}_{r,p}} + \|g\|_{L_r(L_p(\Gamma))} \right) + c T_1^{\frac{1}{r}} \|\tilde{u}\|_{\mathbb{W}_{r,p}}.$$

So for

$$M_1 > c \left(\|u_0\|_{\mathcal{D}_{r,p}} + \|v_0\|_{\mathcal{D}_{r,p}} + \|g\|_{L_r(L_p(\Gamma))} \right)$$

and T_1 sufficiently small we have $\|u\|_{\mathbb{W}_{r,p}} \leq M_1$, hence the solution operator $\tilde{u} \mapsto u$ maps the set $\left\{ u \in \mathbb{W}_{r,p} : \|u\|_{\mathbb{W}_{r,p}} \leq M_1 \right\}$ into itself. The contraction property is shown in the same way: For $\tilde{u}_1, \tilde{u}_2 \in \mathbb{W}_{r,p}$, $\|\tilde{u}_1\|_{\mathbb{W}_{r,p}} \leq M_1$, $\|\tilde{u}_2\|_{\mathbb{W}_{r,p}} \leq M_1$ we get

$$\begin{aligned} (u_1 - u_2)_t - \Delta(u_1 - u_2) =& -\nabla \cdot \{ f(\tilde{u}_1) \nabla v(\tilde{u}_1) - f(\tilde{u}_2) \nabla v(\tilde{u}_2) \} && \text{in } Q, \\ (u_1 - u_2)(0) =& 0 && \text{in } \Omega \end{aligned}$$

and together with (3.5),

$$\begin{aligned}\|u_1-u_2\|_{\mathbb{W}_{r,p}} \leq & c\left(\|\{f(\tilde u_1)-f(\tilde u_2)\}\nabla v(\tilde u_1)\|_{L_r(L_p)}\right.\\ &\left.+\|f(\tilde u_2)\nabla\{v(\tilde u_1)-v(\tilde u_2)\}\|_{L_r(L_p)}\right)\\ \leq & c\Big(L_f\|\tilde u_1-\tilde u_2\|_{C(\bar Q)}\|v(\tilde u_1)\|_{L_r(W^1_p)}\\ &+c_f\|v(\tilde u_1)-v(\tilde u_2)\|_{L_r(W^1_p)}\Big)\\ \leq & c\Big(L_f\|v(\tilde u_1)\|_{L_r(W^1_p)}+c_f\Big)\|\tilde u_1-\tilde u_2\|_{C(\bar Q)}\\ \leq & c\Big(L_f(\|v_0\|_{\mathcal{D}_{r,p}}+\|g\|_{L_r(L_p(\Gamma))}+\|\tilde u_1\|_{L_r(W_p^{-1})})+c_f\Big)\\ &\|\tilde u_1-\tilde u_2\|_{C(\bar Q)}\\ \leq & c(L_fM_1+c_f)\|\tilde u_1-\tilde u_2\|_{C(\bar Q)}.\end{aligned}$$

Now choose some $2<\alpha<r$ such that $\frac{2}{\alpha}+\frac{N}{p}<1$ is still satisfied. Similarly to (3.8) we get

$$\|\tilde u_1-\tilde u_2\|_{C(\bar Q)}\leq c\|\tilde u_1-\tilde u_2\|_{\mathbb{W}_{\alpha,p}}\leq cT_1^{\frac{1}{\alpha}-\frac{1}{r}}\|\tilde u_1-\tilde u_2\|_{\mathbb{W}_{r,p}}$$

and hence

$$\|u_1-u_2\|_{\mathbb{W}_{r,p}}\leq c\,(L_fM_1+c_f)\,T_1^{\frac{1}{\alpha}-\frac{1}{r}}\|\tilde u_1-\tilde u_2\|_{\mathbb{W}_{r,p}}.$$

If T_1 is sufficiently small, the constant becomes smaller than one which proves the contraction property. We have thus shown that there is a $T_1>0$ such that the solution operator $\tilde u\mapsto u$ satisfies the conditions of Banach's fixed point theorem, which means there is a unique solution $(u,v)\in\mathbb{W}^2_{r,p}$ of (3.1) - (3.2) on the time interval $[0,T_1]$. This procedure can be iterated with $u(T_1)\in\mathcal{D}_{r,p}$ (see Lemma 2.3) as new initial value for as long as the solution stays bounded.

(ii) *Boundedness:* Next, we will show that the solution stays bounded for all $t>0$, i.e. $T_{max}=\infty$. To do this, for every $t>0$ we introduce a weighted norm on the spaces $C([0,t];L_p)$ via

$$\|u\|_{\mu,t}:=\max_{s\in[0,t]}e^{-\mu s}\|u(s)\|_{L_p}, \tag{3.9}$$

$\mu>0$, which is obviously equivalent to the canonic norm. For the L_r-

norm on $(0,t)$ we have

$$\|u\|_{L_r(0,t;L_p)} = \left(\int_0^t \|u(s)\|_{L_p}^r \, ds \right)^{\frac{1}{r}}$$

$$= \left(\int_0^t e^{-\mu rs} \|u(s)\|_{L_p}^r e^{\mu rs} \, ds \right)^{\frac{1}{r}} \leq \left(\frac{1}{\mu r} \right)^{\frac{1}{r}} \|u\|_{\mu,t} e^{\mu t}.$$

As we have seen in (3.7), for every $t < T_{max}$ a solution satisfies

$$\|u\|_{C([0,t];L_p)} \leq c\|u\|_{\mathbb{W}_{r,p}} \leq c(u_0, v_0, g) + c\|u\|_{L_r(0,t;L_p)},$$

so in particular it holds that

$$\|u(t)\|_{L_p} \leq c(u_0, v_0, g) + c\|u\|_{L_r(0,t;L_p)}$$

$$\leq c(u_0, v_0, g) + c \left(\frac{1}{\mu r} \right)^{\frac{1}{r}} \|u\|_{\mu,t} e^{\mu t}$$

for every $t < T_{max}$. Multiplying by $e^{-\mu t}$ and taking the maximum over all $t \in [0, T_{max}]$ gives

$$\|u\|_{\mu,T} \leq c(\mu, u_0, v_0, g) + c \left(\frac{1}{\mu r} \right)^{\frac{1}{r}} \|u\|_{\mu,T}.$$

For μ sufficiently large, the second term on the right hand side can be absorbed in the left hand side, so that

$$\|u\|_{\mu,T} \leq c(\mu) \left(\|u_0\|_{\mathcal{D}_{r,p}} + \|v_0\|_{\mathcal{D}_{r,p}} + \|g\|_{L_r(L_p(\Gamma))} \right). \tag{3.10}$$

Hence, the solution stays bounded with respect to $\|\cdot\|_{\mu,T}$ on every interval $[0,T]$, and due to the equivalence of the two norms also with respect to $\|\cdot\|_{C([0,T];L_p)}$.

(iii) *Uniqueness:* Lastly, we need to make sure the solution stays unique on the whole time interval. To this end, assume there are two different solutions (u_1, v_1), (u_2, v_2) of (3.1)-(3.2). Then $w := u_1 - u_2$, $z := v_1 - v_2$ is a solution to

$$w_t = \Delta w - \nabla \cdot \{ f(u_1)\nabla v_1 - f(u_2)\nabla v_2 \} \quad \text{in } Q, \qquad u(0) = 0 \quad \text{in } \Omega,$$

$$z_t = \Delta z - z + w \quad \text{in } Q, \qquad v(0) = 0 \quad \text{in } \Omega.$$

This system has homogeneous initial and boundary conditions so that (w, z) is even differentiable in a classical sense. Hence, we only need to follow the exact same steps as in the proof of Theorem 3.1 in [36] to find that $w \equiv z \equiv 0$ with the help of Gronwall's inequality (A.5).

It remains to be shown that (3.3) holds. With the considerations from above this is simple: With the help of (3.7), (3.4) and (3.10) it follows that

$$\begin{aligned}\|u\|_{\mathbb{W}_{r,p}} + \|v\|_{\mathbb{W}_{r,p}} \leq & c\left(\|u_0\|_{\mathcal{D}_{r,p}} + \|v\|_{\mathbb{W}_{r,p}}\right) \\ \leq & c\left(\|u_0\|_{\mathcal{D}_{r,p}} + \|v_0\|_{\mathcal{D}_{r,p}} + \|g\|_{L_r(L_p(\Gamma))}\right) + c\|u\|_{C([0,T];L_p)} \\ \leq & c\left(\|u_0\|_{\mathcal{D}_{r,p}} + \|v_0\|_{\mathcal{D}_{r,p}} + \|g\|_{L_r(L_p(\Gamma))}\right).\end{aligned}$$

□

Remark 3.2. *This result is not sharp with respect to the boundary term g: In the same way as in* (3.15) *in the proof of Theorem 3.4, if we use the precise spaces and embeddings for the adjoint of the trace operator we can replace $L_p(\Gamma)$ by $L_\sigma(\Gamma)$, $\sigma > \frac{N-1}{N}p$. For the sake of simplicity we skipped this argument in the proof above.*

When dealing with optimal control problem later on, more precisely if we want to guarantee the adjoint equation has a solution in $\mathbb{W}^2_{r,p}$ as well, we will need ∇v to be essentially bounded in time. This can be achieved with the help of semigroup arguments as long as we impose slightly stricter conditions on the data:

Lemma 3.3. *In addition to the conditions of Theorem 3.1 assume that $r > 2p$ and $v_0 \in W^1_p(\Omega)$. Then we have $v \in L_\infty(W^1_p)$ and*

$$\|v\|_{L_\infty(W^1_p)} \leq c\left(\|u_0\|_{\mathcal{D}_{r,p}} + \|v_0\|_{W^1_p} + \|g\|_{L_r(L_p(\Gamma))}\right).$$

for some $c > 0$.

Proof. Let $\{S(t)\}_{t\geq 0}$ be the semigroup generated by the differential operator $-(A+1)$ defined in Definition 2.6. The solution (u, v) of (3.1) - (3.2) solves the integral equation

$$v(t) = S(t)v_0 + \int_0^t S(t-s)u(s)\, ds + \int_0^t S(t-s)\gamma^* g(s)\, ds.$$

The crucial term is the second integral $I(t) := \int_0^t S(t-s)\gamma^* g(s)\, ds$: For every $t \in (0,T)$, with the help of Lemma 2.11 and (2.2) we can estimate

$$\|I(t)\|_{W_p^1} \leq c \int_0^t (t-s)^{-\theta} \|\gamma^* g(s)\|_{H_p^\rho}\, ds \leq c \int_0^t (t-s)^{-\theta} \|g(s)\|_{L_p(\Gamma)}\, ds$$

for $\rho < \frac{1}{p} - 1$ and $\theta := \frac{1}{2} - \frac{\rho}{2} > 1 - \frac{1}{2p}$, and by Young's inequality for convolutions (A.4)

$$\|I\|_{L_\infty(W_p^1)} \leq c \left(\int_0^T t^{-r'\theta}\, dt \right)^{\frac{1}{r'}} \|g\|_{L_r(L_p(\Gamma))}$$

for $\frac{1}{r} + \frac{1}{r'} = 1$. The integral is finite as long as $r'\theta < 1$, so we need a θ satisfying

$$1 - \frac{1}{2p} < \theta < 1 - \frac{1}{r},$$

which exists if $r > 2p$. Hence, once again using Lemma 2.11, we have

$$\|v(t)\|_{W_p^1} \leq c \|v_0\|_{W_p^1} + c \int_0^t \|u(s)\|_{W_p^1}\, ds + \|I(t)\|_{W_p^1}$$

for every $t \in (0,T)$ and by (3.3)

$$\begin{aligned} \|v\|_{L_\infty(W_p^1)} \leq & c\|v_0\|_{W_p^1} + c\|u\|_{L_r(W_p^1)} + c\|g\|_{L_r(L_p(\Gamma))} \\ \leq & c \left(\|u_0\|_{\mathcal{D}_{r,p}} + \|v_0\|_{W_p^1} + \|g\|_{L_r(L_p(\Gamma))} \right). \end{aligned}$$

□

3.2 The linearized equation

The central approach of solving problems in nonlinear optimization is to look for roots of the derivative of the original problem. Solving the optimality system we obtain with the help of Newton's method will even involve derivatives of second order, so it is natural that we will need to be able to solve some kind of linearization of the state system. In order to have it suited for every instance throughout this work, we will formulate it in a rather general way including terms η_1, η_2 on the right hand side which can be chosen as needed. Additionally, when in chapter 7 we want to formulate second order optimality conditions, we will need to be able to bound the solution of the linearized equation with the $L_2(\Sigma)$-norm of the boundary value g. In chapter 8 ,we will need a result saying that the order of integrability of the solution to the linearized equation both in time and space is actually better than that of the boundary value g. Both claims are covered by the below theorem.

Theorem 3.4. *For $p > N$ assume that $\phi_1, \phi_2 \in L_\infty(Q)$, $\psi \in L_\infty(W_p^1)$. For $\alpha > 2(1 + \frac{N}{p-N})$, $\beta \geq 2$ let*

$$\xi_1, \xi_2 \in \mathcal{D}_{\alpha,\beta}, \quad \eta_1, \eta_2 \in L_\alpha(W_\beta^{-1}), \quad g \in L_\nu(L_\sigma(\Gamma))$$

for $1 < \nu \leq \alpha$, $1 < \sigma \leq \beta$ such that

$$\frac{2}{\nu} + \frac{N-1}{\sigma} < \frac{2}{\alpha} + \frac{N}{\beta}. \tag{3.11}$$

The system

$$u_t = \Delta u - \nabla \cdot \{\phi_1 u \nabla \psi + \phi_2 \nabla v\} + \eta_1 \quad \text{in } \Omega \times (0,T), \quad u(0) = \xi_1 \text{ in } \Omega, \tag{3.12}$$

$$v_t = \Delta v - v + u + \gamma^* g + \eta_2 \quad \text{in } \Omega \times (0,T), \quad v(0) = \xi_2 \text{ in } \Omega \tag{3.13}$$

has a unique solution $(u, v) \in \mathbb{W}_{\alpha,\beta} \times \mathbb{W}_{\nu,\beta} \cap L_\alpha(W_\beta^1)$ satisfying

$$\begin{aligned} \|u\|_{\mathbb{W}_{\alpha,\beta}} + \|v\|_{\mathbb{W}_{\nu,\beta}} + \|v\|_{L_\alpha(W_\beta^1)} \leq & c \big(\|\xi_1\|_{\mathcal{D}_{\alpha,\beta}} + \|\xi_2\|_{\mathcal{D}_{\alpha,\beta}} \\ & + \|\eta_1\|_{L_\alpha(W_\beta^{-1})} + \|\eta_2\|_{L_\alpha(W_\beta^{-1})} \\ & + \|g\|_{L_\nu(L_\sigma(\Gamma))} \big) \end{aligned} \tag{3.14}$$

for some constant $c > 0$ depending on ϕ_1, ϕ_2, ψ.

Remark 3.5. *(i) The conditions above can actually be satisfied: If for example $\alpha = \beta$, $\nu = \sigma$ (3.11) becomes $\alpha < \frac{N+2}{N+1}\nu$.*

(ii) In order to cover the case $\nu = \sigma = 2$ i.e. $g \in L_2(\Sigma)$ we need to assume that $p > 2N$, see Chapter 4.

Proof. The proof will be carried out in a similar way as the one of Theorem 3.1. Once again, for every $u \in L_\alpha(W_\beta^{-1})$ the linear equation (3.13) defines a map $u \mapsto v(u) \in \mathbb{W}_{\alpha,\beta}$. Since $g \in L_\nu(L_\sigma(\Gamma))$, it is obvious that $v \in \mathbb{W}_{\nu,\sigma}$. In order to see that v is actually more regular than that, we observe that for a.e. $t \in (0,T)$,

$$\|\gamma^* g(t)\|_{W_\beta^{-1}} \le c\|\gamma^* g(t)\|_{H_\sigma^\rho} \le c\|g(t)\|_{L_\sigma(\Gamma)} \tag{3.15}$$

for $-1 + N(\frac{1}{\sigma} - \frac{1}{\beta}) < \rho < \frac{1}{\sigma} - 1$. The left inequality is due to the embedding $H_\sigma^\rho \hookrightarrow W_\beta^1$ (cf. (2.1)), the right one holds since by (2.2), the adjoint of the trace operator γ^* is linear and continuous from $L_\sigma(\Gamma)$ to $H_\sigma^\rho(\Omega)$. This already implies

$$\|v\|_{\mathbb{W}_{\nu,\beta}} \le c\left(\|\xi_2\|_{\mathcal{D}_{\alpha,\beta}} + \|\eta_2\|_{L_\alpha(W_\beta^{-1})} + \|g\|_{L_\nu(L_\sigma(\Gamma))}\right). \tag{3.16}$$

In order to improve the order of integrability in time, we will make use of semigroup arguments: As in Lemma 3.3, v solves the integral equation

$$v(t) = S(t)v_0 + \int_0^t S(t-s)\{u+\eta_2\}(s)\, ds + \int_0^t S(t-s)\gamma^* g(s)\, ds.$$

From Lemma 2.9 we know that the first two terms satisfy

$$\begin{aligned}\|S(\cdot)\xi_2\|_{\mathbb{W}_{\alpha,\beta}} &\le c\|\xi_2\|_{\mathcal{D}_{\alpha,\beta}},\\ \|\int_0^{\cdot} S(\cdot - s)\{u+\eta_2\}(s))ds\|_{\mathbb{W}_{\alpha,\beta}} &\le c\left(\|u\|_{L_\alpha(W_\beta^{-1})} + \|\eta_2\|_{L_\alpha(W_\beta^{-1})}\right),\end{aligned}$$

so this time the interesting term is $I(t) := \int_0^t S(t-s)\gamma^* g(s)\, ds$. By (3.15) and Lemma 2.11, for

$$\theta := \frac{1-\rho}{2} + \frac{N}{2}(\frac{1}{\sigma} - \frac{1}{\beta}) > 1 - \frac{1}{2\sigma} + \frac{N}{2}(\frac{1}{\sigma} - \frac{1}{\beta}) \tag{3.17}$$

it holds that

$$\|I(t)\|_{W_\beta^1} \le c\int_0^t (t-s)^{-\theta}\|\gamma^* g(s)\|_{H_\sigma^\rho} ds \le c\int_0^t (t-s)^{-\theta}\|g(s)\|_{L_\rho(\Gamma)} ds$$

for $t \in (0,T)$. For ν^* such that $1 + \frac{1}{\alpha} = \frac{1}{\nu^*} + \frac{1}{\nu}$, Young's inequality for convolutions (A.4) gives

$$\|I\|_{L_\alpha(W_\beta^1)} \le c\left(\int_0^T t^{-\nu^*\theta} dt\right)^{\frac{1}{\nu^*}} \|g\|_{L_\nu(L_\sigma(\Gamma))},$$

where the integral is well defined as long as $\nu^*\theta < 1$. Hence we need to be able to find a θ such that (3.17) and

$$\theta < 1 + \frac{1}{\alpha} - \frac{1}{\nu} \tag{3.18}$$

are satisfied. This is guaranteed by (3.11) since

$$1 - \frac{1}{2\sigma} + \frac{N}{2}(\frac{1}{\sigma} - \frac{1}{\beta}) < 1 + \frac{1}{\alpha} - \frac{1}{\nu} \quad \Leftrightarrow \quad \frac{2}{\nu} + \frac{N-1}{\sigma} < \frac{2}{\alpha} + \frac{N}{\beta},$$

which finally implies

$$\|v\|_{L_\alpha(W^1_\beta)} \leq c\left(\|\xi_2\|_{\mathcal{D}_{\alpha,\beta}} + \|u\|_{L_\alpha(W^{-1}_\beta)} + \|\eta_2\|_{L_\alpha(W^{-1}_\beta)} + \|g\|_{L_\nu(L_\sigma(\Gamma))}\right). \tag{3.19}$$

After having dealt with (3.13), we are now going to show that the map $\tilde{u} \mapsto u$,

$$u_t = \Delta u - \nabla\cdot\{\phi_1\tilde{u}\nabla\psi + \phi_2\nabla v(\tilde{u})\} + \eta_1 \qquad u(0) = \xi_1 \tag{3.20}$$

has a unique fixed point. This time we will not have to restrict ourselves to small intervals first. Introducing a weighted norm

$$\|u\|_{\mu,t} := \max_{s\in[0,t]} e^{-\mu s}\|u(s)\|_{\mathcal{D}_{\alpha,\beta}}$$

on the spaces $C([0,t];\mathcal{D}_{\alpha,\beta})$ like in (3.9) right away, this time we will be able to show the fixed point property directly. Once again using (2.7), we estimate

$$\begin{aligned}\|-\nabla\cdot\{\phi_1\tilde{u}\nabla\psi + \phi_2\nabla v(\tilde{u})\}\|_{L_\alpha(W^{-1}_\beta)} \leq & c\|\phi_1\tilde{u}\nabla\psi + \phi_2\nabla v(\tilde{u})\|_{L_\alpha(L_\beta)} \\ \leq & c\|\tilde{u}\|_{L_\alpha(L_\rho)}\|\psi\|_{L_\infty(W^1_p)} + c\|v(\tilde{u})\|_{L_\alpha(W^1_\beta)} \\ \leq & c\|\tilde{u}\|_{L_\alpha(\mathcal{D}_{\alpha,\beta})} + c\|v(\tilde{u})\|_{L_\alpha(W^1_\beta)}\end{aligned}$$

where $\frac{1}{\beta} = \frac{1}{\rho} + \frac{1}{p}$ and $\rho = \infty$ if $\beta \geq p$. In the last step, we used (2.6) to get the embedding $\mathcal{D}_{\alpha,\beta} \hookrightarrow L_\rho$. This holds since by $\alpha > 2(1 + \frac{N}{p-N}) \;\Leftrightarrow\; \frac{2}{\alpha} < 1 - \frac{N}{p}$, there is an $\varepsilon > 0$ such that

$$1 - \frac{2}{\alpha} - \varepsilon - \frac{N}{\beta} > -\frac{N}{\rho} = \frac{N}{p} - \frac{N}{\beta}.$$

Due to (3.19) and maximal parabolic regularity, there is a $c > 0$ such that the solution u of (3.20) satisfies

$$\begin{aligned}\|u\|_{\mathbb{W}_{\alpha,\beta}} \leq & c\left(\|\xi_1\|_{\mathcal{D}_{\alpha,\beta}} + \|\tilde{u}\|_{L_\alpha(\mathcal{D}_{\alpha,\beta})} + \|v(\tilde{u})\|_{L_\alpha(W^1_\beta)} + \|\eta_1\|_{L_\alpha(W^{-1}_\beta)}\right) \\ \leq & c\left(\|\xi_1\|_{\mathcal{D}_{\alpha,\beta}} + \|\eta_1\|_{L_\alpha(W^{-1}_\beta)} + \|\xi_2\|_{\mathcal{D}_{\alpha,\beta}} + \|\eta_2\|_{L_\alpha(W^{-1}_\beta)} + \|g\|_{L_\nu(L_\sigma(\Gamma))}\right) \\ & + c\|\tilde{u}\|_{L_\alpha(\mathcal{D}_{\alpha,\beta})}.\end{aligned}$$

In the case of $\tilde{u}_1, \tilde{u}_2 \in \mathbb{W}_{\alpha,\beta}$, we get

$$\|u_1 - u_2\|_{\mathbb{W}_{\alpha,\beta}} \leq c\|\tilde{u}_1 - \tilde{u}_2\|_{L_\alpha(\mathcal{D}_{\alpha,\beta})}.$$

Now for every $t \in [0,T]$, the self-mapping and contraction property can be shown in the spaces $C([0,t];\mathcal{D}_{\alpha,\beta})$ using $\|\cdot\|_{\mu,t}$ in the same way as boundedness in the previous proof. □

3.3 The adjoint equation

Writing down necessary optimality conditions for the optimal control problem, we will introduce an adjoint state which will play the role of a multiplier to the constraint given by the state equation. This adjoint state is given as the solution of an adjoint equation of the below structure. We could also obtain existence and uniqueness of the adjoint state directly since the adjoint of the linearized control-to-state operator is well defined. However, the regularity results we would get — the adjoint state is an element of the dual space $(\mathbb{W}_{\alpha,\beta})^*$ — are not enough for our purposes. Also, the adjoint system turns out to be rather complex: Here, the second equation (which was rather simple in the state system) is coupled with the first equation by a term of second order, and in the first equation a gradient term appears which causes some additional trouble. Hence, it makes sense to look at the following system separately. Similarly to the previous section, the system includes some terms on the right hand side which we will need later on in this work.

Theorem 3.6. *Assume $p > N$, $\phi_1, \phi_2 \in L_\infty(Q)$ and $\psi \in L_\infty(W_p^1)$. For $2 < \alpha, \beta < \infty$ let*

$$\xi_1, \xi_2 \in \mathcal{D}_{\alpha,\beta}, \qquad \eta_1, \eta_2 \in L_\alpha(W_\beta^{-1}).$$

The system

$$-p_t = \Delta p + \phi_1 \nabla\psi\nabla p + q + \eta_1 \qquad \text{in } \Omega \times (0,T), \quad p(T) = \xi_1 \text{ in } \Omega, \tag{3.21}$$

$$-q_t = \Delta q - q - \nabla \cdot \{\phi_2 \nabla p\} + \eta_2 \qquad \text{in } \Omega \times (0,T), \quad q(T) = \xi_2 \text{ in } \Omega \tag{3.22}$$

has a unique solution $(p,q) \in \mathbb{W}^2_{\alpha,\beta}$ satisfying

$$\begin{aligned}\|p\|_{\mathbb{W}_{\alpha,\beta}} + \|q\|_{\mathbb{W}_{\alpha,\beta}} \leq c\big(&\|\xi_1\|_{\mathcal{D}_{\alpha,\beta}} + \|\xi_2\|_{\mathcal{D}_{\alpha,\beta}} \\ &+ \|\eta_1\|_{L_\alpha(W_\beta^{-1})} + \|\eta_2\|_{L_\alpha(W_\beta^{-1})}\big)\end{aligned} \tag{3.23}$$

where the constant c depends on ϕ_1, ϕ_2, ψ.

Proof. First of all, let us set $\tau := T - t$, $\hat{p}(\tau) := p(T-t)$, $\hat{q}(\tau) := q(T-t)$ etc. This way, the backward-in-time system above can be transformed into a forward system,

$$\begin{aligned} \hat{p}_t =& \Delta\hat{p} + \hat{\phi}_1 \nabla\hat{\psi}\nabla\hat{p} + \hat{q} + \hat{\eta}_1 \qquad && \text{in } \Omega \times (0,T), \qquad && \hat{p}(0) = \xi_1 \text{ in } \Omega, \\ \hat{q}_t =& \Delta\hat{q} - \hat{q} - \nabla \cdot \{\hat{\phi}_2 \nabla\hat{p}\} + \hat{\eta}_2 \qquad && \text{in } \Omega \times (0,T), \qquad && \hat{q}(0) = \xi_2 \text{ in } \Omega. \end{aligned}$$

For the rest of this proof we will work with this system, but skip the $\hat{\cdot}$ for convenience. Even though in this system the second equation (3.22) contains the cross diffusion term, still for every $p \in L_\alpha(W^1_\beta)$ it uniquely defines a $q = q(p) \in \mathbb{W}_{\alpha,\beta}$ satisfying

$$\begin{aligned} \|q\|_{\mathbb{W}_{\alpha,\beta}} \leq& c\left(\|\xi_2\|_{\mathcal{D}_{\alpha,\beta}} + \|p\|_{L_\alpha(W^1_\beta)} + \|\eta_2\|_{L_\alpha(W^{-1}_\beta)}\right) \\ \text{and} \quad \|q_1 - q_2\|_{\mathbb{W}_{\alpha,\beta}} \leq& c\|p_1 - p_2\|_{L_\alpha(W^1_\beta)} \end{aligned} \tag{3.24}$$

for $p_1, p_2 \in L_\alpha(W^1_\beta)$. Once again, this allows us to reduce (3.21)-(3.22) to

$$-p_t = \Delta p + \phi_1 \nabla\psi\nabla p + q(p) + \eta_1 \ \text{ in } Q, \qquad p(T) = \xi_1 \ \text{ in } \Omega. \tag{3.25}$$

As stated before, due to the gradient term on the right hand side this system is a bit more complicated than the others before. The strategy however stays similar: We introduce a weighted norm, this time on $L_\alpha(W^1_\beta)$, via

$$\|p\|_\mu := \|e^{-\mu\cdot}p(\cdot)\|_{L_\alpha(W^1_\beta)},$$

$\mu > 0$, and apply Banach's fixed point theorem, this time to the mild solution of (3.25). So let $\{S(t)\}_{t\geq 0}$ be the semigroup generated by $-A$ (cf. Definition 2.6). For $\tilde{p} \in L_\alpha(W^1_\beta)$, we look at the map $\tilde{p} \mapsto p$ defined by

$$p(t) = S(t)\xi_1 + \int_0^t S(t-s)\{\phi_1\nabla\psi\nabla\tilde{p} + q(\tilde{p})\}(s)\ ds + \int_0^t S(t-s)\eta_1(s)\ ds. \tag{3.26}$$

From Lemma 2.9, for the first and the last term we have

$$\|S(\cdot)\xi_1\|_{\mathbb{W}_{\alpha,\beta}} \leq c\|\xi_1\|_{\mathcal{D}_{\alpha,\beta}}, \quad \|\int_0^\cdot S(\cdot - s)\eta_1(s)ds\|_{\mathbb{W}_{\alpha,\beta}} \leq c\|\eta_1\|_{L_\alpha(W^{-1}_\beta)}.$$

So let us look at $I(t) := \int_0^t S(t-s)\{\phi_1 \nabla\psi\nabla\tilde{p} + q(\tilde{p})\}(s)\, ds$. For $\frac{1}{\rho} := \frac{1}{\beta} + \frac{1}{p}$ and $\theta := \frac{1}{2} + \frac{N}{2}(\frac{1}{\rho} - \frac{1}{\beta}) = \frac{1}{2}(1 + \frac{N}{p})$, (2.11) and the Hölder inequality (A.2) give

$$\begin{aligned}\|I(t)\|_{W^1_\beta} \leq & c\int_0^t (t-s)^{-\theta}\|\phi_1\nabla\psi\nabla\tilde{p}(s)\|_{L_\rho} + \|q(\tilde{p})\|_{W^1_\beta}\, ds \\ \leq & c(\phi_1)\int_0^t (t-s)^{-\theta}\|\psi(s)\|_{W^1_p}\|\tilde{p}(s)\|_{W^1_\beta} + \|q(\tilde{p})\|_{W^1_\beta}\, ds.\end{aligned}$$

Note that due to equivalence of norms, (3.24) also holds with respect to $\|\cdot\|_\mu$ for p and q. Multiplying by $e^{-\mu t}$, we have

$$\begin{aligned}\|e^{-\mu t} I(t)\|_{W^1_\beta} \leq c(\phi_1,\psi) & \int_0^t e^{-\mu(t-s)}(t-s)^{-\theta}\|e^{-\mu s}\tilde{p}(s)\|_{W^1_\beta}\, ds \\ + c & \int_0^t e^{-\mu(t-s)}\|e^{-\mu s} q(\tilde{p}(s))\|_{W^1_\beta}\, ds,\end{aligned}$$

and with the help of Young's inequality for convolutions (A.4),

$$\|I\|_\mu \leq c\int_0^T e^{-\mu t}t^{-\theta}\, dt\|\tilde{p}\|_\mu + c\int_0^T e^{-\mu t}\, dt\|q(\tilde{p})\|_\mu.$$

Both integrals tend to zero if $\mu \to \infty$. Coming back to (3.26), we obtain

$$\begin{aligned}\|p\|_\mu \leq & c(\mu)\left(\|\xi_1\|_{\mathcal{D}_{\alpha,\beta}} + \|\eta_1\|_{L_\alpha(W^{-1}_\beta)}\right) + c(\mu)\|\tilde{p}\|_\mu \\ & + c(\mu)\left(\|\xi_2\|_{\mathcal{D}_{\alpha,\beta}} + \|\tilde{p}\|_\mu + \|\eta_2\|_{L_\alpha(W^{-1}_\beta)}\right).\end{aligned}$$

For μ large enough, this implies $\|p\|_\mu \leq \|\tilde{p}\|_\mu$, and the same estimate

$$\|p_1 - p_2\|_\mu \leq c(\mu)\|\tilde{p}_1 - \tilde{p}_2\|_\mu$$

shows that $\tilde{p} \mapsto p$ is a contraction for μ chosen sufficiently large.

So far, we have shown that there is a unique solution $(p,q) \in L_\alpha(W^1_\beta) \times \mathbb{W}_{\alpha,\beta}$ satisfying

$$\begin{aligned}\|p\|_{L_\alpha(W^1_\beta)} + \|q\|_{\mathbb{W}_{\alpha,\beta}} \leq & c\left(\|\xi_1\|_{W^1_\beta} + \|\xi_2\|_{\mathcal{D}_{\alpha,\beta}}\right. \\ & \left. + \|\eta_1\|_{L_\alpha(W^{-1}_\beta)} + \|\eta_2\|_{L_\alpha(W^{-1}_\beta)}\right).\end{aligned} \tag{3.27}$$

Now that we know a solution exists, we can improve the regularity with the help of maximal parabolic regularity results: We actually have $p \in \mathbb{W}_{\alpha,\beta}$, since

$$\|p\|_{\mathbb{W}_{\alpha,\beta}} \leq \|\xi_1\|_{\mathcal{D}_{\alpha,\beta}} + \|\phi_1 \nabla\psi\nabla p\|_{L_\alpha(W_\beta^{-1})} + \|q\|_{L_\alpha(W_\beta^{-1})} + \|\eta_1\|_{L_\alpha(W_\beta^{-1})}$$

and

$$\begin{aligned}\|\phi_1 \nabla\psi\nabla p\|_{L_\alpha(W_\beta^{-1})} \leq & c\|\phi_1\|_{L_\infty(Q)}\|\nabla\psi\nabla p\|_{L_r(L_\rho)} \\ \leq & c\|\phi_1\|_{L_\infty(Q)}\|\psi\|_{L_\infty(W_p^1)}\|p\|_{L_\alpha(W_\beta^1)}.\end{aligned}$$

Together with (3.27) that gives the assertion. □

Chapter 4

The control-to-state operator

When we start analyzing the optimal control problem, it will be useful to reduce the objective function to just depend on the control. To that end, we introduce the control-to-state operator

$$\mathcal{G} : L_r(L_p(\Gamma)) \to \mathbb{W}^2_{r,p} = \left[L_r(W^1_p) \cap W^1_r(L_p)\right]^2$$

that maps the control $g \in L_r(L_p(\Gamma))$ to the solution (u, v) of the state equation

$$u_t = \Delta u - \nabla \cdot \{f(u)\nabla v\} \quad \text{in } \Omega \times (0, T), \qquad u(0) = u_0 \text{ in } \Omega, \tag{4.1}$$

$$v_t = \Delta v - v + u + \gamma^* g \quad \text{in } \Omega \times (0, T), \qquad v(0) = v_0 \text{ in } \Omega. \tag{4.2}$$

In this chapter, we are going to collect a few properties of this mapping which we are going to need in order to formulate optimality conditions, such as continuous Fréchet-differentiability of $\mathcal{G}$. In the last section, we are going to introduce the solution operator to the adjoint equation. Before we start, let us first state some assumptions which are supposed to hold in general for the optimal control problem. Assume that

$$p > N, \qquad r > 2p, \qquad \frac{2}{r} + \frac{N}{p} < 1, \tag{4.3}$$

$$u_0 \in \mathcal{D}_{r,p}, \qquad v_0 \in W^1_p(\Omega), \qquad u_Q \in L_r(L_p(Q)), \qquad u_\Omega \in \mathcal{D}_{r,p}, \tag{4.4}$$

$$\left.\begin{aligned} &f:\mathbb{R}^+\to\mathbb{R} \text{ twice continuously differentiable,}\\ &f(x)\le c_f,\; f'(x)\le c_{f'}\; f''(x)\le c_{f''} \text{ for all } x\in\mathbb{R}^+\\ &\left.\begin{aligned}|f(x)-f(y)| \le& L|x-y|,\\ |f'(x)-f'(y)| \le& L_{f'}|x-y|,\\ |f''(x)-f''(y)| \le& L_{f''}|x-y|\end{aligned}\right\} \text{ for all } x,y\in\mathbb{R}^+.\end{aligned}\right\} \tag{4.5}$$

Note that the choice of r and p implies that $\mathbb{W}_{r,p} \hookrightarrow C(\bar{Q})$. In what is to come, writing f we will mean the Nemytskii operator induced by the real function f (for more information see e.g. [59] p. 147 ff.). First of all, as simple consequences of Theorem 3.1 we know that the control-to-state operator is bounded and Lipschitz continuous:

Lemma 4.1. *The contol-to-state operator $\mathcal{G}$ is bounded in the sense that*

$$\|u\|_{\mathbb{W}_{r,p}} + \|v\|_{\mathbb{W}_{r,p}} \le c\left(\|u_0\|_{\mathcal{D}_{r,p}} + \|v_0\|_{\mathcal{D}_{r,p}} + \|g\|_{L_r(L_p(\Gamma))}\right)$$

for some $c > 0$.

Lemma 4.2. *The control-to-state operator $\mathcal{G}$ is Lipschitz continuous in the sense that for $(u, v) = \mathcal{G}(g)$, $(u^\delta, v^\delta) = \mathcal{G}(g + \delta)$*

$$\|u^\delta - u\|_{\mathbb{W}_{r,p}} + \|v^\delta - v\|_{\mathbb{W}_{r,p}} \le L(g,\delta)\|\delta\|_{L_r(L_p(\Gamma))}$$

for every $g, \delta \in L_r(L_p(\Gamma))$ and a constant $L > 0$.

Proof. Set $\delta u := u^\delta - u$, $\delta v := v^\delta - v$. Then $(\delta u, \delta v)$ is a solution to the system

$$\begin{aligned} \delta u_t =& \Delta\delta u - \nabla\cdot\{f(u^\delta)\nabla\delta v - f(u)\nabla v\} && \text{in } \Omega\times(0,T), && \delta u(0) = 0 \text{ in } \Omega,\\ \delta v_t =& \Delta\delta v - \delta v + \delta u + \gamma^*\delta && \text{in } \Omega\times(0,T), && \delta v(0) = 0 \text{ in } \Omega. \end{aligned}$$

The right hand side of the first equation can be transformed in the following way:

$$\begin{aligned} f(u^\delta)\nabla v^\delta - f(u)\nabla v =& (f(u^\delta) - f(u))\nabla v^\delta + f(u)\nabla(v^\delta - v)\\ =& -\int_0^1 \frac{d}{d\theta} f(u^\delta + \theta(u - u^\delta))\, d\theta\; \nabla v^\delta + f(u)\nabla(v^\delta - v)\\ =& \int_0^1 f'(u^\delta + \theta(u - u^\delta))\, d\theta\; \delta u \nabla v^\delta + f(u)\nabla\delta v\\ =& \phi\delta u\nabla v^\delta + f(u)\nabla\delta v \end{aligned}$$

with a continuous and bounded function $\phi \in C(\bar{Q})$. This has the same structure as the linearized equation (3.12) - (3.13) with $\phi_1 = \phi$, $\psi = v^\delta$, $\phi_2 = f(u)$, so Theorem 3.4 yields

$$\|\delta u\|_{\mathbb{W}_{r,p}} + \|\delta v\|_{\mathbb{W}_{r,p}} \leq c\|\delta\|_{L_r(L_p(\Gamma))},$$

where the constant depends on g and δ. □

4.1 First Derivative

The control-to-state operator is a nonlinear operator mapping from one function space to another. Hence, in order to compute the derivative, we first need to clarify what we mean by that and generalize the notion of a derivative (cf. e.g. [60] Def III.5.1):

Definition 4.3. *Let X, Y be two Banach spaces and $\mathcal{T} : X \to Y$. $\mathcal{T}$ is Fréchet differentiable in $x \in X$ if there is a linear continuous operator $\mathcal{S} : X \to Y$ and an $r : X \times X \to Y$ such that*

$$\mathcal{T}(x + h) = \mathcal{T}(x) + \mathcal{S}h + r(x, h)$$

for every $h \in X$ and

$$\frac{\|r(x, h)\|_Y}{\|h\|_X} \to 0, \qquad \|h\|_X \to 0.$$

$\mathcal{S}$ is called Fréchet derivative of $\mathcal{T}$ in x. $\mathcal{T}$ is called Fréchet differentiable if the derivative exists for every $x \in X$, and continuously Fréchet differentiable if the map $x \mapsto \mathcal{S}(x) \in \mathcal{L}(X, Y)$ is continuous.

With the help of this definition, the implicit function theorem can be generalized as well (cf. e.g. [60] Satz III.5.4 (e)):

Theorem 4.4. *Let X, Y, Z be Banach spaces and let $U \subset X$, $V \subset Y$ be open. Let $\mathcal{T} : X \times Y \supset U \times V \to Z$ be continuously differentiable, $x_0 \in U$, $y_0 \in V$ such that $\mathcal{T}(x_0, y_0) = 0$ and $y \mapsto \mathcal{T}_y(x_0, y_0)y$ is an isomorphism from $Y \to Z$. Then there are neighbourhoods U_0 of x_0, V_0 of y_0 such that for every $x \in U_0$ there is an $y = y(x) \in V_0$ uniquely defined such that $\mathcal{T}(x, y) = 0$. The function $x \mapsto y(x)$ is continuously differentiable from U_0 to Y with*

$$y_x(x) = -\left(\mathcal{T}_y(x, y(x))\right)^{-1} \mathcal{T}_x(x, y(x)).$$

Following the lines of [34], in order to apply this result to the control-to-state operator it is convenient to reformulate the state equation by defining an operator $\mathcal{A} : \mathbb{W}^2_{r,p} \to \left[L_r(W_p^{-1}) \times \mathcal{D}_{r,p}\right]^2$ via

$$(u,v) \mapsto \mathcal{A}(u,v) := \begin{pmatrix} u_t - \Delta u + \nabla \cdot \{f(u)\nabla v\} \\ u(0) \\ v_t - \Delta v + v - u \\ v(0) \end{pmatrix}. \tag{4.6}$$

Like this, the state equation is equivalent to

$$\mathcal{A}(u,v) = (0, u_0, \gamma^* g, v_0)^\top.$$

If in addition we introduce the map $\mathcal{T} : \mathbb{W}^2_{r,p} \times L_r(L_p(\Gamma)) \to [L_r(W_p^{-1}) \times \mathcal{D}_{r,p}]^2$,

$$\mathcal{T}(u,v,g) := \mathcal{A}(u,v) - (0, u_0, \gamma^* g, v_0)^\top, \tag{4.7}$$

the possible solutions to the state system are in fact given by the zero set of all (u,v,g) such that

$$\mathcal{T}(u,v,g) = 0.$$

Now we can apply the implicit function theorem to show

Theorem 4.5. *The control-to-state operator $\mathcal{G} : L_r(L_p(\Gamma)) \to \mathbb{W}^2_{r,p}$ is continuously Fréchet-differentiable. The derivative $h \mapsto \mathcal{G}'(g)h =: (w,z)$ of $\mathcal{G}$ in $g \in L_r(L_p(\Gamma))$ in direction $h \in L_r(L_p(\Gamma))$ is given by the solution to the system*

$$w_t = \Delta w - \nabla \cdot \{f'(u) w \nabla v + f(u)\nabla z\} \quad \text{in } \Omega \times (0,T), \quad w(0) = 0 \quad \text{in } \Omega, \tag{4.8}$$

$$z_t = \Delta z - z + w + \gamma^* h \quad \text{in } \Omega \times (0,T), \quad z(0) = 0 \quad \text{in } \Omega, \tag{4.9}$$

where $(u,v) = \mathcal{G}(g)$ and we have

$$\|w\|_{\mathbb{W}_{r,p}} + \|z\|_{\mathbb{W}_{r,p}} \leq c(g)\|h\|_{L_r(L_p(\Gamma))}$$

for some $c > 0$ depending on g.

Proof. We need to show that the assumptions of Theorem 4.4 are satisfied, i.e. we need to show three things: The operator $\mathcal{T}$ defined in (4.7) needs to be continuously differentiable with respect to g as well as with respect to (u,v), and the derivative $\mathcal{T}_{(u,v)}$ needs to be continuously invertible on the space $[L_r(W_p^{-1}) \times \mathcal{D}_{r,p}]^2$.

(i) Since $\mathcal{T}$ is linear with respect to g, continuous differentiability in this component is obvious and $\mathcal{T}_g h = (0, 0, \gamma^* h, 0)^\top$ for $h \in L_r(L_p(\Gamma))$.

(ii) Due to (4.5), the Nemytskii operator f is continuously differentiable from $L_\infty(Q)$ to $L_\infty(Q)$, and since we have $\mathbb{W}_{r,p} \hookrightarrow L_\infty(Q) \hookrightarrow L_r(L_p)$ due to (4.3), also from $\mathbb{W}_{r,p}$ to $L_r(L_p)$. Since everything else is linear, we have

$$\mathcal{T}_u(u, v, g)w = \mathcal{A}_u(u, v)w = \begin{pmatrix} w_t - \Delta w + \nabla \cdot \{f'(u)w\nabla v\} \\ w(0) \\ -w \\ 0 \end{pmatrix}$$

for $w \in \mathbb{W}_{r,p}$ and

$$\mathcal{T}_v(u, v, g)z = \mathcal{A}_v(u, v)z = \begin{pmatrix} \nabla \cdot \{f(u)\nabla z\} \\ 0 \\ z_t - \Delta z + z \\ z(0) \end{pmatrix}$$

for $z \in \mathbb{W}_{r,p}$.

(iii) The last thing we need to show is that $\mathcal{T}_{(u,v)} = \mathcal{A}_{(u,v)}$ is continuously invertible, so in other words, for every $(\eta_1, \xi_1 \eta_2, \xi_2) \in [L_r(W_p^{-1}) \times \mathcal{D}_{r,p}]^2$ there is a unique solution $(w, z) \in \mathbb{W}_{r,p}$ of

$$\mathcal{A}_{(u,v)}(u, v) \begin{pmatrix} w \\ z \end{pmatrix} = (\eta_1, \xi_1, \eta_2, \xi_2)^\top$$

satisfying

$$\|w\|_{\mathbb{W}_{r,p}} + \|z\|_{\mathbb{W}_{r,p}} \le c \left(\|\eta_1\|_{L_r(W_p^{-1})} + \|\xi_1\|_{\mathcal{D}_{r,p}} + \|\eta_2\|_{L_r(W_p^{-1})} + \|\xi_2\|_{\mathcal{D}_{r,p}} \right).$$

This is immediately clear by Lemma 3.4, since this is equivalent to (w, z) solving

$$\begin{aligned} w_t =& \Delta w - \nabla \cdot \{f'(u)w\nabla v + f(u)\nabla z\} + \eta_1 && \text{in } Q, \quad w(0) = \xi_1 \text{ in } \Omega, \\ z_t =& \Delta z - z + w + \eta_2 && \text{in } Q, \quad z(0) = \xi_2 \text{ in } \Omega. \end{aligned}$$

$\square$

Since $\mathcal{G}$ is only defined for $g \in L_r(L_p(\Gamma))$, naturally the same is true for its derivative $\mathcal{G}'$ and hence the admissible directions $h \in L_r(L_p(\Gamma))$. However, from Theorem 3.4 we know that the linearized equation remains well defined even for less regular $h \in L_\alpha(L_\beta(\Gamma))$, so that $\mathcal{G}'$ can be extended to an operator mapping from larger spaces $L_\alpha(L_\beta(\Gamma))$ to $\mathbb{W}^2_{\alpha,\beta}$. This is rather convenient when it comes to proving optimality conditions of second order: In Lemma 7.2, the main ingredient for second order optimality conditions, we will want to show that the second derivative of the reduced objective is Lipschitz continuous with an estimate involving the $L_2(\Sigma)$-norm of the direction h, which implies we will need suitable estimates for $\mathcal{G}'$. As we will see now, these estimates are provided by Theorem 3.4, even for general $h \in L_2(\Sigma)$, however imposing a stricter condition on p: Choosing $\nu = \sigma = 2$, we need to be able to find $\alpha, \beta \geq 2$ such that

$$\frac{2}{\alpha} + \frac{N}{p} < 1, \qquad \frac{2}{\alpha} + \frac{N}{\beta} > \frac{N+1}{2}. \tag{4.10}$$

Since $\beta \geq 2$, this can be rewritten to

$$\frac{1}{2} = \frac{N+1}{2} - \frac{N}{2} \leq \frac{N+1}{2} - \frac{N}{\beta} < \frac{2}{\alpha} < 1 - \frac{N}{p},$$

and the interval $(\frac{1}{2}, 1 - \frac{N}{p})$ is nonempty for $p > 2N$.

Lemma 4.6. *Let $p > 2N$ and $r > 2p$. Let $\alpha, \beta > 2$ such that (4.10) holds and $g \in L_r(L_p(\Gamma))$, $h \in L_2(\Sigma)$. The extension of the first derivative of the control-to-state mapping $(w, z) = \mathcal{G}'(g)h$ is bounded in the sense that for some $c > 0$ we have*

$$\|w\|_{\mathbb{W}_{\alpha,\beta}} + \|z\|_{\mathbb{W}_{2,\beta}} + \|z\|_{L_\alpha(W^1_\beta)} \leq c(g)\|h\|_{L_2(\Sigma)}.$$

Proof. Choose $\nu = \sigma = 2$ in Theorem 3.4. □

Lemma 4.7. *Choose r, p, α, β as above and let $g, \delta \in L_r(L_p(\Gamma))$, $h \in L_2(\Sigma)$. Let $(w, z) = \mathcal{G}'(g)h$, $(w^\delta, z^\delta) = \mathcal{G}'(g + \delta)h$. Then*

$$\|w^\delta - w\|_{\mathbb{W}_{\alpha,\beta}} + \|z^\delta - z\|_{\mathbb{W}_{2,\beta}} + \|z^\delta - z\|_{L_\alpha(W^1_\beta)} \leq c(g, \delta)\|\delta\|_{L_r(L_p(\Gamma))}\|h\|_{L_2(\Sigma)}$$

for some $c > 0$ depending on g and δ.

Proof. First of all, note that as in the previous lemma, (w,z) and (w^δ, z^δ) are well defined. Setting $(u,v) = \mathcal{G}(g)$ and $(u^\delta, v^\delta) = \mathcal{G}(g+\delta)$, the difference $(\delta w, \delta z) := (w^\delta, z^\delta) - (w,z)$ solves

$$\begin{aligned}
\delta w_t =& \Delta \delta w - \nabla \cdot \{f'(u)\delta w \nabla v + f(u)\nabla \delta z\} + \eta \quad \text{in } Q, \quad \delta u(0) = 0 \quad \text{in } \Omega,\\
\delta z_t =& \Delta \delta z - \delta z + \delta w \quad \text{in } Q, \quad \delta v(0) = 0 \quad \text{in } \Omega
\end{aligned}$$

with

$$\begin{aligned}
\eta :=& -\nabla \cdot \{(f'(u^\delta) - f'(u)) w^\delta \nabla v^\delta + f'(u) w^\delta \nabla (v^\delta - v)\}\\
&- \nabla \cdot \{(f(u^\delta) - f(u))\nabla z^\delta\}.
\end{aligned}$$

Theorem 3.4 gives

$$\|w^\delta - w\|_{\mathbb{W}_{\alpha,\beta}} + \|z^\delta - z\|_{\mathbb{W}_{2,\beta}} + \|z^\delta - z\|_{L_\alpha(W^1_\beta)} \le c(g,\delta)\|\eta\|_{L_\alpha(W^{-1}_\beta)},$$

so that the crucial part is to find a bound for $\|\eta\|_{L_\alpha(W^{-1}_\beta)}$. To this end, fix $\rho > 1$ by $\frac{1}{\beta} = \frac{1}{\rho} + \frac{1}{p}$. With the help of the Hölder inequality (A.2) and the embedding $W^1_\beta \hookrightarrow L_\rho$, (which works for $p > N$ since $1 - \frac{N}{\beta} \ge -\frac{N}{\rho} = -\frac{N}{\beta} + \frac{N}{p}$, cf. (2.1)) we have

$$\|w\nabla v\|_{L_\alpha(L_\beta)} \le c\|w\|_{L_\alpha(L_\rho)}\|\nabla v\|_{L_\infty(L_p)} \le c\|w\|_{L_\alpha(W^1_\beta)}\|v\|_{L_\infty(W^1_p)}.$$

Since the state v^δ is bounded by a constant depending on the initial values and the control $g + \delta$, we have

$$\begin{aligned}
&\|\eta\|_{L_\alpha(W^{-1}_\beta)}\\
&\quad \le c\left(\|(f'(u^\delta) - f'(u))w^\delta\nabla v^\delta\|_{L_\alpha(L_\beta)} + \|f'(u)w^\delta \nabla(v^\delta - v)\|_{L_\alpha(L_\beta)}\right.\\
&\qquad \left. + \|(f(u^\delta) - f(u))\nabla z^\delta\|_{L_\alpha(L_\beta)}\right)\\
&\quad \le \Big(L_{f'}\|u^\delta - u\|_{C(\bar{Q})}\|w^\delta\|_{L_\alpha(W^1_\beta)}\|v^\delta\|_{L_\infty(W^1_p)}\\
&\qquad + c_{f'}\|w^\delta\|_{L_\alpha(W^1_\beta)}\|v^\delta - v\|_{L_\infty(W^1_p)} + L_f\|u^\delta - u\|_{C(\bar{Q})}\|z^\delta\|_{L_\alpha(W^1_\beta)}\Big)\\
&\quad \le c(g,\delta)\left(\|u^\delta - u\|_{C(\bar{Q})} + \|v^\delta - v\|_{L_r(W^1_p)}\right)\left(\|w^\delta\|_{\mathbb{W}_{\alpha,\beta}} + \|z^\delta\|_{L_\alpha(W^1_\beta)}\right).
\end{aligned}$$

Now Lemma 4.2 and Lemma 4.6 give

$$\begin{aligned}
\|u^\delta - u\|_{C(\bar{Q})} + \|v^\delta - v\|_{L_\infty(W^1_p)} \le& c\|\delta\|_{L_r(L_p(\Gamma))},\\
\|w^\delta\|_{\mathbb{W}_{\alpha,\beta}} + \|z^\delta\|_{L_\alpha(W^1_\beta)} \le& c(g,\delta)\|h\|_{L_2(\Sigma)}
\end{aligned}$$

so that the assertion follows. □

4.2 Second Derivative

In order to derive optimality conditions of second order, of course we need to make sure the control-to-state operator is twice continuously differentiable. Since we applied the implicit function theorem to compute the first derivative, there is not much more to show:

Theorem 4.8. *The control-to-state operator $\mathcal{G}$ is twice continuously differentiable from $L_r(L_p(\Gamma))$ to $\mathbb{W}^2_{r,p}$. The second derivative of $\mathcal{G}$ in $g \in L_r(L_p(\Gamma))$ in directions $h_1, h_2 \in L_r(L_p(\Gamma))$, $h_2 \mapsto \mathcal{G}''(g)[h_1, h_2] =: (\phi, \psi)$, is given by the solution to the system*

$$\begin{aligned} \phi_t =& \Delta\phi - \nabla \cdot \{f'(u)\phi\nabla v + f(u)\nabla\psi\} \\ &- \nabla \cdot \{f''(u)w_1 w_2 \nabla v\} && \text{in } \Omega \times (0,T), \quad \phi(0) = 0 \text{ in } \Omega, \\ &- \nabla \cdot \{f'(u)w_1\nabla z_2 + f'(u)w_2\nabla z_1\} \\ \psi_t =& \Delta\psi - \psi + \phi && \text{in } \Omega \times (0,T), \quad \psi(0) = 0 \text{ in } \Omega. \end{aligned}$$

Proof. We only need to make sure that the operator $\mathcal{A}$ defined in (4.6) is twice continuously Fréchet differentiable. Since the initial values are zero anyway, we can omit those components here. The Nemytskii operator f is twice differentiable in the same spaces as before, so for $w_1, w_2, z_1, z_2 \in \mathbb{W}_{r,p}$, we have

$$\mathcal{A}_{u,u}[w_1, w_2] = \begin{pmatrix} \nabla \cdot \{f''(u)w_1 w_2 \nabla v\} \\ 0 \end{pmatrix}, \quad \mathcal{A}_{u,v}[w_1, z_2] = \begin{pmatrix} \nabla \cdot \{f'(u)w_1\nabla z_2\} \\ 0 \end{pmatrix}$$

$$\mathcal{A}_{v,u}[z_1, w_2] = \begin{pmatrix} \nabla \cdot \{f'(u)w_2\nabla z_1\} \\ 0 \end{pmatrix}, \qquad \mathcal{A}_{v,v}[z_1, z_2] = 0.$$

Since for $\mathcal{T}$ defined in (4.7) we have $\mathcal{T}_{g,g} = \mathcal{T}_{g,(u,v)} = \mathcal{T}_{(u,v),g} = 0$, the second derivative is given by the formula

$$\mathcal{G}''(g)[h_1, h_2] = \mathcal{T}_{(u,v)}(u, v, g)^{-1}\mathcal{T}_{(u,v)^2}(u, v, g)[(w_1, z_1, h_1), (w_2, z_2, h_2)].$$

For $(\phi, \psi) = \mathcal{G}''(g)[h_1, h_2]$ this is exactly the solution to the system above. $\square$

4.3 The adjoint operator

When it comes to deriving first order optimality conditions for the optimal control problem (1.1)-(1.3), we are going to need to solve an adjoint to the state system. Formally, if we want to write the constraint as an operator equation mapping the control to the state we plug into the objective, we do not end up with the control-to-state operator $\mathcal{G}$ itself, but with an operator mapping the control g onto the first component of the solution u and its final values $u(T)$. So if we introduce an operator $\mathcal{S}$ mapping the right hand side (η_w, η_z) of the linearized equation (4.8)-(4.9) to its solution (w, z), its adjoint $\mathcal{S}^*$ maps (η_p, η_q) to the solution (p, q) of the adjoint system and we have

$$\begin{aligned}\begin{pmatrix}0\\g\end{pmatrix} \mapsto \begin{pmatrix}\mathcal{E}_Q & 0\\ \mathcal{E}_\Omega & 0\end{pmatrix} \mathcal{S} \begin{pmatrix}0 & 0\\ 0 & \gamma^*\end{pmatrix}\begin{pmatrix}0\\g\end{pmatrix} &= \begin{pmatrix}\mathcal{E}_Q & 0\\ \mathcal{E}_\Omega & 0\end{pmatrix} \mathcal{S} \begin{pmatrix}0\\ \gamma^* g\end{pmatrix}\\ &= \begin{pmatrix}\mathcal{E}_Q & 0\\ \mathcal{E}_\Omega & 0\end{pmatrix}\begin{pmatrix}w\\z\end{pmatrix} = \begin{pmatrix}w\\ w(T)\end{pmatrix},\end{aligned}$$

where $\mathcal{E}_Q : w \mapsto w$ and $\mathcal{E}_\Omega : w \mapsto w(T)$ are embedding operators. The adjoint to all this hence maps the right hand side η_p and the final value ξ_p of the first component of the adjoint system to the boundary value γq of the second component,

$$\begin{aligned}\begin{pmatrix}\eta_p\\ \xi_p\end{pmatrix} \mapsto \begin{pmatrix}0 & 0\\ 0 & \gamma\end{pmatrix} \mathcal{S}^* \begin{pmatrix}\mathcal{E}_Q^* & \mathcal{E}_\Omega^*\\ 0 & 0\end{pmatrix}\begin{pmatrix}\eta_p\\ \xi_p\end{pmatrix} &= \begin{pmatrix}0 & 0\\ 0 & \gamma\end{pmatrix} \mathcal{S}^* \begin{pmatrix}\mathcal{E}_Q^*\eta_p + \mathcal{E}_\Omega^*\xi_p\\ 0\end{pmatrix}\\ &= \begin{pmatrix}0 & 0\\ 0 & \gamma\end{pmatrix}\begin{pmatrix}p\\ q\end{pmatrix} = \gamma q.\end{aligned}$$

In order to do this rigorously, we would have to carefully check which spaces are involved and for example work in dual spaces $\mathbb{W}^*_{r,p}$. Since this is neither trivial nor particularly helpful, instead we are going to introduce an adjoint system combining the embeddings and the operator $\mathcal{S}^*$, i.e. an operator

$$\mathcal{P}(g) : L_r(W_p^{-1}) \times \mathcal{D}_{r,p} \to \mathbb{W}^2_{r,p}, \qquad (\eta_p, \xi_p) \mapsto (p, q) \tag{4.11}$$

by

$$\begin{aligned} -p_t =& \Delta p + f'(u)\nabla v \nabla p + q + \eta_p \ \text{ in } \Omega \times (0, T), && p(T) = \xi_p \ \text{ in } \Omega,\\ -q_t =& \Delta q - q - \nabla \cdot \{f(u)\nabla p\} \quad \text{ in } \Omega \times (0, T), && q(T) = 0 \quad \text{in } \Omega,\end{aligned}$$

where $(u, v) = \mathcal{G}(g)$ is a solution to the state equation (4.1)-(4.2). Due to Theorem 3.6, this is well defined for $\eta_p \in L_\alpha(W_\beta^{-1})$, $\xi_p \in \mathcal{D}_{\alpha,\beta}$, and the following properties hold:

Lemma 4.9. *Assume that* (4.3) *holds. Let* $\alpha, \beta > 2$ *and* $(u, v) = \mathcal{G}(g)$ *for* $g \in L_r(L_p(\Gamma))$. *The adjoint state is bounded in the sense that*

$$\|p\|_{\mathbb{W}_{\alpha,\beta}} + \|q\|_{\mathbb{W}_{\alpha,\beta}} \leq c(g) \left(\|\xi_p\|_{\mathcal{D}_{\alpha,\beta}} + \|\eta_p\|_{L_\alpha(W_\beta^{-1})} \right)$$

for some $c > 0$ *depending on* g.

Proof. This is an immediate consequence of Theorem 3.6. □

Remark 4.10. *In the optimality system, we will have* $\xi_p = \alpha_1(u(T) - u_\Omega)$ *and* $\eta_p = \alpha_2(u - u_Q)$, *so that the above estimate becomes*

$$\begin{aligned} \|p\|_{\mathbb{W}_{\alpha,\beta}} + \|q\|_{\mathbb{W}_{\alpha,\beta}} \leq c(g) \Big(&\|u_\Omega\|_{\mathcal{D}_{\alpha,\beta}} + \|u_Q\|_{L_\alpha(W_\beta^{-1})} \\ &+ \|u_0\|_{\mathcal{D}_{r,p}} + \|v_0\|_{\mathcal{D}_{r,p}} + \|g\|_{L_r(L_p(\Gamma))} \Big) . \end{aligned}$$

Lemma 4.11. *Assume* (4.3) *holds. Let* $g, \delta \in L_r(L_p(\Gamma))$ *and* $(u, v) := \mathcal{G}(g)$, $(u^\delta, v^\delta) := \mathcal{G}(g + \delta)$. *Choose*

$$\begin{aligned} \xi_p &:= \alpha_1(u(T) - u_\Omega) & \xi_p^\delta &:= \alpha_1(u^\delta(T) - u_\Omega) \\ \eta_p &:= \alpha_2(u - u_Q) & \eta_p^\delta &:= \alpha_2(u^\delta - u_Q). \end{aligned}$$

The solution to the adjoint system is Lipschitz stable with respect to perturbations δ *in the sense that*

$$\|p^\delta - p\|_{\mathbb{W}_{r,p}} + \|q^\delta - q\|_{\mathbb{W}_{r,p}} \leq c(g) \|\delta\|_{L_r(L_p(\Gamma))}. \tag{4.12}$$

for some $c > 0$ *depending on* g.

Proof. Set $\delta p := p^\delta - p$, $\delta q := q^\delta - q$, $\delta u = u^\delta - u$, $\delta v = v^\delta - v$. Then $(\delta p, \delta q)$ solves

$$\begin{aligned} -\delta p_t &= \Delta \delta p + f'(u) \nabla v \nabla \delta p + \delta q + \eta_1 && \text{in } Q, && p(T) = \delta u(T) && \text{in } \Omega, \\ -\delta q_t &= \Delta \delta q - \delta q - \nabla \cdot \{f(u) \nabla \delta p\} + \eta_2 && \text{in } Q, && q(T) = 0 && \text{in } \Omega, \end{aligned}$$

where

$$\begin{aligned} \eta_1 &= (f'(u^\delta) - f'(u)) \nabla v^\delta \nabla p^\delta + f'(u) \nabla \delta v \nabla p^\delta + \alpha_2 \delta u, \\ \eta_2 &= -\nabla \cdot \{(f(u^\delta) - f(u)) \nabla p^\delta\}. \end{aligned}$$

Since for $p > N$ we have

$$\|\nabla v \nabla p\|_{L_r(W_p^{-1})} \leq c\|\nabla v \nabla p\|_{L_r(L_{\frac{p}{2}})} \leq c\|v\|_{L_\infty(W_p^1)}\|p\|_{L_r(W_p^1)},$$

we can estimate

$$\begin{aligned}
\|\eta_1\|_{L_r(W_p^{-1})} \leq & c\left(L_{f'}\|\delta u\|_{C(\bar{Q})}\|v^\delta\|_{L_\infty(W_p^1)}\|p^\delta\|_{L_r(W_p^1)}\right.\\
& \left. + c_{f'}\|\delta v\|_{L_\infty(W_p^1)}\|p^\delta\|_{L_r(W_p^1)}\right)\\
\leq & c(g,\delta)\left(\|\delta u\|_{C(\bar{Q})} + \|\delta v\|_{L_\infty(W_p^1)}\right),\\
\|\eta_2\|_{L_r(W_p^{-1})} \leq & c\|\{f(u^\delta) - f(u)\}\nabla p^\delta\|_{L_r(L_p)}\\
\leq & cL_f\|\delta u\|_{C(\bar{Q})}\|p^\delta\|_{L_r(W_p^1)}\\
\leq & c(g,\delta)\|\delta u\|_{C(\bar{Q})},
\end{aligned}$$

since both v^δ and p^δ are bounded by a constant depending on g, δ and the data u_0, v_0, u_Ω, u_Q. From Theorem 3.6 we have

$$\|\delta p\|_{\mathbb{W}_{r,p}} + \|\delta q\|_{\mathbb{W}_{r,p}} \leq c\left(\|\delta u(T)\|_{\mathcal{D}_{r,p}} + \|\eta_1\|_{L_r(W_p^{-1})} + \|\eta_2\|_{L_r(W_p^{-1})}\right),$$

and by Lemma 4.2

$$\|\delta u\|_{\mathbb{W}_{r,p}} + \|\delta v\|_{\mathbb{W}_{r,p}} \leq c(g,\delta)\|\delta\|_{L_r(L_p(\Gamma))}$$

which implies (4.12). $\square$

Chapter 5

Existence of an optimal control

So far, we have only focused on the pde constraint. Now that we have provided all the results we need to deal with the state system, it is time to turn to the actual optimal control problem (1.1)-(1.3): For $\alpha_1, \alpha_2, \lambda > 0$ and constraints

$$g_a, g_b \in L_r(L_p(\Gamma)) \text{ such that } g_a(x,t) \leq g_b(x,t) \text{ for a.e. } (x,t) \in \Sigma, \tag{5.1}$$

we want to find a solution to

$$J(u,v;g) = \frac{\alpha_1}{2}\|u(T) - u_\Omega\|^2_{L_2(\Omega)} + \frac{\alpha_2}{2}\|u - u_Q\|^2_{L_2(Q)} + \frac{\lambda}{2}\|g\|^2_{L_2(\Sigma)},$$

$$\begin{aligned} u_t =& \Delta u - \nabla \cdot \{f(u)\nabla v\} \text{ in } \Omega \times (0,T), \quad u(0) = u_0 \text{ in } \Omega, \\ v_t =& \Delta v - v + u + \gamma^* g \qquad \text{in } \Omega \times (0,T), \quad v(0) = v_0 \text{ in } \Omega, \end{aligned}$$

$$g \in G_{ad} := \{g \in L_r(0,T;L_p(\Gamma)) : g_a \leq g \leq g_b \text{ a.e. in } \Gamma \times (0,T)\}.$$

Naturally, the first step on the way to finding an optimal solution is making sure such a solution actually exists. Since the control-to-state operator is nonlinear, it is clear that we cannot expect the solution to be unique. Existence however can be shown in a rather standard way (cf. eg. [41], [59]):

Theorem 5.1. *The control problem (1.1)-(1.3) possesses an optimal solution* $\bar{g} \in G_{ad}$.

Proof. First of all, note that obviously the objective is bounded from below, so an infimum and with it an infimal sequence of controls, i.e. a sequence

$\{g_k\}_{k\in\mathbb{N}} \subset G_{ad}$ such that

$$\mathcal{J}(g_k) \to \inf_{g\in G_{ad}} \mathcal{J}(g),$$

surely exist. Since G_{ad} is a bounded, closed and convex subset of the reflexive Banach space $L_r(L_p(\Gamma))$ and hence weakly sequentially compact, there is a subsequence of $\{g_k\}$ that weakly converges to some $\bar{g} \in G_{ad}$,

$$g_k \rightharpoonup \bar{g}, \quad k \to \infty.$$

In order to avoid multiple indices, we will refer to this subsequence by $\{g_k\}$ as well. So let us look at the corresponding state sequence $\{(u_k, v_k)\}_{k\in\mathbb{N}}$ defined by the control-to-state operator. By Lemma 4.1, this sequence is uniformly bounded in $\mathbb{W}^2_{r,p}$, and since the embedding $\mathbb{W}_{r,p} \hookrightarrow C(\bar{Q})$ is compact (cf. [7], [55]), we find a subsequence of $\{u_k\}$ — once again denoted by $\{u_k\}$ — that strongly converges to some $\bar{u} \in C(\bar{Q})$,

$$u_k \to \bar{u}, \quad k \to \infty.$$

So with the right hand side $u_k + \gamma^* g_k$, we can look at v_k as the solution of the linear problem

$$v_{k,t} - \Delta v_k + v_k = u_k + \gamma^* g_k \;\text{ in } \Omega \times (0,T), \qquad v_k(0) = v_0 \text{ in } \Omega.$$

Since the mapping $(u_k + \gamma^* g_k) \mapsto v_k$ is linear and continuous and hence weakly continuous, $\{v_k\}$ weakly converges to some $\bar{v}$ in $\mathbb{W}_{r,p}$,

$$v_k \rightharpoonup \bar{v}, \quad k \to \infty.$$

Now we do the same with the first equation: Since $\{u_k\}$ converges strongly in $C(\bar{Q})$, so does $\{f(u_k)\}$ and the term $R_k := \nabla\cdot\{f(u_k)\nabla v_k\}$ is weakly convergent to some $R \in L_r(W_p^{-1})$. Hence the mapping $R_k \mapsto u_k$, defined as the solution of

$$u_{k,t} - \Delta u_k = R_k \;\text{ in } \Omega \times (0,T), \qquad u_k(0) = u_0 \text{ in } \Omega,$$

yields that $u_k \rightharpoonup \bar{u}$ in $\mathbb{W}_{r,p}$. This way we have found candidates $\bar{g}, \bar{u}, \bar{v}$ that might give an optimal solution to the problem. We still have to make sure though that they actually solve the state equation. To that end, let us look at the variational formulation of the state equation in $\mathbb{W}_{2,2}$. Integrating by parts as in Lemma 2.2, we get

$$\int_0^T \int_\Omega u_k \phi_t + \nabla u_k \nabla \phi \; dxdt = \int_0^T \int_\Omega f(u_k) \nabla v_k \nabla \phi \; dxdt + \int_\Omega u_0 \phi(0) \; dt,$$

$$\int_0^T \int_\Omega v_k \psi_t + \nabla v_k \nabla \psi + v_k \psi \; dxdt = \int_0^T \int_\Omega u_k \psi + \gamma^* g_k \psi \; dxdt + \int_\Omega v_0 \psi(0) \; dt$$

for every $\phi, \psi \in H^1(H^1)$ such that $\phi(T) = \psi(T) = 0$. With the above convergence results $u_k \rightharpoonup \bar{u}$, $v_k \rightharpoonup \bar{v}$ in $\mathbb{W}_{r,p}$ and $f(u_k) \to f(\bar{u})$ in $C(\bar{Q})$, in the limit we have

$$\int_0^T \int_\Omega \bar{u} \phi_t + \nabla \bar{u} \nabla \phi \; dxdt = \int_0^T \int_\Omega f(\bar{u}) \nabla \bar{v} \nabla \phi \; dxdt + \int_\Omega u_0 \phi(0) \; dx,$$

$$\int_0^T \int_\Omega \bar{v} \psi_t + \nabla \bar{v} \nabla \psi + \bar{v} \psi \; dxdt = \int_0^T \int_\Omega \bar{u} \psi + \gamma^* \bar{g} \psi \; dxdt + \int_\Omega v_0 \psi(0) \; dx.$$

What we have shown now is the following: There is a subsequence $\{g_k\}$ of the infimal sequence that, together with its corresponding state sequence $\{(u_k, v_k)\}$, weakly converges to some $\bar{g} \in L_r(L_p(\Gamma))$, $(\bar{u}, \bar{v}) \in \mathbb{W}_{r,p}^2$ such that the triple $(\bar{g}, \bar{u}, \bar{v})$ itself solves the sate equation as well. So it only remains to verify that $(\bar{g}, \bar{u}, \bar{v})$ actually minimizes the objective: This follows from the fact that the objective is continuous and convex and hence weakly lower semi-continuous, i.e.

$$(g_k, u_k, v_k) \rightharpoonup (\bar{g}, \bar{u}, \bar{v}) \quad \Rightarrow \quad \lim \inf_{k \to \infty} J(g_k, u_k, v_k) \geq J(\bar{g}, \bar{u}, \bar{v}).$$

□

Chapter 6

Necessary optimality conditions of first order

After we have established that an optimal solution exists, in this chapter we are going to look at necessary conditions for a control $g \in G_{ad}$ to be optimal. This serves as a basis for many numerical methods of finding an optimal solution. The approach is very similar to the well known KKT conditions in finite dimensional optimization (cf. e.g. [3], [22]). As it was mentioned in chapter 4, it is not necessary to face the difficulties resulting from defining Lagrange multipliers in the dual spaces precisely. Instead, it is well known that the optimality conditions can be represented with an adjoint state which is introduced directly with the help of an adjoint system. For now, the inequality constraints we impose on the control will be kept explicitly without introducing multipliers. Recall the objective is given by

$$J(u,v;g) = \frac{\alpha_1}{2}\|u(T)-u_\Omega\|^2_{L_2(\Omega)} + \frac{\alpha_2}{2}\|u-u_Q\|^2_{L_2(Q)} + \frac{\lambda}{2}\|g\|^2_{L_2(\Sigma)}.$$

We can reduce J to a function only depending on the control by plugging in the control-to-state operator $\mathcal{G}$, i.e. we set $\mathcal{J}(g) := J(\mathcal{G}(g), g)$. The Fréchet-derivative of $\mathcal{G}$ was computed in Theorem 4.5, so the Fréchet-derivative of $\mathcal{J}$ in g in direction h is then given by

$$\mathcal{J}'(g)h = \alpha_1 \langle u(T)-u_\Omega, w(T)\rangle_\Omega + \alpha_2 \langle u-u_Q, w\rangle_Q + \lambda \langle g,h\rangle_\Sigma\,, \qquad (6.1)$$

where $(w, z) = \mathcal{G}'(g)h$ solves the linearized equation

$$w_t = \Delta w - \nabla \cdot \{f'(u)w\nabla v + f(u)\nabla z\} \quad \text{in } \Omega \times (0,T), \quad w(0) = 0 \text{ in } \Omega, \tag{6.2}$$

$$z_t = \Delta z - z + w + \gamma^* h \quad \text{in } \Omega \times (0,T), \quad z(0) = 0 \text{ in } \Omega. \tag{6.3}$$

It is well known and easily seen that it is necessary for $\bar{g}$ to be an optimal solution that the variational inequality

$$\mathcal{J}'(\bar{g})(g - \bar{g}) \geq 0 \qquad \text{for all } g \in G_{ad}$$

must be satisfied. This can be reformulated by introducing an adjoint system,

$$\begin{aligned} -p_t &= \Delta p + f'(\bar{u})\nabla\bar{v}\nabla p + q + \alpha_2(\bar{u} - u_Q) && \text{in } \Omega \times (0,T), \\ p(T) &= \alpha_1(\bar{u}(T) - u_\Omega) && \text{in } \Omega, \end{aligned} \tag{6.4}$$

$$\begin{aligned} -q_t &= \Delta q - q - \nabla \cdot \{f(\bar{u})\nabla p\} && \text{in } \Omega \times (0,T), \\ q(T) &= 0 && \text{in } \Omega, \end{aligned} \tag{6.5}$$

where $(\bar{u}, \bar{v})$ is the solution to the state equation corresponding to the control $\bar{g}$. For $\xi_p := \alpha_1(\bar{u}(T) - u_\Omega)$, $\eta_p := \alpha_2(\bar{u} - u_Q)$, this is the system which defines the operator $\mathcal{P}(g)$ in (4.11). With the help of this we can show that

Lemma 6.1. *Assume* (4.3) *holds. The derivative* (6.1) *of the reduced objective in* $g \in L_r(L_p(\Gamma))$ *in the direction* $h \in L_r(L_p(\Gamma))$ *can be written as*

$$\mathcal{J}'(g)h = \langle \gamma q + \lambda g, h \rangle_\Sigma ,$$

where $q \in \mathbb{W}_{r,p}$ *is the second component of the solution to the system* (6.4)-(6.5).

Proof. We have to show that for $(u, v) = \mathcal{G}(g)$, $(w, z) \in \mathbb{W}^2_{r,p}$ solving (6.2)-(6.3) and $(p, q) \in \mathbb{W}^2_{r,p}$ solving (6.4)-(6.5) it holds that

$$\alpha_1 \langle u(T) - u_\Omega, w(T) \rangle_\Omega + \alpha_2 \langle u - u_Q, w \rangle_Q = \langle \gamma q, h \rangle_\Sigma .$$

The idea is to "test" the variational formulation of the linearized system with the solution to the adjoint system and vice versa. Due to the way the adjoint system is defined, combining these systems will lead to the desired result.

Recall that a generalized solution to (6.2)-(6.3) satisfies

$$\int_0^T \langle w_t, p\rangle_{W_p^{-1},W_{p'}^1} + \langle \nabla w, \nabla p\rangle_\Omega - \langle f'(u)w\nabla v, \nabla p\rangle_\Omega \,dt = \int_0^T \langle f(u)\nabla z, \nabla p\rangle_\Omega \,dt,$$

$$\int_0^T \langle z_t, q\rangle_{W_p^{-1},W_{p'}^1} + \langle \nabla z, \nabla q\rangle_\Omega + \langle z, q\rangle_\Omega \,dt = \int_0^T \langle w, q\rangle_\Omega + \langle \gamma^* h, q\rangle_\Omega \,dt$$

for all $p, q \in L_{r'}(W_{p'}^1)$, where $\frac{1}{r} + \frac{1}{r'} = 1$, $\frac{1}{p} + \frac{1}{p'} = 1$, so in particular for adjoint state $(p, q) \in \mathbb{W}_{r,p}^2$. For (6.4)-(6.5), we choose the linearized state $(w, z) \in \mathbb{W}_{r,p}$ as test functions and integrate by parts along Lemma 2.2 to get

$$\int_0^T \langle w_t, p\rangle_{W_p^{-1},W_{p'}^1} + \langle \nabla p, \nabla w\rangle_\Omega - \langle f'(u)\nabla v\nabla p, w\rangle_\Omega - \langle q, w\rangle_\Omega \,dt$$
$$= \int_0^T \langle \alpha_2(u - u_Q), w\rangle_\Omega \,dt + \langle \alpha_1 u(T) - u_\Omega, w(T)\rangle_\Omega \,dt,$$

$$\int_0^T \langle z_t, q\rangle_{W_p^{-1},W_{p'}^1} + \langle \nabla q, \nabla z\rangle_\Omega + \langle q, z\rangle_\Omega \,dt = \int_0^T \langle f(u)\nabla p, \nabla z\rangle_\Omega \,dt.$$

Now we can compute

$$\begin{aligned}
\alpha_1 \langle u(T) - u_\Omega, w(T)\rangle_\Omega + \alpha_2 \langle u - u_Q, w\rangle_Q
&= \int_0^T \langle p_t, w\rangle_{W_p^{-1},W_{p'}^1} + \langle \nabla p, \nabla w\rangle_\Omega \,dt \\
&\quad - \int_0^T \langle f'(u)\nabla v\nabla p, w\rangle_\Omega - \langle q, w\rangle_\Omega \,dt \\
&= \int_0^T \langle f(u)\nabla z, \nabla p\rangle_\Omega - \langle q, w\rangle_\Omega \,dt \\
&= \int_0^T \langle z_t, q\rangle_\Omega + \langle \nabla q, \nabla z\rangle_\Omega + \langle q, z\rangle_\Omega - \langle q, w\rangle_\Omega \,dt \\
&= \int_0^T \langle w, q\rangle_\Omega + \langle \gamma^* h, q\rangle_\Omega - \langle q, w\rangle_\Omega \,dt = \int_0^T \langle h, \gamma q\rangle_\Gamma \,dt
\end{aligned}$$

which is exactly what we wanted to obtain. □

Putting this together we can now formulate optimality conditions of first order for a control $g \in G_{ad}$, its corresponding state $(u, v) \in \mathbb{W}^2_{r,p}$ and the adjoint state $(p, q) \in \mathbb{W}^2_{r,p}$ to be optimal:

$$\left.\begin{aligned}
u_t =& \Delta u - \nabla \cdot \{f(u)\nabla v\} && \text{in } \Omega \times (0, T) \\
u(0) =& u_0 && \text{in } \Omega \\
v_t =& \Delta v - v + u + \gamma^* g && \text{in } \Omega \times (0, T) \\
v(0) =& v_0 && \text{in } \Omega \\
-p_t =& \Delta p + f'(u)\nabla v \nabla p + q + \alpha_2(u - u_Q) && \text{in } \Omega \times (0, T) \\
p(T) =& \alpha_1(u(T) - u_\Omega) && \text{in } \Omega \\
-q_t =& \Delta q - q - \nabla \cdot \{f(u)\nabla p\} && \text{in } \Omega \times (0, T) \\
q(T) =& 0 && \text{in } \Omega \\
&\langle \gamma q + \lambda g, h - g\rangle_\Sigma \geq 0 && \text{for all } h \in G_{ad}
\end{aligned}\right\} \qquad \text{(FON)}$$

Remark 6.2. *There is an equivalent formulation of the gradient inequality which we will use later on: The optimal control satisfies*

$$g = -\mathbb{P}_{[g_a, g_b]}\left(\frac{1}{\lambda}\gamma q\right) \tag{6.6}$$

where $\mathbb{P} : L_r(L_p(\Gamma)) \to G_{ad}$ *is the projection operator.*

Chapter 7

Necessary and sufficient optimality conditions of second order

Second order optimality conditions for optimal control problems have been studied extensively in the last years, cf. e.g. [13], [24], [23], [45], [37]. If a sufficient optimality condition is satisfied, this allows for fast converging numerical methods such as the SQP method presented in the next chapter, as well as for example for sensitivity analysis of the parameterized problem. The concept is again well known from finite dimensional optimization: Once we have found a candidate for an optimal solution with the help of first order optimality conditions, we take a look the second derivative. If the problem is strictly convex in a neighbourhood of the candidate, we know that we have found a (local) minimizer. Executing this plan however becomes a bit more complicated when working in a function space setting. As we have seen before, for the control-to-state operator to be well defined and differentiable, we need to put restrictions on the order of integrability of $g \in L_r(L_p(\Gamma))$, in particular $r, p > 2$. For a positive definiteness condition like $\mathcal{J}''(g) \geq c\|g\|^2$ on the other hand, we will need to work with the $L_2(\Sigma)$-norm for the control. Luckily, as we have seen in the fourth chapter already, all the estimates we need transfer to this weaker norm. Let us mention that we can actually avoid having to deal with the common phenomenon of a two norm discrepancy here: Many problems are differentiable only in L_∞, which leads to an optimality result of the following form: If the sufficient optimality condition holds, a quadratic growth property can be shown with respect to the L_2-norm, however this property only holds in an L_∞-neighbourhood (quite like in Theorem 7.4 here). Since in our case we can show differentiability in $L_r(L_p(\Gamma))$, $r, p < \infty$, if we impose control constraints in L_∞ this result in fact even holds in an L_2-neighbourhood. Throughout this chapter, we will mainly follow the line of argumentation presented in [59].

Clearly, before we can get started we need to compute the second derivative of the objective. Once again we follow the same strategy as in the previous chapter: We look at the reduced objective $\mathcal{J}(g) = J(\mathcal{G}(g); g)$, compute the derivative and introduce an adjoint state to simplify the representation. For directions $h_1, h_2 \in L_r(L_p(\Gamma))$ we obtain

$$\begin{aligned}\mathcal{J}''(g)[h_1, h_2] =& \alpha_1 \langle w_2(T), w_1(T)\rangle_\Omega + \alpha_2 \langle w_2, w_1\rangle_Q + \lambda \langle h_2, h_1\rangle_\Sigma \\ &+ \alpha_1 \langle u(T) - u_\Omega, \phi(T)\rangle_\Omega + \alpha_2 \langle u - u_Q, \phi\rangle_Q ,\end{aligned}$$

where once again $(w_i, z_i) = \mathcal{G}'(g)h_i$, $i = 1, 2$, is the first derivative of the control-to-state operator, and $(\phi, \psi) = \mathcal{G}''(g)[h_1, h_2]$ is the second derivative given by the solution to the system

$$\begin{aligned}\phi_t =& \Delta\phi - \nabla \cdot \{f'(u)\phi\nabla v + f(u)\nabla\psi\} \\ &- \nabla \cdot \{f''(u)w_1w_2\nabla v\} \qquad \text{in } \Omega \times (0, T), \quad \phi(0) = 0 \text{ in } \Omega, \quad (7.1)\\ &- \nabla \cdot \{f'(u)w_1\nabla z_2 + f'(u)w_2\nabla z_1\} \\ \psi_t =& \Delta\psi - \psi + \phi \qquad \text{in } \Omega \times (0, T), \quad \psi(0) = 0 \text{ in } \Omega. \quad (7.2)\end{aligned}$$

Introducing the adjoint system we obtain:

Lemma 7.1. *Assume* (4.3) *holds. The second derivative of the reduced objective $\mathcal{J}$ in $g \in L_r(L_p(\Gamma))$ in directions $h_1, h_2 \in L_r(L_p(\Gamma))$ is given by*

$$\begin{aligned}\mathcal{J}''(g)[h_1, h_2] =& \alpha_1 \langle w_2(T), w_1(T)\rangle_\Omega + \alpha_2 \langle w_2, w_1\rangle_Q + \lambda \langle h_2, h_1\rangle_\Sigma \\ &+ \langle \nabla p, f''(u)w_2w_1\nabla v + f'(u)w_1\nabla z_2 + f'(u)w_2\nabla z_1\rangle_Q ,\end{aligned}$$

where $(u, v) = \mathcal{G}(g)$ is a solution to the state equation, $(w_i, z_i) = \mathcal{G}'(g)h_i$, $i = 1, 2$ solves the linearized system

$$\begin{aligned}w_{i,t} =& \Delta w_i - \nabla \cdot \{f'(u)w_i\nabla v + f(u)\nabla z_i\} \quad \text{in } \Omega \times (0, T), \quad w_i(0) = 0 \text{ in } \Omega, \\ z_{i,t} =& \Delta z_i - z_i + w_i + \gamma^* h_i \qquad \text{in } \Omega \times (0, T), \quad z_i(0) = 0 \text{ in } \Omega,\end{aligned}$$

and (p,q) solves the adjoint system

$$
\begin{aligned}
-p_t =& \Delta p + f'(u)\nabla v \nabla p + q + \alpha_2(u-u_Q) && \text{in } \Omega\times(0,T),\\
p(T) =& \alpha_1(u(T)-u_\Omega) && \text{in } \Omega,
\end{aligned} \tag{7.3}
$$

$$
\begin{aligned}
-q_t =& \Delta q - q - \nabla\cdot\{f(u)\nabla p\} && \text{in } \Omega\times(0,T),\\
q(T) =& 0 && \text{in } \Omega.
\end{aligned} \tag{7.4}
$$

Proof. We will use the same argumentation as in Lemma 6.1. This time we need to show that

$$
\begin{aligned}
\alpha_1 \langle u(T)-u_\Omega, \phi(T)\rangle_\Omega &+ \alpha_2 \langle u-u_Q, \phi\rangle_Q \\
&= \langle \nabla p, f''(u) w_2 w_1 \nabla v + f'(u) w_1 \nabla z_2 + f'(u) w_2 \nabla z_1\rangle_Q
\end{aligned}
$$

with $(\phi,\psi)\in\mathbb{W}^2_{r,p}$ solving (7.1)-(7.2) and $(p,q)\in\mathbb{W}^2_{r,p}$ solving (7.3)-(7.4), so once again we "test" the variational formulation of each system with the solution to the other. After integrating by parts with respect to time, the adjoint system becomes

$$
\begin{aligned}
\int_0^T \langle \phi_t, p\rangle_{W_p^{-1},W^1_{p'}} &+ \langle \nabla p, \nabla\phi\rangle - \langle f'(u)\nabla v\nabla p, \phi\rangle - \langle q,\phi\rangle \; dt \\
&= \int_0^T \langle \alpha_2(u-u_Q),\phi\rangle\, dt + \langle \alpha_1 u(T) - u_\Omega, \phi(T)\rangle ,
\end{aligned}
$$

$$
\int_0^T \langle \psi_t, q\rangle_{W_p^{-1},W^1_{p'}} + \langle \nabla q, \nabla\psi\rangle + \langle q,\psi\rangle \; dt = \int_0^T \langle f(u)\nabla p, \nabla\psi\rangle ,
$$

and for (7.1)-(7.2) we obtain

$$
\begin{aligned}
\int_0^T \langle \phi_t, p\rangle_{W_p^{-1},W^1_{p'}} &+ \langle \nabla\phi, \nabla p\rangle - \langle f'(u)\phi\nabla v, \nabla p\rangle \; dt \\
&= \int_0^T \langle f(u)\nabla\psi, \nabla p\rangle + \langle I, \nabla p\rangle \; dt,
\end{aligned}
$$

$$
\int_0^T \langle \psi_t, q\rangle_{W_p^{-1},W^1_{p'}} + \langle \nabla\psi, \nabla q\rangle + \langle \psi, q\rangle \; dt = \int_0^T \langle \phi, q\rangle \; dt,
$$

where $I := f''(u)w_2w_1\nabla v + f'(u)w_1\nabla z_2 + f'(u)w_2\nabla z_1$. This leads to

$$\begin{aligned}\alpha_2 \langle u - u_Q, \phi\rangle_Q &+\alpha_1 \langle u(T) - u_\Omega, \phi(T)\rangle \\ &= \int_0^T \langle p_t, \phi\rangle_{W_p^{-1}, W_{p'}^1} + \langle \nabla p, \nabla\phi\rangle - \langle f'(u)\nabla v \nabla p, \phi\rangle - \langle q, \phi\rangle \; dt \\ &= \int_0^T \langle f(u)\nabla\psi, \nabla p\rangle + \langle I, \nabla p\rangle - \langle q, \phi\rangle \; dt \\ &= \int_0^T \langle \psi_t, q\rangle + \langle \nabla q, \nabla\psi\rangle + \langle q, \psi\rangle + \langle I, \nabla p\rangle - \langle q, \phi\rangle \; dt \\ &= \int_0^T \langle \phi, q\rangle + \langle I, \nabla p\rangle - \langle q, \phi\rangle \; dt \\ &= \int_0^T \langle f''(u)w_2w_1\nabla v + f'(u)w_1\nabla z_2 + f'(u)w_2\nabla z_1, \nabla p\rangle \; dt\end{aligned}$$

exactly as asserted. □

For what is to come, it simplifies notation significantly to introduce the Lagrange function. Like in the definition of the adjoint operator, we do not worry about employing the exact dual spaces but note that our choice embeds into them so that everything is well defined. Additionally, from now on we are going to assume that

$$p > 2N, \qquad\qquad r > 2p. \tag{7.5}$$

Although the Lagrange function is well defined without this restriction, as we have seen in Lemma 4.6 and 4.7 already this is crucial for estimates involving the L_2-norm. So let us set

$$Y_{r,p} := \mathbb{W}_{r,p} \times \mathbb{W}_{r,p} \cap L_\infty(W_p^1) \times L_r(L_p(\Gamma)) \times \mathbb{W}_{r,p}^2 \times L_{r'}(L_{p'}(\Gamma))^2 \tag{7.6}$$

and define the *Lagrange function* $\mathcal{L} : Y_{r,p} \to \mathbb{R}$,

$$\begin{aligned}\mathcal{L}(y) = J(u,v,g) + \int_0^T \langle u_t, p\rangle_{W_p^{-1},W_{p'}^1}\,dt + \langle \nabla u, \nabla p\rangle_Q + \langle f(u)\nabla v, \nabla p\rangle_Q \\ + \langle u(0) - u_0, p(0)\rangle_\Omega \\ + \int_0^T \langle v_t, q\rangle_{W_p^{-1},W_{p'}^1}\,dt + \langle \nabla v, \nabla q\rangle_Q + \langle v - u - \gamma^* g, q\rangle_Q \\ + \langle v(0) - v_0, q(0)\rangle_\Omega + \langle \mu_a, g_a - g\rangle_\Sigma + \langle \mu_b, g - g_b\rangle_\Sigma\end{aligned}$$

for $y := (u, v, g, p, q, \mu_a, \mu_b) \in Y_{r,p}$. The second derivative $\mathcal{L}''(y)(w,z,h)^2$ is then given by

$$\begin{aligned}\mathcal{L}''(y)(w,z,h)^2 = \mathcal{J}''(g)h^2 = \alpha_1\|w(T)\|^2_{L_2(\Omega)} + \alpha_2\|w\|^2_{L_2(Q)} + \lambda\|h\|^2_{L_2(\Sigma)} \\ + \left\langle \nabla p, f''(u)w^2\nabla v + 2f'(u)w\nabla z\right\rangle_Q ,\end{aligned} \tag{7.7}$$

where $(w,z) \in \mathbb{W}^2_{r,p}$ solves the linearized equation

$$\begin{aligned} w_t &= \Delta w - \nabla\cdot\{f'(u)w\nabla v + f(u)\nabla z\} \quad \text{in } \Omega\times(0,T), \qquad w(0) = 0 \text{ in } \Omega, \\ z_t &= \Delta z - z + w + \gamma^* h \quad \text{in } \Omega\times(0,T), \qquad z(0) = 0 \text{ in } \Omega\end{aligned}$$

for $h \in L_r(L_p(\Gamma))$. Note that $\mathcal{L}''$ is actually well defined for every $h \in L_2(\Sigma)$.

The next Lemma, the fact that $\mathcal{L}''$ is Lipschitz continuous in y and the difference is bounded by the L_2-norm of the direction h, will be the main step on the way to proving second order sufficient optimality conditions. This becomes necessary due to the use of different norms: For h in the $L_r(L_p(\Gamma))$-norm, this would be a direct consequence of Theorem 4.8, the fact that the control-to-state operator is twice continuously differentiable in that space. In L_2 we need to put some additional effort into this. Before we get started, let us have a look at the terms responsible for the restrictions on r and p fixed in (7.5). For $\rho > 1$ such that $\frac{N}{\rho} = \frac{N}{\beta} - 1$, i.e. such that $\mathbb{W}^1_\beta \hookrightarrow L_\rho$, we can estimate

$$\begin{aligned}\|\nabla v \nabla p w^2\|_{L_1(Q)} &\le c\|v\|_{L_\infty(W_p^1)}\|p\|_{L_r(W_p^1)}\|w\|^2_{L_\alpha(L_\rho)} \\ &\le c\|v\|_{L_\infty(W_p^1)}\|p\|_{L_r(W_p^1)}\|w\|^2_{L_\alpha(W_\beta^1)},\end{aligned} \tag{7.8}$$

$$\begin{aligned}\|\nabla p \nabla z w\|_{L_1(Q)} &\le c\|p\|_{L_r(W_p^1)}\|z\|_{L_\alpha(W_\beta^1)}\|w\|_{L_\alpha(L_\rho)} \\ &\le c\|p\|_{L_r(W_p^1)}\|z\|_{L_\alpha(W_\beta^1)}\|w\|_{L_\alpha(W_\beta^1)},\end{aligned} \tag{7.9}$$

as long as the conditions of the Hölder inequality (A.2),

$$\frac{1}{r}+\frac{2}{\alpha}\leq 1 \qquad \text{and} \qquad \frac{1}{p}+\frac{1}{\beta}+\frac{1}{\rho}=\frac{1}{p}+\frac{2}{\beta}-\frac{1}{N}\leq 1$$

are satisfied. If α,β fulfill the conditions of Lemmas 4.6 and 4.7 this holds: For $p>2N$, the second condition holds as long as $\beta\geq 2$, the first condition is implied by $\frac{2}{\alpha}+\frac{N}{p}<1$ from (4.10) and $r>2p$. We can hence show:

Lemma 7.2. *Assume (7.5) is satisfied. The second derivative of the Lagrange function is Lipschitz continuous in the sense that for every $M>0$ there is an $L=L(M)>0$ such that for every $y^\delta, y\in Y_{r,p}$, $\|y^\delta\|_{Y_{r,p}}+\|y\|_{Y_{r,p}}\leq M$ we have*

$$|\mathcal{L}''(y^\delta)(w^\delta,z^\delta,h)^2-\mathcal{L}''(y)(w,z,h)^2|\leq L(M)\|y^\delta-y\|_{Y_{r,p}}\|h\|^2_{L_2(\Sigma)}$$

for $h\in L_2(\Sigma)$ and $(w,z)=\mathcal{G}'(g)h$, $(w^\delta,z^\delta)=\mathcal{G}'(g^\delta)h$.

Proof. By (7.7), the left hand side reads

$$\begin{aligned}\mathcal{L}''(y^\delta)(w^\delta,&z^\delta,h)^2-\mathcal{L}''(y)(w,z,h)^2\\ =&\alpha_1\left(\|w^\delta(T)\|^2_{L_2(\Omega)}-\|w(T)\|^2_{L_2(\Omega)}\right)+\alpha_2\left(\|w^\delta\|^2_{L_2(Q)}-\|w\|^2_{L_2(Q)}\right)\\ &+\left\langle\nabla p^\delta, f''(u^\delta)(w^\delta)^2\nabla v^\delta+2f'(u^\delta)w^\delta\nabla z^\delta\right\rangle_Q\\ &-\left\langle\nabla p, f''(u)w^2\nabla v+2f'(u)w\nabla z\right\rangle_Q.\end{aligned}$$

For the first bracket, the third binomial formula gives

$$\begin{aligned}\|w^\delta(T)\|^2_{L_2(\Omega)}-\|w(T)\|^2_{L_2(\Omega)}\leq&\|w^\delta(T)+w(T)\|_{L_2(\Omega)}\|w^\delta(T)-w(T)\|_{L_2(\Omega)}\\ \leq&\|w^\delta+w\|_{\mathbb{W}_{2,2}}\|w^\delta-w\|_{\mathbb{W}_{2,2}}\\ \leq&c(g,\delta)\|h\|_{L_2(\Sigma)}\cdot\|g^\delta-g\|_{L_r(L_p(\Gamma))}\|h\|_{L_2(\Sigma)}\\ \leq&c\|g^\delta-g\|_{L_r(L_p(\Gamma))}\|h\|^2_{L_2(\Sigma)}\end{aligned}$$

due to Lemma 4.6 and Lemma 4.7. The same holds for the second bracket,

$$\|w^\delta\|^2_{L_2(Q)}-\|w\|^2_{L_2(Q)}\leq c(g,\delta)\|g^\delta-g\|_{L_r(L_p(\Gamma))}\|h\|^2_{L_2(\Sigma)}.$$

So let us turn to the last part. If we choose α,β according to (4.10), due to

(7.8) and (7.9) we have

$$
\begin{aligned}
|\left\langle\nabla p^\delta, f''(u^\delta)(w^\delta)^2\nabla v^\delta\right\rangle_Q - \left\langle\nabla p, f''(u)(w)^2\nabla v\right\rangle_Q|
\leq & |\left\langle\nabla(p^\delta - p), f''(u^\delta)(w^\delta)^2\nabla v^\delta\right\rangle_Q| \\
& + |\left\langle\nabla p, \{f''(u^\delta) - f''(u)\}(w^\delta)^2\nabla v^\delta\right\rangle_Q| \\
& + |\left\langle\nabla p, f''(u)\{(w^\delta)^2 - w^2\}\nabla v^\delta\right\rangle_Q| \\
& + |\left\langle\nabla p, f''(u)w^2\nabla(v^\delta - v)\right\rangle_Q| \\
\leq & c\Big(c_{f''}\|p^\delta - p\|_{L_r(W_p^1)}\|w^\delta\|^2_{L_\alpha(W_\beta^1)}\|v^\delta\|_{L_\infty(W_p^1)} \\
& + L_{f''}\|p\|_{L_r(W_p^1)}\|u^\delta - u\|_{C(\bar{Q})}\|w^\delta\|^2_{L_\alpha(W_\beta^1)}\|v^\delta\|_{L_\infty(W_p^1)} \\
& + c_{f''}\|p\|_{L_r(W_p^1)}\|w^\delta - w\|_{L_\alpha(W_\beta^1)}\|w^\delta + w\|_{L_\alpha(W_\beta^1)}\|v^\delta\|_{L_\infty(W_p^1)} \\
& + c_{f''}\|p\|_{L_r(W_p^1)}\|w\|^2_{L_\alpha(W_\beta^1)}\|v^\delta - v\|_{L_\infty(W_p^1)}\Big)
\end{aligned}
$$

and

$$
\begin{aligned}
|\left\langle\nabla p^\delta, f'(u^\delta)w^\delta\nabla z^\delta\right\rangle_Q - \langle\nabla p, f'(u)w\nabla z\rangle_Q|
\leq & |\left\langle\nabla(p^\delta - p), f'(u^\delta)w^\delta\nabla z^\delta\right\rangle_Q| + |\left\langle\nabla p, (f'(u^\delta) - f'(u))w^\delta\nabla z^\delta\right\rangle_Q| \\
& + |\left\langle\nabla p, f'(u)(w^\delta - w)\nabla z^\delta\right\rangle_Q| + |\left\langle\nabla p, f'(u)w\nabla(z^\delta - z)\right\rangle_Q| \\
\leq & c\Big(c_{f'}\|p^\delta - p\|_{L_r(W_p^1)}\|w^\delta\|_{L_\alpha(W_\beta^1)}\|z^\delta\|_{L_\alpha(W_\beta^1)} \\
& + L_{f'}\|p\|_{L_r(W_p^1)}\|u^\delta - u\|_{C(\bar{Q})}\|w^\delta\|_{L_\alpha(W_\beta^1)}\|z^\delta\|_{L_\alpha(W_\beta^1)} \\
& + c_{f'}\|p\|_{L_r(W_p^1)}\|w^\delta - w\|_{L_\alpha(W_\beta^1)}\|z^\delta\|_{L_\alpha(W_\beta^1)} \\
& + c_{f'}\|p\|_{L_r(W_p^1)}\|w\|_{L_\alpha(W_\beta^1)}\|z^\delta - z\|_{L_\alpha(W_\beta^1)}\Big).
\end{aligned}
$$

Obviously we have

$$
\begin{aligned}
\|v^\delta\|_{L_r(W_p^1)} + \|p\|_{L_r(W_p^1)} \leq & M, \\
\|u^\delta - u\|_{C(\bar{Q})} + \|v^\delta - v\|_{L_r(W_p^1)} + \|p^\delta - p\|_{L_r(W_p^1)} \leq & c\|y^\delta - y\|_{Y_{r,p}},
\end{aligned}
$$

and once again, Lemma 4.6 and Lemma 4.7 give

$$
\begin{aligned}
\|w\|_{\mathbb{W}_{\alpha,\beta}} + \|w^\delta\|_{\mathbb{W}_{\alpha,\beta}} + \|z^\delta\|_{L_\alpha(W_\beta^1)} \leq & c\|h\|_{L_2(\Sigma)} \\
\|w^\delta - w\|_{\mathbb{W}_{\alpha,\beta}} + \|z^\delta - z\|_{L_\alpha(W_\beta^1)} \leq & c\|g^\delta - g\|_{L_r(L_p(\Gamma))}\|h\|_{L_2(\Sigma)} \\
\leq & c\|y^\delta - y\|_{Y_{r,p}}\|h\|_{L_2(\Sigma)}.
\end{aligned}
$$

Hence, every summand is bounded by $L(M)\|y^\delta - y\|_{Y_{r,p}}\|h\|^2_{L_2(\Sigma)}$ so that the assertion follows. □

Before we formulate sufficient optimality conditions, let us start with what is necessary for a control to be optimal. To that end, define the active set via

$$A_0(g) := \{(x,t) \in \Sigma : |\lambda g(x,t) + \gamma q(x,t)| > 0\}.$$

On this set of active control constraints, the control is already fixed by the projection formula (6.6),

$$g(x,t) = \begin{cases} g_a(x,t) & \text{if } \lambda g(x,t) + \gamma q(x,t) > 0 \\ g_b(x,t) & \text{if } \lambda g(x,t) + \gamma q(x,t) < 0. \end{cases}$$

Hence, it only makes sense to look at second order conditons for the control outside these sets: Set

$$h(x,t) \begin{cases} = 0 & \text{if } (x,t) \in A_0(g) \\ \geq 0 & \text{if } (x,t) \notin A_0(g) \text{ and } g(x,t) = g_a(x,t) \\ \leq 0 & \text{if } (x,t) \notin A_0(g) \text{ and } g(x,t) = g_b(x,t) \end{cases} \tag{7.10}$$

for a.e. $(x,t) \in \Sigma$ and define a cone of admissible directions via

$$C_0(g) := \{h \in L_r(L_p(\Gamma)) : (7.10) \text{ holds } \}.$$

Lemma 7.3. *Let g be an optimal control to* (1.1)-(1.3)*. It holds that*

$$\mathcal{L}''(y)(w,z,h)^2 \geq 0$$

for every $h \in C_0(g)$ and $(w,z) = \mathcal{G}'(g)h$.

When it comes to sufficient optimality conditions now, it is desirable that the gap to the necessary conditions is not too big. One way to do that is to define the strongly active set

$$A_\tau(g) := \{(x,t) \in \Sigma : |\lambda g(x,t) + \gamma q(x,t)| > \tau\},$$

$\tau \geq 0$ and a cone $C_\tau(g)$ in the same way as $C_0(g)$. This condition is rather sharp, however it creates some difficulties when it comes to the convergence analysis of numerical methods solving the optimal control problem, since these active sets need not be the same in different points. In order not to let things get too technical, we are going to work with a stronger condition: We will not put any restrictions on the set of admissible directions at all and simply demand

$$\left.\begin{array}{l}\text{For } p > 2N,\ r > 2p \text{ let } y \in Y_{r,p} \text{ satisfy (FON).}\\ \text{There is a } \kappa > 0 \text{ such that}\\ \mathcal{L}''(y)(w,z,h)^2 \geq \kappa \|h\|^2_{L^2(\Sigma)}\\ \text{for all } \in L_r(L_p(\Gamma)) \text{ and } (w,z) = \mathcal{G}'(g)h.\end{array}\right\} \tag{SSC}$$

Theorem 7.4. *Assume* $\bar{y} \in Y_{r,p}$ *satisfies* (SSC). *There are constants* $\varepsilon > 0$, $\sigma > 0$ *such that for the reduced objective it holds that*

$$\mathcal{J}(g) \geq \mathcal{J}(\bar{g}) + \sigma \|g - \bar{g}\|^2_{L_2(\Sigma)} \tag{7.11}$$

for all $g \in G_{ad}$, $\|g - \bar{g}\|_{L_r(L_p(\Gamma))} < \varepsilon$.

Proof. The proof is fairly standard and can for example be found in [59], so we will just give a sketch here. Let $g \in G_{ad}$. Since $\mathcal{J}$ is twice continuously differentiable, we can write down the Taylor expansion, so for some $\theta > 0$ we have

$$\mathcal{J}(g) = \mathcal{J}(\bar{g}) + \mathcal{J}'(\bar{g})(g - \bar{g}) + \frac{1}{2}\mathcal{J}''(\bar{g} + \theta(g - \bar{g}))(g - \bar{g})^2.$$

For the first order term we have $\mathcal{J}'(\bar{g})(g - \bar{g}) \geq 0$ due to the necessary optimality condition (FON). For the second order term we have

$$\begin{aligned}&\mathcal{J}''(\bar{g} + \theta(g - \bar{g}))(g - \bar{g})^2\\ &\qquad = \mathcal{J}''(\bar{g})(g - \bar{g})^2 + [\mathcal{J}''(\bar{g} + \theta(g - \bar{g})) - \mathcal{J}''(\bar{g})](g - \bar{g})^2\\ &\qquad \geq \kappa \|g - \bar{g}\|^2_{L_2(\Sigma)} - L(M)\|g - \bar{g}\|_{L_r(L_p(\Gamma))}\|g - \bar{g}\|^2_{L_2(\Sigma)}\end{aligned}$$

with κ given in (SSC) and $L(M)$ given in Lemma 7.2. So if $\|g - \bar{g}\|_{L_r(L_p(\Gamma))} < \varepsilon$ with ε so small that $L(M)\varepsilon < \frac{\kappa}{2}$, we have

$$\mathcal{J}''(\bar{g} + \theta(g - \bar{g}))(g - \bar{g})^2 \geq \frac{\kappa}{2}\|g - \bar{g}\|^2_{L_2(\Sigma)}$$

and hence (7.11). □

It is not hard to see that as long as the control constraints are in $L_\infty(\Sigma)$ this holds in an L_2 neighbourhood as well:

Corollary 7.5. *Assume $g_a, g_b \in L_\infty(\Sigma)$. There are constants $\varepsilon' > 0$, $\sigma > 0$ such that*

$$\mathcal{J}(g) \geq \mathcal{J}(\bar{g}) + \sigma \|g - \bar{g}\|^2_{L_2(\Sigma)}$$

for all $g \in G_{ad}$, $\|g - \bar{g}\|_{L_2(\Sigma)} < \varepsilon'$.

Proof. With control constraints in $L_\infty(\Sigma)$ we know that every $g \in G_{ad}$ is in $L_\infty(\Sigma)$ as well which implies there is a $c > 0$ depending on g_a, g_b such that

$$\|g - \bar{g}\|_{L_\infty(\Sigma)} \leq c(g_a, g_b) \qquad \text{for all } g \in G_{ad}.$$

In this case, there is another constant $c' > 0$ depending on $r = \max\{r, p\}$, Σ and $\|\phi\|_{L_\infty(\Sigma)}$ such that

$$\|g - \bar{g}\|_{L_r(L_p(\Gamma))} \leq c\|g - \bar{g}\|_{L_r(\Sigma)} \leq c'\|g - \bar{g}\|_{L_2(\Sigma)},$$

since for $\phi \in L_\infty(\Sigma)$ we have

$$\begin{aligned}\|\phi\|^r_{L_r(\Sigma)} = \int_\Sigma |\phi|^2 |\phi|^{r-2} \leq & \left(\int_\Sigma |\phi|^2\right)^{\frac{r}{2}} \left(\int_\Sigma |\phi|^{r-2}\right)^{\frac{r}{r-2}} \\ \leq & c\|\phi\|^r_{L_2(\Sigma)} \|\phi\|^r_{L_\infty(\Sigma)} |\Sigma|^{\frac{r}{r-2}}.\end{aligned}$$

□

7.1 Consequences of the second order condition

When in the next chapter we want to derive convergence results for an SQP method, we will need the condition (SSC) to hold not only in the optimal solution $\bar{y}$, but also in the iterates y^k (Lemma 8.5). Also, when in Lemma 8.9 we want to show Lipschitz stability of the generalized function, we need to allow for perturbation terms in the linearized equation. Fortunately, both assertions follow from (SSC). We start with the perturbation result:

Corollary 7.6. *Assume $\bar{y}$ satisfies* (SSC). *For α, β chosen according to* (4.10) *let $\delta = (\delta_1, \delta_2, \delta_3, \delta_4) \in [\mathbb{W}_{\alpha,\beta} \times \mathcal{D}_{\alpha,\beta}]^2$. There is a $\kappa' > 0$ such that*

$$\kappa' \|h\|^2_{L_2(\Sigma)} \leq \mathcal{L}''(\bar{y})(\delta w, \delta z, h)^2 + \|\delta\|^2_{[\mathbb{W}_{\alpha,\beta} \times \mathcal{D}_{\alpha,\beta}]^2}$$

holds for all $h \in L_2(\Sigma)$ *and* $(\delta w, \delta z) \in \mathbb{W}_{\alpha,\beta} \times \mathbb{W}_{2,\beta} \cap L_\alpha(W^1_\beta)$ *solving*

$$\begin{aligned} \delta w_t =& \Delta \delta w - \nabla \cdot \{f'(\bar{u})\delta w \nabla \bar{v} + f(\bar{u})\nabla \delta z\} + \delta_1 && \textit{in } \Omega \times (0,T), \\ \delta w(0) =& \delta_2 && \textit{in } \Omega, \end{aligned} \tag{7.12}$$

$$\begin{aligned} \delta z_t =& \Delta \delta z - \delta z + \delta w + \gamma^* h + \delta_3 && \textit{in } \Omega \times (0,T), \\ \delta z(0) =& \delta_4 && \textit{in } \Omega. \end{aligned} \tag{7.13}$$

Proof. We split up the solution to (7.12)-(7.13) into one part depending on the direction h and another one depending on the perturbations δ, so into $(\delta w, \delta z) = (w, z) + (w_\delta, z_\delta)$ solving

$$\begin{aligned} w_t =& \Delta w - \nabla \cdot \{f'(\bar{u}) w \nabla \bar{v} + f(\bar{u})\nabla z\} \text{ in } \Omega \times (0,T), && w(0) = 0 \text{ in } \Omega, \\ z_t =& \Delta z - z + w + \gamma^* h \quad \text{in } \Omega \times (0,T), && z(0) = 0 \text{ in } \Omega, \end{aligned}$$

and

$$\begin{aligned} w_{\delta,t} =& \Delta w_\delta - \nabla \cdot \{f'(\bar{u}) w_\delta \nabla \bar{v} + f(\bar{u})\nabla z_\delta\} + \delta_1 \text{ in } Q, && w_\delta(0) = \delta_2 \text{ in } \Omega, \\ z_{\delta,t} =& \Delta z_\delta - z_\delta + w_\delta + \delta_3 \quad \text{in } Q, && z_\delta(0) = \delta_4 \text{ in } \Omega. \end{aligned}$$

For the bilinear form $\mathcal{L}''$ this means we get

$$\begin{aligned} &|\mathcal{L}''(\bar{y})(\delta w, \delta z, h)^2| \\ &\quad= |\mathcal{L}''(\bar{y})(w, z, h)^2 + 2\mathcal{L}''(\bar{y})(w, z, h)(w_\delta, z_\delta, 0) + \mathcal{L}''(\bar{y})(w_\delta, z_\delta, 0)^2| \\ &\quad\geq |\mathcal{L}''(\bar{y})(w, z, h)^2| - 2|\mathcal{L}''(\bar{y})(w, z, h)(w_\delta, z_\delta, 0)| - |\mathcal{L}''(\bar{y})(w_\delta, z_\delta, 0)^2|. \end{aligned}$$

The first term is coercive due to (SSC),

$$\mathcal{L}''(\bar{y})(w, z, h)^2 \geq \kappa \|h\|^2_{L_2(\Sigma)}.$$

Due to (7.8) and (7.9), for the third term we have

$$\begin{aligned} \mathcal{L}''(\bar{y})(w_\delta, z_\delta, 0)^2 =& \alpha_1 \|w_\delta(T)\|^2_{L_2(\Omega)} + \alpha_2 \|w_\delta\|^2_{L_2(Q)} \\ &+ \left\langle \nabla \bar{p}, f''(\bar{u}) w_\delta^2 \nabla \bar{v} + 2 f'(\bar{u}) w_\delta \nabla z_\delta \right\rangle_Q \\ \leq& c \Big(\|w_\delta\|^2_{\mathbb{W}_{\alpha,\beta}} + L_{f''} \|\bar{p}\|_{L_r(W^1_p)} \|\bar{v}\|_{L_\infty(W^1_p)} \|w_\delta\|^2_{L_r(W^1_\beta)} \\ &+ L_{f'} \|\bar{p}\|_{L_r(W^1_p)} \|w_\delta\|_{L_\alpha(W^1_\beta)} \|z_\delta\|_{L_\alpha(W^1_\beta)} \Big) \\ \leq& c(\bar{g}) \|\delta\|^2_{[\mathbb{W}_{\alpha,\beta} \times \mathcal{D}_{\alpha,\beta}]^2} \end{aligned}$$

since

$$\begin{aligned}\|\bar{p}\|_{L_r(W_p^1)} + \|\bar{v}\|_{L_r(W_p^1)} \leq & c(\bar{g}),\\ \|w_\delta\|_{\mathbb{W}_{\alpha,\beta}} + \|z_\delta\|_{L_\alpha(W_\beta^1)} \leq & c\|\delta\|_{[\mathbb{W}_{\alpha,\beta}\times\mathcal{D}_{\alpha,\beta}]^2}.\end{aligned}$$

Using the same arguments, the second term gives

$$\begin{aligned}\mathcal{L}''(\bar{y})(w,z,h)(w_\delta,z_\delta,0) =&\alpha_1\left\langle w(T), w_\delta(T)\right\rangle + \alpha_2\left\langle w, w_\delta\right\rangle\\ &+\left\langle \nabla\bar{p}, f''(\bar{u})ww_\delta\nabla\bar{v} + f'(\bar{u})(w\nabla z_\delta + w_\delta\nabla z)\right\rangle\\ \leq&\varepsilon\|w\|^2_{\mathbb{W}_{\alpha,\beta}} + c(\varepsilon)\|w_\delta\|^2_{\mathbb{W}_{\alpha,\beta}}\\ &+cL_{f''}\|\bar{p}\|_{L_r(W_p^1)}\|w\|_{L_\alpha(W_\beta^1)}\|w_\delta\|_{L_\alpha(W_\beta^1)}\|\bar{v}\|_{L_\infty(W_p^1)}\\ &+cL_{f'}\|\bar{p}\|_{L_r(W_p^1)}\|w\|_{L_\alpha(W_\beta^1)}\|z_\delta\|_{L_\alpha(W_\beta^1)}\\ &+cL_{f'}\|\bar{p}\|_{L_r(W_p^1)}\|w_\delta\|_{L_\alpha(W_\beta^1)}\|z_\delta\|_{L_\alpha(W_\beta^1)}\\ \leq&\varepsilon c(\bar{g})\left(\|w\|^2_{\mathbb{W}_{\alpha,\beta}} + \|z\|^2_{L_\alpha(W_\beta^1)}\right)\\ &+c(\varepsilon,\bar{g})\left(\|w_\delta\|^2_{\mathbb{W}_{\alpha,\beta}} + \|z_\delta\|^2_{L_\alpha(W_\beta^1)}\right)\\ \leq&\varepsilon c(\bar{g})\|h\|^2_{L_2(\Sigma)} + c(\varepsilon,\bar{g})\|\delta\|^2_{[\mathbb{W}_{\alpha,\beta}\times\mathcal{D}_{\alpha,\beta}]^2}\end{aligned}$$

for some $\varepsilon > 0$ due to Young's inequality (A.3). Alltogether we have

$$|\mathcal{L}''(\bar{y})(\delta w,\delta z,h)^2| \geq(\kappa-\varepsilon c(\bar{g}))\|h\|^2_{L_2(\Sigma)} - c(\varepsilon,\bar{g})\|\delta\|^2_{[\mathbb{W}_{\alpha,\beta}\times\mathcal{D}_{\alpha,\beta}]^2},$$

so that for $\varepsilon > 0$ small enough the assertion follows. □

Corollary 7.7. *Assume $\bar{y}$ satisfies* (SSC). *Let $y \in Y_{r,p}$ and choose α,β according to* (4.10). *There are $\rho > 0$, $\kappa'' > 0$ such that*

$$\mathcal{L}''(y^k)(w,z,h)^2 \geq \kappa''\|h\|^2_{L_2(\Sigma)}$$

holds for all $h \in L_2(\Sigma)$ and $(w,z) \in \mathbb{W}_{\alpha,\beta}\times\mathbb{W}_{2,\beta}\cap L_\alpha(W_\beta^1)$ solving

$$\begin{aligned}w_t =&\Delta w - \nabla\cdot\{f'(u^k)w\nabla v^k + f(u^k)\nabla z\} \quad \text{in } Q, \quad w(0)=0 \text{ in } \Omega, &(7.14)\\ z_t =&\Delta z - z + w + \gamma^* h \quad \text{in } Q, \quad z(0)=0 \text{ in } \Omega &(7.15)\end{aligned}$$

whenever $\|y^k-\bar{y}\|_{Y_{r,p}} < \rho$.

Proof. If we can expand the right hand side to

$$\mathcal{L}''(y^k)(u,v,g)^2 =\mathcal{L}''(\bar{y})(u,v,g)^2 + [\mathcal{L}''(y^k)-\mathcal{L}''(\bar{y})](u,v,g)^2, \qquad (7.16)$$

the second term can easily be dealt with by Lemma 7.2 since

$$|[\mathcal{L}''(y^k) - \mathcal{L}''(\bar{y})](u,v,g)^2| \leq c\|y^k - y\|_{W_{r,p}}\|g\|^2_{L_2(\Sigma)} \leq c(\rho)\|g\|^2_{L_2(\Sigma)}. \quad (7.17)$$

Dealing with the first term, note that (7.14)-(7.15) is linearized in y^k instead of $\bar{y}$ so that we cannot apply (SSC) directly. We can however rewrite the system to meet the conditions of the previous corollary: Set $(\delta w, \delta z) := (w,z) - (\hat{w}, \hat{z})$, where $(\hat{w}, \hat{z})$ solves the familiar linearized system

$$\begin{aligned} \hat{w}_t =& \Delta \hat{w} - \nabla \cdot \{f'(\bar{u})\hat{w}\nabla\bar{v} + f(\bar{u})\nabla\hat{z}\} \text{ in } \Omega \times (0,T), \quad \hat{w}(0) = 0 \text{ in } \Omega, \\ \hat{z}_t =& \Delta\hat{z} - \hat{z} + \hat{w} + \gamma^* h \qquad \text{in } \Omega \times (0,T), \quad \hat{z}(0) = 0 \text{ in } \Omega, \end{aligned}$$

and $(\delta w, \delta z)$ is a solution to

$$\begin{aligned} \delta w_t =& \Delta \delta w - \nabla \cdot \{f'(\bar{u})\delta w \nabla \bar{v} + f(\bar{u})\nabla \delta z\} + \delta \text{ in } Q, \quad \delta w(0) = 0 \text{ in } \Omega, \\ \delta z_t =& \Delta \delta z - \delta z + \delta w \qquad \text{in } Q, \quad \delta z(0) = 0 \text{ in } \Omega, \end{aligned}$$

where $\delta := -\nabla \cdot \{(f'(u^k) - f'(\bar{u}))w\nabla v^k + f'(\bar{u})w\nabla(v^k - \bar{v}) + (f(u^k) - f(\bar{u}))\nabla z\}$. Let us look at δ:

$$\begin{aligned} \|\delta\|_{L_\alpha(W_\beta^{-1})} \leq& c\Big(L_{f'}\|u^k - \bar{u}\|_{C(\bar{Q})}\|w\|_{L_\alpha(W^1_\beta)}\|v^k\|_{L_\infty(W^1_p)} \\ &+ c_{f'}\|w\|_{L_\alpha(W^1_\beta)}\|v^k - \bar{v}\|_{L_\infty(W^1_p)} + L_f\|u^k - \bar{u}\|_{C(\bar{Q})}\|z\|_{L_\alpha(W^1_\beta)}\Big) \\ \leq& c\left(\|u^k - \bar{u}\|_{C(\bar{Q})} + \|v^k - \bar{v}\|_{L_\infty(W^1_p)}\right)\left(\|w\|_{\mathbb{W}_{\alpha,\beta}} + \|z\|_{L_\alpha(W^1_\beta)}\right) \\ \leq& c(\rho)\left(\|w\|_{\mathbb{W}_{\alpha,\beta}} + \|z\|_{L_\alpha(W^1_\beta)}\right). \end{aligned}$$

Since $u = \delta u + \hat{u}$, $v = \delta v + \hat{v}$ and $(\hat{u}, \hat{v})$ solves the linearized equation, we can go on to get

$$\begin{aligned} \|\delta\|_{L_\alpha(W_\beta^{-1})} \leq& c(\rho)\left(\|\delta w\|_{\mathbb{W}_{\alpha,\beta}} + \|\delta z\|_{L_\alpha(W^1_\beta)} + \|\hat{w}\|_{\mathbb{W}_{\alpha,\beta}} + \|\hat{z}\|_{L_\alpha(W^1_\beta)}\right) \\ \leq& c(\rho)\left(\|\delta w\|_{\mathbb{W}_{\alpha,\beta}} + \|\delta z\|_{L_\alpha(W^1_\beta)}\right) + c(\rho)\|h\|_{L_2(\Sigma)}. \end{aligned}$$

So for $\rho > 0$ small enough, this yields

$$\|\delta w\|_{\mathbb{W}_{\alpha,\beta}} + \|\delta z\|_{L_\alpha(W^1_\beta)} \leq c(\rho)\|h\|_{L_2(\Sigma)}.$$

Looking at the proof of the previous corollary, this means we have

$$\begin{aligned} \mathcal{L}''(\bar{y})(\delta w, \delta z, 0)^2 \leq& c(\rho, \bar{g})\|h\|^2, \\ \mathcal{L}''(\bar{y})(\hat{w}, \hat{z}, h)(\delta w, \delta z, 0) \leq& c(\rho, \bar{g})\|h\|^2, \end{aligned}$$

so that altogether, for the second term in (7.16) we get

$$\begin{aligned}|\mathcal{L}''(\bar{y})(w,z,h)^2| \geq &|\mathcal{L}''(\bar{y})(\hat{w},\hat{z},h)^2| \\ &- 2|\mathcal{L}''(\bar{y})(\hat{w},\hat{z},h)(\delta w,\delta z,0)| - |\mathcal{L}''(\bar{y})(\delta w,\delta z,0)^2| \\ \geq &\kappa\|g\|^2_{L_2(\Sigma)} - c(\bar{g},\rho)\|h\|^2_{L_2(\Sigma)}.\end{aligned} \tag{7.18}$$

Putting together (7.16), (7.17) and (7.18) now yields

$$\begin{aligned}|\mathcal{L}''(y^k)(w,z,h)^2| \geq &|\mathcal{L}''(\bar{y})(w,z,h)^2| - [\mathcal{L}''(y^k) - \mathcal{L}''(\bar{y})](w,z,h)^2| \\ \geq &(\kappa - c(\rho))\|h\|^2_{L_2(\Sigma)} \\ \geq &\kappa''\|h\|^2_{L_2(\Sigma)}\end{aligned}$$

for $\rho > 0$ sufficiently small and some $\kappa'' > 0$. □

Chapter 8

Convergence of an SQP method

In this chapter, we are going to turn to the question of how we can find an optimal solution to (1.1)-(1.3) numerically. Typically, this means we are trying to find a solution to (FON). The fact that we could identify a second order sufficient optimality condition allows us, given such a condition holds, to look at sophisticated and fast converging Newton based methods such as the *Sequential Quadratic Programming* algorithm. For this algorithm, we will solve a sequence of linear quadratic optimal control problems,

$$\begin{aligned}
&\min\ J'(u^k, v^k, g^k)\begin{pmatrix} u-u^k \\ v-v^k \\ g-g^k \end{pmatrix} + \frac{1}{2}\mathcal{L}''(y^k)(u-u^k, v-v^k, g-g^k)^2, \\
&u_t = \Delta u - \nabla \cdot \{f'(u^k)(u-u^k)\nabla v^k + f(u^k)\nabla v\} \text{ in } Q \quad u(0)=u_0 \text{ in } \Omega \\
&v_t = \Delta v - v + u + \gamma^* g \qquad\qquad\qquad\qquad\qquad\quad \text{in } Q \quad v(0)=v_0 \text{ in } \Omega \\
&\qquad\qquad g_a \le g \le g_b,
\end{aligned} \tag{QP_k}$$

generating a sequence $\{y^k\}_{k\in\mathbb{N}}$ that quadratically converges to an optimal solution of (1.1)-(1.3). The SQP method is a popular and well known technique for solving nonlinear mathematical programming problems cf. e.g. [3], [22]. It has been successfully applied to infinite dimensional optimization problems in general as in [2], and optimal control problems in particular, cf. e.g. [5], [9], [57]. The central idea is to apply Newton's method to the full KKT system (so including the inequality constraints on the control) of the optimal control problem (1.1)-(1.3), that is to

$$\left.\begin{aligned}
u_t =&\Delta u - \nabla \cdot \{f(u)\nabla v\} && \text{in } \Omega \times (0,T)\\
u(0) =&u_0 && \text{in } \Omega\\
v_t =&\Delta v - v + u + \gamma^* g && \text{in } \Omega \times (0,T)\\
v(0) =&v_0 && \text{in } \Omega\\
-p_t =&\Delta p + f'(u)\nabla v \nabla p + q + \alpha_2(u-u_Q) && \text{in } \Omega \times (0,T)\\
p(T) =&\alpha_1(u(T)-u_\Omega) && \text{in } \Omega\\
-q_t =&\Delta q - q - \nabla \cdot \{f(u)\nabla p\} && \text{in } \Omega \times (0,T)\\
q(T) =&0 && \text{in } \Omega\\
&\lambda g + \gamma q - \mu_a + \mu_b = 0 && \text{in } \Gamma \times (0,T)\\
\mu_a \geq&0, \quad g_a - g \leq 0, \quad \mu_a(g_a - g) = 0 && \text{in } \Gamma \times (0,T)\\
\mu_b \geq&0, \quad g - g_b \leq 0, \quad \mu_b(g - g_b) = 0 && \text{in } \Gamma \times (0,T).
\end{aligned}\right\} \qquad (FON_P)$$

Since the Newton method provides a root of a given term, we need to rewrite this system in an appropriate way. The fact that we have inequality constraints makes this a set valued problem, that is we will reformulate the optimality system in a way that we define a function F and a set valued term N, and instead of (FON_P) look for a solution y of

$$0 \in F(y) + N(y). \tag{GE}$$

This poses the question of how to deal with such a set valued equation, in particular, looking at Newton's method, how to guarantee that the inverse of F' is sufficiently well behaved. One way to do that is to prove strong regularity of the equation, which leads to a generalized implicit function theorem (cf. [15], [52]), as it is done for example in [28], [27]. Even though we will not need the notion of strong regularity, we will largely follow the ideas presented in this work. The main ingredient is to prove Lipschitz stability of the control problem with respect to perturbations. This property of the problem is interesting in its own right for understanding the behaviour of problems and has been analyzed for many problems (cf. e.g. [4], [43], [44], [58]), as well as for example as a means to perform parametric sensitivity analysis (cf. e.g. [26], [29]).

Let us give a short outline of what is to come in this chapter: In section 8.1, we are going to introduce the generalized equation setting for the optimality system and verify some properties we will need, in particular differentiability of the generalized equation and Lipschitz continuity of its derivative. This allows us to linearize (GE) in the optimal solution. In section 8.2, we will show that the Newton iteration

$$0 \in F(y^k) + F'(y^k)(y - y^k) + N(y) \qquad (GEL_k)$$

corresponds to the optimal control problem (QP_k), and that this system is uniquely solvable as long as y^k is close enough to the optimal solution $\bar{y}$. For this we need to assume that the sufficient optimality condition (SSC) holds. In section 8.3, we will prove that the generalized equation is Lipschitz stable with respect to perturbations δ in the sense that given perturbations δ_i and corresponding solutions $y_i = y(\delta_i)$, $i = 1, 2$, of

$$\delta_i \in F(\bar{y}) + F'(\bar{y})(y_i - \bar{y}) + N(y_i),$$

there is a constant $L > 0$ such that

$$\|y_1 - y_2\|_{Y_{r,p}} \leq L\|\delta_1 - \delta_2\|_{Z_{r,p}}$$

for suitable spaces $Y_{r,p}$, $Z_{r,p}$. The last section is devoted to the proof of convergence for the Newton method. To give an idea of why we need the following considerations let us give a rough sketch of the line of argumentation: We can rewrite the Newton iteration (GEL_k) as

$$\begin{aligned} \delta_{k+1} \in& F(\bar{y}) + F'(\bar{y})(y^{k+1} - \bar{y}) + N(y^{k+1}), \\ \delta_{k+1} :=& F(\bar{y}) - F(y^k) + F'(\bar{y})(y^{k+1} - \bar{y}) - F'(y^k)(y^{k+1} - y^k). \end{aligned}$$

Now on the one hand, the Lipschitz stability from section 8.3, which will be proved in Theorem 8.10, gives

$$\|y^{k+1} - \bar{y}\|_{Y_{r,p}} \leq c\|\delta^{k+1}\|_{Z_{r,p}},$$

and on the other hand, since the first derivative of F is Lipschitz continuous, with the help of Corollary 8.4 we will see that

$$\|\delta^{k+1}\|_{Z_{r,p}} \leq c\|y^k - \bar{y}\|_{Y_{r,p}}.$$

Both constants depend on the radius ρ of the neighbourhood of $\bar{y}$ in which the sequence $\{y^k\}_{k\in\mathbb{N}}$ lies. Putting together these two estimates we will obtain convergence as long as we start closely enough to the actual solution, that is if the distance $\|y^0 - \bar{y}\|_{Y_{r,p}}$ is sufficiently small.

8.1 Generalized equation

So let us start by fixing the setting for the generalized equation in which we will work during this chapter. For

$$p > N, \qquad r > 2p, \qquad \frac{2}{r} + \frac{N}{p} < 1 \tag{8.1}$$

as in (4.3), let us define the spaces

$$Y_{r,p} := \mathbb{W}_{r,p} \times \mathbb{W}_{r,p} \cap L_\infty(W_p^1) \times L_r(L_p(\Gamma)) \times \mathbb{W}_{r,p}^2 \times L_{r'}(L_{p'}(\Gamma))^2 \tag{8.2}$$

$$Z_{r,p} := \left[L_r(W_p^{-1}) \times \mathcal{D}_{r,p}\right]^2 \times L_r(L_p(\Gamma)) \times \left[L_r(W_p^{-1}) \times \mathcal{D}_{r,p}\right]^2 \times L_{r'}(L_{p'}(\Gamma))^2 \tag{8.3}$$

where $\frac{1}{p} + \frac{1}{p'} = \frac{1}{r} + \frac{1}{r'} = 1$ (recall that $Y_{r,p}$ was already defined in (7.6)), and a function $F : Y_{r,p} \to Z_{r,p}$ via

$$F(y) = \begin{pmatrix} \langle u_t, \cdot\rangle_{W_p^{-1},W_{p'}^1} + \langle \nabla u, \nabla\cdot\rangle - \langle f(u)\nabla v, \nabla\cdot\rangle \\ u(0) - u_0 \\ \langle v_t, \cdot\rangle_{W_p^{-1},W_{p'}^1} + \langle \nabla v, \nabla\cdot\rangle + \langle v, \cdot\rangle - \langle u, \cdot\rangle + \langle \gamma^* g, \cdot\rangle \\ v(0) - v_0 \\ \lambda g + \gamma^* q - \mu_a + \mu_b \\ \langle -p_t, \cdot\rangle_{W_p^{-1},W_{p'}^1} + \langle \nabla p, \nabla\cdot\rangle - \langle f'(u)\nabla v\nabla p, \cdot\rangle - \langle q, \cdot\rangle - \langle \alpha_2(u-u_Q), \cdot\rangle \\ p(T) - \alpha_1(u(T) - u_\Omega) \\ \langle -q_t, \cdot\rangle_{W_p^{-1},W_{p'}^1} + \langle \nabla q, \nabla\cdot\rangle + \langle q, \cdot\rangle - \langle f(u)\nabla p, \nabla\cdot\rangle \\ q(T) \\ g - g_a \\ g_b - g \end{pmatrix}$$

for $y := (u, v, g, p, q, \mu_a, \mu_b) \in Y_{r,p}$ a.e. in $(0, T)$. We also define a cone

$$N(y) = (\{0\}, \{0\}, \{0\}, \{0\}, \{0\}, N_1(\mu_a), N_1(\mu_b))^T,$$

where

$$N_1(\mu) := \begin{cases} \{h \in L_r(L_p(\Gamma)) : h(\mu - \nu) \geq 0 \text{ a.e. in } \Sigma \text{ for all } \nu \in K\}, & \mu \in K, \\ \emptyset, & \mu \notin K, \end{cases}$$

and $K := \{\mu \in L_{r'}(L_{p'}(\Gamma)) : \mu \geq 0 \text{ a.e. in } \Sigma\}$. First of all, we note that this means we can solve (GE) instead of (FON_P):

Lemma 8.1. *Assume* (8.1) *holds and let* $y \in Y_{r,p}$. *The system* (FON_P) *and the generalized equation* (GE) *are equivalent.*

Proof. The components one to four and six to nine of the generalized equations obviously correspond to the variational formulations of the state system and the adjoint system in (FON_P), the fifth component is exactly the gradient equation. The last two components are equivalent to the complementarity conditions. For the lower bound this can be seen as follows:

"$\Rightarrow$": Assume $\mu_a \in L_{r'}(L_{p'}(\Gamma))$ and $\mu_a \geq 0$, $g_a - g \leq 0$, $\mu_a(g_a - g) = 0$ a.e. in Σ. Then obviously $\mu_a \in K$, so

$$N_1(\mu_a) = \{h \in L_r(L_p(\Gamma)) : h(\mu_a - \nu) \geq 0 \text{ for all } \nu \in K\}.$$

Further we know

$$\begin{aligned} (g_a - g)\nu &\leq 0 \quad \text{a.e. in } \Sigma \text{ for all } \nu \in K \\ \Rightarrow (g_a - g)(\nu - \mu_a) &\leq 0 \quad \text{a.e. in } \Sigma \text{ for all } \nu \in K \\ \Rightarrow (g_a - g)(\mu_a - \nu) &\geq 0 \quad \text{a.e. in } \Sigma \text{ for all } \nu \in K \end{aligned}$$

and so $g_a - g \in N_1(\mu_a)$ or $0 \in g - g_a + N_1(\mu_a)$.

"$\Leftarrow$": Now assume $g_a - g \in N_1(\mu_a)$. Then $\mu_a \in K$ (since $N_1(\mu_a) \neq \emptyset$) and hence $(g_a - g)(\mu_a - \nu) \geq 0$ a.e. in Σ for all $\nu \in K$. Now wherever $\mu_a(x,t) = 0$, we have

$$\begin{aligned} (g_a - g)(-\nu) &\geq 0 \quad \text{a.e. in } \Sigma \text{ for all } \nu \geq 0 \\ \Rightarrow \qquad (g_a - g) &\leq 0 \quad \text{and} \quad \mu_a(g_a - g) = 0 \quad \text{a.e. in } \Sigma. \end{aligned}$$

If instead $\mu_a > 0$ then, in order to have $(g_a - g)(\mu_a - \nu) \geq 0$ for all $\nu \geq 0$, we need $g_a - g = 0$ which implies $\mu_a(g_a - g) = 0$.

For the upper bound this works in the exact same way. □

Since we want to apply Newton's method, we need to be able to linearize this generalized equation. To do this, first we need to make sure F is actually differentiable:

Lemma 8.2. *Assume* (8.1) *holds. Then* $F : Y_{r,p} \to Z_{r,p}$ *is differentiable.*

Proof. The only components involving nonlinear terms are the first, the sixth and the eighth resulting from the variational formulations of the equations for u, p and q. The first one, $\langle f(u)\nabla v, \nabla\cdot\rangle$, has been dealt with already in Theorem 4.5 showing differentiability of the control to state operator. The argumentation relies on the properties of the Nemytzkii operator f and the fact that $\mathbb{W}_{r,p} \hookrightarrow L_\infty(Q)$. The second one, $\langle f'(u)\nabla v\nabla p, \cdot\rangle$, is linear with respect to v and p, and u enters through the Nemytzkii operator f', so here we have

$$\left(\langle f'(\bar{u})\nabla\bar{v}\nabla\bar{p}, \cdot\rangle\right)'(u,v,p) = \langle f''(\bar{u})u\nabla\bar{v}\nabla\bar{p} + f'(\bar{u})\nabla v\nabla\bar{p} + f'(\bar{u})\nabla\bar{v}\nabla p, \cdot\rangle$$

in $L_r(W_p^{-1})$. The third nonlinearity, $\langle f(u)\nabla p, \nabla\cdot\rangle$, has the same structure as the first so that the whole system is indeed differentiable. □

So what does F' acually look like? For $y = (u,v,g,p,q,\mu_a,\mu_b) \in Y_{r,p}$, $\bar{y} = (\bar{u},\bar{v},\bar{g},\bar{p},\bar{q},\bar{\mu}_a,\bar{\mu}_b) \in Y_{r,p}$, the derivative of F in $\bar{y}$ in direction y is given by

$$F'(\bar{y})y = \begin{pmatrix} \langle u_t, \cdot\rangle_{W_p^{-1},W^1_{p'}} + \langle\nabla u, \nabla\cdot\rangle - \langle f'(\bar{u})u\nabla\bar{v} + f(\bar{u})\nabla v, \nabla\cdot\rangle \\ u(0) \\ \langle v_t, \cdot\rangle_{W_p^{-1},W^1_{p'}} + \langle\nabla v, \nabla\cdot\rangle + \langle v, \cdot\rangle - \langle u, \cdot\rangle + \langle\gamma^* g, \cdot\rangle \\ v(0) \\ \lambda g + \gamma^* q - \mu_a + \mu_b \\ \langle -p_t, \cdot\rangle_{W_p^{-1},W^1_{p'}} + \langle\nabla p, \nabla\cdot\rangle - \langle f'(\bar{u})\nabla\bar{v}\nabla p, \cdot\rangle - \langle q, \cdot\rangle \\ -\langle f''(\bar{u})u\nabla\bar{v}\nabla\bar{p} + f'(\bar{u})\nabla v\nabla\bar{p}, \cdot\rangle - \langle\alpha_2 u, \cdot\rangle \\ p(T) - \alpha_1 u(T) \\ \langle -q_t, \cdot\rangle_{W_p^{-1},W^1_{p'}} + \langle\nabla q, \nabla\cdot\rangle + \langle q, \cdot\rangle - \langle f(\bar{u})\nabla p + f'(\bar{u})u\nabla\bar{p}, \nabla\cdot\rangle \\ q(T) \\ g \\ -g \end{pmatrix}$$

a.e. in $(0,T)$.

It is well known from finite dimensional optimization that in order to prove quadratic convergence of the Newton iteration, the derivative F' needs to be Lipschitz continuous. The same is true in the infinite dimensional case. Once again, being able to obtain this property largely depends on the correct choice of the underlying function spaces. Note that in particular, the fact that v is essentially bounded in time is crucial here.

Lemma 8.3. *Assume* (8.1) *holds. The derivative F' is Lipschitz continuous in the sense that for every $M > 0$ and $y_1, y_1, \in Y_{r,p}$, $\|y_1\|_{Y_{r,p}} + \|y_2\|_{Y_{r,p}} \leq M$, there is a constant L(M) such that*

$$\|\{F'(y_1) - F'(y_2)\}y\|_{Z_{r,p}} \leq L(M)\|y\|_{Y_{r,p}}\|y_1 - y_2\|_{Y_{r,p}}$$

for every $y \in Y_{r,p}$.

Proof. Since all the linear terms vanish, we just need to look at the three nonlinear terms from above (for convenience we dropped the minus sign in front of each of them),

$$\begin{aligned}
I =& \langle f'(u_1)u\nabla v_1 + f(u_1)\nabla v, \nabla\cdot\rangle - \langle f'(u_2)u\nabla v_2 + f(u_2)\nabla v, \nabla\cdot\rangle \\
=& \langle \{f'(u_1) - f'(u_2)\}u\nabla v_1 + f'(u_2)u\nabla(v_1 - v_2) + \{f(u_1) - f(u_2)\}\nabla v, \nabla\cdot\rangle \\
II =& \langle f'(u_1)\nabla v_1\nabla p + f''(u_1)u\nabla v_1\nabla p_1 + f'(u_1)\nabla v\nabla p_1, \cdot\rangle \\
&- \langle f'(u_2)\nabla v_2\nabla p + f''(u_2)u\nabla v_2\nabla p_2 + f'(u_2)\nabla v\nabla p_2, \cdot\rangle \\
=& \langle \{f'(u_1) - f'(u_2)\}\nabla v_1\nabla p + f'(u_2)\nabla(v_1 - v_2)\nabla p, \cdot\rangle \\
&+ \langle \{f''(u_1) - f''(u_2)\}u\nabla v_1\nabla p_1 + f''(u_2)u\nabla(v_1 - v_2)\nabla p_1, \cdot\rangle \\
&+ \langle f''(u_2)u\nabla v_2\nabla(p_1 - p_2), \cdot\rangle \\
&+ \langle \{f'(u_1) - f'(u_2)\}\nabla v\nabla p_1 + f'(u_2)\nabla v\nabla(p_1 - p_2), \cdot\rangle \\
III =& \langle f'(u_1)u\nabla p_1 + f(u_1)\nabla p, \nabla\cdot\rangle - \langle f'(u_2)u\nabla p_2 + f(u_2)\nabla p, \nabla\cdot\rangle \\
=& \langle \{f'(u_1) - f'(u_2)\}u\nabla p_1 + f'(u_2)u\nabla(p_1 - p_2) + \{f(u_1) - f(u_2)\}\nabla p, \nabla\cdot\rangle\,.
\end{aligned}$$

Recall from (2.7) that $|\langle\nabla\phi, \nabla\cdot\rangle| \leq c\|\nabla\phi\|_{L_p}$ for $\phi \in W_p^1$ and some $c > 0$. We can estimate

$$\begin{aligned}
\|I\|_{L_r(W_p^{-1})} \leq& c\Big(L_{f'}\|u_1 - u_2\|_{C(\bar{Q})}\|u\|_{C(\bar{Q})}\|v_1\|_{L_r(W_p^1)} \\
&+ c_{f'}\|u\|_{C(\bar{Q})}\|v_1 - v_2\|_{L_r(W_p^1)} + L_f\|u_1 - u_2\|_{C(\bar{Q})}\|v\|_{L_r(W_p^1)}\Big) \\
\leq& c(y_1)\left(\|u\|_{\mathbb{W}_{r,p}} + \|v\|_{\mathbb{W}_{r,p}}\right)\left(\|u_1 - u_2\|_{\mathbb{W}_{r,p}} + \|v_1 - v_2\|_{\mathbb{W}_{r,p}}\right) \\
\leq& c(y_1)\|y\|_{Y_{r,p}}\|y_1 - y_2\|_{Y_{r,p}},
\end{aligned}$$

and in the same way

$$\begin{aligned}\|II\|_{L_r(W_p^{-1})} \leq & c\Big(L_{f'}\|u_1-u_2\|_{C(\bar Q)}\|v_1\|_{L_\infty(W_p^1)}\|p\|_{L_r(W_p^1)}\\ & + c_{f'}\|v_1-v_2\|_{L_\infty(W_p^1)}\|p\|_{L_r(W_p^1)}\\ & + L_{f''}\|u_1-u_2\|_{C(\bar Q)}\|u\|_{C(\bar Q)}\|v_1\|_{L_\infty(W_p^1)}\|p_1\|_{L_r(W_p^1)}\\ & + c_{f''}\|u\|_{C(\bar Q)}\|v_1-v_2\|_{L_\infty(W_p^1)}\|p_1\|_{L_r(W_p^1)}\\ & + c_{f''}\|u\|_{C(\bar Q)}\|v_2\|_{L_\infty(W_p^1)}\|p_1-p_2\|_{L_r(W_p^1)}\\ & + L_{f'}\|u_1-u_2\|_{C(\bar Q)}\|v\|_{L_\infty(W_p^1)}\|p_1\|_{L_r(W_p^1)}\\ & + c_{f'}\|v\|_{L_\infty(W_p^1)}\|p_1-p_2\|_{L_r(W_p^1)}\Big)\\ \leq & c(y_1,y_2)\|y\|_{Y_{r,p}}\|y_1-y_2\|_{Y_{r,p}}.\end{aligned}$$

The third term is identical to the first if we replace v by p, so we get the same estimate with respect to y. □

The following corollary is fairly standard. We will mention it anyway since it will be a crucial argument in the proof of convergence of the Newton iteration in Theorem 8.11.

Corollary 8.4. *Assume* (8.1) *holds and let* $M > 0$, $y, y_1, y_2 \in Y_{r,p}$ *such that* $\|y_1\|_{Y_{r,p}} + \|y_2\|_{Y_{r,p}} \leq M$ *as in the previous lemma.*

(i) With the constant $L(M)$ *from above, we have*

$$\|F(y_1) - F(y_2) - F'(y_2)(y_1 - y_2)\|_{Z_{r,p}} \leq \frac{L(M)}{2}\|y_1 - y_2\|^2_{Y_{r,p}}.$$

(ii) There is a constant c(M,y) such that

$$\begin{aligned}&\|F(y_1) + F'(y_1)(y - y_1)\\ &\qquad -F(y_2) - F'(y_2)(y - y_2)\|_{Z_{r,p}} \leq c(M, y)\|y_1 - y_2\|_{Y_{r,p}}\end{aligned}$$

Proof. (i) Follows as an easy computation from the integral mean value theorem using the Lipschitz continuity of the derivative.

(ii) Relies on the Lipschitz continuity of F' as well and can be seen as follows:

$$\begin{aligned}
\|F(y_1) + F'(y_1)(y - y_1) - F(y_2) - F'(y_2)(y - y_2)\|_{Z_{r,p}} \\
\leq &\|F(y_1) - F(y_2)\|_{Z_{r,p}} + \|(F'(y_1) - F'(y_2))y\|_{Z_{r,p}} \\
&+ \|(F'(y_2) - F'(y_1))y_1\|_{Z_{r,p}} + \|F'(y_2)(y_2 - y_1)\|_{Z_{r,p}} \\
\leq &c\|y_1 - y_2\|_{Y_{r,p}} + c\|y_1 - y_2\|_{Y_{r,p}}\|y\|_{Y_{r,p}} \\
&+ \|y_2 - y_1\|_{Y_{r,p}}\|y_1\|_{Y_{r,p}} + c\|y_2 - y_1\|_{Y_{r,p}} \\
\leq &c(y, y_1)\|y_1 - y_2\|_{Y_{r,p}}.
\end{aligned}$$

□

8.2 The linear-quadratic subproblem

After we have shown that the linearization of (GE) is well defined, let us now look at the equation we have to solve to compute the Newton iterates. In each step, the new iterate y^{k+1} is defined as the solution of the generalized equation

$$0 \in F(y^k) + F'(y^k)(y - y^k) + N(y), \qquad (GEL_k)$$

where $F(y^k) + F'(y^k)(y - y^k)$ is given by

$$\begin{pmatrix}
\langle u_t, \cdot\rangle_{W_p^{-1}, W_{p'}^1} + \langle \nabla u, \nabla \cdot\rangle - \left\langle f'(u^k)(u - u^k)\nabla v^k + f(u^k)\nabla v, \nabla \cdot\right\rangle \\
u(0) - u_0 \\
\langle v_t, \cdot\rangle_{W_p^{-1}, W_{p'}^1} + \langle \nabla v, \nabla \cdot\rangle + \langle v, \cdot\rangle - \langle u, \cdot\rangle + \langle \gamma^* g, \cdot\rangle \\
v(0) - v_0 \\
\lambda g + \gamma^* q - \mu_a + \mu_b \\
\langle -p_t, \cdot\rangle_{W_p^{-1}, W_{p'}^1} + \langle \nabla p, \nabla \cdot\rangle - \left\langle f'(u^k)\nabla v^k \nabla p, \cdot\right\rangle - \langle q, \cdot\rangle \\
- \left\langle f''(u^k)(u - u^k)\nabla v^k \nabla p^k + f'(u^k)\nabla(v - v^k)\nabla p^k, \cdot\right\rangle - \langle \alpha_2(u - u_Q), \cdot\rangle \\
p(T) - \alpha_1(u(T) - u_\Omega) \\
\langle -q_t, \cdot\rangle_{W_p^{-1}, W_{p'}^1} + \langle \nabla q, \nabla \cdot\rangle + \langle q, \cdot\rangle - \left\langle f(u^k)\nabla p + f'(u^k)(u - u^k)\nabla p^k, \nabla \cdot\right\rangle \\
q(T) \\
g - g_a \\
g_b - g
\end{pmatrix}$$

a.e. in $[0, T]$. This raises two questions: First of all, does this equation have a unique solution, at least as long as y^k is not too far away from the optimal solution $\bar{y}$? And secondly, how can we find this solution, since it is not exactly obvious how to tackle such a set valued equation? The first question can be answered positively as long as the condition (SSC) holds and y^k is sufficiently close to $\bar{y}$. The second question leads us to the quadratic subproblem (QP_k) mentioned in the introduction,

$$\begin{aligned} &\min\ J'(u^k, v^k, g^k)\begin{pmatrix} u-u^k \\ v-v^k \\ g-g^k \end{pmatrix} + \frac{1}{2}\mathcal{L}''(y^k)(u-u^k, v-v^k, g-g^k)^2, \\ u_t &= \Delta u - \nabla\cdot\{f'(u^k)(u-u^k)\nabla v^k + f(u^k)\nabla v\} \text{ in } Q \quad u(0)=u_0 \text{ in } \Omega \\ v_t &= \Delta v - v + u + \gamma^* g \qquad\qquad \text{in } Q \quad v(0) = v_0 \text{ in } \Omega \\ &\qquad g_a \le g \le g_b, \end{aligned} \tag{QP_k}$$

where

$$\begin{aligned} J'(u^k, v^k, g^k)\begin{pmatrix} u-u^k \\ v-v^k \\ g-g^k \end{pmatrix} =& \alpha_1 \left\langle u^k(T) - u_\Omega, u(T) - u^k(T)\right\rangle_\Omega \\ &+ \alpha_2 \left\langle u^k - u_Q, u - u^k\right\rangle_Q + \lambda\left\langle g^k, g - g^k\right\rangle_\Sigma, \\ \mathcal{L}''(y^k)(u-u^k, v-v^k, g-g^k)^2 =& \alpha_1\|u(T) - u^k(T)\|^2_{L_2(\Omega)} + \alpha_2\|u-u^k\|^2_{L_2(Q)} \\ &+ \lambda\|g-g^k\|^2_{L_2(\Sigma)} \\ &+ \left\langle \nabla p^k, f''(u^k)(u-u^k)^2\nabla v^k\right\rangle_Q \\ &+ \left\langle \nabla p^k, 2f'(u^k)(u-u^k)\nabla(v-v^k)\right\rangle_Q. \end{aligned}$$

Lemma 8.5. *Assume $\bar{y} \in Y_{r,p}$ satisfies* (SSC). *There is a $\rho > 0$ such that for all $y^k \in Y_{r,p}$, $\|y^k - \bar{y}\|_{Y_{r,p}} \le \rho$ there is a unique optimal control $g \in L_r(L_p(\Gamma))$ to (QP_k) with corresponding state $(u, v) \in \mathbb{W}^2_{r,p}$.*

Proof. Since the constraints are linear, we only have to check if the problem is convex and hence weakly lower semicontinuous. In that case, existence and uniqueness of an optimal solution is a standard result (cf. e.g. [59] Satz 2.14, [41] I Theorem 1.1). Since the linear parts drop out, the second derivative of the objective with respect to (u, v, g) in direction (w, z, h) is given by

$$\begin{aligned} \mathcal{L}''(y^k)(w, z, h)^2 = \alpha_1\|w(T)\|^2_{L_2(\Omega)} + \alpha_2\|w\|^2_{L_2(Q)} + \lambda\|h\|^2_{L_2(\Sigma)} \\ + \left\langle \nabla p^k, f''(u^k)w^2\nabla v^k + 2f'(u^k)w\nabla z\right\rangle_Q, \end{aligned}$$

where

$$w_t = \Delta w - \nabla \cdot \{f'(u^k) w \nabla v^k + f(u^k)\nabla z\} \text{ in } Q, \qquad u(0) = 0 \text{ in } \Omega, \tag{8.4}$$
$$z_t = \Delta z - z + w + \gamma^* h \qquad \text{ in } Q, \qquad v(0) = 0 \text{ in } \Omega. \tag{8.5}$$

By Corollary 7.7, (SSC) implies there are $\rho > 0$, $\kappa'' > 0$ such that

$$\mathcal{L}''(y^k)(w,z,h)^2 \geq \kappa'' \|h\|^2_{L_2(\Sigma)}$$

for all $h \in L_r(L_p(\Gamma))$ whenever $\|y^k - y\|_{Y_{r,p}} \leq \rho$, which implies convexity of the problem. □

Lemma 8.6. *Assume $\bar{y} \in Y_{r,p}$ satisfies* (SSC)*, $y^k \in Y_{r,p}$, $\|y^k - \bar{y}\|_{Y_{r,p}} \leq \rho$ in accordance with the previous Lemma and let $y^* = (u^*, v^*, g^*, p^*, q^*, \mu_a^*, \mu_b^*) \in Y_{r,p}$ solve (GEL_k). Then (u^*, v^*, g^*) solves (QP_k) with adjoint states and multipliers $(p^*, q^*, \mu_a^*, \mu_b^*)$. If conversely $(u^*, v^*, g^*) \in \mathbb{W}^2_{r,p} \times L_r(L_p(\Gamma))$ is a solution of (QP_k) with corresponding adjoint states and multipliers $(p^*, q^*, \mu_a^*, \mu_b^*)$, then $y^* = (u^*, v^*, g^*, p^*, q^*, \mu_a^*, \mu_b^*)$ solves (GEL_k).*

Proof. The first four components of (GEL_k) are exactly the variational formulation of the state system of (QP_k). So let us look at the optimality system of (QP_k) and compare it to the other components. The first derivative of the objective with respect to (u, v, g) in direction (w, z, h) is given by

$$\begin{aligned}\alpha_1 \langle u(T) - u_\Omega, w(T)\rangle_\Omega + \alpha_2 \langle u - u_Q, w\rangle_Q + \lambda \langle g, h\rangle_\Sigma \\ + \left\langle f''(u^k)(u - u^k)\nabla v^k \nabla p^k + f'(u^k)\nabla(v - v^k)\nabla p^k, w\right\rangle_Q \\ + \left\langle f'(u^k)(u - u^k)\nabla p^k, \nabla z\right\rangle_Q,\end{aligned}$$

where (w, z) again solves (8.4)-(8.5). If we apply Lemma 6.1 with the adjoint state from components six to nine of (GEL_k), it is not difficult to see that we end up with $\langle \lambda g + \gamma^* q, h\rangle_\Sigma$. Hence, due to Lemma 8.1 the gradient equation and the complementarity conditions are given by components five, nine and ten of (GEL_k). Note that the adjoint equation is well defined as well: Theorem 3.6 requires

$$\eta_1 = f''(u^k)(u - u^k)\nabla v^k \nabla p^k + f'(u^k)\nabla(v - v^k) \in L_r(W_p^{-1})$$

which has been shown in the proof of Lemma 8.3. □

8.3 Lipschitz stability

In this section, we want to analyze what we can say about the behaviour of the solution to the generalized equation if we add a perturbation parameter δ,

$$\delta \in F(\bar{y}) + F'(\bar{y})(y - \bar{y}) + N(y). \tag{$GE(\delta)$}$$

First of all, we have to make sure the generalized equation remains uniquely solvable, that is we will see that for every $\delta \in Z_{r,p}$ there is a unique solution $y = y(\delta) \in Y_{r,p}$. Once we have done that, we want to show that the solution $y = y(\delta)$ depends on δ in a Lipschitz stable way, that is we want to show there is an $L > 0$ such that for $\delta_1, \delta_2 \in Z_{r,p}$ and corresponding solutions $y_1 = y(\delta_1), y_2 = y(\delta_2) \in Y_{r,p}$, we have

$$\|y_1 - y_2\|_{Y_{r,p}} \leq L\|\delta_1 - \delta_2\|_{Z_{r,p}}.$$

Since the proof of Lipschitz stability relies on (SSC), at first this can typically only be shown with respect to the L_2 norm of the control. This will be done in Lemma 8.9. Based on that, we will then be able to exploit the fact that the projection formula (6.6) provides an improvement in regularity for the optimal control, which allows us to gradually improve the stability estimate to stronger spaces. Due to the regularity results from chapter 3, as before we need $\alpha, \beta, \nu, \sigma \geq 2$ satisfying the restrictions

$$\frac{2}{\alpha} + \frac{N}{p} < 1, \qquad\qquad \frac{2}{\alpha} + \frac{N}{\beta} > \frac{2}{\nu} + \frac{N-1}{\sigma} \tag{8.6}$$

known from (3.12) (or (4.10) for $\nu = \sigma = 2$). In addition, we need to adjust the solution spaces for v, p and q: For $\frac{1}{\tilde{\alpha}} = \frac{1}{\alpha} + \frac{1}{r}$, we introduce

$$\mathcal{Y}_{\alpha,\beta} := \mathbb{W}_{\alpha,\beta} \times \mathbb{W}_{\nu,\beta} \cap L_\alpha(W^1_\beta) \times L_\nu(L_\sigma(\Gamma)) \times \mathbb{W}^2_{\tilde{\alpha},\beta} \times L_\nu(L_\sigma(\Gamma))^2 \tag{8.7}$$

(note that $\tilde{\alpha} > 2$ since $\frac{1}{\alpha} + \frac{1}{r} < \frac{1}{\alpha} + \frac{N}{2p} < \frac{1}{2}$). Having established this framework, we will proceed in the same way as we did in the previous section by defining a linear quadratic optimal control problem that corresponds to $(GE(\delta))$: For

$\delta = (\delta_1, ..., \delta_{11}) \in Z_{\alpha,\beta}$ we look at

$$
\begin{aligned}
\min \ & J'(\bar u, \bar v, \bar g) \begin{pmatrix} u - \bar u \\ v - \bar v \\ g - \bar g \end{pmatrix} + \frac{1}{2}\mathcal{L}''(\bar y)(u - \bar u, v - \bar v, g - \bar g)^2 \\
& \qquad + \langle \delta_7, u(T)\rangle_\Omega + \langle \delta_9, v(T)\rangle_\Omega + \langle \delta_6, u\rangle_Q + \langle \delta_8, v\rangle_Q + \langle \delta_5, g\rangle_\Sigma , \\
u_t =& \Delta u - \nabla \cdot \{f'(\bar u)(u - \bar u)\nabla \bar v + f(\bar u)\nabla v\} + \delta_1 \text{ in } Q, \quad u(0) = u_0 + \delta_2 \text{ in } \Omega, \\
v_t =& \Delta v - v + u + \gamma^* g + \delta_3 \qquad \text{ in } Q, \quad v(0) = v_0 + \delta_4 \text{ in } \Omega, \\
& g_a + \delta_{10} \le g \le g_b - \delta_{11},
\end{aligned} \tag{$QP(\delta)$}
$$

where once again

$$
\begin{aligned}
J'(\bar u, \bar v, \bar g) \begin{pmatrix} u - \bar u \\ v - \bar v \\ g - \bar g \end{pmatrix} =& \alpha_1 \langle \bar u(T) - u_\Omega, u(T) - \bar u(T)\rangle_\Omega \\
& + \alpha_2 \langle \bar u - u_Q, u - \bar u\rangle_Q + \lambda \langle \bar g, g - \bar g\rangle_\Sigma , \\
\mathcal{L}''(\bar y)(u - \bar u, v - \bar v, g - \bar g)^2 =& \alpha_1 \|u(T) - \bar u(T)\|^2_{L_2(\Omega)} + \alpha_2 \|u - \bar u\|^2_{L_2(Q)} \\
& + \lambda \|g - \bar g\|^2_{L_2(\Sigma)} + \left\langle \nabla \bar p, f''(\bar u)(u - \bar u)^2 \nabla \bar v \right\rangle_Q \\
& + \langle \nabla \bar p, 2f'(\bar u)(u - \bar u)\nabla(v - \bar v)\rangle_Q .
\end{aligned}
$$

Lemma 8.7. *Assume that $\bar y \in Y_{r,p}$ satisfies* (SSC)*, $\alpha, \beta, \nu, \sigma$ are chosen according to* (8.6) *and $\delta \in Z_{\alpha,\beta}$. There is a unique optimal control $g \in L_\nu(L_\sigma(\Gamma))$ to $(QP(\delta))$ with corresponding state $(u, v) \in \mathbb{W}_{\alpha,\beta} \times \mathbb{W}_{\nu,\beta} \cap L_\alpha(W^1_\beta)$.*

Proof. The proof works in the same way as Lemma 8.5 by computing the second derivative of the problem. Since δ only enters linearly, it does not appear any more in the second derivative, hence we can apply (SSC) directly to obtain convexity of the problem. □

Lemma 8.8. *Assume $\bar y \in Y_{r,p}$ satisfies* (SSC)*), $\alpha, \beta, \nu, \sigma$ are chosen according to* (8.6) *and $\delta \in Z_{\alpha,\beta}$. Assume $y^* = (u^*, v^*, g^*, p^*, q^*, \mu^*_a, \mu^*_b) \in \mathcal{Y}_{\alpha,\beta}$ solves $(GE(\delta))$. Then (u^*, v^*, g^*) solves $(QP(\delta))$ with adjoint states and multipliers $(p^*, q^*, \mu^*_a, \mu^*_b)$. If conversely $(u^*, v^*, g^*) \in \mathbb{W}_{\alpha,\beta} \times \mathbb{W}_{\nu,\beta} \cap L_\alpha(W^1_\beta) \times L_\nu(L_\sigma(\Gamma))$ is a solution to $(QP(\delta))$ with corresponding adjoint states and multipliers $(p^*, q^*, \mu^*_a, \mu^*_b)$, then $y^* = (u^*, v^*, g^*, p^*, q^*, \mu^*_a, \mu^*_b)$ solves $(GE(\delta))$.*

Proof. Again, this can be shown in the exact same way as the proof of Lemma 8.6. Here, the first derivative of the objective with respect to (u, v, g) in direction (w, z, h) is given by

$$\begin{aligned}\alpha_1 \langle u(T) - u_\Omega, w(T)\rangle_\Omega &+ \alpha_2 \langle u - u_Q, w\rangle_Q + \lambda \langle g, h\rangle_\Sigma \\ &+ \langle f''(\bar{u})(u - \bar{u})\nabla\bar{v}\nabla\bar{p} + f'(\bar{u})\nabla(v - \bar{v}), w\rangle_Q \\ &+ \langle f'(\bar{u})(u - \bar{u})\nabla\bar{p}, \nabla z\rangle_Q + \langle \delta_5, h\rangle_\Omega \\ &+ \langle \delta_6, w\rangle_Q + \langle \delta_7, w(T)\rangle_\Omega + \langle \delta_8, z\rangle_Q + \langle \delta_9, z(T)\rangle_\Omega\end{aligned}$$

where (w, z) solves the linearized equation with homogeneous inital values and boundary value h. □

Let us now look at the first order optimality system of $(QP(\delta))$ given by

$$\left.\begin{aligned}
u_t =&\Delta u - \nabla\cdot\{f'(\bar{u})(u-\bar{u})\nabla\bar{v} + f(\bar{u})\nabla v\} + \delta_1 && \text{in } Q,\\
u(0) =&u_0 + \delta_2 && \text{in } \Omega,\\
v_t =&\Delta v - v + u + \gamma^* g + \delta_3 && \text{in } Q,\\
v(0) =&v_0 + \delta_4 && \text{in } \Omega,\\
-p_t =&\Delta p + f'(\bar{u})\nabla\bar{v}\nabla p + q + f''(\bar{u})(u-\bar{u})\nabla\bar{v}\nabla\bar{p} && \text{in } Q,\\
&+ f'(\bar{u})\nabla(v-\bar{v})\nabla\bar{p} + \alpha_2(u-u_Q) + \delta_6 &&\\
p(T) =&\alpha_1(u(T) - u_\Omega) + \delta_7 && \text{in } \Omega,\\
-q_t =&\Delta q - q - \nabla\cdot\{f'(\bar{u})(u-\bar{u})\nabla\bar{p} + f(\bar{u})\nabla p\} + \delta_8 && \text{in } Q,\\
q(T) =&\delta_9 && \text{in } \Omega,\\
&\lambda g + \gamma q - \mu_a + \mu_b + \delta_5 = 0 && \text{in } \Sigma,\\
\mu_a \geq& 0, \quad g_a + \delta_{10} - g \leq 0, \quad \mu_a(g_a + \delta_{10} - g) = 0 && \text{in } \Sigma,\\
\mu_b \geq& 0, \quad g - g_b - \delta_{11} \leq 0, \quad \mu_b(g - g_b - \delta_{11}) = 0 && \text{in } \Sigma.
\end{aligned}\right\} \quad (FON_\delta)$$

This is the basis for the following result:

Lemma 8.9. *Assume $\bar{y} \in Y_{r,p}$ satisfies* (SSC), $\nu = \sigma = 2$ *and α, β are chosen according to* (8.6)*. There is an $L > 0$ such that for every $\delta, \delta' \in Z_{\alpha,\beta}$, the respective solutions $y^\delta, y^{\delta'} \in \mathcal{Y}_{\alpha,\beta}$ of $(GE(\delta))$ satisfy*

$$\|y^{\delta'} - y^\delta\|_{\mathcal{Y}_{\alpha,\beta}} \leq L\|\delta' - \delta\|_{Z_{\alpha,\beta}}.$$

Proof. For convenience, let us set $\delta y := y^{\delta'} - y^{\delta}$. δy then solves the state system

$$\begin{aligned} \delta u_t =& \Delta\delta u - \nabla\cdot\{f'(\bar u)\delta u\nabla\bar v + f(\bar u)\nabla\delta v\} + \delta_1' - \delta_1 && \text{in } \Omega\times(0,T),\\ \delta u(0) =& \delta_2' - \delta_2 && \text{in } \Omega,\\ \delta v_t =& \Delta\delta v - \delta v + \delta u + \gamma^*\delta g + \delta_3' - \delta_3 && \text{in } \Omega\times(0,T),\\ \delta v(0) =& \delta_4' - \delta_4 && \text{in } \Omega, \end{aligned}$$

adjoint system

$$\begin{aligned} -\delta p_t =& \Delta\delta p + f'(\bar u)\nabla\bar v\nabla\delta p + \delta q + f'(\bar u)\nabla\delta v\nabla\bar p\\ &+ f''(\bar u)\delta u\nabla\bar v\nabla\bar p + \alpha_2\delta u + \delta_6' - \delta_6 && \text{in } \Omega\times(0,T),\\ \delta p(T) =& \alpha_1\delta u(T) + \delta_7' - \delta_7 && \text{in } \Omega,\\ -\delta q_t =& \Delta\delta q - \delta q - \nabla\cdot\{f(\bar u)\nabla\delta p + f'(\bar u)\delta u\nabla\bar p\} + \delta_8' - \delta_8 && \text{in } \Omega\times(0,T),\\ \delta q(T) =& \delta_9' - \delta_9 && \text{in } \Omega \end{aligned}$$

and complementarity system

$$\begin{aligned} \lambda\delta g + \tau\delta q - \delta\mu_a + \delta\mu_b + \delta_5' - \delta_5 &= 0\\ \mu_a^{\delta'} \geq 0, \quad \mu_a^{\delta}\geq 0, \quad g_a + \delta_{10}' - g^{\delta'} \leq 0, \quad g_a + \delta_{10} - g^{\delta} &\leq 0\\ \mu_b^{\delta'} \geq 0, \quad \mu_b^{\delta}\geq 0, \quad g^{\delta'} - g_b - \delta_{11}' \leq 0, \quad g^{\delta} - g_b - \delta_{11} &\leq 0\\ \delta\mu_a(g_a + \delta_{10} - g) + \mu_a^{\delta'}(\delta_{10} - \delta_{10}' - \delta g) &= 0\\ \delta\mu_b(g - g_b - \delta_{11}) + \mu_b^{\delta'}(\delta g - (\delta_{11}' - \delta_{11})) &= 0 \end{aligned}$$

in Σ. The proof will have two main ingredients: In a first step, it is a simple consequence of Theorem 3.4, Theorem 3.6 and Lemma B.1 that the solutions to the state system $(\delta u, \delta v)$, the adjoint system $(\delta p, \delta q)$ and the multipliers $(\delta\mu_a, \delta\mu_b)$ can be bounded by the L_2-norm of δg and the perturbations that occur in these equations,

$$\|\delta y\|_{\mathcal{Y}_{\alpha,\beta}} \leq c(\bar g)\|\delta g\|_{L_2(\Sigma)} + c\|\delta' - \delta\|_{Z_{\alpha,\beta}}. \tag{8.8}$$

As a second step, "testing" the state system with the adjoint state and vice versa allows us to show

$$\mathcal{L}''(\bar y)(\delta u, \delta v, \delta g)^2 \leq \varepsilon\|\delta y\|^2_{\mathcal{Y}_{\alpha,\beta}} + c(\varepsilon)\|\delta' - \delta\|^2_{Z_{\alpha,\beta}} \tag{8.9}$$

for $\varepsilon > 0$. This, together with Corollary 7.6, can then be put together to

$$\|\delta y\|^2_{\mathcal{Y}_{\alpha,\beta}} \le c\left(\|\delta g\|^2_{L_2(\Sigma)} + \|\delta' - \delta\|^2_{Z_{\alpha,\beta}}\right) \le \varepsilon\|\delta y\|^2_{\mathcal{Y}_{\alpha,\beta}} + c(\varepsilon)\|\delta' - \delta\|^2_{Z_{\alpha,\beta}}.$$

So let us start by showing that (8.8) holds. Since α and β are chosen according to (8.6), it immediately follows from Theorem 3.4 that

$$\begin{aligned}\|\delta u\|_{\mathbb{W}_{\alpha,\beta}} + \|\delta v\|_{\mathbb{W}_{2,\beta}} + \|\delta v\|_{L_\alpha(W^1_\beta)} \le & c\,\big(\|\delta g\|_{L_2(\Sigma)} \\ & + \|\delta_1' - \delta_1\|_{L_\alpha(W^{-1}_\beta)} + \|\delta_2' - \delta_2\|_{\mathcal{D}_{\alpha,\beta}} \\ & + \|\delta_3' - \delta_3\|_{L_\alpha(W^{-1}_\beta)} + \|\delta_4' - \delta_4\|_{\mathcal{D}_{\alpha,\beta}}\Big).\end{aligned}$$

For the adjoint system, we can apply Theorem 3.6 with

$$\begin{aligned}\xi_1 =& \alpha_1\delta u(T) + \delta_7' - \delta_7,\\ \xi_2 =& \delta_9' - \delta_9,\\ \eta_1 =& f'(\bar u)\nabla\delta v\nabla\bar p + f''(\bar u)\delta u\nabla\bar v\nabla\bar p + \alpha_2\delta u + \delta_6' - \delta_6,\\ \eta_2 =& -\nabla\cdot\{f'(\bar u)\delta u\nabla\bar p\} + \delta_8' - \delta_8.\end{aligned}$$

ξ_1 and ξ_2 obviously fit into the setting, and η_1 and η_2 are sufficiently regular as well: For $\rho > 1$ such that $\frac{1}{\rho} = \frac{1}{\alpha} + \frac{2}{p}$, due to $p > 2N$ the embedding $L_\rho \hookrightarrow W^{-1}_p$ holds, so that due to $\frac{1}{\tilde\alpha} = \frac{1}{\alpha} + \frac{1}{r}$, the Hölder inequality (A.2) gives

$$\begin{aligned}\|\eta_1\|_{L_{\tilde\alpha}(W^{-1}_\beta)} \le & c\left(c_{f'}\|\delta v\|_{L_\alpha(W^1_\beta)}\|\bar p\|_{L_r(W^1_p)} + c_{f''}\|\delta u\|_{L_\alpha(L_\beta)}\|\bar v\|_{L_\infty(W^1_p)}\|\bar p\|_{L_r(W^1_p)}\right.\\ & \left. + \alpha_2\|\delta u\|_{L_\alpha(L_\beta)} + \|\delta_6' - \delta_6\|_{L_\alpha(W^{-1}_\beta)}\right)\\ \le & c(\bar g)\left(\|\delta u\|_{\mathbb{W}_{\alpha,\beta}} + \|\delta v\|_{L_\alpha(W^1_\beta)}\right) + c\|\delta_6' - \delta_6\|_{L_\alpha(W^{-1}_\beta)},\\ \|\eta_2\|_{L_{\tilde\alpha}(W^{-1}_\beta)} \le & c\|f'(\bar u)\delta u\nabla\bar p\|_{L_\alpha(L_\beta)} + c\|\delta_8' - \delta_8\|_{L_\alpha(W^{-1}_\beta)}\\ \le & cc_{f'}\|\delta u\|_{L_\alpha(W^1_\beta)}\|\bar p\|_{L_r(W^1_p)} + c\|\delta_8' - \delta_8\|_{L_\alpha(W^{-1}_\beta)}\\ \le & c(\bar g)\|\delta u\|_{\mathbb{W}_{\alpha,\beta}} + c\|\delta_8' - \delta_8\|_{L_\alpha(W^{-1}_\beta)}.\end{aligned}$$

This implies

$$\begin{aligned}\|\delta p\|_{\mathbb{W}_{\tilde\alpha,\beta}} + \|\delta q\|_{\mathbb{W}_{\tilde\alpha,\beta}} \le & c(\bar g)\left(\|\delta u\|_{\mathbb{W}_{\alpha,\beta}} + \|\delta v\|_{L_\alpha(W^1_\beta)}\right) + c\left(\|\delta_6' - \delta_6\|_{L_\alpha(W^{-1}_\beta)}\right.\\ & \left. + \|\delta_7' - \delta_7\|_{\mathcal{D}_{\alpha,\beta}} + \|\delta_8' - \delta_8\|_{L_\alpha(W^{-1}_\beta)} + \|\delta_9' - \delta_9\|_{\mathcal{D}_{\alpha,\beta}}\right),\end{aligned}$$

so that together with

$$\|\delta\mu_a\|_{L_2(\Sigma)} + \|\delta\mu_b\|_{L_2(\Sigma)} \le c\left(\|\delta g\|_{L_2(\Sigma)} + \|\delta q\|_{L_\alpha(W^1_\beta)} + \|\delta_5' - \delta_5\|_{L_2(\Sigma)}\right),$$

due to Lemma B.1 we have shown that (8.8) holds. So let us turn to (8.9). Since $\delta u, \delta v, \delta p, \delta q \in \mathbb{W}_{2,2}$, we can use $(\delta p, \delta q)$ as test functions for $(\delta u, \delta v)$ and vice versa, and multiply the gradient equation with δg:

$$\int_0^T \langle \delta u_t, \delta p\rangle_{H^{-1},H^1} + \langle \nabla \delta u, \nabla \delta p\rangle_\Omega \; dt = \int_0^T \langle f'(\bar u)\delta u \nabla \bar v + f(\bar u)\nabla \delta v, \nabla \delta p\rangle_\Omega + \langle \delta_1' - \delta_1, \delta p\rangle_\Omega \; dt, \tag{8.10}$$

$$\int_0^T \langle \delta v_t, \delta q\rangle_{H^{-1},H^1} + \langle \nabla \delta v, \nabla \delta q\rangle_\Omega + \langle \delta v, \delta q\rangle_\Omega \; dt = \int_0^T \langle \delta u, \delta q\rangle_\Omega + \langle \delta g, \gamma \delta q\rangle_\Gamma + \langle \delta_3' - \delta_3, \delta q\rangle_\Omega \; dt, \tag{8.11}$$

$$\begin{aligned}\int_0^T - \langle \delta p_t, \delta u\rangle_{H^{-1},H^1} + \langle \nabla \delta p, \delta u\rangle_\Omega \; dt &= \int_0^T \langle f'(\bar u)\nabla \bar v \nabla \delta p + \delta q + f''(\bar u)\delta u \nabla \bar v \nabla \bar p + f'(\bar u)\nabla \delta v \nabla \bar p, \delta u\rangle_\Omega \\ &\quad + \alpha_2 \langle \delta u, \delta u\rangle_\Omega + \langle \delta_6' - \delta_6, \delta u\rangle_\Omega \; dt,\end{aligned} \tag{8.12}$$

$$\int_0^T - \langle \delta q_t, \delta v\rangle_{H^{-1},H^1} + \langle \nabla \delta q, \delta v\rangle_\Omega + \langle \delta q, \delta v\rangle_\Omega \; dt = \int_0^T \langle f'(\bar u)\delta \nabla \bar p + f(\bar u)\nabla \delta p, \nabla \delta v\rangle_\Omega + \langle \delta_8' - \delta_8, \delta v\rangle_\Omega \; dt, \tag{8.13}$$

$$\lambda \|\delta g\|^2_{L_2(\Sigma)} + \langle \gamma \delta q, \delta g\rangle_\Sigma + \langle -\delta\mu_a + \delta\mu_b + \delta_5' - \delta_5, \delta g\rangle_\Sigma = 0. \tag{8.14}$$

We add up equations (8.10) and (8.12) as well as equations (8.11) and (8.13):

$$\begin{aligned}\int_0^T \langle \delta u_t, \delta p\rangle_{W_p^{-1},W_{p'}^1} + \langle \delta p_t, \delta u\rangle_{W_p^{-1},W_{p'}^1} \; dt &= \int_0^T \langle f(\bar u)\nabla \delta v, \nabla \delta p\rangle_\Omega - \langle f''(\bar u)\delta u \nabla \bar v \nabla \bar p + f'(\bar u)\nabla \delta v \nabla \bar p, \delta u\rangle_\Omega \\ &\quad - \langle \delta q, \delta u\rangle_\Omega - \alpha_2 \|\delta u\|^2_{L_2(\Omega)} + \langle \delta_1' - \delta_1, \delta p\rangle_\Omega - \langle \delta_6' - \delta_6, \delta u\rangle_\Omega \; dt,\end{aligned}$$

$$\int_0^T \langle \delta v_t, \delta q \rangle_{W_p^{-1}, W_{p'}^1} + \langle \delta q_t, \delta v \rangle_{W_p^{-1}, W_{p'}^1} \; dt$$
$$= \int_0^T \langle \delta u, \delta q \rangle_\Omega - \langle f'(\bar{u})\delta u \nabla \bar{p} + f(\bar{u}) \nabla \delta p, \nabla \delta v \rangle_\Omega$$
$$+ \langle \delta g, \gamma \delta q \rangle_\Gamma + \langle \delta_3' - \delta_3, \delta q \rangle_\Omega - \langle \delta_8' - \delta_8, \delta v \rangle_\Omega \; dt.$$

Adding these two and subtracting equation (8.14) from above yields

$$\int_0^T \langle \delta u_t, \delta p \rangle + \langle \delta p_t, \delta u \rangle + \langle \delta v_t, \delta q \rangle + \langle \delta q_t, \delta v \rangle \; dt$$
$$= - \langle f''(\bar{u})\delta u \nabla \bar{v} \nabla \bar{p} + 2 f'(\bar{u}) \nabla \delta v \nabla \bar{p}, \delta u \rangle_Q - \alpha_2 \|\delta u\|^2_{L_2(Q)} - \lambda \|\delta g\|^2_{L_2(\Sigma)}$$
$$+ \langle \delta_1' - \delta_1, \delta p \rangle_Q + \langle \delta_3' - \delta_3, \delta q \rangle - \langle \delta_5' - \delta_5, \delta g \rangle_Q - \langle \delta_6' - \delta_6, \delta u \rangle_Q$$
$$- \langle \delta_8' - \delta_8, \delta v \rangle_Q - \langle -\delta\mu_a + \delta\mu_b, \delta g \rangle_\Sigma .$$

We now stop to take a closer look at the left hand side. With the help of the integration by parts formula, Lemma 2.2, we get

$$\int_0^T \langle \delta u_t, \delta p \rangle + \langle \delta p_t, \delta u \rangle + \langle \delta v_t, \delta q \rangle + \langle \delta q_t, \delta v \rangle \; dt$$
$$= \langle \delta u(T), \delta p(T) \rangle_\Omega - \langle \delta u(0), \delta p(0) \rangle_\Omega + \langle \delta v(T), \delta q(T) \rangle_\Omega - \langle \delta v(0), \delta q(0) \rangle_\Omega$$
$$= \alpha_1 \|\delta u(T)\|^2_{L_2(\Omega)} + \langle \delta_7' - \delta_7, \delta u(T) \rangle_\Omega - \langle \delta_2' - \delta_2, \delta p(0) \rangle_\Omega$$
$$+ \langle \delta_9' - \delta_9, \delta v(T) \rangle_\Omega - \langle \delta_4' - \delta_4, \delta q(0) \rangle_\Omega .$$

Putting this together and rearranging a bit yields

$$\begin{aligned}
\alpha_1 \|\delta u(T)\|^2_{L_2(\Omega)} + \alpha_2 \|\delta u\|^2_{L_2(Q)} + \lambda \|\delta g\|^2_{L_2(\Sigma)} \\
+ \langle f''(\bar{u})\delta u \nabla \bar{v} \nabla \bar{p} + 2 f'(\bar{u}) \nabla \delta v \nabla \bar{p}, \delta u \rangle_Q \\
= \langle \delta_1' - \delta_1, \delta p \rangle_Q + \langle \delta_2' - \delta_2, \delta p(0) \rangle_\Omega \\
+ \langle \delta_3' - \delta_3, \delta q \rangle_Q + \langle \delta_4' - \delta_4, \delta q(0) \rangle_\Omega \\
- \langle \delta_5' - \delta_5, \delta g \rangle_\Sigma - \langle \delta_6' - \delta_6, \delta u \rangle_Q \\
- \langle \delta_7' - \delta_7, \delta u(T) \rangle_\Omega - \langle \delta_8' - \delta_8, \delta v \rangle_Q \\
- \langle \delta_9' - \delta_9, \delta v(T) \rangle_\Omega - \langle -\delta\mu_a + \delta\mu_b, \delta g \rangle_\Sigma .
\end{aligned} \tag{8.15}$$

The left hand side happens to be exactly $\mathcal{L}''(\bar{y})(\delta u, \delta v, \delta g)^2$. On the right hand side, every term except for the last can be split up with Cauchy's and Young's inequalities (A.1), (A.3) in the fashion of

$$|\langle \phi, \psi \rangle_{V^*,V}| \leq \|\phi\|_{V^*}\|\psi\|_V \leq c(\varepsilon)\|\phi\|_{V^*}^2 + \varepsilon\|\psi\|_V^2$$

for $\varepsilon > 0$. For $\delta u, \delta p, \delta q$ we end up with the $\mathbb{W}_{\alpha,\beta}$-norms like

$$\begin{aligned}\langle \delta_6' - \delta_6, \delta u\rangle_Q + \langle \delta_7' - \delta_7, \delta u(T)\rangle_\Omega \leq & c(\varepsilon)\|\delta_6' - \delta_6\|_{L_\alpha(W_\beta^{-1})}^2 + \varepsilon\|\delta u\|_{L_\alpha(W_\beta^1)}^2 \\ & + c(\varepsilon)\|\delta_7' - \delta_7\|_{L_\beta}^2 + \varepsilon\|\delta u(T)\|_{L_\beta}^2 \\ \leq & c(\varepsilon)\left(\|\delta_6' - \delta_6\|_{L_\alpha(W_\beta^{-1})}^2 + \|\delta_7' - \delta_7\|_{\mathcal{D}_{\alpha,\beta}}^2\right) \\ & + \varepsilon\|\delta u\|_{\mathbb{W}_{\alpha,\beta}}^2,\end{aligned}$$

in the case of δv we get the same in $\mathbb{W}_{2,\beta}$. Due to Lemma B.1, the last term satisfies

$$\begin{aligned}|\langle -\delta\mu_a + \delta\mu_b, \delta g\rangle_\Sigma| \leq & c(\varepsilon)\left(\|\delta_{10}' - \delta_{10}\|_{L_2(\Sigma)}^2 + \|\delta_{11}' - \delta_{11}\|_{L_2(\Sigma)}^2\right) \\ & + \varepsilon\left(\|\delta\mu_a\|_{L_2(\Sigma)}^2 + \|\delta\mu_b\|_{L_2(\Sigma)}^2\right).\end{aligned}$$

Together with the obvious estimate

$$\langle \delta_5' - \delta_5, \delta g\rangle_\Sigma \leq c(\varepsilon)\|\delta_5' - \delta_5\|_{L_2(\Sigma)}^2 + \varepsilon\|\delta g\|_{L_2(\Sigma)}^2,$$

it follows from (8.15) that (8.9) holds. We are almost done now: (8.8) together with (8.9) yields

$$\begin{aligned}\|\delta y\|_{\mathcal{Y}_{\alpha,\beta}}^2 \leq c\|\delta g\|_{L_2(\Sigma)}^2 + c\|\delta' - \delta\|_{\mathcal{Z}_{\alpha,\beta}}^2 \leq & \frac{c}{\kappa}\mathcal{L}''(\bar{y})(\delta u, \delta v, \delta g)^2 + c\|\delta' - \delta\|_{Z_{\alpha,\beta}}^2 \\ \leq & c(\varepsilon)\|\delta y\|_{\mathcal{Y}_{\alpha,\beta}}^2 + c(\varepsilon)|\delta' - \delta\|_{Z_{\alpha,\beta}}^2,\end{aligned}$$

so that for $\varepsilon > 0$ sufficiently small the assertion follows. □

This result can now gradually be improved with respect to the order of integrability to end up in the desired spaces $Y_{r,p}$ and $Z_{r,p}$:

Theorem 8.10. *Assume $\bar{y} \in Y_{r,p}$ satisfies* (SSC). *Let $\delta', \delta \in Z_{r,p}$ and let $y^{\delta'} = y(\delta'), y^\delta = y(\delta) \in Y_{r,p}$ be the corresponding solutions to $(GE(\delta))$. There is an $L > 0$ such that*

$$\|y^{\delta'} - y^\delta\|_{Y_{r,p}} \leq c\|\delta' - \delta\|_{Z_{r,p}}. \tag{8.16}$$

Proof. Let $\delta y := y^{\delta'} - y^{\delta}$ as in the previous lemma. We need to combine three arguments to prove this result: Firstly, in the same way as (8.8), from Theorems 3.4 and 3.6 and Lemma B.1 it follows that

$$\|\delta y\|_{\mathcal{Y}_{\alpha,\beta}} \leq c\|\delta g\|_{L_\nu(L_\sigma(\Gamma))} + c\|\delta' - \delta\|_{Z_{\alpha,\beta}} \tag{8.17}$$

for $\nu, \sigma \geq 2$ and $\frac{2}{\alpha} + \frac{N}{\beta} > \frac{2}{\nu} + \frac{N-1}{\sigma}$. Secondly, Lemma 8.9 implies that

$$\|\delta g\|_{L_2(\Sigma)} \leq c\|\delta' - \delta\|_{Z_{\alpha,\beta}} \tag{8.18}$$

for $\frac{2}{\alpha} + \frac{N}{\beta} > \frac{1}{2}(N+1)$. Thirdly, we have

$$\|\delta g\|_{L_\alpha(L_\beta(\Gamma))} \leq c\|\delta q\|_{L_\alpha(W^1_\beta)} + c\|\delta'_5 - \delta_5\|_{L_\alpha(L_\beta(\Gamma))} \tag{8.19}$$

for $\alpha, \beta \geq 2$. The third estimate comes as a simple observation from the projection formula for the optimal control: the optimal solution g^δ to $(QP(\delta))$ satisfies

$$g^\delta(x,t) = \mathbb{P}_{[g_a,g_b]}\left(-\frac{1}{\lambda}\gamma q^\delta + \delta_5\right)(x,t) \qquad \text{f.a.a } (x,t) \in \Sigma.$$

The projection operator $\mathbb{P}$ is Lipschitz continuous with Lipschitz constant 1, so that for almost every $(x,t) \in \Sigma$ we have

$$|\delta g(x,t)| \leq |(\frac{1}{\lambda}\gamma\delta q + \delta'_5 - \delta_5)(x,t)|$$

and hence

$$\begin{aligned}\|\delta g\|_{L_\alpha(L_\beta(\Gamma))} \leq& \frac{1}{\lambda}\|\gamma\delta q\|_{L_\alpha(L_\beta(\Gamma))} + \|\delta'_5 - \delta_5\|_{L_\alpha(L_\beta(\Gamma))}\\ \leq& c\|\delta q\|_{L_\alpha(W^1_\beta)} + \|\delta'_5 - \delta_5\|_{L_\alpha(L_\beta(\Gamma))}.\end{aligned}$$

Now we can turn to proving the actual result: From (8.17) and (8.18), it follows that

$$\begin{aligned}\|\delta y\|_{\mathcal{Y}_{\alpha,\beta}} \leq& c\|\delta g\|_{L_2(\Sigma)} + c\|\delta' - \delta\|_{Z_{\alpha,\beta}}\\ \leq& c\|\delta' - \delta\|_{Z_{\alpha,\beta}} + c\|\delta' - \delta\|_{Z_{\alpha,\beta}} \leq c\|\delta' - \delta\|_{Z_{\alpha,\beta}}\end{aligned}$$

for $\alpha, \beta > 2$ such that $\frac{2}{\alpha} + \frac{N}{\beta} > \frac{N+1}{2}$. This can be considered as something like an induction basis for the following proof, that is to say that based on this, together with (8.17) and (8.19) we can gradually increase the integration indices α, β in the "induction step": For $\alpha' > \alpha$ and $\beta' > \beta$ such that

$$\frac{2}{\alpha'} + \frac{N}{\beta'} > \frac{2}{\alpha} + \frac{N-1}{\beta} \qquad \text{and} \qquad \frac{1}{\alpha} = \frac{1}{\alpha'} + \frac{1}{r}$$

(due to the non-symmetric definition of $\mathcal{Y}_{\alpha,\beta}$) we have

$$\begin{aligned} \|(\delta u, \delta v, \delta p, \delta q)\|_{\mathcal{Y}_{\alpha',\beta'}} \leq & c\|\delta g\|_{L_\alpha(L_\beta(\Gamma))} + c\|\delta' - \delta\|_{Z_{\alpha',\beta'}} \\ \leq & c\|\delta q\|_{L_\alpha(W^1_\beta)} + c\|\delta'_5 - \delta_5\|_{L_\alpha(L_\beta(\Gamma))} + c\|\delta' - \delta\|_{Z_{\alpha',\beta'}} \\ \leq & c\|\delta y\|_{\mathcal{Y}_{\alpha,\beta}} + c\|\delta'_5 - \delta_5\|_{L_\alpha(L_\beta(\Gamma))} + c\|\delta' - \delta\|_{Z_{\alpha',\beta'}} \\ \leq & c\|\delta' - \delta\|_{Z_{\alpha,\beta}} + c\|\delta' - \delta\|_{Z_{\alpha',\beta'}} \\ \leq & c\|\delta' - \delta\|_{Z_{\alpha',\beta'}}. \end{aligned}$$

We can iterate this argument until $\alpha' = r$, $\beta' = p$, so in particular we have

$$\|\delta q\|_{\mathbb{W}_{r,p}} \leq c\|\delta' - \delta\|_{Z_{r,p}}. \tag{8.20}$$

At this stage, we can improve the estimate and show that it actually holds for $Y_{r,p}$ instead of $\mathcal{Y}_{r,p}$. Lemma 3.4, Lemma 3.6 and Lemma B.1 give

$$\|\delta y\|_{Y_{r,p}} \leq c\|\delta g\|_{L_r(L_p(\Gamma))} + c\|\delta' - \delta\|_{Z_{r,p}}, \tag{8.21}$$

and putting together (8.19) and (8.20),

$$\begin{aligned} \|\delta g\|_{L_r(L_p(\Gamma))} \leq & c\|\delta q\|_{L_r(W^1_p))} + \|\delta'_5 - \delta_5\|_{L_r(L_p(\Gamma)} \\ \leq & c\|\delta' - \delta\|_{Z_{r,p}}. \end{aligned} \tag{8.22}$$

Now (8.16) immediately follows from (8.21) and (8.22). □

8.4 Convergence result

Finally, we can put together the considerations of the previous sections to prove the central result of this chapter:

Theorem 8.11. *Assume $\bar{y} \in Y_{r.p}$ satisfies* (SSC) *(so in particular it is a solution to* (FON)*). There are a radius $\rho > 0$ and a constant $c_{SQP} > 0$ such that for every $y^0 \in Y_{r,p}$, $\|y^0 - \bar{y}\|_{Y_{r,p}} \leq \rho$, the sequence $\{y^k\}_{k\in\mathbb{N}}$ defined by (GEL_k) is well defined in $Y_{r,p}$ and that $\|y^k - \bar{y}\|_{Y_{r,p}} < \rho$ for every $k \in \mathbb{N}$. It satisfies $y^k \to \bar{y}$, $k \to \infty$ and*

$$\|y^{k+1} - \bar{y}\|_{Y_{r,p}} \leq C_{SQP}\|y^k - \bar{y}\|^2_{Y_{r,p}}. \tag{8.23}$$

Proof. Choose $\rho > 0$ sufficiently small (we will fix during the proof what that means) and assume that $y^k \in Y_{r,p}$ and $\|y^k - \bar{y}\|_{Y_{r,p}} < \rho$ for some $k \in \mathbb{N}$. Assuming that ρ is chosen according to Lemma 8.5, this Lemma guarantees the new iterate $y^{k+1} \in Y_{r,p}$ is well defined and given as the solution of

$$0 \in F(y^k) + F'(y^k)(y^{k+1} - y^k) + N(y^{k+1}). \tag{8.24}$$

First, we will show that

$$\|y^{k+1} - \bar{y}\|_{Y_{r,p}} \leq \rho. \tag{8.25}$$

To do this, note that (8.24) can be rewritten as

$$\begin{aligned}
\delta_{k+1} \in& F(\bar{y}) + F'(\bar{y})(y^{k+1} - \bar{y}) + N(y^{k+1}), \\
\delta_{k+1} :=& F(\bar{y}) - F(y^k) + F'(\bar{y})(y^{k+1} - \bar{y}) - F'(y^k)(y^{k+1} - y^k).
\end{aligned}$$

The idea of this proof is the following: The results from section 8.1 give us upper bounds for $\|\delta^{k+1}\|_{Z_{r,p}}$, Theorem 8.10 delivers a lower bound. Since y^{k+1} only depends on the initial data and y^k and hence on ρ, from Corollary 8.4 we get

$$\begin{aligned}
\|\delta_{k+1}\|_{Z_{r,p}} =& \|F(\bar{y}) - F(y^k) + F'(\bar{y})(y^{k+1} - \bar{y}) - F'(y^k)(y^{k+1} - y^k)\|_{Z_{r,p}} \\
\leq& c\|y^k - \bar{y}\|_{Y_{r,p}} \\
\leq& c\rho,
\end{aligned} \tag{8.26}$$

and

$$\begin{aligned}
\|\delta_{k+1}\|_{Z_{r,p}} =& \|F(\bar{y}) - F(y^k) + F'(\bar{y})(y^{k+1} - \bar{y}) - F'(y^k)(y^{k+1} - y^k)\|_{Z_{r,p}} \\
\leq& \|F(\bar{y}) - F(y^k) - F'(y^k)(\bar{y} - y^k)\|_{Z_{r,p}} \\
&+ \|(F'(\bar{y}) - F'(y^k))(y^{k+1} - \bar{y})\|_{Z_{r,p}} \\
\leq& c_1\|y^k - \bar{y}\|^2_{Y_{r,p}} + c_2\|y^k - \bar{y}\|_{Y_{r,p}}\|y^{k+1} - \bar{y}\|_{Y_{r,p}}.
\end{aligned} \tag{8.27}$$

The lower bound from Theorem 8.10 reads

$$\|y^{k+1} - \bar{y}\|_{Y_{r,p}} \leq L\|\delta_{k+1}\|_{Z_{r,p}}. \tag{8.28}$$

This can be put together to

$$\begin{aligned}\|y^{k+1}-\bar{y}\|_{Y_{r,p}} \leq & L\|\delta_{k+1}\|_{Z_{r,p}}\\ \leq & L(c_1\|y^k-\bar{y}\|^2_{Y_{r,p}}+c_2\|y^k-\bar{y}\|_{Y_{r,p}}\|y^{k+1}-\bar{y}\|_{Y_{r,p}})\\ \leq & L(c_1\rho+c_2\|y^{k+1}-\bar{y}\|_{Y_{r,p}})\rho\\ \leq & L(c_1\rho+c_2L\|\delta_{k+1}\|_{Z_{r,p}})\rho\\ \leq & L(c_1+c_2Lc)\rho^2,\end{aligned}$$

so that if ρ is chosen such that

$$L(c_1+c_2Lc)\rho<1,$$

(8.25) is established, and by induction we have $\|y^k-\bar{y}\|_{Y_{r,p}} \leq \rho$ for all $k \in \mathbb{N}$. Now (8.23) is simple: Once again using (8.27) and (8.28) and making sure that $Lc_2\rho < 1$, we have

$$\begin{aligned}\|y^{k+1}-\bar{y}\|_{Y_{r,p}} \leq & L(c_1\|y^k-\bar{y}\|^2_{Y_{r,p}}+c_2\|y^k-\bar{y}\|_{Y_{r,p}}\|y^{k+1}-\bar{y}\|_{Y_{r,p}})\\ \leq & L(c_1\|y^k-\bar{y}\|^2_{Y_{r,p}}+c_2\rho\|y^{k+1}-\bar{y}\|_{Y_{r,p}})\\ \leq & c_{SQP}\|y^k-\bar{y}\|^2_{Y_{r,p}},\end{aligned}$$

where $c_{SQP}=\frac{Lc_1}{1-Lc_2\rho}$ and hence (8.23). □

Chapter 9

Numerical example

In the final chapter, we want to illustrate what we derived analytically and present a numerical example. For convenience, we are going to restrict ourselves to one dimension in space and modify the state system and the objective a bit. This does not change the structure of the problem, however it simplifies finding an analytical solution significantly. We fix the sensitivity function to $f(u) := u(1-u)$, that is we include volume filling effects into the model. On the interval $\Omega := [0, \pi]$ and for $T := 1$, we fix the following coefficients: We choose $\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = \lambda = 1$ and set

$$
\begin{aligned}
u_0(x) =& \sin^2 x, \qquad v_0(x) = \sin x, \\
e_u(x,t) =& e^t(5\sin^2 x - 2) + e^{2t}\sin x(3\cos^2 x - 1) + e^{3t}\sin^3 x(5\sin^2 x - 4), \\
e_v(x,t) =& e^t \sin x(3 - \sin x), \\
u_\Omega(x) =& e(\sin^2 x - \cos x), \qquad v_\Omega(x) = e(\sin x - \cos x), \\
u_Q(x,t) =& e^t(\sin^2 x + \cos x) - e^{2t}\sin x\cos x + 2e^{3t}\sin^3 x\cos x, \\
v_Q(x,t) =& e^t(\sin x - \cos x) + 3e^{2t}\sin^2 x\cos x - 5e^{3t}\sin^4 x\cos x \\
g_\Sigma(0,t) =& 0, \qquad g_\Sigma(\pi,t) = -2e^t.
\end{aligned}
$$

for $x \in (0,\pi)$ and $t \in [0,1]$. It is easily checked that again for $x \in (0,\pi)$ and $t \in [0,1]$,

$$
\begin{aligned}
g(0,t) =& -e^t, \qquad u(x,t) = e^t\sin^2 x, \qquad p(x,t) = e^t\cos x, \\
g(\pi,t) =& -e^t, \qquad v(x,t) = e^t\sin x, \qquad q(x,t) = e^t\cos x
\end{aligned}
$$

provide the optimal control, state and adjoint state to the problem

$$
\begin{aligned}
\min & \frac{1}{2}\|u(T)-u_\Omega\|^2_{L_2(\Omega)} + \frac{1}{2}\|u-u_Q\|^2_{L_2(Q)} + \frac{1}{2}\|v(T)-v_Q\|^2_{L_2(\Omega)} \\
& + \frac{1}{2}\|v-v_Q\|^2_{L_2(Q)} + \frac{1}{2}\|g-g_\Sigma\|^2_{L_2(\Sigma)}, \\
u_t &= u_{xx} - (f(u)v_x)_x + e_u \quad \text{in } \Omega\times(0,T), \quad u(0)=u_0 \text{ in } \Omega, \\
v_t &= v_{xx} - v + u + e_v + \gamma^* g \quad \text{in } \Omega\times(0,T), \quad v(0)=v_0 \text{ in } \Omega, \\
g &\in G_{ad} := \{g \in L_r(0,T;L_p(\Gamma)) : g_a \le g \le g_b \text{ a.e. in } \Gamma\times(0,T)\}.
\end{aligned}
\tag{9.1}
$$

Assuming that an iterate $(u^k, v^k, g^k, p^k, q^k)$ has been computed, in each step of the SQP algorithm we solve the linear-quadratic subproblem (QP_k) introduced in the last chapter, in this case

$$
\begin{aligned}
\min\ & \left\langle u^k(T)-u_\Omega, u(T)-u^k(T)\right\rangle_\Omega + \left\langle u^k-u_Q, u-u^k\right\rangle_Q \\
& + \left\langle g^k-g_\Sigma, g-g^k\right\rangle_\Sigma \\
& + \frac{1}{2}\left(\|u(T)-u^k(T)\|^2_{L_2(\Omega)} + \|u-u^k\|^2_{L_2(Q)} + \|g-g^k\|^2_{L_2(\Sigma)}\right) \\
& + \frac{1}{2}\left\langle p^k_x, f''(u^k)(u-u^k)^2 v^k_x + 2f'(u^k)(u-u^k)(v_x-v^k_x)\right\rangle_Q ,
\end{aligned}
\tag{9.2}
$$

$$
\begin{aligned}
u_t &= \Delta u - \left(f'(u^k)(u-u^k)v^k_x + f(u^k)v\right)_x + e_u \text{ in } Q, \quad u(0)=u_0 \text{ in } \Omega, \\
v_t &= \Delta v - v + u + e_v + \gamma^* g \quad \text{in } Q, \quad v(0)=v_0 \text{ in } \Omega,
\end{aligned}
\tag{9.3}
$$

$$
g_a \le g \le g_b. \tag{9.4}
$$

The simplest form of the algorithm looks as follows:

Algorithm 9.1 (SQP Algorithm)**.**

(1) Fix $(u^0, v^0, g^0, p^0, q^0)$*, set* $k = 0$*;*

(2) If $(u^k, v^k, g^k, p^k, q^k)$ *is a KKT point of* (9.1)*: STOP;*

(3) Solve (9.2)-(9.4) *to obtain* $(u^{k+1}, v^{k+1}, g^{k+1}, p^{k+1}, q^{k+1})$*;*

(4) Set $k = k + 1$*, go to (2).*

Note that in general this is a local method, that is we cannot expect global convergence. There are several ways to globalize the algorithm however, for example by adding a line search or just by first performing a few steps of the gradient method in order to get close enough to the solution (cf. e.g. [22]).

Since this is not necessary for our example, we are not going to go into detail here.

So we are left with the question of how to solve the linear-quadratic subproblem (QP_k). Here, we have to pay particular attention to two issues: How do we discretize the problem and how do we treat the inequality constraints? Let us start with the first: In general, there are two possible strategies which do not necessarily lead to the same result. Either we first optimize, that is we write down the first order optimality system for the continuous problem and then discretize this system, or we discretize first and then look at the optimality system for the discrete problem. Due to the fact that the adjoint equation

$$\begin{aligned} -p_t =& p_{xx} + f'(u^k)v_x^k p_x + q + u - u_Q \\ &+ f''(u^k)(u-u^k)v_x^k p_x^k \qquad\qquad \text{in } Q, \quad p(T) = u(T) - u_\Omega \text{ in } \Omega, \\ &+ f'(u^k)(v_x - v_x^k)p_x^k \\ -q_t =& q_{xx} - q - \big(f(u^k)p_x\big)_x \\ &- \big(f'(u^k)(u-u^k)p_x^k\big)_x + v - v_Q \qquad \text{in } Q, \quad q(T) = v(T) - v_\Omega \text{ in } \Omega \end{aligned} \tag{9.5}$$

has to be solved backwards in time, in particular the time discretization needs to be chosen with care. A good strategy can be found in [8]: For both the state equation and the adjoint equation, the Crank-Nicolson method is applied, however, the state is evaluated at the end points of each time interval whereas the adjoint state and the control are evaluated in the center of each interval. To stay consistent, in the objective the integrals only involving the state are discretized with the help of the trapezoidal rule, for the integrals involving the control and the adjoint state the midpoint rule is chosen. In space, a second order finite difference scheme is applied.

This brings us to the next question, what do we do with the control constraints, written with the help of the projection formula,

$$g = -\mathbb{P}_{[g_a, g_b]}\left(\gamma q - g_\Sigma\right). \tag{9.6}$$

Here, the primal dual active set strategy (PDAS) has proven to be a very efficient strategy (cf. e.g. [12], [38], [59]). The general idea is the following: In every step of the iteration, a set of active constraints is determined, i.e. a set of points where the constraint is assumed to hold with equality. Hence, the control is fixed in these points and the system is solved only on the remaining inactive set. After that, the active set is modified in a suitable way. It should be noted that during the iteration, the method produces solutions which are not feasible. The first feasible one is in fact the solution. We proceed as follows:

Algorithm 9.2 (Primal Dual Active Set Algorithm)**.**

(1) Fix $(u^0, v^0, g^0, p^0, q^0)$*,* $\mu^0 := -\left(g^0 - g_\Sigma + \frac{1}{\lambda}\gamma q^0\right)$ *and set* $j = 1$*;*

(2) Determine active and inactive sets

$$\begin{aligned}\mathcal{A}_a^{j+1} :=& \{(x,t) \in \Gamma \times (0,T) : g^j(x,t) + \mu^j(x,t) < g_a(x,t)\},\\ \mathcal{A}_b^{j+1} :=& \{(x,t) \in \Gamma \times (0,T) : g^j(x,t) + \mu^j(x,t) > g_b(x,t)\},\\ \mathcal{I}^{j+1} :=& \Sigma \setminus \left(\mathcal{A}_a^{j+1} \cap \mathcal{A}_b^{j+1}\right);\end{aligned}$$

(3) If $j \geq 1$ *and* $\mathcal{A}_a^{j+1} = \mathcal{A}_a^j$*,* $\mathcal{A}_b^{j+1} = \mathcal{A}_b^j$*: STOP;*

(4) Solve the system (9.3), (9.5), (9.6)*, where the projection formula is replaced by*

$$g(x,t) = \begin{cases} g_a(x,t) & \text{on } \mathcal{A}_a^{j+1},\\ g_\Sigma(x,t) - \gamma q(x,t) & \text{on } \mathcal{I}^{j+1},\\ g_b(x,t) & \text{on } \mathcal{A}_b^{j+1},\end{cases} \tag{9.7}$$

to obtain $(u^{j+1}, v^{j+1}, g^{j+1}, p^{j+1}, q^{j+1})$*;*

(5) Set $\mu^{j+1} = -\left(g^{j+1} - g_\Sigma + \gamma q^{j+1}\right)$*,* $j = j+1$*, go to (2).*

In practice, we can use the indicator functions of the active and inactive sets to compute (9.7) and solve

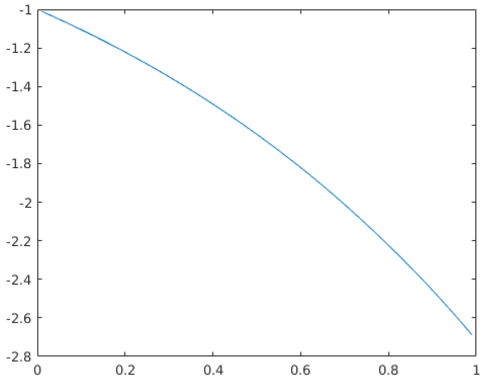
$$g^k + \chi_{\mathcal{I}^k}\left(\frac{1}{\lambda}\gamma q^k - g_\Sigma\right) = \chi_{\mathcal{A}_a^k} g_a + \chi_{\mathcal{A}_b^k} g_b \tag{9.8}$$

instead.

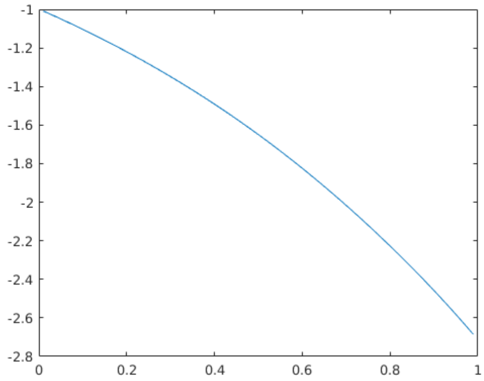
Finally, let us look at the numerical results: For a mesh with $N_x = 200$ points in space and $N_t = 400$ points in time we observed the following behaviour:

k	$\|g^k - g^5\|_{L_r(0,T)}$	$\|u^k - u^5\|_{L_r(W_p^1)}$	$\|v^k - v^5\|$	$\|y^k - y^5\|$	$\frac{\|y^k - y^5\|}{\|y^{k-1} - y^5\|^2}$
1	2.06e+0	4.31e+0	4.53e+0	4.53e+0	0
2	3.68e-1	1.60e+0	4.69e-1	1.72e+0	1.86e-2
3	2.94e-2	1.63e-1	2.65e-2	1.82e-1	3.16e-2
4	2.36e-3	1.33e-3	2.71e-3	2.47e-3	1.51e-2
5	1.27e-5	7.12e-6	1.44e-5	1.20e-5	1.34e-1

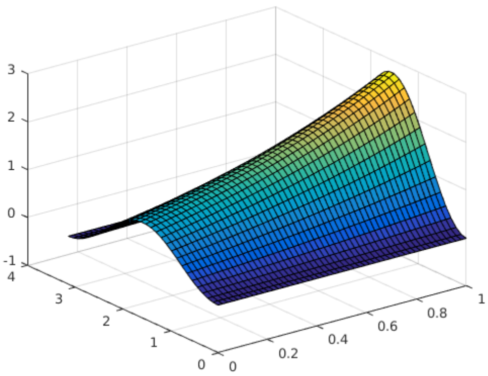
In the last step of the iteration, the convergence rate slows down since the level of the discretization error was reached already. In the last two components of the table, y includes the adjoint states p and q, both, like u and v, evaluated in the $L_r(W_p^1)$-norm ($r = 3$, $p = 7$). On the next page, the plots of the 5th iteration can be found (plotted with $N_x = 30$, $N_t = 50$).



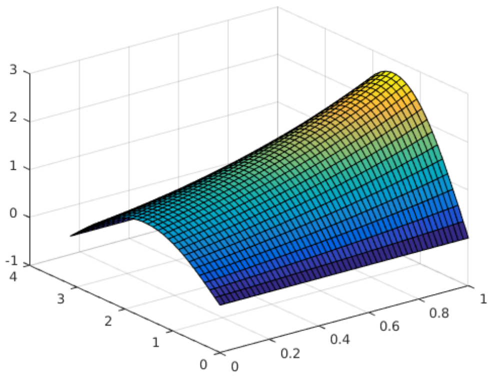
(a) Control $g(t, 0)$



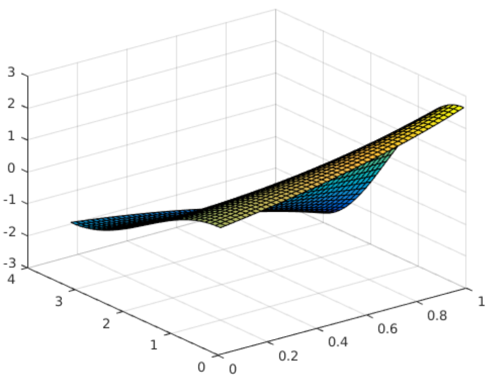
(b) Control $g(t, \pi)$



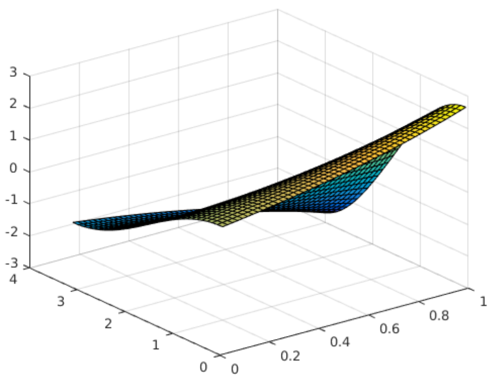
(c) State u



(d) State v



(e) Adjoint state p



(f) Adjoint state q

Appendix A

Calculus facts

Here we will collect some well known inequalities that are used frequently during this work. These can be found for example in [18] and [60].

Cauchy's inequality

For $u, v \in \mathbb{R}$ it holds that

$$uv \leq \frac{u^2}{2} + \frac{v^2}{2}. \tag{A.1}$$

(Generalized) Hölder inequality

Let $1 \leq p, q \leq \infty$ and $r \geq 1$ such that $\frac{1}{p} + \frac{1}{q} = \frac{1}{r}$. Let $u \in L_p(\Omega)$, $v \in L_q(\Omega)$. Then $uv \in L_r(\Omega)$ and

$$\|u \cdot v\|_{L_r(\Omega)} \leq \|u\|_{L_p(\Omega)} \|v\|_{L_q(\Omega)}. \tag{A.2}$$

Young's inequality

Let $u, v \in \mathbb{R}$, $1 < p, q < \infty$ such that $\frac{1}{p} + \frac{1}{q} = 1$ and $\varepsilon > 0$. Then

$$uv \leq \varepsilon u^p + c(\varepsilon) v^q, \tag{A.3}$$

where $c(\varepsilon) = \frac{1}{(p\varepsilon)^{\frac{q}{p}} q}$.

Young's inequality for convolutions

Let $1 \leq p, q \leq \infty$ and $r \geq 1$ such that $1 + \frac{1}{r} = \frac{1}{p} + \frac{1}{q}$. Let $f \in L_p(\mathbb{R})$, $g \in L_q(\mathbb{R})$ and let

$$(f * g)(t) := \int_{-\infty}^{\infty} f(s) g(t-s)\, ds, \qquad t \in \mathbb{R}$$

be the convolution of f and g. Then $f * g \in L_r(\mathbb{R})$ and

$$\|f * g\|_{L_r} \leq \|f\|_{L_p} \|g\|_{L_q}. \tag{A.4}$$

Gronwall's inequality

Assume $\phi \in C^1([0,T])$, $\psi \in L_\infty(0,T)$ are nonnegative. If

$$\phi' \leq \psi \cdot \phi \text{ on } [0,T] \text{ and } \phi(0) = 0, \text{ then } \phi \equiv 0 \text{ on } [0,T]. \tag{A.5}$$

Appendix B

Auxiliary results

In chapter 8, we will need some technical estimates for the complementarity system of the perturbed optimal control problem. In order not to break the train of thought there, we postponed this to the appendix:

Lemma B.1. *Let $r, p \geq 2$. Let $g_a, g_b \in L_r(L_p(\Gamma))$, $g_a(x,t) \leq g_b(x,t)$ for a.e. $(x,t) \in \Sigma$ and $\delta_5, \delta_5', \delta_{10}, \delta_{10}', \delta_{11}, \delta_{11}' \in L_r(L_p(\Gamma))$. Let $g^\delta, g^{\delta'} \in L_r(L_p(\Gamma))$ and $q^\delta, q^{\delta'} \in L_r(W_p^1)$, $\mu_a^\delta, \mu_a^{\delta'}, \mu_b^\delta, \mu_b^{\delta'} \in L_r(L_p(\Gamma))$ such that the following complementarity systems and gradient equations are satisfied:*

$$\begin{aligned}
\mu_a^\delta \geq& 0 \quad g_a + \delta_{10} - g^\delta \leq 0 \quad \mu_a^\delta(g_a + \delta_{10} - g^\delta) = 0 \\
\mu_b^\delta \geq& 0 \quad g^\delta - g_b - \delta_{11} \leq 0 \quad \mu_b^\delta(g^\delta - g_b - \delta_{11}) = 0 \\
&\lambda g^\delta + \gamma q^\delta + \delta_5 - \mu_a^\delta + \mu_b^\delta = 0 \\
\mu_a^{\delta'} \geq& 0 \quad g_a + {\delta'}_{10} - g^{\delta'} \leq 0 \quad \mu_a^{\delta'}(g_a + \delta_{10}' - g^{\delta'}) = 0 \\
\mu_b^{\delta'} \geq& 0 \quad g^{\delta'} - g_b - \delta_{11}' \leq 0 \quad \mu_b^{\delta'}(g^{\delta'} - g_b - \delta_{11}') = 0 \\
&\lambda g^{\delta'} + \gamma q^{\delta'} + \delta_5' - \mu_a^{\delta'} + \mu_b^{\delta'} = 0.
\end{aligned}$$

Then for $\delta g := g^{\delta'} - g^\delta$, $\delta\mu_a := \mu_a^{\delta'} - \mu_a^\delta$, $\delta\mu_b := \mu_b^{\delta'} - \mu_b^\delta$ and every $\varepsilon > 0$ there is a constant $c(\varepsilon) > 0$ such that

$$\begin{aligned}
|\langle \delta\mu_a, \delta g \rangle_\Sigma| \leq& \varepsilon \|\delta\mu_a\|_{L_2(\Sigma)}^2 + c(\varepsilon)\|\delta_{10}' - \delta_{10}\|_{L_2(\Sigma)}^2, \\
|\langle \delta\mu_b, \delta g \rangle_\Sigma| \leq& \varepsilon \|\delta\mu_b\|_{L_2(\Sigma)}^2 + c(\varepsilon)\|\delta_{11}' - \delta_{11}\|_{L_2(\Sigma)}^2,
\end{aligned}$$

and

$$\|\delta\mu_a\|_{L_r(L_p(\Gamma))} + \|\delta\mu_b\|_{L_r(L_p(\Gamma))} \leq c\Big(\|\delta g\|_{L_r(L_p(\Gamma))} + \|\delta q\|_{L_r(W_p^1)} + \|\delta_5' - \delta_5\|_{L_r(L_p(\Gamma))}\Big).$$

Proof. We will just show the computation for the lower bound g_a, the result for the upper bound follows in the same way. We have

$$\begin{aligned}
\langle \delta\mu_a, \delta g\rangle_\Sigma &= \left\langle \mu_a^{\delta'} - \mu_a^\delta, g^{\delta'} - g^{\delta'}\right\rangle \\
&= \left\langle \mu_a^{\delta'} - \mu_a^\delta, (g^{\delta'} - g_a - \delta_{10}') + (\delta_{10}' - \delta_{10}) + (g_a + \delta_{10} - g^\delta)\right\rangle \\
&= \left\langle \mu_a^{\delta'}, g^{\delta'} - g_a - \delta_{10}'\right\rangle - \left\langle \mu_a^\delta, g^{\delta'} - g_a - \delta_{10}'\right\rangle \\
&\quad + \left\langle \mu_a^{\delta'} - \mu_a^\delta, \delta_{10}' - \delta_{10}\right\rangle \\
&\quad + \left\langle \mu_a^{\delta'}, g_a + \delta_{10} - g^\delta\right\rangle - \left\langle \mu_a^\delta, g_a + \delta_{10} - g^\delta\right\rangle \\
&\leq \langle \delta\mu_a, \delta_{10}' - \delta_{10}\rangle,
\end{aligned}$$

since the first and last term are zero by definition, and the second and fourth are nonpositive. Hence, Cauchy's and Young's inequality give

$$\begin{aligned}
|\langle \delta\mu_a, \delta g\rangle_\Sigma| &\leq \|\delta\mu_a\|_{L_2(\Sigma)}\|\delta_{10}' - \delta_{10}\|_{L_2(\Sigma)} \\
&\leq \varepsilon\|\delta\mu_a\|_{L_2(\Sigma)}^2 + c(\varepsilon)\|\delta_{10}' - \delta_{10}\|_{L_2(\Sigma)}^2,
\end{aligned}$$

and in the same way

$$|\langle \delta\mu_b, \delta g\rangle_\Sigma| \leq \varepsilon\|\delta\mu_b\|_{L_2(\Sigma)}^2 + c(\varepsilon)\|\delta_{11}' - \delta_{11}\|_{L_2(\Sigma)}^2.$$

Now, from the gradient equation and the sign condition for $\mu_a^\delta, \mu_b^\delta, \mu_a^{\delta'}, \mu_b^{\delta'}$ we know (writing $z^+ = \frac{1}{2}(z + |z|)$, $z^- = \frac{1}{2}(|z| - z)$)

$$\begin{aligned}
\mu_a^\delta &= (\lambda g^\delta + \gamma q^\delta + \delta_5)^+, & \mu_b^\delta &= (\lambda g^\delta + \gamma q^\delta + \delta_5)^-, \\
\mu_a^{\delta'} &= (\lambda g^{\delta'} + \gamma q^{\delta'} + \delta_5')^+, & \mu_b^{\delta'} &= (\lambda g^{\delta'} + \gamma q^{\delta'} + \delta_5')^-,
\end{aligned}$$

so

$$\begin{aligned}
\delta\mu_a &= (\lambda g^{\delta'} + \gamma q^{\delta'} + \delta_5')^+ - (\lambda g^\delta + \gamma q^\delta + \delta_5)^+ \leq (\lambda\delta g + \gamma\delta q + (\delta_5' - \delta_5))^+, \\
\delta\mu_b &\leq (\lambda\delta g + \gamma\delta q + (\delta_5' - \delta_5))^-,
\end{aligned}$$

and hence

$$\begin{aligned}
\|\delta\mu_a\|_{L_r(L_p(\Gamma))} &\leq c\Big(\|\delta g\|_{L_r(L_p(\Gamma))} + \|\delta q\|_{L_r(W_p^1)} + \|\delta_5' - \delta_5\|_{L_r(L_p(\Gamma))}\Big), \\
\|\delta\mu_b\|_{L_r(L_p(\Gamma))} &\leq c\Big(\|\delta g\|_{L_r(L_p(\Gamma))} + \|\delta q\|_{L_r(W_p^1)} + \|\delta_5' - \delta_5\|_{L_r(L_p(\Gamma))}\Big).
\end{aligned}$$

□

Bibliography

[1] R. A. Adams and J. J. F. Fournier. *Sobolev spaces.* Academic Press, Boston, 2003.

[2] W. Alt. The Lagrange-Newton method for infinite-dimensional optimization problems. *Numer. Funct. Anal. Optim.*, 11(3-4):201–224, 1990.

[3] W. Alt. *Nichtlineare Optimierung.* Vieweg, Braunschweig/Wiesbaden, 2002.

[4] W. Alt, R. Griesse, N. Metla, and A. Rösch. Lipschitz stability for elliptic optimal control problems with mixed control-state constraints. *Optimization*, 59(5-6):833–849, 2010.

[5] W. Alt, R. Sontag, and F. Tröltzsch. An SQP method for optimal control of weakly singular Hammerstein integral equations. *Appl. Math. Optim.*, 33(3):227–252, 1996.

[6] H. Amann. *Linear and Quasilinear Parabolic Problems.* 1995.

[7] H. Amann. Compact embeddings of vector-valued Sobolev and Besov spaces. *Glas. Mat. Ser. III*, 35(55):161–177, 2000.

[8] T. Apel and T. Flaig. Crank–Nicolson Schemes for Optimal Control Problems with Evolution Equations. *SIAM J. Numer. Anal.*, 50(3):1484–1512, 2012.

[9] N. Arada, J.-P. Raymond, and F. Tröltzsch. On an augmented Lagrangian SQP method for a class of optimal control problems in Banach spaces. *Comput. Optim. Appl.*, 22(3):369–398, 2002.

[10] P. Auscher, N. Badr, R. Haller-Dintelmann, and J. Rehberg. The square root problem for second-order, divergence form operators with mixed boundary conditions on L^p. *J. Evol. Eq.*, 15(1):165–208, 2015.

[11] J. Bergh and J. Löfström. *Interpolation Spaces. An introduction.* Springer-Verlag, Berlin-New York, 1976.

[12] M. Bergounioux, K. Ito, and K. Kunisch. Primal-Dual Strategy for Constrained Optimal Control Problems. *SIAM J. Control Optim.*, 37(4):1176–1194, 1999.

[13] E. Casas and F. Tröltzsch. Second-order necessary and sufficient optimailty conditions for optimization problems and applications to control theory. *SIAM J. Optim.*, 13(2):406–431, 2002.

[14] S. Childress and J. Percus. Nonlinear aspects of chemotaxis. *Math. Biosci.*, 56(3-4):217–237, 1981.

[15] A. L. Dontchev. Implicit function theorems for generalized equations. *Math. Programming*, 70(1):91–106, 1995.

[16] G. Dore. L^p regularity for abstract differential equations. *Functional analysis and related topics, Lecture Notes in Mathematics*, 1540:25–38, 1993.

[17] H. Egger, J.-F. Pietschmann, and M. Schlottbom. Identification of chemotaxis models with volume-filling. *SIAM J. Appl. Math.*, 75(2):275–288, 2015.

[18] L. C. Evans. *Partial Differential Equations.* American Math. Society, Providence, Rhode Island, 1998.

[19] K. R. Fister and C. M. McCarthy. Optimal control of a chemotaxis system. *Quart. Appl. Math.*, 61(2):193–211, 2003.

[20] A. Friedman. *Partial Differential Equations.* Holt, Rinehart and Winston, 1969.

[21] H. Gajewski and K. Zacharias. Global behaviour of a reaction-diffusion system modelling chemotaxis. *Math. Nachr.*, 195:77–114, 1998.

[22] C. Geiger and C. Kanzow. *Theorie und Numerik restringierter Optimierungsaufgaben.* Springer-Verlag, Berlin, Heidelberg, 2002.

[23] H. Goldberg and F. Tröltzsch. Second order optimality conditions for a class of control problems governed by non-linear integral equations with application to parabolic boundary control. *Optimization*, 20(5):687–698, 1989.

[24] H. Goldberg and F. Tröltzsch. Second order optimality conditions for nonlinear parabolic boundary control problems. *Optimal control of partial differential equations, Lect. Notes Control Inform. Sci.*, 149:93–103, 1991.

[25] J. A. Griepentrog, H. C. Kaiser, K. Gröger, and J. Rehberg. Interpolation for function spaces related to mixed boundary value problems. *Math. Nachr.*, 241:110–120, 2002.

[26] R. Griesse. Parametric sensitivity analysis in optimal control of a reaction diffusion system. I. Solution differentiability. *Numer. Funct. Anal. Optim.*, 25(1-2):93–117, 2004.

[27] R. Griesse, N. Metla, and A. Rösch. Convergence Analysis of the SQP method for nonlinear mixed-constrained elliptic optimal control problems. *ZAMM Z. Angew. Math. Mech.*, 88(10):776–792, 2008.

[28] R. Griesse, N. Metla, and A. Rösch. Local quadratic convergence of SQP for elliptic optimal control problems with mixed control-state constraints. *Control Cybernet.*, 39(3):717–738, 2010.

[29] R. Griesse and S. Volkwein. Parametric sensitivity analysis for optimal boundary control of a 3D reaction-diffusion system. *Large-Scale Nonlinear Optimization, Nonconvex Optim. Appl. , 83*, pages 127–149, 2006.

[30] P. Grisvard. *Elliptic problems in nonsmooth domains.* Pitman, Boston, 1985.

[31] R. Haller-Dintelmann and J. Rehberg. Maximal parabolic regularity for divergence operators including mixed boundary conditions. *J. Differential Equations*, 247(5):1354–1396, 2009.

[32] T. Hillen and K. Painter. Global existence for a parabolic chemotaxis model with prevention of overcrowding. *Adv. in Appl. Math.*, 26(4):280–301, 2001.

[33] T. Hillen and K. Painter. A user's guide to PDE models for chemotaxis. *J. Math. Biol.*, 58(1-2):183–217, 2009.

[34] D. Hoemberg, C. Meyer, J. Rehberg, and W. Ring. Optimal control for the thermistor problem. *SIAM J. Control Optim.*, 48(5):3449–3481, 2009.

[35] D. Horstmann. From 1970 until present: the Keller-Segel model in chemotaxis and its consequences. *Jahresber. Deutsch. Math.-Verein*, 106(2):51–69, 2004.

[36] D. Horstmann and M. Winkler. Boundedness vs. blow-up in a chemotaxis system. *J. Differential Equations*, 215(1):52–107, 2005.

[37] A. Ioffe. Necessary and sufficient conditions for a local minimum. I: A reduction theorem and first order conditions. *SIAM J. Control Optim.*, 17(2):245–250, 1979.

[38] K. Ito and K. Kunisch. *Lagrange multiplier approach to variational problems and applications.* SIAM, Philadelphia, 2008.

[39] W. Jäger and S. Luckhaus. On explosions of solutions to a system of partial differential equations modelling chemotaxis. *Trans. Amer. Math. Soc.*, 329(2):819–824, 1992.

[40] E. F. Keller and L. A. Segel. Initiation of slime mold aggregation viewed as an instability. *J. Theoretical Biology*, 26(3):399–415, 1970.

[41] J. L. Lions. *Optimal control of systems governed by partial differential equations.* Springer, Berlin, Heidelberg, 1971.

[42] A. Lunardi. *Analytic semigroups and optimal regularity in parabolic problems.* Birkhäuser/Springer, Basel, 1995.

[43] K. Malanowski and F. Tröltzsch. Lipschitz stability of solutions to parametric optimal control problems for parabolic equations. *Z. Anal. Anwendungen*, 18(2):469–489, 1999.

[44] K. Malanowski and F. Tröltzsch. Lipschitz stability of solutions to parametric optimal control for elliptic equations. *Control and Cybernet.*, 29(1):237–256, 2000.

[45] H. Maurer and J. Zowe. First and second order necessary and sufficient optimality conditions for infinite-dimensional programming problems. *Math. Programming*, 16(1):98–110, 1979.

[46] K. Painter and T. Hillen. Volume-filling and quorum-sensing in models for chemosensitive movement. *Can. Appl. Math. Quart.*, 10(4):501–543, 2002.

[47] C. S. Patlak. Random walk with persistence and external bias. *Bull. Math. Biophys.*, 15(3):311–338, 1953.

[48] A. Pazy. *Semigroups of linear operators and applications to partial differential equations.* Springer-Verlag, New York, 1983.

[49] B. Perthame. *Transport equations in Biology.* Birkhäuser, Basel, 2007.

[50] J. Prüss. Maximal regularity for abstract parabolic problems with inhomogeneous boundary data in L_p-spaces. *Math. Bohem.*, 127(2):311–327, 2002.

[51] J. Prüss. *Evolutionary integral equations and applications.* Birkhäuser/Springer, Basel, 2012.

[52] S. Robinson. Strongly regular generalized equations. *Math. Oper. Res.*, 5(1):43–62, 1980.

[53] S.-u. Ryu. Optimal control for a parabolic system modelling chemotaxis. *Trends Math.*, 6(1):45–49, 2003.

[54] R. Seeley. Interpolation in L^p with boundary conditions. *Studia Math*, 44:47–60, 1972.

[55] J. Simon. Compact sets in the space $L^p(0,T;B)$. *Ann. Math. Pura Appl. (4)*, 146:65–96, 1986.

[56] H. Triebel. *Interpolation theory, function spaces, differential operators.* Johann Ambrosius Barth, Heidelberg, 1978.

[57] F. Tröltzsch. On the Lagrange-Newton-SQP method for the optimal control of semilinear parabolic equations. *SIAM J. Control Optim.*, 38(1):294–312, 1999.

[58] F. Tröltzsch. Lipschitz stability of solutions of linear-quadratic parabolic control problems with respect to perturbations. *Dynam. Contin. Discrete Impuls. Systems*, 7(2):289–306, 2000.

[59] F. Tröltzsch. *Optimale Steuerung partieller Differentialgleichungen*. Vieweg+Teubner, Wiesbaden, 2009.

[60] D. Werner. *Funktionalanalysis*. Springer-Verlag, Berlin, 2007.

[61] J. Wloka. *Partielle Differentialgleichungen*. Teubner-Verlag, Leipzig, 1982.