



SPACE-TIME DISCRETIZATION OF OPTIMAL CONTROL OF BURGERS EQUATION  
USING BOTH DISCRETIZE-THEN-OPTIMIZE AND OPTIMIZE-THEN-DISCRETIZE  
APPROACHES

A THESIS SUBMITTED TO  
THE GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES  
OF  
MIDDLE EAST TECHNICAL UNIVERSITY

BY

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IN PARTIAL FULFILLMENT OF THE REQUIREMENTS  
FOR  
THE DEGREE OF DOCTOR OF PHILOSOPHY  
IN  
MATHEMATICS

JUNE 2011

Approval of the thesis:

**SPACE-TIME DISCRETIZATION OF OPTIMAL CONTROL OF BURGERS  
EQUATION USING BOTH DISCRETIZE-THEN-OPTIMIZE AND  
OPTIMIZE-THEN-DISCRETIZE APPROACHES**

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# ABSTRACT

## SPACE-TIME DISCRETIZATION OF OPTIMAL CONTROL OF BURGERS EQUATION USING BOTH DISCRETIZE-THEN-OPTIMIZE AND OPTIMIZE-THEN-DISCRETIZE APPROACHES

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June 2011, 113 pages

Optimal control of PDEs has a crucial place in many parts of sciences and industry. Over the last decade, there have been a great deal in, especially, control problems of elliptic problems. Optimal control problems of Burgers equation that is as a simplified model for turbulence and in shock waves were recently investigated both theoretically and numerically. In this thesis, we analyze the space-time simultaneous discretization of control problem for Burgers equation. In literature, there have been two approaches for discretization of optimization problems: optimize-then-discretize and discretize-then-optimize. In the first part, we follow optimize-then-discretize approach. It is shown that both distributed and boundary time dependent control problem can be transformed into an elliptic pde. Numerical results obtained with adaptive and non-adaptive elliptic solvers of COMSOL Multiphysics are presented for both the unconstrained and the control constrained cases. As for second part, we consider discretize-then-optimize approach. Discrete adjoint concept is covered. Optimality conditions, KKT-system, lead to a saddle point problem. We investigate the numerical treatment for the obtained saddle point system. Both direct solvers and iterative methods are consid-

ered. For iterative methods, preconditioners are needed. The structures of preconditioners for both distributed and boundary control problems are covered. Additionally, an a priori error analysis for the distributed control problem is given. We present the numerical results at the end of each chapter.

Keywords: Optimal control, Burgers equation, COMSOL, all-at-once method

## ÖZ

### AYRIKLAŞTIRDIKTAN SONRA EN İYİLEŞTİRMEK VE EN İYİLEŞTİRDİKTEN SONRA AYRIKLAŞTIRMAK YÖNTEMLERİ KULLANILARAK, BURGERS DENKLEMLERİNİN OPTİMAL KONTROL PROBLEMLERİNİN UZAY-ZAMAN EŞZAMANLI AYRIKLAŞTIRILMASI

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Haziran 2011, 113 sayfa

Bilim ve endüstrinin birçok dalında kısmi türevli denklemlerin en iyilemeli kontrol problemleri önemli bir yere sahiptir. Süregelen çalışmaların önemli bir kısmı eliptik denklemlerin kontrol problemine yöneliktir. Türbülans ve şok dalgalarının basit bir denklemleri olarak Burgers denklemlerinin kontrol teorisi üzerine de son yıllarda hem teorik hem de nümeriksel çalışmalar yapılmıştır. Bu tezde, Burgers denklemlerinin kontrol problemlerinin uzay-zaman eşzamanlı ayrıklaştırması üzerinde odaklanmaktadır. Optimizasyon problemlerinde genelde iki farklı yaklaşım takip edilmektedir: en iyileştirdikten sonra ayrıklaştırma ve ayrıklaştırdıktan sonra en iyileştirme. Hem dağıtılan hem de sınır kontrollü zamana bağlı en iyilemeli kontrol problemin eliptik bir probleme dönüşebildiği gösterilmiştir. Tezin ilk bölümünde, COMSOL paket programı kullanılarak hem kısıtlamasız hem de kontrol kısıtlamalı problemler için sayısal sonuçlar elde edildi. İkinci kısımda, ayrıklaştırdıktan sonra en iyileştirme yaklaşımı izlendi. Ayrık adjoint kavramı üzerinde duruldu. En iyileme koşulları, Karush-Kuhn-Tucker sistemi, bir semer nokta problemi oluşturdu. Elde edilen sistem için uygun sayısal yöntem araştırıldı. Hem doğrudan çözen metotlar hem de yinelemeli yöntemler incelenmiştir.

Anahtar Kelimeler: Optimal kontrol, zamana baęlı Burgers denklemi, COMSOL, tek adımda çözüm yöntemi

*To my mother and my husband*

## ACKNOWLEDGMENTS

It is a pleasure to thank the many people who made this thesis possible.

I gratefully acknowledge Prof. Dr. Bülent Karasözen for his advice, supervision, and crucial contribution to this thesis. Also, I offer my regards for his patience.

I acknowledge Gazi University for having a chance to work as a research assistance during my phd education. I wish to extend my warmest thanks to all members of the department mathematics.

I thank the members of my graduate committee for their guidance and suggestions. I gratefully acknowledge Prof. Dr. Gerhard Wilhelm Weber for his contributions when revising my thesis.

I acknowledge TÜBİTAK for its financial support for a period in USA. During that period, I have to thank Prof.Dr. R.H.W. Hoppe for giving me the opportunity to work in University of Houston.

My special gratitude is due to my mother, Kiraz Özdemir, for her loving support during my life. I owe my loving thanks to my father, Osman Özdemir, for his supporting. I would like to thank the many people. Without my mother-in-law and father-in-law, Leyla Yılmaz and Arif Yılmaz, support I would not have finished the degree.

Words fail me to express my appreciation to my husband, Aydın Yılmaz. He has been persistent confidence in me and taken the load off my shoulder. I owe my every achievement to him.

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# CHAPTER 1

## INTRODUCTION

Optimal control theory has been an important field of applied mathematics. It is a mathematical optimization technique usually used to create control policies. The optimal control consists of a set of equations describing the paths of the variables that take the cost functional to a minimum. The cost functional is basically a function of variables related to state and control. Optimal control has found applications in numerous field including process control, robotics, bioengineering, economics, finance, etc.. The set of equation in a control problem may be an ordinary or partial differential equations. In many cases, the modeling of the problems by an ordinary differential equation are not adequate. Fluid flows, electromagnetic waves, diffusion and many other physical quantities can be modeled by partial differential equations(PDE).

There have been many researches related optimal control of PDE's. The optimal control of heating process, two phase problems and fluid flows were discussed in [58]. The control theory of linear and semi-linear partial differential equations are covered in that work. Necessary functional analysis and first-second order optimality conditions are derived. The work [21] provides a modern introduction to optimal control of PDE's. Beside a deep coverage for functional analysis and optimal control theory for some certain problems, it gives an introduction to discrete concepts in control problems.

An optimal control problem is called a constrained problem if the state or control variable is bounded. It is said to be control constrained and state constrained problem if control variable and state variable are bounded, respectively. The problem is said to be unconstrained

if there does not exist any bounds for the variables. For the unconstrained problem, it is standard to find necessary optimality conditions. Sufficient conditions are investigated for control constrained problem by Bonnans [5], Casas, Unger and Tröltzsch [7], Goldberg and Tröltzsch [14]. For the state constrained problems sufficient optimality conditions are considered in Casas, Tröltzsch and Unger [9], Raymond and Tröltzsch [46], Casas and Mateos [8], Casas, De los Reyes and Tröltzsch [10]. We refer to Bergounioux, Ito and Kunisch [3] or Bergounioux and Kunisch [4] for associated numerical methods.

Many of the works consist of optimal control of elliptic problems. There have been some researches concerning control of parabolic problems [1, 16, 30, 31, 32, 41]. However, the optimal control of nonlinear equations has a more recent history [60, 61, 62]. Also, there have been some works related control problem of Navier-Stokes equations as [15, 19, 51, 63].

Burgers equation plays an important role in fluid dynamics as a first approximation to complex diffusion convection phenomena. It was used as a simplified model for turbulence and in shock waves. Analysis and numerical approximation of optimal control problems for Burgers equation are important for the development of numerical methods for optimal control of more complicated models in fluid dynamics like Navier-Stokes equations.

Recently, several papers appeared dealing with the optimal control of the Burgers equation. A detailed analysis of distributed and boundary control of stationary and unsteady Burgers equation and the approximation of the optimality system with augmented Lagrangian SQP (sequential quadratic programming) method are given in [66]. In [50], the SQP, primal-dual active set and semi-smooth Newton methods are compared for the distributed control problems related with the stationary Burgers equation with pointwise control constraints. Distributed control problems for the unsteady Burgers equation with and without control constraints are investigated numerically using SQP methods in [20, 57, 68]. Different time integration methods like the implicit Euler and Crank-Nicholson methods were considered for solving the adjoint equations arising from the optimal control of the unsteady Burger equation in [36]. In contrast to linear parabolic control problems, the optimal control problem for the Burgers equation is a non-convex problem with multiple local minima due to the nonlinearity

of the differential equation. Numerical methods can only compute minima close to the starting points [57].

For the discretization of the optimal control problems there are two different approaches: *optimize-then-discretize* and *discretize-then-optimize*. In the *optimize-then-discretize* approach, first the necessary optimality conditions are established on the continuous level consisting of the state, adjoint and the optimality equations, and then these equations are discretized usually by finite elements. The optimality system consists of the state and adjoint equations as coupled by an algebraic equation. Usually, this system is integrated iteratively forward and backward in time by gradient based algorithms. It is known that this requires storage of data containing the state and adjoint variables computed at discrete time point, which would be infeasible for two and three dimensional problems. Another approach which appeared recently in the literature is to solve both equations at once as systems of coupled elliptic equation in space and time. The transformation of the optimality system into an elliptic PDE for linear parabolic optimal control problems with pointwise control constraints was considered in [37, 38, 39, 40]. This approach treats the coupled optimality system in the whole space-time cylinder, where the time variable was interpreted as additional space variable. It is also known as one-shot approach. As for numerical solutions a specialized FEM package, called COMSOL multiphysics, was used. The simulation and modeling package COMSOL allows an easy way to define, discretize and solve stationary and time-dependent partial differential equations. For a simple linear parabolic equation, Neitzel, Prüfert and Slawig successfully used this package to get numerical results. We refer to [38] for a detailed COMSOL scripts. The advantages of COMSOL Multiphysics in adaptive and non adaptive solvers, discretizations, and post processing strategies were used in their works. The one-shot approach with space-time discretization was applied to the distributed optimal control problem with the unsteady Burgers equation in [71].

In the discretize-then-optimize approach the state equation is discretized and then the optimality system for the finite dimensional optimization problem is derived. Treating the control and state as independent of optimization variables the discrete optimality conditions yield a

$$\text{system } \underbrace{\begin{pmatrix} E & L^T \\ L & 0 \end{pmatrix}}_{\mathcal{A}} x = b.$$

This system is usually is a kind of saddle point problem, where  $\mathcal{A}$  is symmetric and has sparse structure. This kind of system usually requires preconditioning. There have been many works concerning block iterative solutions of  $\mathcal{A}x = b$  [12, 33, 34, 35]. Recently, Wathen, Stoll and Rees have made many researches related to all-at-once preconditioning of linear control problems [47, 48, 49, 52, 53]. The structure of the control constrained problems are covered. They showed how to handle control constraints. Different preconditioning methods were covered. Especially elliptic problems were worked since it is easy to implement without having memory problems. However, considering parabolic problems if every time step is considered in a block matrix then the system  $\mathcal{A}x = b$  is obtained. This is done for heat equation in [34, 52]. For the non linear control problems it is not as easy as in the linear case. In [2], control problem of steady Navier-Stokes equation was considered. In every linearization step, an Oseen problem was solved. But a detailed implementation was not given.

In this work, we consider the all-at-once type solutions of unsteady control problems for Burgers equation by using both *optimize-then-discretize* and *discretize-then-optimize* approaches. We first cover some related functional analytical results and provide a discussion for the existence and uniqueness results of the Burgers equation. Then, we can consider this work in two main parts:

In the first part of the thesis, we use *optimize-then-discretize* approach to solve control problem. We transform the parabolic problem into an elliptic problem by linearizing the state equation. We cover both distributed and boundary control problems. We use different linearization techniques for the distributed and boundary control problems. We show the existence of the solutions to transformed elliptic equation in both distributed and boundary control problems. Both unconstrained and control constrained problems are considered. For implementation of the control constraints projection method is used. After obtaining elliptic problem, we use COMSOL Multiphysics for numerical solutions. We discuss the mesh independence issue and verify in the numerical results.

For the second part we focus on *discretize-then-optimize* approach. We provide a detailed dis-

cussion for finite element discretization and time approximations. In order to have a symmetric saddle point problem, we apply Crank-Nicolson time approximation to linearized problem and semi-implicit time scheme to nonlinear control problem. Both distributed and boundary control problems are covered. We use active set algorithm to handle control constraints. After obtaining the saddle point system, we use both direct solver and an iterative solver for implementation. Moreover, we provide an a priori error analysis for the distributed control problem. We check the order of convergence in the numerical treatment part.

## CHAPTER 2

### PRELIMINARY RESULTS

In this chapter, we cover some functional analysis preliminaries with basic theoretical results. Then we give the existence and uniqueness results for the control problem of Burgers equation. Moreover we discuss some known methods for the optimization problem such as: the gradient method and the active set strategy.

#### 2.1 Functional Analysis Preliminaries

We now introduce the function spaces that we shall use in our work. We use the same notations as [44].

##### 2.1.1 $L^p$ spaces

Let  $\Omega$  be an open set contained in  $\mathbb{R}^d$ ,  $d \geq 1$ . For  $1 \leq p < \infty$ , consider the set of measurable functions  $w$  such that

$$\int_{\Omega} |w(x)|^p dx < \infty$$

and, when  $p = \infty$ ,

$$\sup\{|w(x)| \mid x \in \Omega\}.$$

These spaces are denoted by  $L^p(\Omega)$  with the associated norm being

$$\|w\|_{L^p(\Omega)} := \left( \int_{\Omega} |w(x)|^p dx \right)^{1/p}, \quad 1 \leq p < \infty,$$

and, when  $p = \infty$ ,

$$\|w\|_{L^\infty(\Omega)} := \sup \{ |w(x)| \mid x \in \Omega \}.$$

***The Hölder inequality.***

If  $1 \leq p < \infty$ , the dual space of  $L^p(\Omega)$  is given by  $L^{p'}(\Omega)$ , with  $(1/p) + (1/p') = 1$ . The following inequality holds

$$\left| \int_{\Omega} w(x)v(x)dx \right| \leq \|w\|_{L^p(\Omega)} \|v\|_{L^{p'}(\Omega)}.$$

For  $p = 2$ , the Hölder inequality is called as Cauchy-Schwarz inequality.

**2.1.2 Sobolev spaces**

The classical Sobolev space  $W^{k,p}(\Omega)$ ,  $k$  is non-negative integer and  $1 \leq p \leq \infty$ , on a domain  $\Omega \subset \mathbb{R}^d$  is defined as

$$W^{k,p}(\Omega) := \left\{ w \in L^p(\Omega) \mid D^\sigma w \in L^p(\Omega) \text{ for each non-negative multi-index } \sigma \text{ such that } |\sigma| \leq k \right\}$$

with the norm

$$\|w\|_{k,p,\Omega} := \left( \sum_{|\sigma| \leq k} \|D^\sigma w\|_{L^p(\Omega)}^p \right)^{1/p}.$$

For the case  $p = 2$  we write  $H^k(\Omega) = W^{k,2}(\Omega)$ . We denote the subspace of  $H^1(\Omega)$  vanishing on  $\partial\Omega$  as  $H_0^1(\Omega)$ . The space  $H^1(\Omega)$  is associated with the following norm:

$$\|w\|_1 := \sqrt{\|w\|^2 + \|\nabla w\|^2}.$$

Similarly, we can consider the time dependent case. We introduce  $Q = (0, T) \times \Omega$  and

$$L^q(0, T; W^{k,p}(\Omega)) := \left\{ w : (0, T) \rightarrow W^{k,p}(\Omega) \mid w \text{ is measurable} \right. \\ \left. \text{and satisfies } \int_0^T \|w(t)\|_{k,p,\Omega}^q dt < \infty \right\}$$

for  $1 \leq q < \infty$  with the norm

$$\|w(t)\|_{L^q(0,T;W^{k,p}(\Omega))} := \left( \int_0^T \|w(t)\|_{k,p,\Omega}^q dt \right)^{1/q}.$$

For a Banach space  $V$ , the space  $H^1(0, T; V)$  can be defined as

$$H^1(0, T; V) := \left\{ w \in L^2(0, T; V) \mid \frac{\partial w}{\partial t} \in L^2(0, T; V) \right\}.$$

### 2.1.3 Some inequalities

In this part, we recall some inequalities that we shall use in the following chapters.

**Young's inequality.**

Let  $a, b \in [0, \infty)$  and  $\epsilon > 0$ . Then, we have

$$ab \leq \frac{1}{\epsilon^p} \frac{a^p}{p} + \epsilon^q \frac{b^q}{q}, \text{ where } 1 < p < \infty \text{ and } \frac{1}{p} + \frac{1}{q} = 1.$$

**Poincaré-Friedrichs inequality.**

There exists a constant  $C(|\Omega|) > 0$  such that

$$\|w\| \leq C \|\nabla w\| \quad \forall w \in \Omega.$$

**Gronwall lemma** [44].

Let  $w \in L^1(t_0, T)$  be a non-negative function,  $f$  and  $g$  be continuous functions in  $[t_0, T]$ . If  $g$  satisfies

$$g(t) \leq f(t) + \int_{t_0}^t w(\tau)g(\tau)d\tau \quad \forall t \in [t_0, T],$$

then,

$$g(t) \leq f(t) + \int_{t_0}^t w(s)f(s) \exp\left(\int_s^t w(\tau)d\tau\right), \quad \forall t \in [t_0, T].$$

If  $g$  is non-decreasing, then,

$$g(t) \leq f(t) \exp\left(\int_{t_0}^t w(\tau)d\tau\right), \quad \forall t \in [t_0, T].$$

**Discrete Gronwall lemma** [44].

Let  $k_n$  be a non-negative sequence,  $f$  and the sequence  $p_n$  satisfies

$$\begin{cases} f_0 \leq g_0 \\ f_n \leq g_0 + \sum_{s_0}^{n-1} p_s + \sum_{s_0}^{n-1} k_s f_s, \quad n \geq 1, \end{cases}$$

then,  $f_n$  satisfies

$$\begin{cases} f_1 \leq g_0(1 + k_0) + p_0 \\ f_n \leq g_0 \prod_{s=0}^{n-1} (1 + k_s) + \sum_{s_0}^{n-2} p_s \prod_{\tau=s_0+1}^{n-1} (1 + k_\tau) + p_{n-1}, \quad n \geq 2, \end{cases}$$

if for  $n \geq 0$  with  $g_0 \geq 0$  and  $p_n \geq 0$  it follows

$$f_n \leq \left(g_0 + \sum_{s_0}^{n-1} p_s\right) \exp\left(\sum_{s_0}^{n-1} k_s\right).$$

## 2.2 Unconstrained optimal control of unsteady Burgers equation

We first summarize the existence and uniqueness of solutions of the unsteady Burgers equation following [57, 67, 70]. Then, we discuss both the distributed and boundary control prob-

lems. After deriving optimality conditions, we obtain the optimality system.

### 2.2.1 Distributed control

Given  $\Omega = (0, 1)$  and  $T > 0$ , we define  $Q = (0, T) \times \Omega$  and  $\Sigma = (0, T) \times \partial\Omega$ . Let  $H = L^2(\Omega)$  and  $V = H_0^1(\Omega)$  be Hilbert spaces. We make use of the following Hilbert space:

$$W(0, T) = \{\varphi \in L^2(0, T; V); \varphi_t \in L^2(0, T; V^*)\},$$

where  $V^*$  denotes the dual space of  $V$ . The inner product in the Hilbert space  $V$  is given with the natural inner product in  $H$  as

$$(\varphi, \psi)_V = (\varphi', \psi')_H, \text{ for } \varphi, \psi \in V.$$

The expression  $\varphi(t)$  stands for  $\varphi(t, \cdot)$ , considered as function in  $\Omega$  only when  $t$  is fixed.

We consider the unsteady viscous Burgers equation

$$y_t + yy_x - \nu y_{xx} = f + bu \text{ in } Q \tag{2.1}$$

with homogenous Dirichlet boundary conditions

$$y(t, 0) = 0 \text{ on } \Sigma,$$

and with the initial condition

$$y(0) = y_0 \text{ in } \Omega,$$

where  $f \in L^2(Q)$  is a fixed forcing term,  $\nu = \frac{1}{Re} > 0$  denotes the viscosity parameter and  $Re$  is the Reynolds number. The location and intensity of the controls  $u \in L^2(Q)$  are expressed by the function  $b \in L^\infty(Q)$ . For example  $b$  might be chosen as

$$bu = \begin{cases} u & \text{in } \tilde{\Omega}, \\ 0 & \text{in } \Omega \setminus \tilde{\Omega}, \end{cases}$$

where  $\tilde{\Omega}$  is the set of active controls [50, 57, 66].

For the unsteady Burgers equation (2.1) with the corresponding initial and boundary conditions there exists a weak solution  $y \in W(0, T)$  satisfying

$$\langle y_t(t), \varphi \rangle_{V^*, V} + \nu (y_t(t), \varphi)_V + (y(t)y_x(t), \varphi)_H = ((f + bu)(t), \varphi)_H$$

for all  $\varphi \in V$ , and  $t \in [0, T]$ , and  $(y(0), \chi)_H = (y_0, \chi)$  for all  $\chi \in H$  [57].

The distributed control problem for Burgers equation without inequality constraints and with homogeneous Dirichlet boundary conditions can be stated as follows [66]:

$$\min J(y, u) = \frac{1}{2} \|y - y_d\|_Q^2 + \frac{\alpha}{2} \|u\|_Q^2 \quad (\text{P1})$$

$$\begin{aligned} \text{subject to } y_t - \nu y_{xx} + yy_x &= f + bu & \text{in } Q, \\ y &= 0 & \text{on } \Sigma, \\ y(0) &= y_0 & \text{in } \Omega, \end{aligned} \quad (2.2)$$

with the regularization parameter  $\alpha > 0$ . Here,  $y$  and  $u$  denote the state and control variables,  $y_d$  is the desired state.

In order to show the existence of the optimal solutions, the operator  $e : X \rightarrow Y$  (see [67], p. 130) was introduced by

$$e(y, u) = (e_1(y, u), e_2(y, u)) = (y_t - \nu y_{xx} + yy_x - f - bu, y(0) - y_0),$$

where  $X = W(V) \times L^2(\bar{\Omega})$  and  $Y = L^2(V) \times H$  identified with  $Y^* = L^2(V^*) \times H$  the dual of  $Y$ . Then, the optimal control system above can be interpreted as a minimization problem with equality constraints

$$\text{minimize } J(y, u), \quad \text{such that } e(y, u) = 0.$$

Let  $(y^*, u^*)$  be an optimal solution. It was proved that there exist Lagrange multipliers  $p^*$  and  $\lambda^*$  satisfying the first-order necessary optimality conditions [20, 66, 67]

$$\mathcal{L}'(y^*, u^*, p^*, \lambda^*) = 0, \quad e(y^*, u^*) = 0$$

with the Lagrangian

$$\mathcal{L}(y, u, p, \lambda) = J(y, u) - (e_1(y, u), p)_{L^2(V^*), L^2(V)} - (e_2(y, u), \lambda)_H.$$

First-order optimality conditions lead to the following optimality system:

$$\begin{aligned} y_t^* - \nu y_{xx}^* + y^* y_x^* &= f + bu^* & \text{in } Q, \\ y^*(t, 0) = y^*(t, 1) &= 0 & \text{on } \Sigma, \\ y^*(0) &= y_0 & \text{in } \Omega, \end{aligned} \quad (2.3)$$

$$\begin{aligned}
p_t^* + \nu p_{xx}^* + y^* p_x^* &= y_d - y^* && \text{in } Q, \\
p^*(t, 0) = p^*(t, 1) &= 0 && \text{on } \Sigma, \\
p^*(T) &= 0 && \text{in } \Omega,
\end{aligned} \tag{2.4}$$

with the gradient condition

$$\alpha u^* + p^* = 0.$$

Here,  $u^*$  is the optimal control and  $y^*$  denotes the associated optimal state,  $p^*$  is the adjoint state.

The adjoint equation (2.4) can be transformed by the time transformation  $\tau = T - t$  into an initial-boundary value problem

$$\begin{aligned}
-p_\tau^* + y^* p_x^* + \nu p_{xx}^* &= \tilde{y}_d - \tilde{y}^* && \text{in } Q, \\
p^*(\tau, 0) = p^*(\tau, 1) &= 0 && \text{on } \Sigma, \\
p^*(\tau = 0) &= 0 && \text{in } \Omega,
\end{aligned}$$

where  $\tilde{y}^*(\tau, x) = y^*(T - t, x)$ .

There are different approaches in order to solve the optimality system (2.3) and (2.4): integrating the state equation (2.3) forward in time and the adjoint equation (2.4) backward in time by an iterative method, and solving the whole optimality system as an elliptic pde by taking time as an additional space variable.

### 2.2.2 Boundary control

We consider the unsteady Burgers equation with Robin boundary conditions

$$y_t + yy_x - \nu y_{xx} = f \text{ in } Q \tag{2.5}$$

with Robin boundary conditions

$$\begin{aligned}
y_t + yy_x - \nu y_{xx} &= f \text{ in } Q, \\
\nu y_x(\cdot, 0) + \sigma_0 y(\cdot, 0) &= u \text{ in } (0, T), \\
\nu y_x(\cdot, 1) + \sigma_1 y(\cdot, 1) &= v \text{ in } (0, T),
\end{aligned}$$

$$y(0, \cdot) = y_0 \text{ in } \Omega,$$

with  $\sigma_0, \sigma_1 \in L^\infty(0, T)$  and  $f \in L^2(Q)$ ,  $y_0 \in L^2(\Omega)$  is the forcing function, and  $u, v \in L^2(0, T)$ .

Special cases of the optimal control problems for the Burgers equation were considered for the Neumann boundary conditions ( $\sigma_0 = \sigma_1 = 0$ ) in [36] and the Dirichlet boundary conditions  $y(\cdot, 0) = u$ ,  $y(\cdot, 1) = v$  in [24, 45].

The results about the existence and uniqueness of the unsteady Burgers equation (2.5) are summarized below [68].

Let  $H = L^2(\Omega)$  be a Hilbert space, then we make use of the following Hilbert space

$$W(0, T) = \{\varphi \in L^2(0, T; H^1(\Omega)); \varphi_t \in L^2(0, T; H^1(\Omega)^*\},$$

where  $H^1(\Omega)^*$  denotes the dual space of  $H^1(\Omega)$ . The expression  $\varphi(t)$  stands for  $\varphi(t, \cdot)$ , considered as function in  $\Omega$  only when  $t$  is fixed.

There exists a weak solution  $y \in W(0, T)$  of the state equation (3.11) satisfying (Theorem 2.2, [70])

$$\begin{aligned} & \langle y_t(t), \varphi \rangle_{H^1(\Omega)^*, H^1(\Omega)} + \sigma_1(t)y(t, 1)\varphi(1) - \sigma_0(t)y(t, 0)\varphi(0) + \int_{\Omega} v y_x(t) \varphi' + y(t)y_x(t)\varphi dx \\ & = \int_{\Omega} f(t)\varphi dx + v(t)\varphi(1) - u(t)\varphi(0) \end{aligned}$$

for all  $\varphi \in H^1(\Omega)$ ,  $t \in [0, T]$ , and  $y(0) = y_0$  in  $L^2(\Omega)$ , where  $\langle \cdot, \cdot \rangle_{H^1(\Omega)^*, H^1(\Omega)}$  denotes the dual pair associated with  $H^1(\Omega)$  and its dual.

We consider the following optimal control problem for the unsteady Burgers equation with Robin boundary conditions [70]

$$\min J(y, u, v) = \frac{1}{2} \int_Q (y - y_d)^2 dx + \frac{1}{2} \int_0^T \beta_u |u|^2 + \beta_v |v|^2 dt \quad (\text{Pb1})$$

subject to

$$\begin{aligned}
y_t + yy_x - \nu y_{xx} &= f & \text{in } Q, \\
\nu y_x(\cdot, 0) + \sigma_0 y(\cdot, 0) &= u & \text{in } (0, T), \\
\nu y_x(\cdot, 1) + \sigma_1 y(\cdot, 1) &= v & \text{in } (0, T), \\
y(0, \cdot) &= y_0 & \text{in } \Omega.
\end{aligned} \tag{2.6}$$

The first order optimality conditions for the optimal control problem (Pb1) given in [70] are summarized below.

Abstract formulation of the control problem (Pb1) is given by introducing the Hilbert spaces

$$X = W(0, T) \times L^2(0, T) \times L^2(0, T), \quad Y = L^2(0, T; H^1(\Omega)) \times L^2(\Omega).$$

Let  $\tilde{e} : X \rightarrow L^2(0, T; H^1(\Omega)^*)$  be defined by

$$\begin{aligned}
\langle \tilde{e}(y, u, v), p \rangle_{L^2(0, T; H^1(\Omega)^*), L^2(0, T; H^1(\Omega))} &= \int_0^T \langle y_t(t), p(t) \rangle_{H^1(\Omega)^*, H^1(\Omega)} dt + \\
&\int_0^T \int_{\Omega} \nu y_x p_x + (yy_x - f) p dx dt + \int_0^T (\sigma_1 y(\cdot, 1) - v) p(\cdot, 1) + (u - \sigma_0 y(\cdot, 0)) p(\cdot, 0) dt
\end{aligned}$$

for  $p \in L^2(0, T; H^1(\Omega))$ . We set  $e : X \rightarrow Y$ ,  $(y, u, v) \mapsto (\mathcal{N}\tilde{e}(y, u, v), y(0) - y_0)$  where  $\mathcal{N} : H^1(\Omega)^* \rightarrow H^1(\Omega)$  is the Neumann solution operator, that is for  $g \in H^1(\Omega)^*$  the function  $w = \mathcal{N}g$  solves

$$\int_{\Omega} (w_x \varphi_x + w \varphi) dx = \langle g, \varphi \rangle_{H^1(\Omega)^*, H^1(\Omega)} \text{ for all } \varphi \in H^1(\Omega).$$

There exists at least one globally optimal solution  $z^* = (y^*, u^*, v^*)$  of (1-3) (Theorem 2.6, [70]).

We introduce now the Lagrangian functional  $L$  to obtain the optimality conditions as

$$\begin{aligned}
L(y, u, v, p) &= J(y, u, v) - \int_0^T \langle y(t), p(t) \rangle_{H^1(\Omega)^*, H^1(\Omega)} dt \\
&- \int_0^T \int_{\Omega} (\nu y_x p_x + yy_x - f) p dx dt - \int_0^T (\sigma_1 y(\cdot, 1) - v) p(\cdot, 1) + (u - \sigma_0 y(\cdot, 0)) p(\cdot, 0) dt.
\end{aligned}$$

For each  $p \in W(0, T)$  the Lagrangian is twice continuously Fréchet-differentiable with respect to  $z = (y, u, v) \in X$  and its second derivative is Lipschitz continuous. The first order optimality conditions are obtained by the taking the partial derivatives of the Lagrangian with respect to the state variable  $y$ , to the adjoint variable  $p$  and to the control variables  $u$  and  $v$ .

Let  $z^* = (y^*, u^*, v^*)$  be a local solution to control constrained problem (Pb1). Then there exist  $p^* \in W(0, T) \times L^2(\Omega)$  satisfying

$$\begin{aligned} p_t^* + v p_{xx}^* + p^* p_{*x}^* &= y_d - y^* \quad \text{in } Q, \\ v p_x^*(t, 0) + (y^*(t, 0) + \sigma_0) p^*(t, 0) &= 0 \quad \text{in } (0, T), \\ v p_x^*(t, 1) + (y^*(t, 1) + \sigma_1) p^*(t, 1) &= 0 \quad \text{in } (0, T), \\ p^*(T) &= 0, \end{aligned} \tag{2.7}$$

with the gradient equations

$$p^*(\cdot, 0) + \beta_u u^* = 0, \tag{2.8}$$

$$-p^*(\cdot, 1) + \beta_v v^* = 0. \tag{2.9}$$

We note that the optimal control problem (Pb1) is a non-convex optimization problem, so that different local minima might occur. We do not consider the global solutions of (Pb1), numerical methods considered in the next sections can find a local minimum close to its starting value.

## 2.3 Constrained optimal control problem of Burgers equation

### 2.3.1 Distributed control

We consider now distributed optimal control problem with pointwise bilateral control constraints [57]

$$\min J(y, u) = \frac{1}{2} \|y - z\|_Q^2 + \frac{\alpha}{2} \|u\|_Q^2 \tag{P2}$$

$$\text{subject to } y_t + y y_x - v y_{xx} = f + bu \quad \text{in } Q,$$

$$y = 0 \quad \text{in } \Sigma,$$

$$y(\cdot, \cdot) = y_0 \quad \text{in } \Omega,$$

$$u_a(t, x) \leq u(t, x) \leq u_b(t, x) \quad \text{in } Q.$$

First-order necessary conditions for the optimality system of the local solution  $(y^*, u^*)$  have to be satisfied with the adjoint variable  $p^*$  in form of the optimality system including the control

constraints  $u^* \in U_{ad} = \{u \in L_2(Q) : u_a(t, x) \leq u(t, x) \leq u_b(t, x)\}$ . Because of the pointwise constraints, additionally we have the variational inequality [57]

$$\int_Q (\alpha u^* + b p^*)(u - u^*) dx dt \geq 0 \text{ for all } u \in U_{ad}. \quad (2.10)$$

The last inequality can be expressed in the form of a projection [57]:

$$u^*(t, x) = P_{[u_a(t, x), u_b(t, x)]} \left( \frac{-b(t, x)}{\alpha} p^*(t, x) \right).$$

First order optimality conditions for the control constrained Burgers equation are stated as follows [57]:

$$\begin{aligned} y_t - \nu y_{xx} + y y_x &= f + bu & \text{in } Q, \\ y(t, 0) = y(t, 1) &= 0 & \text{on } \Sigma, \\ y(0) &= y_0 & \text{in } \Omega, \end{aligned} \quad (2.11)$$

$$\begin{aligned} p_t + \nu p_{xx} + y p_x &= y_d - y & \text{in } Q, \\ p(t, 0) = p(t, 1) &= 0 & \text{on } \Sigma, \\ p(T) &= 0 & \text{in } \Omega, \end{aligned} \quad (2.12)$$

with the gradient condition

$$\alpha u + p + \mu_b - \mu_a = 0.$$

and complementary slackness conditions

$$\begin{aligned} (\mu_a, u_a - u)_{L^2(Q)} &= 0, \quad u \geq u_a \quad \mu_a \geq 0 \quad a.e. \text{ in } Q, \\ (\mu_b, u - u_b)_{L^2(Q)} &= 0, \quad u \leq u_b \quad \mu_b \geq 0 \quad a.e. \text{ in } Q. \end{aligned} \quad (2.13)$$

In [50], different solution algorithms like primal dual-SQP, SQP-primal dual methods and semi smooth Newton method are applied and compared for solving the optimality system of the steady Burgers equation with control constraints.

### 2.3.2 Boundary control

Since the control constraints are present, then

$$(u, v) \in U_{ad} \times V_{ad} \subset L^2(0, T) \times L^2(0, T). \quad (2.14)$$

The sets of admissible controls are given by

$$U_{ad} = \{u \in L^\infty(0, T) : u_a \leq u \leq u_b, \text{ a.e. in } (0, T)\},$$

$$V_{ad} = \{v \in L^\infty(0, T) : v_a \leq v \leq v_b, \text{ a.e. in } (0, T)\},$$

with  $u_a, u_b, v_a, v_b \in L^\infty(0, T)$  and  $u_a \leq u_b$  and  $v_a \leq v_b$  almost everywhere (a.e.) in  $Q$ ,

and the subset  $K_{ad}$  is defined as

$$\emptyset \neq K_{ad} = W(0, T) \times U_{ad} \times V_{ad} \subset X.$$

Now the optimal control problem can be written as equality constrained optimization problem:

$$\min J(x) \text{ subject to } x \in K_{ad} \text{ and } e(x) = 0. \quad (\text{Pb2})$$

Let  $z^* = (y^*, u^*, v^*) \in K_{ad}$  be a local solution to control constrained problem (Pb2). Then, there exist  $p^* \in W(0, T) \times L^2(\Omega)$  and  $(\mu, \xi) \in L^2(0, T) \times L^2(0, T)$  satisfying

$$\begin{aligned} p_t^* + \nu p_{xx}^* + p^* p_x^* &= y_Q - y^* \quad \text{in } Q, \\ \nu p_x^*(t, 0) + (y^*(t, 0) + \sigma_0) p^*(t, 0) &= 0 \quad \text{in } (0, T), \\ \nu p_x^*(t, 1) + (y^*(t, 1) + \sigma_1) p^*(t, 1) &= 0 \quad \text{in } (0, T), \\ p^*(T) &= 0, \end{aligned} \quad (2.15)$$

with the gradient equations

$$p^*(\cdot, 0) + \beta_u u^* + \mu = 0, \quad (2.16)$$

$$-p^*(\cdot, 1) + \beta_v v^* + \xi = 0. \quad (2.17)$$

## 2.4 The sequential or iterative approach: the gradient method

In order to implement optimality system we give a summary of well-known gradient based method. This kind of methods are usually used to solve optimization problems. Although it may cost to compute gradient, this method provides an efficient and fast solver.

After introducing the control to state operator  $G : L^2(Q) \rightarrow H$  that assigns to each  $u \in L^2(Q)$  of the corresponding Burgers solution  $y(u)$ , the functional  $J(G(u), u)$  will be minimized by the gradient method:

$$\left( \frac{d}{du} J(G(u), u), h \right) = (G(u) - y_d, Gh) + \alpha(u, h) = (G^*(G(u) - y_d), h) + \alpha(u, h),$$

where  $h \in L^2(Q)$  is a directional vector. The descent direction is given by

$$v = G^*(G(u) - y_d) + \alpha u.$$

The adjoint state is  $p := G^*(G(u) - y_d) = G^*(y - y_d)$ . We use the gradient method as described in [38] where for the Burgers equation at each iteration step a nonlinear system of equation is to be solved.

The following algorithm is implemented:

*Algorithm 1 (Gradient Method in function space)*

1. Choose  $\epsilon > 0$ . Choose  $u_{old}$  arbitrarily.
2. Initialize  $y_{old}$  by solving  $y_{old} = G(u_{old})$ .
3. while  $v > \epsilon$
4. solve the adjoint equation  $p = G^*(G(u_{old}) - y_d)$
5. set  $v = p + \kappa(u_{old} - u_d)$

for  $k = 1, 2, \dots$

$$\text{padding-left: 80px; } u_{new} = u_{old} + \sigma v$$

solve the state equation  $y_{new} = G(u_{new})$

if  $J(y_{new}, u_{new}) < J(y_{old}, u_{old})$

break

end

set  $\sigma = \sigma/2$

end

7. set  $u_{old} = u_{new}, y_{old} = y_{new}$ .

8. end

## 2.5 Active set strategy to implement control constraints

There have been significant changes in methods for solving nonlinear constrained problems. Most of them are based on SQP (sequential quadratic programming) [17, 23, 25, 56, 57]. The SQP-algorithm is sequential and each of its iterations requires the solution of a quadratic minimization problem subject to linearized constraints. For the numerical treatment of the control constraints we apply the well-known method, primal dual active set strategy. This method was proposed by Bergounioux, Ito, and Kunisch [3, 4, 27]. For a general class of problems it has been shown that primal dual active set strategy and semi-smooth Newton methods lead to the same algorithms [28, 51].

A reformulation of the complementary conditions (3.9) can be stated as

$$\mu = \max(0, \mu + (\bar{u} - u_b)) + \min(0, \mu + (\bar{u} - u_a)).$$

The following sets are defined

$$A^- := \{\vec{x} \in Q : \mu + c(u - u_a) < 0\}$$

and

$$A^+ := \{\vec{x} \in Q : \mu + c(u - u_b) > 0\},$$

where  $c > 0$ .

***The primal-Dual Active Set Strategy.***

1. Initialize  $u_0, \mu_0$  and  $n := 0$  and choose  $c > 0$
2. **while**  $n < 1$  or  $\|residual\| > tol$  **do**

Determine the active sets

Solve the equality constrained problem

Update Lagrange multiplier  $\mu$

Evaluate residual

Set  $n := n + 1$

3. **end while**

## CHAPTER 3

### OPTIMIZE-THEN-DISCRETIZE APPROACH USING SPACE-TIME DISCRETIZATION

The optimality system of an optimal control problem is usually integrated iteratively forward and backward in time by gradient based algorithms. Another approach which appeared recently in the literature is to solve both equations at once as systems of coupled elliptic equation in space and time. The transformation of the optimality system into an elliptic pde for linear parabolic distributed optimal control problems with pointwise control constraints was considered in [37, 38, 39, 40]. For distributed optimal control of the unsteady Burgers equation the same approach was used in [71]. It was shown there, that by linearizing the Burgers equation, the forward-backward system containing the state and adjoint equations can be expressed by an elliptic boundary value problem in space-time domain. The elliptic system is then simultaneously discretized in space and time.

This chapter is organized as follows. In Section 1, by using Cole-Hopf transformation the elliptic boundary value problem in space-time domain is obtained for distributed control problem of the unsteady Burgers equation. We obtain biharmonic equation. Because the linear distributed control problems are studied in [39, 40] we do not cover the existence and uniqueness steps for the distributed problem. In Section 2, we consider the boundary control problem. Since the Cole-Hopf transformation yields a nonlinearity in boundary for boundary case we use Taylor approximation for linearizing the boundary control problem. Control constrained and unconstrained problems are covered for both distributed and boundary control problems. Finally, we give the numerical results in Section 3. We compare the gradient-based method and one-shot-approach.

### 3.1 Distributed control problem

The results obtained in this section are studied in [71].

In the sequential approach, the optimality system is solved iteratively using the gradient method. The control variable  $u$  is first initialized and the state equation is solved for  $y$  forwards; the adjoint equation backwards for  $p$  until convergence. In the one-shot approach, the optimality system in the whole space-time cylinder is solved as an elliptic equation by interpreting the time as an additional space variable. This approach was used in [37, 38, 39, 42] by deriving a biharmonic pde from the optimality system for parabolic linear pde control problems. Therefore we will use the nonlinear Cole-Hopf transformation which converts the Burgers equation to a linear parabolic problem.

Cole-Hopf transformation is a Backlund transformation between Burgers equation and the linear heat equation, and it was used to show the existence of the equivalent optimal control problems for the Burgers equation and the transformed linear parabolic pde in [65].

Using the change of variable  $\tilde{y}(x, t) = y(x, t) - y_d(x)$  and instead of  $\tilde{y}(x, t)$  we use  $y(x, t)$ , then, the optimal control problem (P1) defined in Chapter 2 can be stated as follows [65]:

$$\begin{aligned} \min \quad J(y, u) &= \frac{1}{2} \|y\|_Q^2 + \frac{\alpha}{2} \|u\|_Q^2 \\ \text{subject to} \quad y_t - \nu y_{xx} + yy_x + (y y_d)_x + y_d(y_d)_x - \nu(y_d)_{xx} &= u \quad \text{in } Q, \\ y(t, 1) = y(t, 0) &= 0 \quad \text{on } \Sigma, \\ y(0, x) &= y_0(x) \quad \text{in } \Omega. \end{aligned} \quad (3.1)$$

The optimal control problem with a linear diffusion type equation is obtained using the Cole-Hopf transformation [65]

$$y(t, x) = -2\nu \frac{\phi_x}{\phi} = -2\nu(\ln(\phi(t, x)))_x.$$

Substituting this in (3.1), multiplying both side by  $\frac{\phi^2}{2\nu}$  and integrating with respect to  $x$ , we obtain

$$\int_Q \phi_x(\phi_t - \nu\phi_{xx}) - \int_Q \phi(\phi_t - \nu\phi_{xx})_x = \int_Q \phi(\phi_x y_d)_x - \phi_x^2 y_d + \frac{\phi^2}{2}(y_d)_{xx} - \frac{\phi^2}{4\nu}(y_d^2)_x + \frac{\phi^2}{2\nu}u.$$

Integration by parts with  $\phi_x(t, 0) = \phi_x(t, 1) = 0$ ,  $\phi(0, x) = 0$  leads to

$$2 \int_Q \phi_x(\phi_t - \nu\phi_{xx}) = -2 \int_Q \phi_x^2 y_d - \int_Q \phi \phi_x (y_d)_x + \int_Q \frac{1}{2\nu} \phi \phi_x y_d^2 + \int_Q \frac{\phi^2}{2\nu} u,$$

and we obtain

$$\phi_t - \nu\phi_{xx} = -\phi_x y_d - \frac{1}{2}\phi(y_d)_x + \frac{\phi}{4\nu}y_d^2 + \frac{\phi^2}{4\nu\phi_x}u.$$

Optimal control problem becomes

$$\min J(\phi, u) = \frac{1}{2} \|-2\nu(\ln(\phi(t, x)))_x\|_Q^2 + \frac{\alpha}{2} \|u\|_Q^2 \quad (3.2)$$

$$\begin{aligned} \text{subject to } \phi_t - \nu\phi_{xx} + y_d\phi_x - g(x)\phi - m(x, t)\phi &= 0 & \text{in } Q, \\ \phi_x(t, 1) = \phi_x(t, 0) &= 0 & \text{on } \Sigma, \\ \phi(0, x) &= \phi_0(x) & \text{in } \Omega, \end{aligned}$$

where

$$g(x) = \frac{1}{4\nu}y_d^2 - \frac{1}{2}(y_d)_x, \quad m(x, t) = -\frac{1}{2\nu} \left( \int_{\Omega} u dx \right).$$

Because the cost function in (3.2) is a complicated expression, a simplified equivalent form was used in [65]. Let  $J[\phi, u]$  be given by (3.2) and

$$C[\phi, u] = \frac{1}{2} \|\phi\|_Q^2 + \frac{\alpha}{2} \|u\|_Q^2.$$

A function  $\phi^*$  is defined as  $P$ -optimal if  $P[\phi^*] = \min_{\phi} P[\phi]$ . Let  $u^*$  be a fixed control function. Then  $\phi^*$  is  $C$ -optimal implies  $\phi^*$  is  $J$ -optimal also, (see Theorem 1 in [65]). That is

$$C[\phi^*, u^*] = \min J[\phi, u^*] \Rightarrow J[\phi^*, u^*] = \min J[\phi, u^*].$$

The transformed optimal control problem with state and adjoint equations is now given by

$$\min J(\phi, u) = \frac{1}{2} \|\phi\|_Q^2 + \frac{\alpha}{2} \|u\|_Q^2$$

$$\begin{aligned} \text{subject to } \phi_t - \nu\phi_{xx} + y_d\phi_x - g(x)\phi - m(x, t)\phi &= 0 & \text{in } Q, \\ \phi_x(t, 1) = \phi_x(t, 0) &= 0 & \text{on } \Sigma, \\ \phi(0, x) &= \phi_0(x) & \text{in } \Omega, \end{aligned} \quad (3.3)$$

$$\begin{aligned} \psi_t + \nu\psi_{xx} + (y_d\psi)_x + g(x)\psi + m(x, t)\psi - \phi &= 0 & \text{in } Q, \\ \psi_x(t, 1) = \psi_x(t, 0) &= 0 & \text{on } \Sigma, \\ \psi(T, x) &= 0 & \text{in } \Omega. \end{aligned} \quad (3.4)$$

It was shown in [42] that the optimality system for linear parabolic containing equations can be transformed to a biharmonic elliptic pde. The existence and uniqueness of the weak solutions of the optimality systems and its regularization was proved [42]. Following the

same approach we will show that after the Cole-Hopf transformation of the Burgers equation the optimality system (3.3)-(3.4) is equivalent to an elliptic pde. For this purpose, we use the same function spaces defined in [42] as:

$$H^{1,0}(Q) = L^2(0, T, H^1(\Omega)),$$

$$H^{k,1}(Q) = L^2(0, T, H^k(\Omega)) \cap H^{1,0}(0, T, L^2(\Omega)).$$

On  $H^{2,1}(Q)$  we use the inner product

$$(u, v)_{H^{2,1}(Q)} := \int \int_Q uv + \frac{d}{dt}u \frac{d}{dt}v + \nabla u \nabla v + \sum_{i,j=1}^N \left( \frac{\partial^2 u}{\partial x_i \partial x_j} \frac{\partial^2 v}{\partial x_i \partial x_j} \right) dx dt,$$

and natural norm

$$\|u\|_{H^{2,1}(Q)} = \left( \|u\|^2 + \left\| \frac{d}{dt}u \right\|^2 + \|\partial u\|^2 + \sum_{i,j} \left\| \frac{d^2 u}{dx_i dx_j} \right\|^2 \right)^{1/2}.$$

**Theorem 3.1.1** (Biharmonic equation in  $H^{2,1}(Q)$ )

Let  $(\phi, \psi, u)$  are smooth solution of the control problem (3.3-3.4) with  $\phi, \psi \in H^{2,1}(Q), u \in L^2(\Omega)$ . Then  $\psi$  satisfies the following elliptic pde:

$$-\psi_{tt} + v^2 \Delta^2 \psi + c_4 \Delta \psi + c_3 \psi_{xt} + c_2 \psi_x + c_1 \psi_t + c_0 \psi = 0, \quad (3.5)$$

with the boundary conditions

$$\psi_t + v \psi_{xx} + (y_d)_x \psi + (g + m) \psi = 0 \text{ on } \Sigma,$$

$$\psi_x(t, 1) = \psi_x(t, 0) = 0, \quad \psi(T, x) = 0, \quad (3.6)$$

$$\psi_t + v \psi_{xx} + (y_d \psi)_x + (g + m) \psi = y_0 \text{ in } \Omega,$$

where

$$c_0 = v(y_d)_{xxx} + v(g + m)_{xx} - y_d(y_d)_{xx} - y_d(g + m)_x + (g + m)(y_d)_x + (g + m)^2 - m_t - (y_d)_{tx},$$

$$c_1 = g - (y_d)_x,$$

$$c_2 = 2v(g_x + m_x) + 3v(y_d)_{xx} - 2y_d(y_d)_x - (y_d)_t,$$

$$c_3 = -2y_d,$$

$$c_4 = 3v(y_d)_x + 2v(g(x) + m(x, t)) - y_d^2.$$

**Proof.** Take the derivative of the adjoint equation with respect to  $t$

$$-\psi_{tt} = \nu\psi_{xxt} + (y_d\psi)_{xt} + (g\psi + m\psi)_t - \phi_t,$$

inserting  $\phi_t$  in the state equation, yielding,

$$\psi_{tt} + \nu\psi_{xxt} + (y_d\psi)_{xt} + (g\psi + m\psi)_t = \nu\phi_{xx} - y_d\phi_x + (g + m)\phi,$$

and using the adjoint equation to eliminate  $\phi$  give

$$\psi_{tt} + \nu\psi_{xxt} + (y_d\psi)_{xt} + (g\psi + m\psi)_t = \nu(\psi_t + \nu\psi_{xx} + (y_d\psi)_x + g(x)\psi + m(x,t)\psi)_{xx}$$

$$-y_d(\psi_t + \nu\psi_{xx} + (y_d\psi)_x + g(x)\psi + m(x,t)\psi)_x + (g + m)(\psi_t + \nu\psi_{xx} + (y_d\psi)_x + g(x)\psi + m(x,t)\psi).$$

After taking derivatives and simplifying, we obtain the elliptic pde (3.5). Applying the boundary conditions of  $\phi$  and  $\psi$  in Eq. (3.3) and Eq. (3.4), the boundary conditions are obtained for the elliptic pde (3.5). ■

### 3.1.1 Inequality constrained problem and regularization

We consider now distributed optimal control problem with pointwise bilateral control constraints [57]

$$\min J(y, u) = \frac{1}{2} \|y - z\|_Q^2 + \frac{\alpha}{2} \|u\|_Q^2$$

$$\text{subject to } y_t + yy_x - \nu y_{xx} = f + bu \text{ in } Q,$$

$$y = 0 \text{ in } \Sigma,$$

$$y(\cdot, \cdot) = y_0 \text{ in } \Omega,$$

$$u_a(t, x) \leq u(t, x) \leq u_b(t, x) \text{ in } Q.$$

First-order necessary conditions for the optimality system of the local solution  $(y^*, u^*)$  have to be satisfied with the adjoint variable  $p^*$  in form of the optimality system including the control constraints  $u^* \in U_{ad} = \{u \in L_2(Q) : u_a(t, x) \leq u(t, x) \leq u_b(t, x)\}$ . Because of the pointwise constraints, additionally we have the variational inequality [57]

$$\int_Q (\alpha u^* + bp^*)(u - u^*) dxdt \geq 0 \text{ for all } u \in U_{ad}.$$

The last inequality can be expressed in the form of a projection [57]:

$$u^*(t, x) = P_{[u_a(t,x), u_b(t,x)]} \left( \frac{-b(t, x)}{\alpha} p^*(t, x) \right).$$

First order optimality conditions for the control constrained Burgers equation are stated as follows [57]

$$\begin{aligned} y_t - \nu y_{xx} + yy_x &= f + bu & \text{in } Q, \\ y(t, 0) = y(t, 1) &= 0 & \text{on } \Sigma, \\ y(0) &= y_0 & \text{in } \Omega, \end{aligned} \tag{3.7}$$

$$\begin{aligned} p_t + \nu p_{xx} + yp_x &= y_d - y & \text{in } Q, \\ p(t, 0) = p(t, 1) &= 0 & \text{on } \Sigma, \\ p(T) &= 0 & \text{in } \Omega, \end{aligned} \tag{3.8}$$

with the gradient condition

$$\alpha u + p + \mu_b - \mu_a = 0,$$

and complementary slackness conditions

$$\begin{aligned} (\mu_a, u - u_a)_{L^2(Q)} &= 0, \quad u \geq u_a \quad \mu_a \geq 0 \quad \text{in } Q, \\ (\mu_b, u - u_b)_{L^2(Q)} &= 0, \quad u \leq u_b \quad \mu_b \geq 0 \quad \text{in } Q. \end{aligned} \tag{3.9}$$

In [50], different solution algorithms like primal dual-SQP, SQP-primal dual methods and semi smooth Newton method are applied and compared for solving the optimality system the steady Burgers equation with control constraints. We will apply the projection method in [39]. This method is an implementation of the active set strategy as a semi smooth Newton method [28]. The projection method replaces the complementary slackness conditions by a projection. In other words, we will find equivalent conditions to the complementary slackness conditions.

After getting an equivalent form of complementary conditions, we have to solve the following system of equations

$$\begin{aligned} y_t - \nu y_{xx} + yy_x &= f + bu & \text{in } Q, \\ y(t, 0) = y(t, 1) &= 0 & \text{on } \Sigma, \\ y(0) &= y_0 & \text{in } \Omega, \end{aligned}$$

$$\begin{aligned} p_t + \nu p_{xx} + yp_x &= y_d - y & \text{in } Q, \\ p(t, 0) = p(t, 1) &= 0 & \text{on } \Sigma, \\ p(T) &= 0 & \text{in } \Omega, \end{aligned}$$

$$\alpha u + p + \mu_b - \mu_a = 0,$$

$$\mu_a = \max(0, p + \alpha u_a), \quad \mu_b = \max(0, -p - \alpha u_b).$$

### 3.2 Boundary control problem

We recall (Pb2)

$$\min J(y, u, v) = \frac{1}{2} \int_Q (y - y_d)^2 dx + \frac{1}{2} \int_0^T \beta_u |u|^2 + \beta_v |v|^2 dt \quad (3.10)$$

subject to

$$\begin{aligned} y_t + yy_x - \nu y_{xx} &= f & \text{in } Q, \\ \nu y_x(\cdot, 0) + \sigma_0 y(\cdot, 0) &= u & \text{in } (0, T), \\ \nu y_x(\cdot, 1) + \sigma_1 y(\cdot, 1) &= v & \text{in } (0, T), \\ y(0, \cdot) &= y_0 & \text{in } \Omega, \end{aligned} \quad (3.11)$$

and

$$(u, v) \in U_{ad} \times V_{ad} \subset L^2(0, T) \times L^2(0, T). \quad (3.12)$$

For the control constraint case, the sets of admissible controls are given by

$$U_{ad} = \{u \in L^\infty(0, T) : u_a \leq u \leq u_b, \text{ a.e. in } (0, T)\},$$

$$V_{ad} = \{v \in L^\infty(0, T) : v_a \leq v \leq v_b, \text{ a.e. in } (0, T)\},$$

with  $u_a, u_b, v_a, v_b \in L^\infty(0, T)$  and  $u_a \leq u_b$  and  $v_a \leq v_b$  almost everywhere (a.e.) in  $Q$ .

#### 3.2.1 Linearization of the Burgers equation

In order to apply the one-shot approach, Burgers equation is linearized and the linearized parabolic problem is interpreted as an elliptic equation. Before we present the linearized state equation, we denote  $\mathbf{u} = (u, v)^T$ ,  $\sigma = (\sigma_0, \sigma_1)^T$ . We consider the state equation

$$\begin{aligned} y_t - \nu y_{xx} + yy_x &= f & \text{in } Q, \\ \nu y_x + \sigma y &= \mathbf{u} & \text{in } (0, T), \\ y(0, \cdot) &= y_0(x) & \text{in } \Omega \end{aligned} \quad (3.13)$$

The Cole-Hopf transformation is used in [71] to linearize Burgers equation with homogeneous Dirichlet boundary conditions. Because this leads to a nonlinearity in the boundary, we apply standard linearization of [55] to the state equation by using Taylor expansions. The nonlinear term  $yy_x$  in can be written as  $yy_x = \frac{1}{2}(y^2)_x$ .

Taylor expansion of the product of functions  $p(t)q(t)$  at  $(k + 1)$  up to the second order terms can be written as

$$\begin{aligned} p^{k+1}q^{k+1} &= p^kq^k + \left[\frac{\partial}{\partial p}(pq)^k\right](p^{k+1} - q^k) + \left[\frac{\partial}{\partial q}(pq)^k\right](q^{k+1} - q^k) + \mathcal{O}(\delta p^2, \delta q^2) \\ &= p^{k+1}q^k + p^kq^{k+1} - p^kq^k + \mathcal{O}(\delta p^2, \delta q^2), \end{aligned}$$

where  $\delta p = p^{k+1} - p^k$  and  $\delta q = q^{k+1} - q^k$ . Then  $(y^2)_x^{k+1}$  can be linearized as

$$\begin{aligned} (y^2)_x^{k+1} &= (y^{k+1}y^k + y^ky^{k+1} - y^ky^k)_x \\ &= y_x^{k+1}y^k + y^{k+1}y_x^k + y_x^ky^{k+1} + y^ky_x^{k+1} - y_x^ky^k - y^ky_x^k \\ &= 2y_x^{k+1}y^k + 2y^{k+1}y_x^k - 2y_x^ky^k + \mathcal{O}(\delta y_x^2, \delta y^2). \end{aligned} \quad (3.14)$$

Inserting in the state equation (2.5) gives

$$y_t^{k+1} - \nu y_{xx}^{k+1} + y_x^{k+1}y^k + y^{k+1}y_x^k - y_x^ky^k = f, \quad (3.15)$$

where  $y_x^k = \eta$ ,  $y^k = \beta$ ,  $f = \tilde{f} - y_x^ky^k$ . We obtain by defining  $\bar{y} = y^{k+1}$  and denoting  $\bar{y} = y$ , with  $\tilde{y} = y^{k+1} - y_d$  the linearized state equation

$$\begin{aligned} \tilde{y}_t - \nu \tilde{y}_{xx} + \beta \tilde{y}_x + \eta \tilde{y} &= \tilde{f} - \frac{d}{dt}y_d + \nu(y_d)_{xx} - \eta y_d - \beta \frac{d}{dx}y_d, \\ \nu \tilde{y}_x + \sigma \tilde{y} &= \mathbf{u} - \nu(y_d)_x - \sigma y_d \quad \text{in } (0, T), \\ \tilde{y}(0, \cdot) &= y_0(x) - y_d. \end{aligned} \quad (3.16)$$

In order to handle the boundary control problem, the initial condition has to be homogenized as in [71] with  $y = \tilde{y} + \delta$  where  $\delta$  satisfies the necessary boundary conditions

$$\begin{aligned} y_t - \nu y_{xx} + \beta y_x + \eta y &= s \quad \text{in } Q, \\ \nu y_x + \sigma y &= \mathbf{u} \quad \text{in } (0, T), \\ y(0, \cdot) &= 0 \quad \text{in } \Omega, \end{aligned} \quad (3.17)$$

where  $s = \tilde{f} - \frac{d}{dt}y_d + \nu y_d - \eta y_d - \beta \frac{d}{dx}y_d + \frac{d}{dt}\delta - \nu \delta_{xx} + \beta \delta_x + \eta \delta$ .

Then, corresponding adjoint system becomes

$$\begin{aligned} -p_t - \nu p_{xx} + \eta p - \beta p_x &= y \quad \text{in } Q, \\ \nu p_x + (\sigma + \beta)p &= 0 \quad \text{in } (0, T), \\ p(T, \cdot) &= 0 \quad \text{in } \Omega. \end{aligned} \quad (3.18)$$

### 3.2.2 Equivalence to the biharmonic pde

It was shown in [40, 42] that the optimality system for linear parabolic equations can be transformed to a  $H^{2,1}$ -elliptic pde. Similarly for the distributed control problem with the unsteady Burgers equation [71], the linearized optimality system was transformed to a  $H^{2,1}$ -elliptic pde in the adjoint variable  $p$ , so that the time variable can be treated as an additional space variable as in [40, 42, 71]. Following the approach in [42] we will prove the existence and uniqueness of the weak solutions of the optimality conditions and their regularization. In fact, a control problem subject to the following linear parabolic problem

$$\begin{aligned} y_t + \nu y_{xx} + c_0 y &= u & \text{in } Q, \\ \vec{n} \cdot \nabla y &= g & \text{in } (0, T), \\ y(0) &= y_0 & \text{in } \Omega, \end{aligned}$$

was studied in [40, 42]. In this section we will extend works in [40, 42] to a control problem having a linearized parabolic pde as constraint. Since we handle boundary control problem, the main difference from [40, 42] is non homogeneous boundary terms. So that our results will be an extension of [40, 42] to a linearized boundary control problem.

We introduce two Hilbert spaces that we need in the weak formulation of the optimality system.

#### Definition 3.2.1

$$H^{2,1}(Q) := L^2(0, T, H^2(\Omega)) \cap H^1(0, T, L^2(\Omega))$$

is a Hilbert space with the inner product

$$(u, v)_{H^{2,1}(Q)} := \iint_Q uv + \frac{\partial}{\partial t} u \frac{\partial}{\partial t} v + \nabla u \nabla v + \sum_{i,j=1}^N \left( \frac{\partial^2 u}{\partial x_i \partial x_j} \frac{\partial^2 v}{\partial x_i \partial x_j} \right) dx dt,$$

and with the natural norm

$$\|u\|_{H^{2,1}(Q)} = \left( \|u\|^2 + \left\| \frac{\partial}{\partial t} u \right\|^2 + \|\nabla u\|^2 + \sum_{i,j} \left\| \frac{\partial^2 u}{\partial x_i \partial x_j} \right\|^2 \right)^{1/2},$$

$$\bar{H}^{2,1}(Q) := \{u \in H^{2,1}(Q) : \nu u_x + (\beta + \sigma)u = 0 \text{ and } u(T) = 0\}.$$

The Laplace and gradient operator are given by  $\Delta = \frac{\partial^2}{\partial x^2}$  and  $\nabla = \frac{\partial}{\partial x}$ , respectively. Since  $H^1(0, T)$  is continuously embedded in  $C(0, T)$ , for  $u \in H^{2,1}(Q)$  the functions  $u(0) := u(0, \cdot)$ ,  $u(T) := u(T, \cdot)$  both are well defined in  $L^2(\Omega)$ . The space  $\bar{H}^{2,1}(Q)$  is an analog to the space used in [6] for a problem with homogenous Dirichlet boundary conditions.

For  $u, v \in H^{2,1}(Q)$  we define

$$(u, v)_{H_{\Delta}^{2,1}(Q)} := \iint_Q (uv + u_t v_t + \nabla u \cdot \nabla v + \Delta u \Delta v) dx dt$$

which is clearly an inner product on  $H^{2,1}(Q)$ . And a norm on  $H^{2,1}(Q)$  is defined as

$$\|u\|_{H_{\Delta}^{2,1}} = \left( \|u\|^2 + \left\| \frac{\partial}{\partial t} u \right\|^2 + \|\nabla u\|^2 + \|\Delta u\|^2 \right)^{1/2}.$$

**Theorem 3.2.2** *Let  $(y, u, p)$  be smooth solution of the control problem (3.17)-(3.18) with  $y, p \in \bar{H}^{2,1}(Q)$  and  $u \in L^2(0, T)$ . Then  $p$  satisfies the following PDE*

$$-p_{tt} + v^2 \Delta^2 p - (2\eta v + \beta^2) \Delta p - 2\beta p_{xt} + \eta^2 p = s, \quad \text{in } Q \quad (3.19a)$$

with the boundary conditions

$$-v^2 \nabla(\Delta p) - v(\beta + \sigma) \Delta p + (v\eta - \sigma\beta) \nabla p + \beta p_t + \sigma \eta p = \mathbf{u} \quad \text{in } (0, T), \quad (3.19b)$$

$$v \nabla p + (\sigma + \beta) p = 0 \quad \text{in } (0, T), \quad (3.19c)$$

$$-p_t(0, \cdot) - v \Delta p(0, \cdot) - \beta \nabla p(0, \cdot) + \eta p(0, \cdot) = 0 \quad \text{in } \Omega, \quad (3.19d)$$

$$p(T, \cdot) = 0 \quad \text{in } \Omega. \quad (3.19e)$$

**Proof.** Taking the derivative of the adjoint equation with respect to  $t$

$$-p_{tt} - v \frac{d}{dt} \Delta p + \eta p_t - \beta \frac{d}{dt} p_x = y_t,$$

and inserting  $y_t$  in the state equation, we obtain

$$-p_{tt} - v \frac{d}{dt} \Delta p + \eta p_t - \beta \frac{d}{dt} p_x = v \Delta y - \beta \nabla y - \eta y + s.$$

We eliminate  $y$  by using the adjoint equation (3.18)

$$\begin{aligned} -p_{tt} &- v \frac{d}{dt} \Delta p + \eta p_t - \beta \frac{d}{dt} \nabla p = v \Delta(-p_t - v \Delta p + \eta p - \beta \nabla p) \\ &- \beta \nabla(-p_t - v \Delta p + \eta p - \beta \nabla p) - \eta(-p_t - v \Delta p + \eta p - \beta \nabla p) + s. \end{aligned}$$

After taking derivatives and simplifying, we obtain the elliptic pde (3.19a).

We evaluate  $y = -p_t - \nu\Delta p + \eta p - \beta\nabla p$  on the boundary to obtain

$$\nu(-p_{tx} - \nu\nabla(\Delta)p - \beta\Delta p + \eta\nabla p) + \sigma(-p_t - \nu\Delta p - \beta\nabla p + \eta p) = \mathbf{u}.$$

Using the original boundary condition  $\nu\nabla p + (\sigma + \beta)p = 0$ , (3.19b) and (3.19c) are obtained.

By setting  $t = 0$  gives  $y = -p_t - \nu\Delta p - \beta\nabla p + \eta p = 0$  and  $t = T$  we get (3.19d) and (3.19e). ■

**Lemma 3.2.3** *The solution  $p$  of the equation (3.19a) satisfies*

$$a[p, w] = F(w) \quad \forall w \in \bar{H}^{2,1}(Q),$$

where  $F(w) = \iint_Q sw dx dt + \int_0^T \mathbf{u}w|_0^1 dt$  and

$$\begin{aligned} a[p, w] &= \iint_Q \left( \frac{d}{dt}p \frac{d}{dt}w + \nu^2 \Delta p \Delta w + (2\eta\nu + \beta^2) \nabla p \nabla w + \eta^2 p w + 2\beta \nabla p \frac{d}{dt}w \right) dx dt \\ &+ \int_{\Omega} (p_t(0, x) + 2\beta \nabla p(x, 0))w(x, 0) dx + \int_0^T (\gamma p + \beta p_t)w|_0^1 dt \end{aligned}$$

**Proof.** We apply a test function  $w \in \bar{H}^{2,1}(Q)$  to (3.19a) to obtain the weak form

$$\iint_Q -\frac{d^2}{dt^2}pw + \nu^2 \Delta^2 pw - \beta^2 \Delta pw - 2\beta p_{xt}w + \eta^2 p w dx dt = \iint_Q sw dx dt.$$

Integration by parts yields

$$\begin{aligned} &\iint_Q -\frac{d^2}{dt^2}pw + \nu^2 \Delta^2 pw - (2\eta\nu + \beta^2) \Delta pw - 2\beta p_{xt}w + \eta^2 p w dx dt \\ &= - \int_{\Omega} \frac{d}{dt}pw|_0^T dx + \iint_Q \frac{d}{dt}p \frac{d}{dt}w dx dt + \int_0^T \nu^2 \nabla(\Delta p)w|_0^1 dt - \int_0^T \nu^2 \Delta p \nabla w|_0^1 dt \\ &+ \iint_Q \nu^2 \Delta p \Delta w dx dt - (2\eta\nu + \beta^2) \int_0^T \nabla p w|_0^1 dt + \iint_Q (2\eta\nu + \beta^2) \nabla p \nabla w dx dt \\ &- 2\beta \int_{\Omega} \nabla p w|_0^T dx + \iint_Q 2\beta \nabla p \frac{d}{dt}w dx dt + \iint_Q \eta^2 p w dx dt. \end{aligned}$$

From the boundary conditions  $\nu w_x + (\sigma + \beta)w = 0$ , we obtain  $\nabla w = -\frac{\sigma + \beta}{\nu}w$ . Using  $\nu^2 \nabla(\Delta p) + \nu(\sigma + \beta)\Delta p = (\nu\eta - \sigma\beta)\nabla p + \beta p_t + \sigma\eta p - u$  and  $\nabla p = -\frac{\sigma + \beta}{\nu}p$  and letting  $\gamma = \frac{\eta\nu(\beta + 2\sigma) + \sigma\beta(\sigma + 2\beta)}{\nu}$  gives

$$\int_0^T (\nu^2 \nabla(\Delta p) + \nu(\sigma + \beta)\Delta p - (2\nu\eta + \beta^2)\nabla p)w|_0^1 dt = \int_0^T (\gamma p + \beta p_t - \mathbf{u})w|_0^1 dt.$$

Also,  $w(x, T) = 0$  implies

$$-\int_{\Omega} \frac{d}{dt} pw \Big|_0^T dx - 2\beta \int_{\Omega} \nabla pw \Big|_0^T dx = \int_{\Omega} \left( \frac{d}{dt} p(x, 0) + 2\beta \nabla p(x, 0) \right) w(\cdot, 0) dx.$$

Defining

$$F(w) := \iint_Q sw + \int_0^T \mathbf{u}w \Big|_0^1 dt$$

gives the desired result. ■

**Lemma 3.2.4** *The bilinear form is  $H^{2,1}$ -elliptic, i.e. there is a constant  $c > 0$  such that*

$$a[v, v] \geq c \|v\|_{H_{\Delta}^{1,2}(Q)}^2$$

for all  $v \in \tilde{H}^{2,1}(Q)$ .

**Proof.** By choosing  $v \in H^{2,1}(Q)$  we evaluate  $a[v, v]$ .

$$\begin{aligned} a[v, v] &= \iint_Q \left( \left( \frac{d}{dt} v \right)^2 + v^2 (\Delta v)^2 + (2\eta v + \beta^2) (\nabla v)^2 + \eta^2 v^2 + 2\beta \nabla v \frac{d}{dt} v \right) dx dt \\ &+ \int_{\Omega} \left( -v \Delta v(0, x) + \beta \nabla v(x, 0) + \eta v(x, 0) \right) v(x, 0) dx + \int_0^T (\gamma v + \beta v_t) v \Big|_0^1 dt. \end{aligned}$$

The last term becomes

$$\int_0^T (\gamma v + \beta v_t) v \Big|_0^1 dt = \int_0^T \gamma v v \Big|_0^1 dt + \int_0^T \beta v_t v \Big|_0^1 dt = \int_0^T \gamma v v \Big|_0^1 dt - \frac{\beta}{2} v^2(0, \cdot) \Big|_0^1.$$

Also

$$\begin{aligned} &\int_{\Omega} \left( -v \Delta v + \beta \nabla v + \eta v \right) v dx \\ &= -v \nabla v v \Big|_0^1 + v \int_{\Omega} \nabla v \nabla v dx + \beta \int_{\Omega} \nabla v v dx + \eta \int_{\Omega} v v dx \\ &= (\beta + \sigma) v v \Big|_0^1 + v \int_{\Omega} \nabla v \nabla v dx + \frac{\beta}{2} v^2 \Big|_0^1 + \eta \int_{\Omega} v v dx, \end{aligned}$$

where all terms above are evaluated at  $t = 0$ .

For the ellipticity we need the following assumptions:

- appropriate choice of  $\sigma$  gives  $\gamma v v \Big|_0^1 \geq 0$  and  $(\beta + \sigma) v v \Big|_0^1 \geq 0$ ,
- $\beta \nabla v \frac{d}{dt} v \leq 0$  in  $Q$ .

By using these assumptions, we obtain

$$\begin{aligned} a[v, v] &\geq \min \{1, v^2, 2\eta v + \beta^2, \eta^2\} \iint_Q \left( \left( \frac{d}{dt} v \right)^2 + (\Delta v)^2 + (\nabla v)^2 + v^2 \right) dx dt \\ &= c \|v\|_{H_{\Delta}^{2,1}(Q)}^2 \geq c \|v\|_{H^{2,1}(Q)}^2, \end{aligned}$$

which proves the  $H^{2,1}$  ellipticity ■

**Lemma 3.2.5** *The bilinear form  $a[v, w]$  is bounded in  $\bar{H}^{2,1}(Q)$ , i.e.,*

$$a[v, w] \leq c \|v\|_{H^{2,1}(Q)} \|w\|_{H^{2,1}(Q)}$$

for all  $v, w \in \bar{H}^{2,1}(Q)$ .

**Proof.** The proof is similar to the Lemma 3.5. in [40, 42].

In the following let  $c$  be a generic constant. We have  $v, w \in H^{2,1}(Q) \hookrightarrow C([0, T], H^1(\Omega))$ .

Using the inner product on the space  $H^{2,1}(Q)$  we obtain

$$\begin{aligned} |(\nabla v(0), w(0))_{L^2(\Omega)}| &\leq \|\nabla v(0)\|_{L^2(\Omega)} \|w(0)\|_{L^2(\Omega)} \\ &\leq c \|v(0)\|_{H^1(\Omega)} \|w(0)\|_{H^1(\Omega)} \\ &\leq c \|v\|_{C(0,T;H^1(\Omega))} \|w\|_{C(0,T;H^1(\Omega))} \\ &\leq c \|v\|_{H^{2,1}(Q)} \|w\|_{H^{2,1}(Q)}. \end{aligned}$$

By a similar argument, the terms  $|(\frac{d}{dt}v(0), w(0))_{L^2(\Omega)}|$ ,  $|\gamma(v, w)_{L^2(0,T)}|$ ,  $|\frac{d}{dt}v, w)_{L^2(0,T)}|$  and  $|2\beta(\nabla v, w_t)_{L^2(Q)}|$  are bounded by  $c\|v\|_{H^{2,1}(Q)}\|w\|_{H^{2,1}(Q)}$ .

Proceeding the same structure as in [42], the bilinear form can be bounded as

$$|a[v, w]| \leq c \|v\|_{H^{2,1}(Q)} \|w\|_{H^{2,1}(Q)}.$$

■

Using the Lemma 3.2.4, Lemma 3.2.5 and the Lax-Milgram theorem the main theorem can be stated as

**Theorem 3.2.6** *By continuity and coercivity of  $a$ , for all  $F \in (\bar{H}^{2,1}(Q))^*$  the bilinear equation*

$$a[p, w] = F(w) \quad \forall w \in \bar{H}^{2,1}(Q)$$

has a unique solution  $p \in \bar{H}^{2,1}(Q)$ .

### 3.2.3 Inequality constrained problem and regularization

In this subsection, we consider the regularization of inequality constrained optimal control problems.

We first describe the optimality system in terms of projections, which is a source of non-differentiability when solving the optimality systems. We therefore introduce a regularized projection formula in the following subsection and show convergence of the associated solutions. The projection defined below differs in space from the projection defined in [42].

**Definition 3.2.7** *Let  $a, b, z \in \mathbb{R}$  be given real numbers. We define the projection*

$$\mathbb{P}_{[a,b]}[z] := \pi_{[a(t),b(t)]}\{z(t)\} \quad \forall t \in (0, T).$$

*Let us state without proof some helpful properties of the projection.*

*The projection  $\mathbb{P}_{[a,b]}[z]$  satisfies*

$$(i) \quad -\mathbb{P}_{[a,b]}[-z] = \mathbb{P}_{[-b,-a]}[z],$$

$$(ii) \quad \mathbb{P}_{[a,b]}[z] \text{ is strongly monotone increasing, i.e., by } z_1 < z_2 \text{ follows } \mathbb{P}_{[a,b]}[z_1] \leq \mathbb{P}_{[a,b]}[z_2] \\ \text{and } \mathbb{P}_{[a,b]}[z_1] = \mathbb{P}_{[a,b]}[z_2] \text{ iff } z_1 = z_2,$$

$$(iii) \quad \mathbb{P}_{[a,b]}[z] \text{ is continuous and measurable.}$$

From variational inequality we have

$$u^* = \mathbb{P}_{[u_a(t),u_b(t)]}\left\{\frac{p(0,t)}{\beta_u}\right\} \text{ and } v^* = \mathbb{P}_{[v_a(t),v_b(t)]}\left\{-\frac{p(1,t)}{\beta_v}\right\}.$$

Similar to Theorem 3.2.2, we obtain the biharmonic pde

$$-p_{tt} + v^2 \Delta^2 p - (2\eta v + \beta^2) \Delta p - 2\beta p_{xt} + \eta^2 p = s \quad (3.20)$$

with the boundary conditions

$$\begin{aligned} -v^2 \nabla(\Delta p) - v(\beta + \sigma) \Delta p + (v\eta - \sigma\beta) \nabla p + \beta p_t + \sigma \eta p &= \mathbb{P}_{[u_a(t),u_b(t)]}\left\{\frac{p(0,t)}{\beta_u}\right\}, \\ -v^2 \nabla(\Delta p) - v(\beta + \sigma) \Delta p + (v\eta - \sigma\beta) \nabla p + \beta p_t + \sigma \eta p &= \mathbb{P}_{[v_a(t),v_b(t)]}\left\{-\frac{p(1,t)}{\beta_v}\right\}, \\ v p_x + (\sigma + \beta) p &= 0, \\ -p_{0,\cdot} - v p_{xx}(0, \cdot) - \beta p_x(0, \cdot) + \eta p(0, \cdot) &= 0, \\ p(T, \cdot) &= 0. \end{aligned}$$

**Theorem 3.2.8** *We define the operators as*

$A = A_1 + A_2$ ,  $\langle A_1 r, w \rangle = a[r, w]$  and weak formulation of (3.20) as

$$\langle A_2 r, w \rangle = \int_0^T \left( \mathbb{P}_{[-v_b, -v_a]} \left\{ \frac{r(1, t)}{\beta_v} \right\} w(1, t) + \mathbb{P}_{[u_a, u_b]} \left\{ \frac{r(0, t)}{\beta_u} \right\} w(0, t) \right) dt.$$

Then biharmonic form is equivalent to

$$Ap = \bar{F}, \quad (3.21)$$

where  $\bar{F} = \iint_Q sw dx dt$

**Lemma 3.2.9** *The operator  $A$  defined in Theorem 1 is strongly monotone, coercive, and hemi-continuous.*

**Proof.** Let us first show that  $A$  is strongly monotone. From Lemma 3.2.4 we have

$$\langle A_1(w_1 - w_2), w_1 - w_2 \rangle = a[w_1 - w_2, w_1 - w_2] \geq c \|w\|_{H^{1,2}(Q)}^2.$$

By monotonicity of the projection we have

$$\int_0^T \left( \mathbb{P}_{[u_a, u_b]} \left\{ -\frac{w_1(0, t)}{\beta_u} \right\} - \mathbb{P}_{[u_a, u_b]} \left\{ \frac{w_2(0, t)}{\beta_u} \right\} \right) (v_1(0, t) - v_2(0, t)) dt \geq 0.$$

Similarly,

$$\int_0^T \left( \mathbb{P}_{[-v_b, -v_a]} \left\{ \frac{w_1(1, t)}{\beta_v} \right\} - \mathbb{P}_{[-v_b, -v_a]} \left\{ \frac{w_2(1, t)}{\beta_v} \right\} \right) (v_1(1, t) - v_2(1, t)) dt \geq 0.$$

To prove coercivity we have to estimate  $\langle A_2 w, w \rangle$ . We observe first that

$$\mathbb{P}_{[u_a, u_b]} \left\{ \frac{w}{\beta_u} \right\} w = \begin{cases} u_a w & \text{in } \Sigma_{u_a} := \{t \in (0, T) : w < u_a\}, \\ u_b w & \text{in } \Sigma_{u_b} := \{t \in (0, T) : w > u_b\}, \\ \frac{w^2}{\beta_u} & \text{in } (0, T) \setminus \{\Sigma_{u_a} \cup \Sigma_{u_b}\}. \end{cases} \quad (3.22)$$

Similarly

$$\mathbb{P}_{[-v_b, -v_a]} \{w\} w = \begin{cases} -v_a w & \text{in } \Sigma_{v_a} := \{t \in (0, T) : w > -v_a\}, \\ -v_b w & \text{in } \Sigma_{v_b} := \{t \in (0, T) : w < -v_b\}, \\ \frac{w^2}{\beta_v} & \text{in } (0, T) \setminus \{\Sigma_{v_a} \cup \Sigma_{v_b}\}. \end{cases} \quad (3.23)$$

Hence,

$$\begin{aligned}
& \int_0^T \left( \mathbb{P}_{[u_a, u_b]} \left\{ \frac{w(0, t)}{\beta_u} \right\} w(0, t) \right) dt \\
&= \int_{\Sigma_{u_a}} u_a(0, t) w(0, t) dt + \int_{\Sigma_{u_b}} u_b(0, t) w(0, t) dt + \int_{(0, T) \setminus \{\Sigma_{u_a} \cup \Sigma_{u_b}\}} w(0, t)^2 dt \\
&\geq \int_{\Sigma_{u_a}} u_a(t, 0) w(t, 0) dt + \int_{\Sigma_{u_b}} u_b(t, 0) w(t, 0) dt
\end{aligned}$$

and, similarly,

$$\int_0^T \left( \mathbb{P}_{[-v_b, -v_a]} \left\{ \frac{w(t, 1)}{\beta_v} \right\} w(t, 1) \right) dt \geq - \int_{\Sigma_{v_a}} v_a(t, 1) w(t, 1) dt - \int_{\Sigma_{v_b}} v_b(t, 1) w(t, 1) dt.$$

From Theorem 3.2.8 we have

$$\begin{aligned}
\langle Aw, w \rangle &= \langle A_1 w, w \rangle + \langle A_2 w, w \rangle \\
&= a[w, w] + \int_0^T \left( \mathbb{P}_{[-v_b, -v_a]} \left\{ \frac{w(t, 1)}{\beta_v} \right\} w(t, 1) \right) dt + \int_0^T \left( \mathbb{P}_{[u_a, u_b]} \left\{ \frac{w(t, 0)}{\beta_u} \right\} w(t, 0) \right) dt \\
&\geq c \|w\|_{H^{2,1}(Q)}^2 - \int_{\Sigma_{v_a}} v_a(t, 1) w(t, 1) dt - \int_{\Sigma_{v_b}} v_b(t, 1) w(t, 1) dt \\
&\quad + \int_{\Sigma_{u_a}} u_a(t, 0) w(t, 0) dt + \int_{\Sigma_{u_b}} u_b(t, 0) w(t, 0) dt.
\end{aligned}$$

If the integrals  $\int_{\Sigma_{u_a}} u_a(t, 0) w(t, 0) dt$  and  $\int_{\Sigma_{u_b}} u_b(t, 0) w(t, 0) dt$  are positive then

$$\langle Aw, w \rangle \geq c \|w\|_{H^{2,1}(Q)}^2 - (\|v_a\|_{L^2(\Sigma_{v_a})} + \|v_b\|_{L^2(\Sigma_{v_b})}) \|w\|_{H^{2,1}(Q)}.$$

We get

$$\frac{\langle Aw, w \rangle}{\|w\|_{H^{2,1}(Q)}} \geq c \|w\|_{H^{2,1}(Q)} - \frac{c_{a,b} \|w\|_{H^{2,1}(Q)}}{\|w\|_{H^{2,1}(Q)}}$$

with  $c_{a,b} = \|v_a\|_{L^2(\Sigma_{v_a})} + \|v_b\|_{L^2(\Sigma_{v_b})}$ .

Similarly, if the integrals are negative then

$$c_{a,b} = \|v_a\|_{L^2(\Sigma_{v_a})} + \|v_b\|_{L^2(\Sigma_{v_b})} + \|u_a\|_{L^2(\Sigma_{u_a})} + \|u_b\|_{L^2(\Sigma_{u_b})},$$

and if one of them is negative and the other is positive then the constants are

$$c_{a,b} = \|v_a\|_{L^2(\Sigma_{v_a})} + \|v_b\|_{L^2(\Sigma_{v_b})} \text{ or } c_{a,b} = \|u_a\|_{L^2(\Sigma_{u_a})} + \|u_b\|_{L^2(\Sigma_{u_b})}.$$

The hemi-continuity of  $A$  can be shown as in [37]. ■

Now we are able to use the main theorem on monotone operators to show the existence of a unique solution of (3.21).

**Theorem 3.2.10** *The biharmonic equation (3.21) has a unique solution  $p \in \bar{H}^{2,1}(Q)$  for all  $\bar{F} \in (\bar{H}^{2,1}(Q))^*$ .*

**Proof.** This follows by applying Theorem 4.1 from [58] to

$$Ap = \bar{F},$$

where  $A$  is defined in Theorem 1 ■

### 3.3 Implementation details

Numerical solutions are obtained with equation based modeling and simulation environment COMSOL Multiphysics. This software provides an easy discretization and a fast solution for both steady and unsteady time dependent control problems. We show that the finite element package of COMSOL Multiphysics can be used for solving time-dependent non-linear optimal control problems after transforming to a linear problem. When the optimality conditions are available in for of PDE's, the specialized finite elements solvers can be easily implementable.

Quadratic finite elements are used for the state  $y$  and the adjoint variable  $p$ . We use two different solvers of COMSOL Multiphysics; **adaption**, which solves the elliptic PDE using adaptive mesh refinement , and the **femnlm** that solves nonlinear problems without adaptation.

```
fem.xmesh=meshextend(fem);
fem=adaption(fem);
OR fem.sol=femnlm(fem);
```

The **fem** structure in COMSOL Multiphysics contains the geometry of the domain, the coefficients of the **PDE's**, etc. As an example we give the following lines from the one-shot approach for control constrained problem:

```
fem.form='general'; fem.globalexpr= {'u' '-(p+mu)/alpha' };
fem.equ.ga= { { {'-nu*yx' '0'} {'-nu*px' '0'} {'0' '0'} } };
```

```

fem.equ.f= { {'-ytime-(p+mu)/alpha-y*yx' 'ptime+y-zd(x,time)+y*px'
...'(1/alpha)*mu-max(0,-0.3-(1/alpha)*p)' } };
fem.bnd.ind=[1 2 3 2];
%Boundary conditions
fem.bnd.r= { {'y-y0(x)' 0 0 };{'y' 'p' 0 }; {0 'p' 0 } };
fem.bnd.g= { {0 0 0 }; {0 0 0 };{0 0 0 } };
% Postprocessing
postplot(fem,'tridata','y','triz','y')

```

For the control constrained problem we used quadratic finite elements like in the unconstrained case for state and adjoint state variables, but for the Lagrange multiplier  $\mu$ , linear finite elements are taken as in [39].

The projection method [38] that is an implementation of the active set strategy as a semi-smooth Newton method [28] for a boundary control problem is implemented in COMSOL multiphysics as

```

fem.globalexpr={'mu_a' 'max(0,ua(time)*alpha0-p)'
'mu_b' 'max(0,-ub(time)*alpha0+p)' '$\xi_a$'
'max(0,va(time)*alpha1+p)' '$\xi_b$' 'max(0,-vb(time)*alpha1-p)'}

```

### 3.3.1 Mesh independence

We obtain a finite dimensional optimal control problem by using finite element methods. If we let  $x^k$  and  $x_h^k$  be the solutions to infinite and finite dimensional problems respectively, it is natural to ask about the behaviours of solutions as  $h \rightarrow 0$ . We say that the solution method is mesh independent if the convergence behavior of  $x^k$  and  $x_h^k$  gets more alike when  $h \rightarrow 0$ . The mesh independence of Newton-like methods are studied in [22]. Similarly, the mesh independence of SQP and semi-smooth Newton methods are analyzed in [67] and [64], respectively.

The built-in nonlinear solver *femnlm* is an affine invariant form of the damped Newton method. In order to show the mesh-independence as in [66], we use the relative error es-

timator in *femnlm*, according this the nonlinear iterations terminate.

The solver *femnlm* we use is an affine invariant form of the damped Newton method. We used different tolerances to end the algorithm. The value in the relative tolerance edit field applies to a convergence criterion based on a weighted Euclidean norm for the estimated relative error; the solver iterations stop when the relative error is less than the relative tolerance.

Let  $U$  be the current approximation to the true solution vector, and let  $E$  be the estimated error in this vector. The software stops the iterations when the relative tolerance exceeds the relative error computed as the weighted Euclidean norm :

$$err = \left( \frac{1}{N} \sum_{i=1}^N (|E_i|/W_i)^2 \right)^{1/2} .$$

Here,  $N$  is the number of degrees of freedom and  $W_i = \max(|U_i|, S_i)$ , where  $S_i$  denotes the scaling which is the average of  $|U_j|$  for all degrees of freedom  $j$ .

Mesh-independence was observed numerically for the one-shot approach for the unconstrained and control constrained problems.

### 3.4 Numerical Results

Parabolic optimal control problems with and without constraints were solved using COMSOL Multiphysics [37, 38, 39, 40]. COMSOL Multiphysics was used in [71] for the solution of distributed optimal control of the unsteady Burgers equation.

Both classical gradient based approach solving the state equation forward in time and the adjoint equation backward in time and solving the the whole optimality system as an biharmonic equation produces satisfactory results for the Burgers equation.

**Run 3.1** (*Distributed control problem without control constraint*)

We have chosen the following optimal control problem in [66] with the parameters  $\alpha = 0.05$ ,  $\nu = 0.01$ ,  $f = 0$ , with the desired state  $y_d(t, x) = y_0$  and with the initial condition

$$y_0 = \begin{cases} 1 & \text{in } (0, \frac{1}{2}], \\ 0 & \text{otherwise.} \end{cases}$$

The numerical results for different space and time meshes are given in Table 3.1. The same

Table 3.1: Gradient method for the unconstrained optimal control problem.

$\Delta x_{max} = \Delta t_{max}$	$\ J(y_h, u_h)\ _Q$	# iterations
$2^{-2}$	0.09393	22
$2^{-3}$	0.06725	32
$2^{-4}$	0.07233	46
$2^{-5}$	0.06926	73
$2^{-6}$	0.06778	74
$2^{-7}$	0.06716	53
$2^{-8}$	0.06687	117
$2^{-9}$	0.06674	126

problem was solved in [66] with augmented Lagrangian SQP method, and for a given tolerance  $\epsilon$ , mesh-independence, the convergence of the number of steps required in the finite dimensional optimization methods for sufficiently small meshes and for different mesh-sizes, was observed numerically. In our case, the convergence of the gradient method is controlled by the difference of the current value of  $J(u)$  and the average of the last and first values of  $J(u)$  as in [38]. Therefore, a similar behavior for the number of iterations as in [66] is given in Table 3.1.

Figure 1 shows the computed optimal control  $u_h$ , the computed optimal state  $y_h$  and the associated adjoint state  $u_h$  for the one-shot approach with adaptation for  $h = \Delta x_{max} = 2^{-6}$ . The numerical solutions obtained by the gradient method and by the one-shot approach without adaptation are similar to those in Figure 3.1. The adaptive mesh for  $h = \Delta x_{max} = 2^{-4}$  is given in Figure 3.2. The numerical results for the optimal control and optimal state shown in the Figure 3.1 are similar to those obtained in [66].

The numerical results for different mesh sizes are given in Table 3.2.

As indicated in [67], when a solution method is applied to a nonlinear equation and to a finite

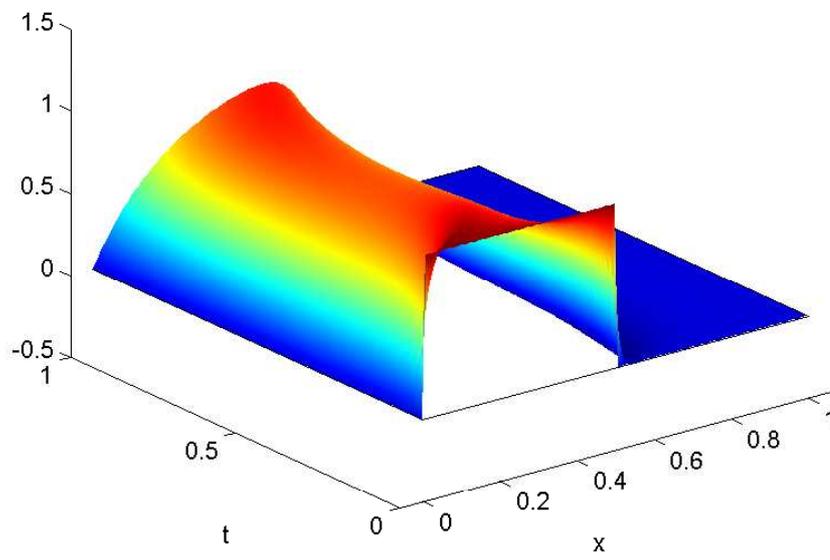
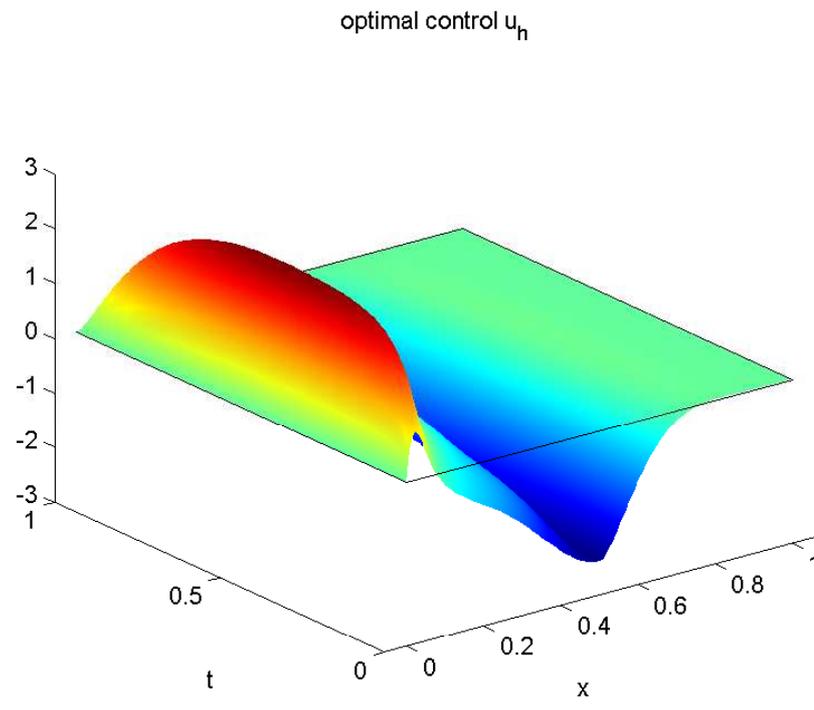


Figure 3.1: One-shot approach with adaptation for the unconstrained problem with distributed control.

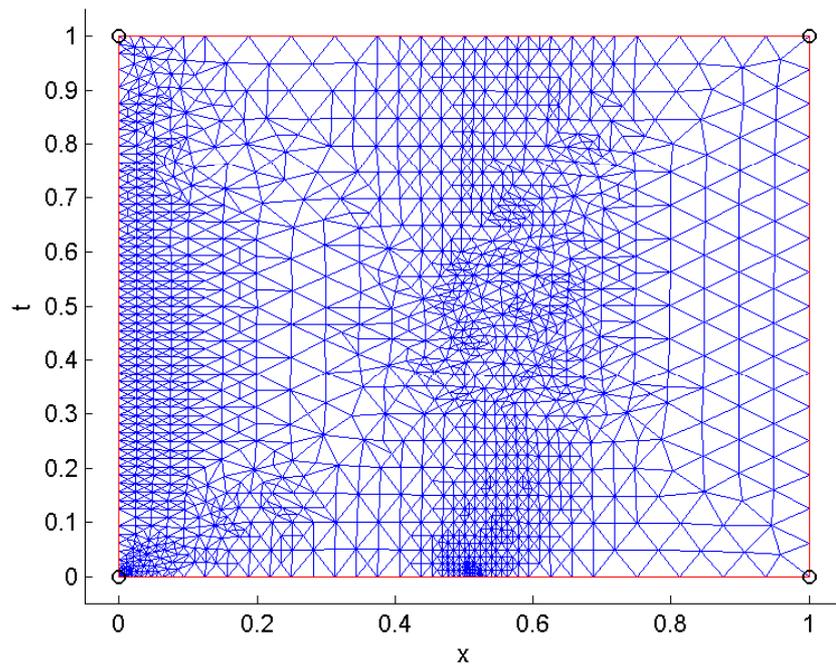


Figure 3.2: Adaptive mesh of the one-shot approach for the unconstrained problem with distributed control.

Table 3.2: One-shot approach for the unconstrained control problem with distributed control.

$\Delta x_{\max}$	$\ J(y, u)\ _Q$ with adaption	$\ J(y, u)\ _Q$ with femlin
$2^{-2}$	0.0683	0.0276
$2^{-3}$	0.0663	0.0651
$2^{-4}$	0.0667	0.0686
$2^{-5}$	0.0667	0.0671
$2^{-6}$	0.0667	0.0669
$2^{-7}$	0.0667	0.0667

dimensional discretization of the equation, the behavior of the discretized process is asymptotically the same. As a consequence of this, the number of steps required needed to satisfy a given stopping criterion to converge, tends asymptotically to a constant value, which is known as mesh-independence. In Table 3.3, for different mesh-sizes and tolerances the number of iterations are given. For sufficiently small mesh-sizes and tolerances, mesh-independence can be observed numerically.

Table 3.3: Mesh independence for Run 3.1.

tol \ $\Delta x_{\max}$	$2^{-2}$	$2^{-3}$	$2^{-4}$	$2^{-5}$	$2^{-6}$	$2^{-7}$
1e-1	4	4	4	4	4	4
1e-3	5	5	5	5	5	5
1e-5	5	5	5	5	5	5
1e-7	6	6	6	6	6	6
1e-9	6	6	6	6	6	6
1e-11	6	6	6	6	6	6

**Run 3.2.** (*Distributed control problem with control constraint*)

We consider the unilaterally control constrained bounded problem ( $u \leq u_b$ ) with the initial condition  $y_0 = \sin(13x)$ ,  $\nu = 0.1$ ,  $u_b = 0.3$  and regularization parameter  $\alpha = 0.01$  in [50]. The desired state is taken as the initial condition  $y_d = y_0$ .

As for the unconstrained optimal control of Burgers equation, we use one shot approach and iterative approach.

In the following code, the state equation is solved using the iterative approach:

```
fem.equ.f = { {'u-y*yx';0;0;0;0} }
fem=femdiff(fem)
fem.bnd.r = { {'y';0;0;0;0} }
fem.xmesh = meshextend(fem)
fem.sol = femtime(fem,'solcomp',{'y'},'outcomp',
{'y','p','u','uold','mu'},'u',fem.sol,'tlist',[0,1],
... 'tout','tsteps','maxstep', 2^(-6))
```

Similarly, we have solve for adjoint, control and Lagrange multiplier variables. For a detailed COMSOL script we refer to [38] and [39].

Numerical results of the gradient method are given in Table 3.4:

Table 3.4: Gradient method for the control constrained problem.

$\Delta x_{max} = \Delta t_{max}$	$\ J(y_h, u_h)\ _Q$	# iterations
$2^{-2}$	0.2466	55
$2^{-3}$	0.2155	52
$2^{-4}$	0.2082	65
$2^{-5}$	0.2023	219
$2^{-6}$	0.2006	524
$2^{-7}$	0.2004	489
$2^{-8}$	0.2003	580

Table 3.5: One-shot approach for Run 2.

$\Delta x_{max}$	$\ J(y, u)\ _Q$ with adaption	$\ J(y, u)\ _Q$ with femnlin
$2^{-2}$	0.1994	0.1684
$2^{-3}$	0.2000	0.1985
$2^{-4}$	0.2002	0.2000
$2^{-5}$	0.2003	0.2002
$2^{-6}$	0.2003	0.2003

From Table 3.6, the mesh-independence can be also observed numerically for the control constrained problem as in [50] by using SQP methods.

In Figure 3.3, the computed solutions are given for the control constraint problem for  $\Delta x_{max} =$

Table 3.6: Mesh independence for Run 3.2.

tol \ $\Delta x_{max}$	$2^{-2}$	$2^{-3}$	$2^{-4}$	$2^{-5}$	$2^{-6}$
1e-1	4	4	4	4	4
1e-3	5	5	5	5	5
1e-5	6	6	6	6	6
1e-7	6	6	6	6	6
1e-9	7	7	7	7	7
1e-11	7	7	7	7	7

$2^{-6}$ . The numerical solutions obtained by the gradient method and by the one-shot approach without adaptation are similar to those in Figure 3.3. The adaptive mesh for  $h = \Delta x_{max} = 2^{-4}$  is given in Figure 3.4.

The numerical solutions for the optimal control and optimal state in Figure 3.3, are similar to those in [50].

**Run 3.3** (*Boundary control problem with control constraint*)

We have chosen the space-time domain as  $Q = (0, 1) \times (0, 1)$ . We consider a Robin-type boundary control problem with  $\beta_u = 0.05, \beta_v = 0.01, \sigma_0 = -0.1, \sigma_1 = 0$ . The viscosity parameter is  $\nu = 0.05$ . The initial condition is taken as  $y_0(\cdot, 0) = \sin(6x)$  and the desired state is  $y_d(x, t) = y_0(\cdot, 0)$ . The bounds for the pointwise bilateral control constraints are:

$$u_a = -0.04, u_b = 0.06, v_a = -0.04, v_b = 0.05.$$

A similar problem without inequality constraints is examined in [36].

We note that the controls are not discretized. This concept is studied in [21]. The variational discretization concept is introduced. The state and adjoint state are discretized but an explicit discretization is avoided for controls. Variational discretization considered in [21] allows the easiest analysis of the discretization error. This discretization approach can be understood as a generalization of the discretize-then optimize approach in which it avoids discretization of the control space  $U$ .

The control variables on the boundary are defined in COMSOL as

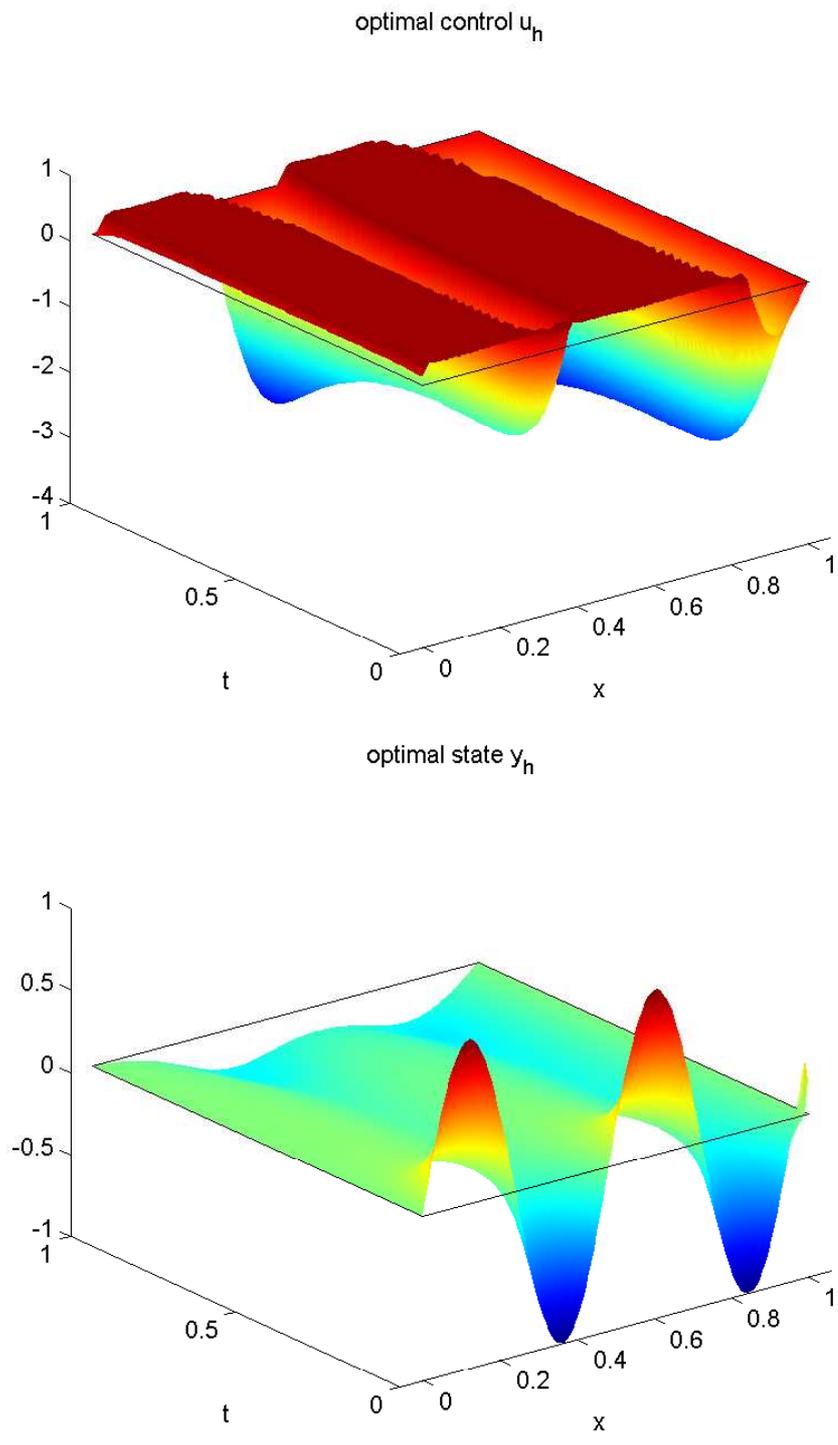


Figure 3.3: One-shot approach with adaptation for the control constrained problem.

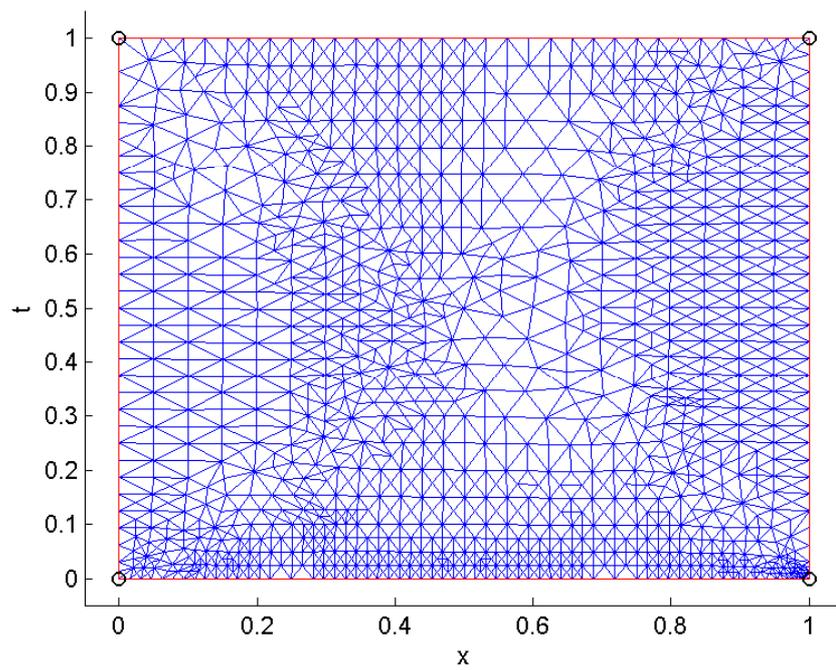


Figure 3.4: Adaptive mesh of the one-shot approach for the control constrained problem.

```
fem.globalexpr={'u' '(p+mu0-mu1)/alpha0'
'v' '(-p+eta0-eta1)/alpha1' 'mu0' 'max(0,ua(time)*alpha0-p)'
'mu1' 'max(0,-ub(time)*alpha0+p)' 'eta0'
'max(0,va(time)*alpha1+p)' 'eta1' 'max(0,-vb(time)*alpha1-p)'}'
```

The Robin-type boundary conditions,  $\vec{n} \cdot (\nabla y) + \alpha y = g$ , are implemented as follows:

```
fem.bnd.r={{'y-y0(x)' 0};{0 0};{0 'p'};{0 0}}
fem.bnd.g={{0 0};{'v/nu' 'y*p/nu'};{0 0}
{'(-u-0.1*y)/nu' '(-y+0.1)*p/nu'}}
```

We have chosen the same step size for in space and time, i.e.,  $h = \Delta_x = \Delta_t$ . The computed optimal state and control variables are denoted by  $\bar{y}_h$  and  $\bar{u}_h$  respectively. Here, the subindex  $h$  indicates the computed state and control variables with step sizes  $h$ .

Finally the postprocessing follows as

```
figure(1)
postplot(fem,'tridata','y','triz','y')
figure(2)
postplot(fem,'liny','u','bd1',4)
hold on
postplot(fem,'liny','v','bd1',4)
```

Since the exact solution of the optimal control problem under consideration is not known, the values of the cost functional  $J$  are listed in Table 3.7. for a sequence of uniformly refined meshes with  $h$  tending to zero.

We give the numerical results of the one-shot approach in Table 3.7

In [66], the mesh independence is obtained with respect to a stopping criteria defined in that paper.

Table 3.7: Run 3.3

$h_{\max}$	$\ J(\bar{y}_h, \bar{u}_h)\ $ <b>femlin</b>	$\ J(\bar{y}_h, \bar{u}_h)\ $ <b>adaption</b>
$2^{-2}$	3.8556e-2	3.8560e-2
$2^{-3}$	1.7930e-1	1.8192e-1
$2^{-4}$	3.9390e-2	3.9326e-2
$2^{-5}$	3.8772e-2	3.8709e-2
$2^{-6}$	3.8735e-2	3.8718e-2

Table 3.8: Run 3.3: mesh independence.

$h_{\max}$	$2^{-3}$	$2^{-4}$	$2^{-5}$	$2^{-6}$	$2^{-7}$
tol=1e-3	6	7	7	6	7
tol=1e-5	6	8	7	7	7
tol=1e-7	7	8	8	7	8
tol=1e-9	7	8	8	7	8
tol=1e-11	7	9	8	7	8

The optimal state  $y(t)$ , the optimal controls  $u(t)$ ,  $v(t)$  and the adaptive mesh are given in Figures 3.5-3.7, computed with the one-shot approach with the adaptive solver for  $h_{\max}$ .

For a comparison we give the numerical results of iterative method that is covered in [38, 71].

Table 3.9: Run 3.3: Iterative solution results.

$h$	$(\ J(\bar{y}_h, \bar{u}_h)\ )$	# of iterations
$2^{-2}$	1.0096e-1	12
$2^{-3}$	5.4849e-2	12
$2^{-4}$	4.4446e-2	25
$2^{-5}$	3.3385e-2	49
$2^{-6}$	3.1437e-2	63

**Run 3.4.** (Boundary control problem with control constraint)

We solve the boundary control problem in [70], Run 8.1, p.24. The same space-time domain

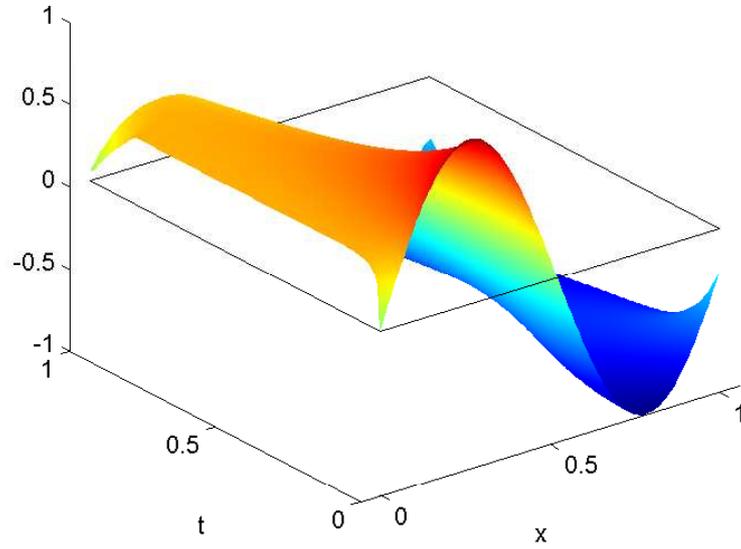


Figure 3.5: Run 3.3: optimal state

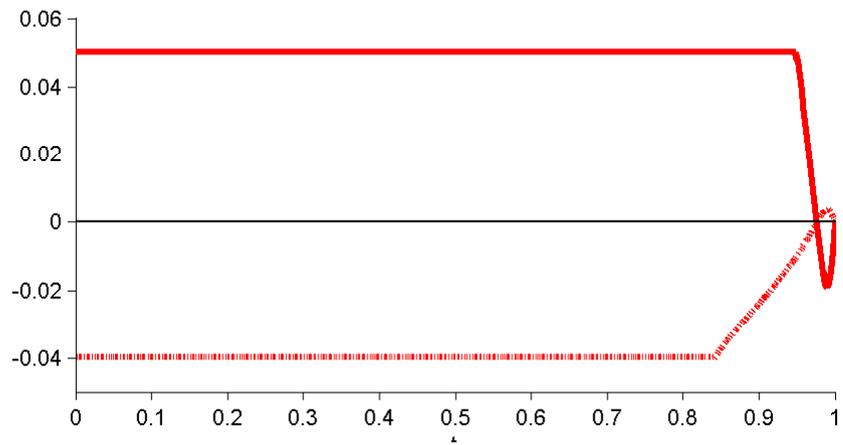


Figure 3.6: Run 3.3. optimal controls: (solid lines)  $v(t)$ , (dotted lines)  $u(t)$

is used as in above example. We consider a Robin-type boundary control problem with  $\beta_u = 0.05, \beta_v = 0.01, \sigma_0 = -0.1, \sigma_1 = 0$ . The viscosity parameter is  $\nu = 0.05$ . The initial condition is given by

$$y_0(\cdot, 0) = \begin{cases} 1 & \text{in } (0, \frac{1}{2}], \\ 0 & \text{otherwise.} \end{cases}$$

The desired state is  $y_Q(x, t) = y_0(\cdot, 0)$ . The bounds for the unilaterally constraint pointwise control constraints are:

$$u_a(t) = \begin{cases} -0.2 & \text{in } [0, 0.5], \\ -0.1 + 5(t - 0.52) & \text{in } [0.5, 0.52], \\ -0.1 & \text{in } [0.52, 1], \end{cases}$$

and

$$u_b = 0, v_a = -0.25, v_b = 0.$$

We note that since  $u_a$  is not given exactly in ([70], Run 8.1 p. 24), we here solve a slightly different problem. The results are almost the same. The cost function is computed as 0.0638 in cited paper. For our case the numerical results are presented in the following tables and in the Figure 4.

Table 3.10: Run 3.4.

$h_{\max}$	$\ J(\bar{y}_h, \bar{u}_h)\ $ <b>femnlm</b>	$\ J(\bar{y}_h, \bar{u}_h)\ $ <b>adaption</b>
$2^{-2}$	8.0100e-2	6.760e-2
$2^{-3}$	1.7930e-1	1.7930e-1
$2^{-4}$	6.7900e-2	6.4900e-2
$2^{-5}$	6.5500e-2	6.4900e-2
$2^{-6}$	6.5300e-2	6.4900e-2

Letting  $h_{\max} = 2^{-4}$  mesh-independence can be seen from Table 3.11.

We remark that because of the restrictions in Lemma 2 the choices of box constraints and initial condition effect the existence of solutions in both examples. That is randomly chosen initial values can not guarantee existence of solutions.

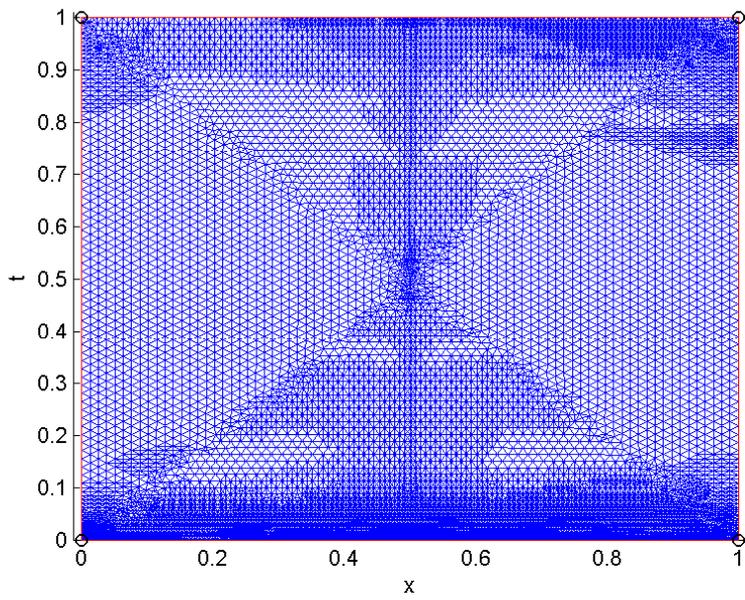


Figure 3.7: Run 3.4: adaptive mesh

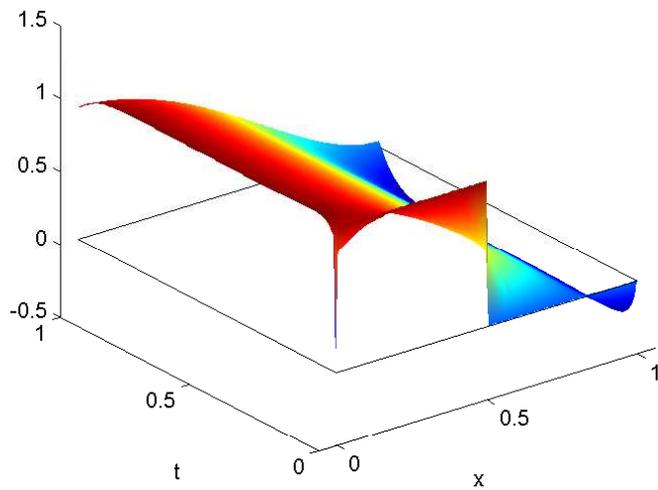


Figure 3.8: Run 3.4.: optimal state

Table 3.11: Run 3.4 : mesh independence

$h_{\max}$	$2^{-3}$	$2^{-4}$	$2^{-5}$	$2^{-6}$	$2^{-7}$
tol=1e-3	13	9	9	9	9
tol=1e-5	13	10	10	10	10
tol=1e-7	13	10	10	11	11
tol=1e-9	13	11	11	11	11
tol=1e-11	13	11	11	12	12

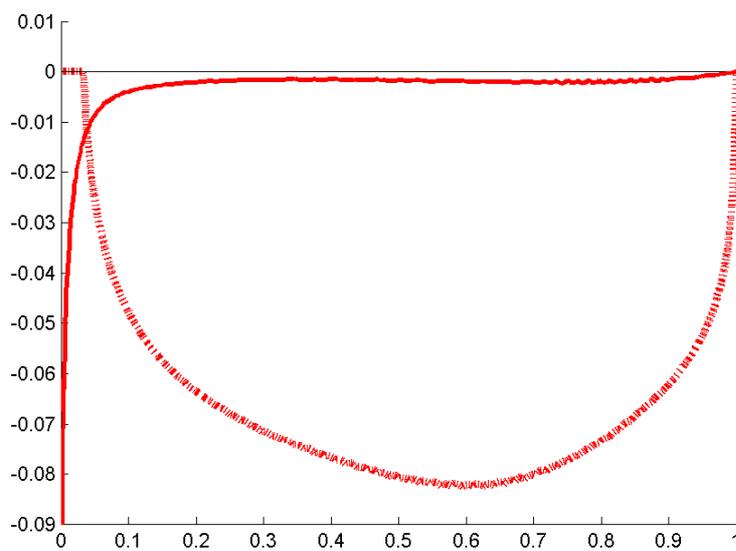


Figure 3.9: Run 3.4.: optimal controls: (solid lines)  $v(t)$ , (dotted lines)  $u(t)$

## CHAPTER 4

### DISCRETIZE-THEN-OPTIMIZE APPROACH: ONE-SHOT METHOD

In this chapter, we follow the *discretize-then-optimize* approach. This approach was successfully applied to optimal control problem of Burgers equation with non-linear conjugate gradient method in [13]. We will show by applying the *discretize-then-optimize* to Burgers equation, the so called all-at-once type solution of the control problem leads to a saddle system point problem with a symmetric, positive definite matrix  $A$ . The system  $\mathcal{A}x = b$  is usually very large, sparse and bad conditioned.

The all-at-once approach was applied to elliptic linear optimal control problems in [48, 49, 47]. In [52] the all-at-once approach was applied to parabolic control problems.

We consider in this chapter both linearized and nonlinear control problem because of nonlinearity in the state equation. This leads to different control problems after semidiscretization in space. Standard linear finite element approach is used for the space discretization. In first section we consider the unconstrained and control constrained distributed control problems. After linearization of the nonlinear term, we use Crank-Nicolson scheme for time discretization. In the second part of the first section, the nonlinear state equation is discretized. We use then semi-implicit time approach to obtain fully discrete scheme. At the end of the first section we provide an a priori error analysis for the distributed control problem of Burgers equation in order to see the accuracy order of all-at-once approach. The saddle point system is solved either directly by using sparse LU-decomposition or by the iterative solver MINRES (minimum residual method). The second section covers the boundary control problems. Numerical results confirm the a priori error estimates and mesh independence of the solutions

## 4.1 The distributed control problem

### 4.1.1 Semi-discretization of the linearized state equation

We consider the linearized Burgers equation (3.17) from Chapter 3:

$$\begin{aligned} y_t - \nu y_{xx} + (\bar{y}y)_x &= \bar{y}\bar{y}_x + u & \text{in } Q, \\ y &= 0 & \text{on } \Sigma, \\ y(0) &= y_0 & \text{in } \Omega. \end{aligned}$$

The state  $y$ , linearized state  $\bar{y}$  and control  $u$  are discretized by using standard Galerkin method with linear finite elements on the interval  $(0, 1)$  with  $n$  uniform subdivisions.

$$y(x, t) \sim \sum_{j=0}^n y_j(t)\phi_j(x), \quad \bar{y}(x, t) \sim \sum_{k=0}^n \bar{y}_k(t)\phi_k(x), \quad \text{and } u(x, t) \sim \sum_{l=0}^n u_l(t)\phi_l(x).$$

The test functions for the homogeneous Dirichlet boundary conditions. The weak formulation of the linearized Burgers equation becomes then

$$\begin{aligned} & \int_0^1 \frac{\partial}{\partial t} \left( \sum_{j=0}^n y_j \phi_j \right) \phi_i dx + \nu \int_0^1 \frac{\partial}{\partial x} \left( \sum_{j=0}^n y_j \phi_j \right) \frac{d}{dx} \phi_i dx + \int_0^1 \frac{\partial}{\partial x} \left( \sum_{k=0}^n \bar{y}_k \phi_k \sum_{j=0}^n y_j \phi_j \right) \phi_i dx \\ &= \int_0^1 \left( \sum_{k=0}^n \bar{y}_k \phi_k \right) \frac{\partial}{\partial x} \left( \sum_{k=0}^n \bar{y}_k \phi_k \right) \phi_i dx + \int_0^1 \left( \sum_{l=0}^n u_l \phi_l \right) \phi_i dx, \quad i = 1, \dots, n+1. \end{aligned} \quad (4.1)$$

The semi-discrete system of ordinary differential equations are given by defining the vectors

$$\mathbf{y} = (y_1(t), \dots, y_{n+1}(t)), \quad \mathbf{u} = (u_1(t), \dots, u_{n+1}(t)) \text{ and } \bar{\mathbf{y}} = (\bar{y}_1(t), \dots, \bar{y}_{n+1}(t)),$$

$$M\mathbf{y}_t + S\mathbf{y} + C(\bar{\mathbf{y}})\mathbf{y} = q(\bar{\mathbf{y}}) + M\mathbf{u}, \quad (4.2)$$

with the matrices  $S, M \in \mathbb{R}^{(n+1) \times (n+1)}$  are defined as

$$S := \frac{\nu}{h} \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}, \quad M := \frac{h}{6} \begin{pmatrix} 4 & 1 & & & \\ 1 & 4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & & 1 & 4 & 1 \\ & & & & 1 & 4 \end{pmatrix},$$

$$C(\bar{\mathbf{y}}) := \frac{1}{6} \begin{pmatrix} \bar{y}_1 - 4\bar{y}_0 & \bar{y}_0 + 2\bar{y}_1 & 0 & \dots & 0 \\ -(2\bar{y}_0 + \bar{y}_1) & \bar{y}_2 - \bar{y}_0 & \bar{y}_1 + 2\bar{y}_2 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -(2\bar{y}_{n-2} + \bar{y}_{n-1}) & \bar{y}_n - \bar{y}_{n-2} & \bar{y}_{n-1} + 2\bar{y}_n \\ 0 & \dots & 0 & -(2\bar{y}_{n-1} + \bar{y}_n) & 4\bar{y}_n - \bar{y}_{n-1} \end{pmatrix}$$

and

$$q(\mathbf{y}) := \frac{1}{6} \begin{pmatrix} y_1^2 + y_0 y_1 - 2y_0^2 \\ \vdots \\ y_i^2 + y_{i-1}(y_i - y_{i-2}) - y_{i-2}^2 \\ \vdots \\ 2y_n^2 - y_n y_{N-1} - y_{N-1}^2 \end{pmatrix} \in \mathbb{R}^{n+1}.$$

The semi-discrete control problem can be formulated as

$$\begin{aligned} \min \quad J_h &= \int_0^T \frac{1}{2} (\mathbf{y} - \mathbf{y}_d)^T M (\mathbf{y} - \mathbf{y}_d) dt + \int_0^T \frac{\alpha}{2} \mathbf{u}^T M \mathbf{u} dt & (4.3) \\ \text{subject to} \quad M \mathbf{y}_t + S \mathbf{y} + C(\bar{\mathbf{y}}) \mathbf{y} &= q(\bar{\mathbf{y}}) + M \mathbf{u}, \\ \mathbf{y}(0) &= \mathbf{y}_0. \end{aligned}$$

#### 4.1.2 Time discretization using Crank-Nicolson scheme

The Crank-Nicolson scheme is one of the most used method for the time discretization of the Burgers equation, which is an implicit and second order method, [44].

Given  $0 = t_0 < t_1 < \dots < t_{N+1} = T$ , we define

$$\Delta t_i = t_{i+1} - t_i, \quad i = 0, \dots, N, \quad \text{with } \Delta t_{-1} = \Delta t_{N+1} = 0.$$

Application of the Crank-Nicolson scheme to 4.3 gives

$$\begin{aligned} & \left( M + \frac{\Delta t_i}{2} S + \frac{\Delta t_i}{2} C(\bar{\mathbf{y}}^{i+1}) \right) \mathbf{y}^{i+1} + \left( -M + \frac{\Delta t_i}{2} S + \frac{\Delta t_i}{2} C(\bar{\mathbf{y}}^i) \right) \mathbf{y}^i \\ &= \frac{\Delta t_i}{2} (q(\bar{\mathbf{y}}^{i+1}) + q(\bar{\mathbf{y}}^i)) + \frac{\Delta t_i}{2} M (\mathbf{u}^i + \mathbf{u}^{i+1}) \end{aligned} \quad (4.4)$$

$$\mathbf{y}(0) = \mathbf{y}_0 \quad i = 0, \dots, N.$$

We define

$$Y = (\mathbf{y}^1, \dots, \mathbf{y}^N) \text{ and } U = (\mathbf{u}^1, \dots, \mathbf{u}^N),$$

where  $\mathbf{y}^i$  and  $\mathbf{u}^i$  correspond to vector valued functions at the time step  $i$ .

Then the full-discrete system in matrix-vector form becomes

$$\mathcal{K}Y - \frac{\Delta t}{2}\mathcal{M}U = \frac{\Delta t}{2} \underbrace{\begin{pmatrix} q(\bar{\mathbf{y}}^0) + q(\bar{\mathbf{y}}^1) \\ q(\bar{\mathbf{y}}^1) + q(\bar{\mathbf{y}}^2) \\ \vdots \\ q(\bar{\mathbf{y}}^{N-1}) + q(\bar{\mathbf{y}}^N) \end{pmatrix}}_Q + \underbrace{\begin{pmatrix} (-M + \frac{\Delta t}{2}S + \frac{\Delta t}{2}C(\bar{\mathbf{y}}^0))\mathbf{y}_0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}}_d$$

with

$$\mathcal{K} = \begin{pmatrix} Z_1 & & & & & \\ \bar{Z}_2 & Z_2 & & & & \\ & \ddots & \ddots & & & \\ & & \ddots & \ddots & & \\ & & & \bar{Z}_N & Z_N & \end{pmatrix} \text{ and } \mathcal{M} = \begin{pmatrix} M & & & & & \\ M & M & & & & \\ & \ddots & \ddots & & & \\ & & & M & M & \\ & & & & M & M \end{pmatrix},$$

where

$$Z_i = M + \frac{\Delta t}{2}S + \frac{\Delta t}{2}C(\bar{\mathbf{y}}^{i+1}), \quad \bar{Z}_i = -M + \frac{\Delta t}{2}S + \frac{\Delta t}{2}C(\bar{\mathbf{y}}^i)$$

for  $i = 2, \dots, N$ .

Thus, we obtain the representation of the unsteady Burgers equation with Dirichlet boundary conditions in the following form

$$\mathcal{K}Y - \frac{\Delta t}{2}\mathcal{M}U = \frac{\Delta t}{2}Q + d.$$

For discretization of the cost function, we use the trapezoidal rule

$$\min_{\mathbf{u}_1, \dots, \mathbf{u}_N} \sum_{i=0}^{N+1} \frac{\Delta t_i + \Delta t_{i+1}}{2} \left( \frac{1}{2}(\mathbf{y} - \mathbf{y}_d)^T M(\mathbf{y} - \mathbf{y}_d) + \frac{\alpha}{2} \mathbf{u}^T M \mathbf{u} \right). \quad (4.5)$$

When we collect every time step in a block, the functional  $J_h(Y, U)$  can be stated as

$$J_h(Y, U) = \frac{\Delta t}{2}(Y - Y_d)^T \mathcal{M}_{1/2}(Y - Y_d) + \frac{\alpha \Delta t}{2} U^T \mathcal{M}_{1/2} U$$

with the matrix

$$\mathcal{M}_{1/2} = \begin{pmatrix} \frac{1}{2}M & & & \\ & M & & \\ & & \ddots & \\ & & & \frac{1}{2}M \end{pmatrix} \in \mathbb{R}^{(n+1) \times N, (n+1) \times N}.$$

**Remark 1.** If rectangular rule instead of trapezoidal rule is used  $\mathcal{M}_{1/2}$  has the last block to be 0.

Both trapezoidal and rectangular rules give the same results. Therefore, we have performed our computations with the trapezoidal rule.

The optimality system containing first order optimality conditions is obtained by introducing the extended Lagrangian containing the Lagrange multiplier  $P$  [58].

$$\begin{aligned} L(Y, U, P) : &= \frac{\Delta t}{2}(Y - Y_d)^T \mathcal{M}_{1/2}(Y - Y_d) + \frac{\alpha \Delta t}{2} U^T \mathcal{M}_{1/2} U \\ &+ P^T (-\mathcal{K}Y + \Delta t \mathcal{M}U + Q + d). \end{aligned} \quad (4.6)$$

The optimality conditions are given as

$$\nabla_Y L(Y^*, U^*, P^*) = \Delta t \mathcal{M}_{1/2}(Y^* - Y_d) - \mathcal{K}^T P^* = 0,$$

$$\nabla_P L(Y^*, U^*, P^*) = -\mathcal{K}Y^* + \Delta t \mathcal{M}U^* + Q + d = 0,$$

$$\nabla_U L(Y^*, U^*, P^*) = \alpha \Delta t \mathcal{M}_{1/2} U^* + \Delta t \mathcal{M}P^* = 0.$$

The first optimality condition gives the discrete adjoint equation

$$-\mathcal{K}^T P^* = \Delta t \mathcal{M}_{1/2}(Y^* - Y_d). \quad (4.7)$$

**Remark 2.** The matrix formulation of discrete adjoint (4.7) corresponds to a backward Euler scheme as

$$-\frac{p^{i+1} - p^i}{\Delta t} - \Delta p^i = y^i - y_d.$$

This scheme is not consistent with the continuous adjoint mentioned in Chapter 1. Another difference occurs at time level  $t = T$ . When the trapezoidal rule is used the system (4.8) shows that  $p$  is not necessarily equal to 0 at  $t = T$ . This obstacle can be overcome by letting  $\Delta t \rightarrow 0$ . However, we remark that when rectangular rule is used, the final block of the matrix  $\mathcal{M}_{1/2}$  is 0. This shows that final time condition of discrete adjoint is satisfied. Numerically, there is not big differences when we choose sufficiently small  $\Delta t$ .

Finally, the optimality system can be written as

$$\underbrace{\begin{pmatrix} \mathcal{M} & 0 & -\mathcal{K}^T \\ 0 & \alpha\Delta t\mathcal{M}_{1/2} & \frac{\Delta t}{2}\mathcal{M} \\ -\mathcal{K} & \frac{\Delta t}{2}\mathcal{M} & 0 \end{pmatrix}}_{\mathcal{T}} \begin{pmatrix} Y \\ U \\ P \end{pmatrix} = \begin{pmatrix} \mathcal{M}_{1/2}Y_d \\ 0 \\ Q + d \end{pmatrix}. \quad (4.8)$$

The solution of the above system will be handled in the implementation part.

#### 4.1.3 Time discretization with the semi-implicit method

We give first the space discretization of the nonlinear state equation using linear finite elements

$$\begin{aligned} & \int_0^1 \frac{\partial}{\partial t} \left( \sum_{j=0}^n y_j \phi_j \right) \phi_i dx + \nu \int_0^1 \frac{\partial}{\partial x} \left( \sum_{j=0}^n y_j \phi_j \right) \frac{d}{dx} \phi_i dx \\ & + \int_0^1 \frac{\partial}{\partial x} \left( \sum_{j=0}^n y_j \phi_j \right) \left( \sum_{j=0}^n y_j \phi_j \right) \phi_i dx = \int_0^1 \left( \sum_{l=0}^n u_l \phi_l \right) \phi_i dx, \end{aligned}$$

where  $i = 1, \dots, n + 1$ .

Using the vector valued variables defined in the previous subsection, we get

$$M\mathbf{y}_t + S\mathbf{y} + q(\mathbf{y}) = M\mathbf{u}. \quad (4.9)$$

Then, semi-discrete control problem follows as

$$\min J_h = \int_0^T \frac{1}{2}(\mathbf{y} - \mathbf{y}_d)^T M(\mathbf{y} - \mathbf{y}_d) dt + \int_0^T \frac{\alpha}{2} \mathbf{u}^T M \mathbf{u} dt \quad (4.10)$$

$$\text{subject to } M\mathbf{y}_t + S\mathbf{y} + q(\mathbf{y}) = M\mathbf{u},$$

$$\mathbf{y}(0) = \mathbf{y}_0,$$

where  $M$  and  $S$  are mass and stiffness matrices, respectively.

Semi-implicit time approximation [44] consists in evaluating the diffusive part  $y_{xx}$ , at the time level  $t_{i+1}$ , whereas the remaining parts are considered at time  $t_i$ . When this scheme is applied to a non-linear advection, it provides an efficient linearization. Full discretization of the Burgers equation with Dirichlet boundary conditions can be stated as

$$\begin{cases} \frac{1}{\Delta t}(y_h^{i+1} - y_h^i, \phi_h) + \nu(\nabla y_h^{i+1}, \nabla \phi_h) + (y_h^i \nabla y_h^i, \phi_h) = (f(t_{i+1}), \phi_h), \\ y_h^0 = y_{0,h}, \text{ for any } \phi_h \in V_h, \text{ for } i = 0, \dots, N. \end{cases}$$

Discretizing the variables we obtain

$$\begin{aligned} (M + \Delta t S)\mathbf{y}^{i+1} - M\mathbf{y}^i + \Delta t q(\mathbf{y}^i) &= \Delta t M \mathbf{u}^{i+1}, \\ \mathbf{y}(0) &= \mathbf{y}_0 \text{ for } i = 0, \dots, N. \end{aligned} \quad (4.11)$$

Let  $\tilde{Q} = (q(\mathbf{y}^1), \dots, q(\mathbf{y}^N))$  for  $N$  time-steps. Then

$$\underbrace{\begin{pmatrix} Z & & & & \\ -M & Z & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & -M & Z \end{pmatrix}}_{\tilde{\mathcal{K}}} Y - \tilde{\mathcal{M}} U = \underbrace{\begin{pmatrix} -M\mathbf{y}^0 + \Delta t q(\mathbf{y}^0) \\ 0 \\ \vdots \\ 0 \end{pmatrix}}_{\tilde{d}} + \tilde{Q},$$

where  $Z = M + \Delta t S$ , and  $\tilde{\mathcal{M}} = \text{blockdiag}\{M, \dots, M\}$ .

Optimality conditions result in the optimality system as

$$\begin{pmatrix} \tilde{\mathcal{M}} & 0 & -\tilde{\mathcal{K}}^T \\ 0 & \alpha \Delta t \mathcal{M}_{1/2} & \Delta t \tilde{\mathcal{M}} \\ -\tilde{\mathcal{K}} & \Delta t \tilde{\mathcal{M}} & 0 \end{pmatrix} \begin{pmatrix} Y \\ U \\ P \end{pmatrix} = \begin{pmatrix} \mathcal{M}_{1/2} Y_d \\ 0 \\ \tilde{d} + \tilde{Q} \end{pmatrix}. \quad (4.12)$$

#### 4.1.4 Solution of the optimality system

In general, there exists two general approaches for solving optimization problems. The first is to use an existing PDE solver for the constraints to compute  $y$  as a function of  $u$  and evaluate cost function  $J(y(u), u)$ . This approach is referred to as the "black-box" approach. In other words, an existing algorithm for the solution of the state equation is embedded into an optimization loop. To obtain an efficient and fast optimization algorithm, gradients are required. Computation of the gradients can be done by adjoint or sensitivity approaches. When the PDE is non-linear as for the Burgers equation, the state equation has to be solved several times, which might be costly.

The second approach is all-at-once methods. This method treats the control and state variable as independent of optimization variables. The obvious advantage of all-at-once approach is avoiding the repeated solution of (non-linear) state equation. Optimization algorithms of this class requires the solution of the linearized state equations. In recent years, there have been an interest in all-at-once type methods for solving optimal control problems. There are many concerning elliptic problems [53, 2, 33, 47, 49]. However there are only a few published results for parabolic problems [52, 13, 35, 34].

To implement an optimization problem, the gradient based methods are usually applied. Although their performance is efficient and fast it is usually cost to compute gradients. Because all-at-once methods treat the control and state as independent optimization variables, the optimization problem is explicitly constrained. That is the state  $Y$ , the control  $U$  and the adjoint state  $P$  can be solved explicitly. The systems (4.8) and (4.12) solve the optimization variables in one-step. We note that they are very large and contain zero blocks because of the matrices  $M$  and  $S$  coming from the finite element discretizations. Indeed, the discretization of many problems lead to large dimensional systems which are usually of saddle-point type. In recent years, many efficient solution methods were developed for optimal control problems using all-at-once type methods [48, 49, 34, 35, 52, 53].

Both (4.8) and (4.12) lead to a saddle point type problem. A saddle point problem is  $Ax = b$

with

$$A = \begin{pmatrix} E & L^T \\ L & C \end{pmatrix},$$

where the matrix  $A$  is a symmetric and indefinite, which is usually bad conditioned and invertible when  $L$  has full rank. The matrix  $C$  is usually 0.

For Crank-Nicolson discretization (4.8), we have

$$E := \begin{pmatrix} \mathcal{M} & 0 \\ 0 & \alpha\Delta t\mathcal{M}_{1/2} \end{pmatrix}.$$

By defining

$$x := \begin{pmatrix} Y \\ U \\ P \end{pmatrix}, \quad L := \begin{pmatrix} -\mathcal{K} & \Delta t\mathcal{M} \end{pmatrix} \quad \text{and} \quad b := \begin{pmatrix} \mathcal{M}Y_d \\ 0 \\ d \end{pmatrix}$$

we obtain the saddle point formulation. It is also called KKT-matrix, which corresponds to Karush-Kuhn-Tucker first order necessary optimality conditions. Similar saddle point system is also obtained for the semi-implicit discretization (4.12) with a different matrix  $E$ .

For a saddle point system both direct solver and iterative methods can be considered. When the dimension of the problem is not huge, direct solver can be used. That is the system  $Ax = b$  can be solved by sparse LU-decomposition. Direct solvers are faster than the iterative solvers. However when the dimension of the problem is large then an iterative solver has to be used because of memory problems. In the following subsection, we present first the direct solver.

#### 4.1.4.1 Direct Solver

Since we have one-dimensional parabolic problem, the optimality system  $\mathcal{A}x = b$  can be solved directly by using sparse LU decomposition. We note that due to the linearization there has to be an outer iteration in the solution algorithm. The direct solution of  $\mathcal{A}x = b$  can be summarized as follows:

##### *Direct solver for the all-at-once method with Crank-Nicolson discretization*

1. Given  $U_0, Y_0, tol > 0$ . Set  $k = 0$
2. Set  $done = inf$
3. While  $done > tol$ 
  - 3.1 Set  $k = k + 1$
  - 3.2 Update  $\mathcal{K}$  using computed  $Y$ , in the place of  $\bar{Y}$
  - 3.3 By using LU decomposition solve

$$\begin{pmatrix} \mathcal{M} & 0 & -\tilde{\mathcal{K}}^T \\ 0 & \alpha\Delta t\mathcal{M}_{1/2} & \frac{\Delta t}{2}\tilde{\mathcal{M}} \\ -\tilde{\mathcal{K}} & \frac{\Delta t}{2}\tilde{\mathcal{M}} & 0 \end{pmatrix} \begin{pmatrix} Y \\ U \\ P \end{pmatrix} = \begin{pmatrix} \mathcal{M}Y_d \\ 0 \\ \tilde{Q} + \tilde{d} \end{pmatrix} \quad (4.13)$$

$$3.4 \text{ Set } done = \|Y_{k+1} - Y_k\| + \|P_{k+1} - P_k\| + \|U_{k+1} - U_k\|$$

4. End while.

We note that the block matrix  $\mathcal{K}$  depends on  $\bar{Y}$ , i.e. it has to be updated after every calculation of the state variable.

#### 4.1.4.2 Iterative method

Generally, the KKT matrix is bad conditioned. When an iterative solver is used, the convergence may be slow. In this case, preconditions must be used to accelerate the convergence. A preconditioner is a matrix that transforms the saddle point problem into a system having better spectral property. The preconditioned solver will then solve an equivalent system  $\mathcal{P}^{-1}\mathcal{A}X = \mathcal{P}^{-1}F$ . The matrix  $\mathcal{P}$  has to be cheap to be inverted and has to cluster the eigenvalues of  $\mathcal{P}^{-1}\mathcal{A}$  [2, 18].

We note that when  $A$  is nonsingular then the following block triangular factorization holds

$$\begin{pmatrix} E & L^T \\ L & 0 \end{pmatrix} = \begin{pmatrix} I & 0 \\ LE^{-1} & I \end{pmatrix} \begin{pmatrix} E & 0 \\ 0 & S \end{pmatrix} \begin{pmatrix} I & E^{-1}L^T \\ 0 & I \end{pmatrix},$$

where  $S = LE^{-1}L^T$  is the Schur complement of  $E$ . This factorization gives an idea about preconditioning. As for solution method various preconditioned Krylov subspace methods or multilevel methods can be considered to increase the convergence rate [2, 12, 33]. Among the Krylov subspace methods there are several preconditioning techniques:

- CG, MINRES, and SYMMLQ require positive semi definiteness,
- SQMR requires symmetric matrix,
- GMRES.

We use the minimal residual method (MINRES) for solving the saddle point problem (4.13). MINRES computes a sequence  $X_k$  for each residual  $r_k = AX_k - B$  by constructing the following Krylov subspace

$$\text{span} \{r_0, Ar_0, A^2r_0, \dots, A^k r_0\},$$

where  $k = 1, 2, \dots$  denotes iteration number. Within the MINRES algorithm the residual norm  $\|r_k\|$  is minimized over the Krylov subspace.

For elliptic problems the preconditioners for the MINRES algorithm have the following:

$$\mathcal{P} = \begin{pmatrix} A & 0 \\ 0 & S \end{pmatrix},$$

with  $S = BA^{-1}B^T$ . For the matrix

$$\mathcal{A} = \begin{pmatrix} \mathcal{M} & 0 & -\mathcal{K}^T \\ 0 & \alpha\Delta t\mathcal{M}_{1/2} & \Delta t\mathcal{M} \\ -\mathcal{K} & \Delta t\mathcal{M} & 0 \end{pmatrix},$$

the following preconditioner is proposed in [52]

$$\mathcal{P} = \begin{pmatrix} \mathcal{M} & 0 & 0 \\ 0 & \alpha\Delta t\mathcal{M} & 0 \\ 0 & 0 & S \end{pmatrix}$$

with  $S^{-1} := \mathcal{K}^{-T}\mathcal{M}\mathcal{K}^{-1}$ .

### 4.1.5 Control constrained problem

In case of box constraints for the control variable

$$u_a(t, x) \leq u(t, x) \leq u_b(t, x) \text{ in } Q,$$

the variational inequality gives rise to the following optimality condition (see Chapter 1, Eq. 2.10)

$$(U - U^*)^T \nabla_U L(Y^*, U^*, P^*) = (U - U^*)^T (\alpha \Delta t \mathcal{M}_{1/2} U^* + \Delta t \mathcal{M} P^*) \geq 0. \quad (4.14)$$

Similar to unconstrained problem the augmented Lagrange function is introduced [58]

$$\begin{aligned} L(Y, U, P, \mu_a, \mu_b) := & \frac{\Delta t}{2} (Y - Y_d)^T \mathcal{M}_{1/2} (Y - Y_d) + \frac{\alpha \Delta t}{2} U^T \mathcal{M}_{1/2} U \\ & + P^T (-\mathcal{K}Y + \Delta t \mathcal{M}U + d) + \mu_a^T (U_a - U) + \mu_b^T (U - U_b), \end{aligned}$$

where  $\mu_a$  and  $\mu_b$  represent the Lagrange multipliers for the inequality constraints on the control variable defined as

$$\mu_a := (\alpha \Delta t \mathcal{M}_{1/2} U^* + \Delta t \mathcal{M} P^*)^+ \text{ and } \mu_b := (\alpha \Delta t \mathcal{M}_{1/2} U^* + \Delta t \mathcal{M} P^*)^-.$$

We consider an extension of theorem in [58] about the optimality conditions to  $N$  time-steps.

**Theorem 4.1.1** *For an optimal solution  $(y^*, u^*)$ , there exists Lagrange multipliers  $p$ ,  $\mu_a$ , and  $\mu_b$  such that*

$$\begin{aligned} \nabla_y L(y^*, u^*, p^*, \mu_a, \mu_b) &= 0, \\ \nabla_u L(y^*, u^*, p^*, \mu_a, \mu_b) &= 0, \\ \mu_a &\geq 0, \mu_b \geq 0, \\ \mu_a^T (u_a - u^*) &= \mu_b^T (u^* - u_b) = 0. \end{aligned}$$

#### 4.1.5.1 Active set method

The optimality system with the control constraints are solved usually with the active set methods. This method was introduced in [3]. For a detailed discussion of active set methods we

refer [3, 58].

We define the following sets

$$A_+ := \{i \in \{1, \dots, N\} : (U^* - \mu)_i > (U_b)_i\},$$

$$A_- := \{i \in \{1, \dots, N\} : (U^* - \mu)_i < (U_a)_i\},$$

$$I := \{1, 2, \dots, N\} \setminus (A_+ \cup A_-).$$

Then, the optimality system [26] can be written as

$$\begin{aligned} \Delta t \mathcal{M}_{1/2} (Y^* - Y_d) - \mathcal{K}^T P^* &= 0, \\ -\mathcal{K} Y^* + \frac{\Delta t}{2} \tilde{\mathcal{M}} U^* &= d, \\ \alpha \Delta t \mathcal{M}_{1/2} U^* + \frac{\Delta t}{2} \chi_I \tilde{\mathcal{M}} P^* &= \alpha \Delta t \mathcal{M}_{1/2} (\chi_{A_-} U_a + \chi_{A_+} U_b), \end{aligned}$$

where  $\chi$  denotes the characteristic function of the given set. The following algorithm consists of the solution procedure of active set strategy applied to inequality constrained problem with semi-implicit discretization.

***Inequality constrained problem with active set strategy.***

1. Solve

$$\begin{pmatrix} \mathcal{M} & 0 & -\mathcal{K}^T \\ 0 & \alpha \Delta t \mathcal{M}_{1/2} & \Delta t \chi_I \tilde{\mathcal{M}} \\ -\mathcal{K} & \Delta t \mathcal{M} & 0 \end{pmatrix} \begin{pmatrix} Y \\ U \\ P \end{pmatrix} = \begin{pmatrix} \mathcal{M} Y_d \\ \alpha \Delta t \mathcal{M}_{1/2} (\chi_{A_-} U_a + \chi_{A_+} U_b) \\ d + Q \end{pmatrix}$$

2. Set  $A_+ = \{x \in Q : -\alpha \Delta t \mathcal{M}_{1/2} U_a - \frac{\Delta t}{2} \tilde{\mathcal{M}} P < 0\}$

3. Set  $A_- = \{x \in Q : -\alpha \Delta t \mathcal{M}_{1/2} U_b - \frac{\Delta t}{2} \tilde{\mathcal{M}} P > 0\}$

4. Set  $I = Q \setminus (A_+ \cup A_-)$ .

It is similar for Crank-Nicolson scheme. We change just the matrix formulation.

#### 4.1.6 A priori error analysis of the control problem

Error analysis of optimal control problems has a recent history. Hinze and Tröltzsch provide error estimations for optimization variables considering different discretization techniques for control variable [21]. Maidner and Vexler examine a priori error analysis for optimal control problems using discontinuous Galerkin methods in space and time [30, 31, 32]. In this subsection, we first find error estimations for Burgers equation. Then we consider the discrete adjoint and show the stability and convergence of adjoint state. Then, an error estimation for control variable is given. At the end of subsection, we obtain error bounds for control constrained problems.

##### 4.1.6.1 Error analysis for the state equation

In this subsection, we shall show the stability and convergence for both semi-discretized and fully discretized Burgers equation. We first let the control  $u = 0$  to analyze Burgers equation. We later find error estimates for control  $u$ .

Burgers equation with homogeneous Dirichlet boundary conditions follows

$$\begin{aligned} y_t - \nu y_{xx} + yy_x &= f & \text{in } Q, \\ y(t, 0) = y(t, 1) &= 0 & \text{on } \Sigma, \\ y(0) &= y_0 & \text{in } \Omega. \end{aligned} \tag{4.15}$$

Now we multiply both sides of the state equation (4.15) by a test function  $w \in H_0^1(\Omega)$  to get

$$(y_t, w) + \nu(y_x, w_x) + (yy_x, w) = (f, w) \quad \forall w \in H_0^1(\Omega) \quad a.e. \ t \in [0, T],$$

where  $(\cdot, \cdot)$  is the inner product in  $L^2(\Omega)$ . We assume  $y_0(x) \in L^\infty(\Omega)$  and  $f(x, t) \in L^\infty(Q)$ . The weak formulation follows

$$\begin{aligned} (y_t, w) + \nu(y_x, w_x) + (yy_x, w) &= (f, w) \quad \forall w \in H_0^1(\Omega), \\ y(0, \cdot) &= y_0(x). \end{aligned}$$

##### 4.1.6.2 Semi-discretization

After selecting the space  $\mathcal{S}_h \subset H_0^1(\Omega)$ , we let  $y^h(t) \in \mathcal{S}_h$  satisfying

$$\begin{aligned}
(y_t^h, w) + \nu(y_x^h, w_x) + (y^h y_x^h, w) &= (f, w) \quad \forall w \in H_0^1(\Omega), \\
y^h(0, \cdot) &= y_{0h},
\end{aligned} \tag{4.16}$$

where  $|y_{0h}|_{L^\infty(\Omega)} \leq |y_0|_{L^\infty(\Omega)}$ .

We assume that the polynomials of degree  $\leq p$  over any mesh have the following property

$$\inf_{\chi \in \mathcal{S}_h} \{ \|v - \chi\| + h \|\nabla(v - \chi)\| \} \leq Ch^s \|v\|_s \tag{4.17}$$

for  $1 \leq s \leq p + 1 = r$  and  $v \in H^s(\Omega) \cup H_0^1(\Omega)$ , where  $\|\cdot\|_s$  is the norm on  $H^s$ . Then, the problem (4.16) has at least a solution [Lemma 4.3, p. 52 of [29]].

**Theorem 4.1.2 (Stability)** *The approximate solution  $y^h$  of (4.16) is stable. For any  $t > 0$ ,*

$$\|y^h(t)\|^2 + 2\nu \int_0^t \|\nabla y^h(\tau)\|^2 d\tau \leq \|y^h(0)\|^2 + \left| \int_0^t (f, y^h) d\tau \right|$$

and

$$\sup_{0 \leq t \leq T} \|y^h\| \leq C(f, y_0)$$

for a constant  $C$  that does not depend on  $h$ .

**Proof.** We take  $w^h = y^h$  in (4.16). Then

$$(y_t^h, y^h) + \nu(y_x^h, y_x^h) + (y^h y_x^h, y^h) = (f, y^h)$$

$$\Rightarrow \frac{1}{2} \frac{d}{dt} \|y^h\|^2 + \nu \|\nabla y^h\|^2 = (f, y^h).$$

We obtain the first result after taking integral from 0 to  $t$ . Taking supremum of each side and applying Cauchy-Schwarz inequality on the right hand side gives the second result. ■

**Theorem 4.1.3 (Convergence)** Let  $y^h$  and  $y$  be solutions of (4.16) and (4.15), respectively. Then,

$$\|y^h(t) - y(t)\| \leq C\|y_{0h} - y_0\| + h^{r-1}$$

with  $C = C(y)$ .

**Proof.** For the purpose of the proof we introduce the Ritz projection  $P_1$  from  $H_0^1(\Omega)$  into  $\mathcal{S}_h$  as the orthogonal projection with respect to the inner product  $(v_x, u_x)$  so that :

$$((P_1 u)_x, w_x) = (u_x, w_x) \quad \forall w \in \mathcal{S}_h.$$

This projection has the following properties ([54])

$$\|(P_1 v - v)_x\| \leq \bar{C} h^{s-1} \|v\|_s,$$

$$\|P_1 v - v\| \leq \bar{C} h^s \|v\|_s,$$

for  $1 \leq s \leq r$  and  $v \in H^s(\Omega) \cap H_0^1(\Omega)$ .

Let

$$y^h - y = (y^h - P_1 y) + (P_1 y - y) = v^h + \rho.$$

The second term is bounded by the properties of the projection  $P_1$ ,

$$\|\rho(t)\| \leq C_1(y) h^r \quad \text{and} \quad \|\rho_x\| \leq C_1(y) h^{r-1}.$$

Then, it is enough to estimate  $v^h$ . We note that

$$\begin{aligned} & (v_t^h, w) + \nu(v_x^h, w_x) \\ &= (y_t^h, w) + \nu(y_x^h, w_x) - (P_1 y_t, w) - \nu((P_1 y)_x, w_x) \\ &= -(y_x^h, w) - (P_1 y_t, w) - \nu(y_x, w_x) \\ &= -(y_x^h, w) - (P_1 y_t, w) + (y_t, w) + (y y_x, w) \\ &= (y y_x - y_x^h, w) + (y_t - P_1 y_t, w) \\ &= -(\rho_t, w) + (y(y - y^h)_x - y_x^h(y - y^h), w). \end{aligned}$$

Let  $w = v^h$ . Then, by Young's inequality we get

$$\begin{aligned}
& \frac{1}{2} \frac{d}{dt} \|v^h\|^2 + \nu \|v_x^h\|^2 \\
&= -(\rho_t, v^h) + (y(y - y^h)_x - y_x^h(y - y^h), v^h) \\
&\leq \|\rho_t\| \|v^h\| + |(y(y - y^h)_x, v^h)| + |(y_x^h(y - y^h), v^h)| \\
&\leq C\epsilon \|v_x^h\|^2 + \frac{C}{\epsilon} \|\rho_t\|^2 + |(y(y - y^h)_x, v^h)| + |(y_x^h(y - y^h), v^h)|,
\end{aligned}$$

and,  $y^h - y = v^h - \rho$  implies that

$$\begin{aligned}
|(y(y - y^h)_x, v^h)| &\leq \underbrace{|(y\rho_x, v^h)|}_{L_1} + \underbrace{|(yv_x^h, v^h)|}_{L_2} \\
|(y_x^h(y - y^h), v^h)| &\leq \underbrace{|(y_x^h\rho, v^h)|}_{L_3} + \underbrace{|(y_x^h v^h, v^h)|}_{L_4}.
\end{aligned}$$

For a trilinear term defined by  $b(y, u, v) = \int_Q y u_x v dx dt$  the following estimates can be used [11]:

$$\begin{aligned}
|b(y, u, v)| &\leq C \|y\|^{1/2} \|y_x\|^{1/2} \|u_x\| \|v\|, \\
|b(y, y, v)| &\leq C \|y_x\|^{3/2} \|y\|^{1/2} \|u_x\|.
\end{aligned}$$

Then, by using Young's inequality

$$\begin{aligned}
L_1 &= |(y\rho_x, v^h)| \\
&\leq C \|v^h\|^{1/2} \|v_x^h\|^{1/2} \|\rho_x\| \|y\| \\
&\leq C\epsilon_1 \|v_x^h\|^2 + \frac{C}{\epsilon_1} \|\rho_x\|^2 \|y\|^2,
\end{aligned}$$

and,

$$\begin{aligned}
L_2 &= |(yv_x^h, v^h)| \\
&\leq C \|v^h\|^{1/2} \|v_x^h\|^{3/2} \|y\| \\
&\leq C\epsilon_2 \|v_x^h\|^2 + \frac{C}{\epsilon_2^3} \|v^h\|^2 \|y\|^4.
\end{aligned}$$

Similarly, we obtain

$$\begin{aligned}
L_3 &= |(y_x^h\rho, v^h)| \\
&\leq C \|\rho_x\| \|y_x^h\| \|v_x^h\| \\
&\leq C\epsilon_3 \|v_x^h\|^2 + \frac{C}{\epsilon_3} \|\rho_x\|^2 \|y_x^h\|^2.
\end{aligned}$$

Writing  $y^h = v^h + P_1 y$  and using  $(y_x^h y^h, y^h) = 0$  give

$$\begin{aligned} ((v^h + P_1 y)_x v^h, v^h) &= (v_x^h v^h, v^h) + ((P_1 y)_x v^h, v^h) \\ &= ((P_1 y)_x v^h, v^h). \end{aligned}$$

Using the definition of the projection operator  $P_1$  and letting  $w = P_1 y$  we get  $\|(P_1 y)_x\| \leq C\|y_x\|$ . Then,

$$\begin{aligned} L_4 &\leq C\|v^h\|^{1/2}\|v_x^h\|^{3/2}\|(P_1 y)_x\| \\ &\leq C\|v^h\|^{1/2}\|v_x^h\|^{3/2}\|y_x\| \\ &\leq C\epsilon_4\|v_x^h\|^2 + \frac{C}{\epsilon_4}\|v^h\|^2\|y_x\|^4. \end{aligned}$$

It follows that

$$\begin{aligned} &\frac{1}{2} \frac{d}{dt} \|v^h\|^2 + \nu \|v_x^h\|^2 \\ &\leq C\epsilon \|v_x^h\|^2 + \frac{C}{\epsilon} \|\rho_t\|^2 + L_1 + L_2 + L_3 + L_4 \\ &\leq C\epsilon \|v_x^h\|^2 + \frac{C}{\epsilon} \|\rho_t\|^2 + C\epsilon_1 \|v_x^h\|^2 + \frac{C}{\epsilon_1} \|\rho_x\|^2 \|y\|^2 + C\epsilon_2 \|v_x^h\|^2 + \frac{C}{\epsilon_2} \|v^h\|^2 \|y\|^4 \\ &\quad + C\epsilon_3 \|v_x^h\|^2 + \frac{C}{\epsilon_3} \|\rho_x\|^2 \|y_x^h\|^2 + C\epsilon_4 \|v_x^h\|^2 + \frac{C}{\epsilon_4} \|v^h\|^2 \|y_x\|^4. \end{aligned}$$

Letting  $\epsilon = \epsilon_1 = \epsilon_2 = \epsilon_3 = \epsilon_4 = \frac{\nu}{5C}$  gives

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|v^h\|^2 &\leq C(\nu) \{ \|\rho_t\|^2 + \|\rho_x\|^2 (\|y\|^2 + \|y_x^h\|^2) + \|v^h\|^2 (\|y\|^4 \\ &\quad + \|y_x\|^4) + \|\rho\|^2 + \|v^h\|^2 \|y_x\|^4 + \|y_x^h\|^2 \|v^h\|^2 \}. \end{aligned}$$

Integrating over  $[0, t]$ ,  $t \leq T$  implies that

$$\begin{aligned} \|v^h(t)\|^2 &\leq \|v^h(0)\|^2 + C(\nu) \int_0^t \{ \|\rho_t\|^2 + \|\rho_x\|^2 (\|y\|^2 + \|y_x^h\|^2) + \|v^h\|^2 (\|y\|^4 \\ &\quad + \|y_x\|^4) + \|\rho\|^2 \} d\tau. \end{aligned}$$

Cauchy-Schwarz inequality and Theorem 4.1.2 give the following

$$\begin{aligned} & \int_0^T \|\rho_x\|^2 (\|y\|^2 + \|y_x^h\|^2) d\tau \\ & \leq C \|\rho_x\|_{L^4(0,T;L^2(\Omega))}^2 (\|y\|_{L^4(0,T;L^2(\Omega))}^2 + \|y_x^h\|_{L^4(0,T;L^2(\Omega))}^2). \end{aligned}$$

By assumption  $y, y_x \in L^4(0, T; L^2(\Omega))$ , Gronwall's inequality, see Chapter 2, shows that

$$\|v^h(t)\|^2 \leq \bar{C} \|v^h(0)\|^2 + \bar{C}(v) \int_0^t \{\|\rho_t\|^2 + \|\rho_x\|^2 + \|\rho\|^2\} d\tau.$$

Also,

$$\begin{aligned} \|v^h(0)\| & \leq \|y_{0h} - P_1 y(0)\| \\ & \leq \|y_{0h} - y_0\| + \|P_1 y(0) - y_0\| \\ & \leq \|y_{0h} - y(0)\| + \tilde{C} h^r \|y_0\|_r. \end{aligned}$$

Thus,

$$\|v^h(t)\| \leq C (\|y_{0h} - y_0\| + h^{r-1}),$$

which completes the proof. ■

#### 4.1.6.3 Fully discretization

We formulate two different fully discrete finite element schemes arising from Crank-Nicolson and semi-implicit time approaches.

Similar to linearized Burgers equation in Chapter 3, Eq. (3.17), we can write the linear problem with homogenous Dirichlet boundary conditions as

$$\begin{aligned}
y_t - \nu y_{xx} + \beta y_x + \gamma y &= \tilde{f} & \text{in } Q, \\
y &= 0 & \text{on } \Sigma, \\
y(0) &= y_0 & \text{in } \Omega.
\end{aligned}$$

**Scheme 1 :** (Crank-Nicolson method) Given Find  $y_h^i \in V_h$  such that

$$\left\{ \begin{aligned}
&\frac{1}{\Delta t}(y_h^{i+1} - y_h^i, w_h) + \frac{\nu}{2}(\nabla y_h^{i+1} + \nabla y_h^i, \nabla w_h) - \frac{\beta}{2}(y_h^{i+1} + y_h^i, \nabla w_h) \\
&\quad + \frac{\gamma}{2}(y_h^{i+1} + y_h^i, w_h) = \frac{1}{2}(\tilde{f}(t_i) + \tilde{f}(t_{i+1}), w_h), \\
&y_h^0 = y_{0,h}, \text{ for any } w_h \in V_h.
\end{aligned} \right. \quad (4.18)$$

**Scheme 2 :** (Semi-implicit time approximation) For each  $i = 0, \dots, N-1$  evaluate the second order term at the time level  $t_{i+1}$ , whereas the remaining parts considered at the time  $t_n$ . Find  $y_h^i$  such that

$$\left\{ \begin{aligned}
&\frac{1}{\Delta t}(y_h^{i+1} - y_h^i, w_h) + \nu(\nabla y_h^{i+1}, \nabla w_h) + (y_h^i \nabla y_h^i, w_h) = (f(t_{i+1}), w_h), \\
&y_h^0 = y_{0,h}, \text{ for any } w_h \in V_h.
\end{aligned} \right. \quad (4.19)$$

We consider first Crank-Nicolson scheme. The error estimates are covered in [44] for the linear parabolic problems with Crank-Nicolson scheme. So that we refer to [44] for the proofs of the stability and convergence results.

**Theorem 4.1.4** (*Stability of the Crank-Nicolson scheme*) Let  $y_{0,h}$  be given and  $n > 0$ . Then, approximate solution of (4.18) is stable and satisfies

$$\|y_h^n\|^2 \leq C(\|y_{0,h}\|^2 + \frac{T}{2\nu} \|f\|_{L^2(0,T;\Omega)}^2),$$

with a constant  $C$  independent of  $h$  and  $n$

**Theorem 4.1.5** (*Convergence of the Crank-Nicolson scheme*)

Assume that  $y_0 \in H_0^1(\Omega)$  and the solution to (3.11) is such that  $\frac{\partial y}{\partial t} \in L^2(0, T; H_0^1(\Omega))$  and  $\frac{\partial^2 y}{\partial t^2} \in L^2(0, T; L^2(\Omega))$ . Then  $y_h^n$  satisfies

$$\begin{aligned} \|y_h^n - y(t_n)\|^2 &\leq \|(I - P_1)y(t_n)\|^2 + \exp(C^* t_n) \left\{ \|y_{h,0} - P_1 y_0\|^2 \right. \\ &\quad \left. + \frac{C}{\nu} \left\| \int_{t_n}^{t_{i+1}} (I - P_1) \frac{\partial y}{\partial t}(s) ds \right\|^2 + \frac{C(\Delta t)^4}{\nu} \left\| \int_{t_n}^{t_{i+1}} \frac{\partial^3 y}{\partial t^3}(s) ds \right\|^2 \right\}, \end{aligned}$$

where  $C^*$  and  $C$  only depend on  $\nabla y$  and  $\nu$ .

**Remark.** As a corollary of the Theorem we can state that the expected order of convergence is  $O(h + k^2)$ .

Now, we shall obtain the stability and convergence of the semi-implicit scheme.

**Theorem 4.1.6** (Stability of semi-implicit scheme) *The solutions to Scheme 2 is unconditionally stable and*

$$\|y_h^n\|^2 \leq C^* (\|y_{0,h}\|^2 + \frac{TC}{2\nu} \|f\|_{L^2(0,T;\Omega)}^2), \quad (4.20)$$

where  $C$  and  $C^*$  are constants independent of  $h, \Delta t$  and  $\nu$ .

**Proof.**

Letting  $w_h = y_h^{i+1}$  gives

$$\begin{aligned} &\frac{1}{2\Delta t} \|y_h^{i+1}\|^2 - \frac{1}{2\Delta t} \|y_h^i\|^2 + \frac{1}{2\Delta t} \|y_h^{i+1} - y_h^i\|^2 + \nu \|y_h^{i+1}\|^2 \\ &= -(y_h^i \nabla y_h^i, y_h^{i+1}) + (f(t_{i+1}), y_h^{i+1}) \\ &\leq |(y_h^i \nabla y_h^i, y_h^{i+1})| + |(f(t_{i+1}), y_h^{i+1})|. \end{aligned}$$

Note that, using Young inequality implies

$$|(y_h^i \nabla y_h^i, y_h^{i+1})| \leq \frac{C}{2\epsilon} \|y_h^i\|^2 \|\nabla y_h^i\|^2 + \frac{\epsilon}{2} \|\nabla y_h^{i+1}\|^2,$$

and

$$|(f(t_{i+1}), y_h^{i+1})| \leq \frac{C}{2\epsilon} \|f(t_{i+1})\|^2 + \frac{\epsilon}{2} \|\nabla y_h^{i+1}\|^2.$$

It follows that

$$\begin{aligned} \frac{1}{2\Delta t} \|y_h^{i+1}\|^2 - \frac{1}{2\Delta t} \|y_h^i\|^2 + \frac{1}{2\Delta t} \|y_h^{i+1} - y_h^i\|^2 + \nu \|y_h^{i+1}\|^2 \\ \leq \frac{C}{2\epsilon} \|y_h^i\|^2 \|\nabla y_h^i\|^2 + \frac{\epsilon}{2} \|\nabla y_h^{i+1}\|^2 + \frac{C}{2\epsilon} \|f(t_{i+1})\|^2 + \frac{\epsilon}{2} \|\nabla y_h^{i+1}\|^2. \end{aligned}$$

Choosing  $\epsilon = \nu$  gives

$$\frac{1}{2\Delta t} \|y_h^{i+1}\|^2 - \frac{1}{2\Delta t} \|y_h^i\|^2 \leq \frac{C}{2\nu} \|y_h^i\|^2 \|\nabla y_h^i\|^2 + \frac{C}{2\nu} \|f(t_{i+1})\|^2.$$

Let now  $m$  be a fixed index,  $1 \leq m \leq N$ . Summing over  $n$  from 0 to  $m-1$ , we find

$$\|y_h^m\|^2 \leq \|y_{0,h}\|^2 + \frac{C\Delta t}{2\nu} \sum_{n=0}^{m-1} \left( \|y_h^n\|^2 \|\nabla y_h^n\|^2 + \frac{\Delta t C}{2\nu} \|f(t_{n+1})\|^2 \right).$$

We use discrete Gronwall inequality to get

$$\|y_h^m\|^2 \leq \left( \|y_{0,h}\|^2 + \frac{TC}{2\nu} \|f\|_{L^2(0,T;\Omega)}^2 \right) \exp \left( \frac{CT}{2\nu} \sum_{n=0}^{m-1} \|\nabla y_h^n\|^2 \right).$$

We let  $C^* = \exp \left( \frac{CT}{2\nu} \sum_{n=0}^{m-1} \|\nabla y_h^n\|^2 \right)$  to get

$$\|y_h^m\|^2 \leq C^* \left( \|y_{0,h}\|^2 + \frac{TC}{2\nu} \|f\|_{L^2(0,T;\Omega)}^2 \right),$$

■

**Theorem 4.1.7** (Convergence of semi-implicit scheme)

Assume that  $y_0 \in H_0^1(\Omega)$  and the solution to (4.15) is such that  $\frac{\partial y}{\partial t} \in L^2(0, T; H_0^1(\Omega))$  and  $\frac{\partial^2 y}{\partial t^2} \in L^2(0, T; L^2(\Omega))$ . Then,  $y_h^n$  satisfies

$$\begin{aligned} & \|y_h^n - y(t_n)\|^2 \\ & \leq \|(I - P_1)y(t_n)\|^2 + \exp(C^* t_n) \left\{ \|y_{h,0} - P_1 y_0\|^2 + \frac{C}{\nu} \left\| \int_{t_n}^{t_{i+1}} (I - P_1) \frac{\partial y}{\partial t}(s) ds \right\|^2 \right. \\ & \quad \left. + \frac{C(\Delta t)^2}{\nu} \left\| \int_{t_n}^{t_{i+1}} \frac{\partial^2 y}{\partial t^2}(s) ds \right\|^2 + \frac{(\Delta t)^2 \tilde{C}(\nabla y(t_i))}{\nu} \left\| \int_{t_n}^{t_{i+1}} \frac{\partial y}{\partial t}(s) ds \right\|^2 \right\}, \end{aligned}$$

where  $C^*$  only depends on  $\nabla y$  and  $\nu$ .

**Proof.**

We define  $e^i = y_h^i - y(t_i)$ . Let  $\eta^i = y_h^i - P_1 y(t_i)$ . Then,  $e^i = \eta^i + P_1 y(t_i) - y(t_i)$ . Since

$$\|P_1 y(t_i) - y(t_i)\| \leq Ch \|y(t_i)\|,$$

$\eta^i$  is bounded. We have

$$\begin{aligned} & \frac{1}{\Delta t} (\eta^{i+1} - \eta^i, w_h) + \nu (\nabla \eta_h^{i+1}, \nabla w_h) \\ & = -\frac{1}{\Delta t} (P_1 y(t_{i+1}) - P_1 y(t_i), w_h) - \nu (\nabla P_1 y(t_{i+1}), \nabla w_h) - (y_h^i \nabla y_h^i, w_h) + (f(t_{i+1}), w_h). \end{aligned}$$

Also, we note that by definition of  $P_1$ ,

$$\begin{aligned} \nu (\nabla (P_1 y(t_{i+1})), \nabla w_h) & = \nu (\nabla y(t_{i+1}), \nabla w_h) \\ & = -\left(\frac{\partial}{\partial t} y(t_{i+1}), w_h\right) - (y(t_{i+1}) \nabla y(t_{i+1}), w_h) + (u(t_{i+1}), w_h). \end{aligned} \tag{4.21}$$

Then,

$$\begin{aligned} & \frac{1}{\Delta t} (\eta^{i+1} - \eta^i, w_h) + \nu (\nabla \eta_h^{i+1}, \nabla w_h) \\ & = -\frac{1}{\Delta t} (P_1 y(t_{i+1}) - P_1 y(t_i), w_h) + \left(\frac{\partial}{\partial t} y(t_{i+1}), w_h\right) + (y(t_{i+1}) \nabla y(t_{i+1}), w_h) - (y_h^i \nabla y_h^i, w_h). \end{aligned}$$

The first two terms of the right hand-side can be written as

$$\begin{aligned}
& -\frac{1}{\Delta t}(P_1(y(t_{i+1})) - P_1(y(t_i), w_h) + (\frac{\partial}{\partial t}y(t_{i+1}), w_h)) \\
& = \frac{1}{\Delta t}(\int_{t_n}^{t_{i+1}} (I - P_1) \frac{\partial y}{\partial t}(s) ds, w_h) + (\frac{\partial y}{\partial t}(t_{i+1}) - \frac{y(t_{i+1}) - y(t_i)}{\Delta t}, w_h) \\
& = \frac{1}{\Delta t}(\int_{t_n}^{t_{i+1}} (I - P_1) \frac{\partial y}{\partial t}(s) ds, w_h) + \Delta t(\int_{t_n}^{t_{i+1}} \frac{\partial^2 y}{\partial t^2}(s) ds, w_h).
\end{aligned}$$

Let  $w_h = \eta^{i+1}$ . It follows that

$$\begin{aligned}
& \frac{1}{2\Delta t}\|\eta^{i+1}\|^2 - \frac{1}{2\Delta t}\|\eta^i\|^2 + \nu\|\nabla\eta_h^{i+1}\|^2 \\
& \leq \frac{1}{\Delta t}|(\int_{t_n}^{t_{i+1}} (I - P_1) \frac{\partial y}{\partial t}(s) ds, \eta^{i+1})| + \Delta t|(\int_{t_n}^{t_{i+1}} \frac{\partial^2 y}{\partial t^2}(s) ds, \eta^{i+1})| \\
& \quad + |(y(t_{i+1})\nabla y(t_{i+1}) - y_h^i\nabla y_h^i, \eta^{i+1})|.
\end{aligned}$$

Consider the term  $(y(t_{i+1})\nabla y(t_{i+1}) - y_h^i\nabla y_h^i, \eta^{i+1})$ . Adding and subtracting terms yield

$$\begin{aligned}
& (y(t_{i+1})\nabla y(t_{i+1}), \eta^{i+1}) - (y_h^i\nabla y_h^i, \eta^{i+1}) \\
& = -\frac{1}{2}(y(t_{i+1})y(t_{i+1}) - y_h^iy_h^i, \nabla\eta^{i+1}) \\
& = -\frac{1}{2}((y(t_{i+1}) - y(t_i))y(t_{i+1}) + (y(t_i) - y_h^i)y_h^i + y(t_i)(y(t_{i+1}) - y_h^i), \nabla\eta^{i+1}).
\end{aligned}$$

Also,

$$(y(t_{i+1}) - y_h^i) = (y(t_{i+1}) - y(t_i) + y(t_i) - y_h^i).$$

Then, using the boundedness of  $\nabla y_h^i$  we get

$$\begin{aligned}
& |(y(t_{i+1})\nabla y(t_{i+1}), \eta^{i+1}) - (y_h^i\nabla y_h^i, \eta^{i+1})| \\
& \leq C\|\nabla\eta^{i+1}\|(\|\nabla y(t_{i+1})\|\|y(t_{i+1}) - y(t_i)\| + \|\nabla y_h^i\|\|y(t_i) - y_h^i\| \\
& \quad + \|\nabla y(t_i)\|\|y(t_{i+1}) - y(t_i)\| + \|\nabla y(t_i)\|\|y(t_i) - y_h^i\|) \\
& \leq C(\nabla y(t_i))\|\nabla\eta^{i+1}\|\|y(t_{i+1}) - y(t_i)\| + \bar{C}(\nabla y(y_i))\|\nabla\eta^{i+1}\|\underbrace{\|y(t_i) - y_h^i\|}_{\eta^i}.
\end{aligned}$$

Now, using  $y(t_{i+1}) - y(t_i) = \Delta t \int_{t_n}^{t_{i+1}} \frac{\partial y}{\partial t}(s) ds$

$$\begin{aligned}
& \frac{1}{2\Delta t} \|\eta^{i+1}\|^2 - \frac{1}{2\Delta t} \|\eta^i\|^2 + \nu \|\nabla \eta_h^{i+1}\|^2 \\
& \leq \frac{1}{\Delta t} \left| \left( \int_{t_n}^{t_{i+1}} (I - P_1) \frac{\partial y}{\partial t}(s) ds, \eta^{i+1} \right) \right| + \Delta t \left| \left( \int_{t_n}^{t_{i+1}} \frac{\partial^2 y}{\partial t^2}(s) ds, \eta^{i+1} \right) \right| \\
& \quad + \Delta t C(\nabla y(t_i)) \|\nabla \eta^{i+1}\| \left\| \int_{t_n}^{t_{i+1}} \frac{\partial y}{\partial t}(s) ds \right\| + \bar{C}(\nabla y(t_i)) \|\nabla \eta^{i+1}\| \|\eta^i\| \\
& \leq \frac{C}{\nu \Delta t} \left\| \int_{t_n}^{t_{i+1}} (I - P_1) \frac{\partial y}{\partial t}(s) ds \right\|^2 + \frac{\nu}{4} \|\nabla \eta^{i+1}\|^2 + \frac{C \Delta t}{\nu} \left\| \int_{t_n}^{t_{i+1}} \frac{\partial^2 y}{\partial t^2}(s) ds \right\|^2 + \frac{\nu}{4} \|\nabla \eta^{i+1}\|^2 \\
& \quad + \frac{\Delta t \bar{C}(\nabla y(t_i))}{\nu} \left\| \int_{t_n}^{t_{i+1}} \frac{\partial y}{\partial t}(s) ds \right\|^2 + \frac{\nu}{4} \|\nabla \eta^{i+1}\|^2 + \frac{\bar{C}(\nabla y(t_i))}{\nu} \|\eta^i\|^2 + \frac{\nu}{4} \|\nabla \eta^{i+1}\|^2.
\end{aligned}$$

Then,

$$\begin{aligned}
\|\eta^{i+1}\|^2 - \|\eta^i\|^2 & \leq \frac{C}{\nu} \left\| \int_{t_n}^{t_{i+1}} (I - P_1) \frac{\partial y}{\partial t}(s) ds \right\|^2 + \frac{C(\Delta t)^2}{\nu} \left\| \int_{t_n}^{t_{i+1}} \frac{\partial^2 y}{\partial t^2}(s) ds \right\|^2 \\
& \quad + \frac{(\Delta t)^2 \bar{C}(\nabla y(t_i))}{\nu} \left\| \int_{t_n}^{t_{i+1}} \frac{\partial y}{\partial t}(s) ds \right\|^2 + \frac{\Delta t \bar{C}(\nabla y(t_i))}{\nu} \|\eta^i\|^2.
\end{aligned}$$

Summing over  $n$  from 0 to  $m - 1$  and using discrete Gronwall inequality imply that

$$\begin{aligned}
\|\eta^n\|^2 & \leq \|\eta_{0h}\|^2 + \exp(C^* t_n) \left\{ \frac{C}{\nu} \left\| \int_{t_n}^{t_{i+1}} (I - P_1) \frac{\partial y}{\partial t}(s) ds \right\|^2 \right. \\
& \quad \left. + \frac{C(\Delta t)^2}{\nu} \left\| \int_{t_n}^{t_{i+1}} \frac{\partial^2 y}{\partial t^2}(s) ds \right\|^2 + \frac{(\Delta t)^2 \bar{C}(\nabla y(t_i))}{\nu} \left\| \int_{t_n}^{t_{i+1}} \frac{\partial y}{\partial t}(s) ds \right\|^2 \right\}.
\end{aligned}$$

■

#### 4.1.6.4 Error analysis for the control problem

We first obtain weak formulation of the discrete adjoint with respect to both time approaches.

We obtain error estimations for adjoint then.

#### 4.1.6.5 Discrete adjoint and error estimates

In this subsection, the semi-implicit scheme is covered in detail and the results for the Crank-Nicolson scheme are presented only.

The optimality conditions obtained in Eqn. (4.11) leads to an adjoint for each time step as:

$$\begin{aligned} (M + \Delta t S)\mathbf{p}^i - M\mathbf{p}^{i+1} &= \Delta t M(\mathbf{y}^i - \mathbf{y}_d) \\ \mathbf{p}(T) &= 0 \text{ for } i = N, \dots, 1. \end{aligned}$$

This corresponds to a weak formulation following as

$$\begin{cases} \frac{1}{\Delta t}(p_h^i - p_h^{i+1}, w_h) + \nu(\nabla p_h^i, \nabla w_h) = (y(t_i) - y_d(t_i), w_h), \\ p_h^T = 0, \text{ for any } w_h \in V_h. \end{cases} \quad (4.22)$$

**Theorem 4.1.8** (*Stability with respect to Semi-implicit scheme*) *The solution to (4.23) is stable and satisfies*

$$\|p_h^n\|^2 \leq C^*(\|p_{T,h}\|^2 + \frac{TC}{2\nu}\|f\|_{L^2(0,T;\Omega)}^2).$$

**Proof.** We let  $w_h = p_h^i$ . We perform the same strategy as in Theorem 3 and result follows. ■

Now we find an error bound for adjoint variable.

**Theorem 4.1.9** (*Convergence for the semi-implicit scheme*)

Assume that the solution to (4.23) is such that  $\frac{\partial p}{\partial t} \in L^2(0, T; H_0^1(\Omega))$  and  $\frac{\partial^2 p}{\partial t^2} \in L^2(0, T; L^2(\Omega))$ . Then  $p_h^n$ , satisfies

$$\begin{aligned} \|p_h^n - p(t_n)\|^2 &\leq \|(I - P_1)p(t_n)\|^2 + \exp(T) \left\{ \frac{C}{\nu} \left\| \int_0^{t_n} (I - P_1) \frac{\partial y}{\partial t}(s) ds \right\|^2 \right. \\ &\quad \left. + \frac{C(\Delta t)^2}{\nu} \left\| \int_0^{t_n} \frac{\partial^2 p}{\partial t^2}(s) ds \right\|^2 + (\Delta t)^2 \|y(t_i) \nabla p(t_i)\|^2 \right\}, \end{aligned}$$

where  $C^*$  only depends on  $\nabla y$  and  $\nu$ .

**Proof.** Since  $y_h^n$  is stable then for simplicity let us consider the following weak formulation

$$\frac{1}{\Delta t}(p_h^i - p_h^{i+1}, w_h) + \nu(\nabla p_h^i, \nabla w_h) = (\tilde{f}, w_h)$$

Following the same procedure as in the proof of convergence theorem of state equation, for  $i = N, \dots, 1$  we get

$$\begin{aligned} & \frac{1}{\Delta t}(\eta^i - \eta^{i+1}, w_h) + \nu(\nabla \eta_h^i, \nabla w_h) \\ &= -\frac{1}{\Delta t}(P_1 p(t_i) - P_1 p(t_{i+1}), w_h) - \nu(\nabla P_1 p(t_i), \nabla w_h) + (\tilde{f}(t_i), w_h). \end{aligned}$$

Using the definition of  $P_1$  and continuous adjoint equation given by

$$\begin{aligned} p_t^* + \nu \Delta p^* + y^* \nabla p^* &= y_d - y^* & \text{in } Q, \\ p^*(t, 0) = p^*(t, 1) &= 0 & \text{on } \Sigma, \\ p^*(T) &= 0 & \text{in } \Omega. \end{aligned}$$

It follows that

$$\begin{aligned} & \frac{1}{\Delta t}(\eta^i - \eta^{i+1}, w_h) + \nu(\nabla \eta_h^i, \nabla w_h) \\ &= -\frac{1}{\Delta t}(P_1 p(t_i) - P_1 p(t_{i+1}), w_h) + \left(\frac{\partial}{\partial t} p(t_i), w_h\right) + (y(t_i) \nabla p(t_i), w_h), \end{aligned}$$

then,

$$\begin{aligned} & \frac{1}{2\Delta t} \|\eta^i\|^2 - \frac{1}{2\Delta t} \|\eta^{i+1}\|^2 + \frac{1}{2\Delta t} \|\eta^i - \eta^{i+1}\|^2 + \nu \|\nabla \eta_h^i\|^2 \\ & \leq \frac{1}{\Delta t} \left| \left( \int_{t_{i+1}}^{t_i} (I - P_1) \frac{\partial p}{\partial t}(s) ds, \eta^i \right) \right| + \Delta t \left| \left( \int_{t_{i+1}}^{t_i} \frac{\partial^2 p}{\partial t^2}(s) ds, \eta^i \right) \right| + |(y(t_i) \nabla p(t_i), \eta^i)|. \end{aligned}$$

Considering the term  $(y(t_i) \nabla p(t_i), \eta^i)$  gives

$$\begin{aligned} & |(y(t_i) \nabla p(t_i), \eta^i)| \\ &= |(y(t_i) \nabla p(t_i), \eta^i - \eta^{i+1} + \eta^{i+1})| \\ &\leq |(y(t_i) \nabla p(t_i), \eta^i - \eta^{i+1})| + |(y(t_i) \nabla p(t_i), \eta^{i+1})| \\ &\leq \frac{\Delta t}{2} \|y(t_i) \nabla p(t_i)\|^2 + \frac{1}{2\Delta t} \|\eta^i - \eta^{i+1}\|^2 + \frac{\Delta t}{2} \|y(t_i) \nabla p(t_i)\|^2 + \frac{1}{2\Delta t} \|\eta^{i+1}\|^2. \end{aligned}$$

Then,

$$\begin{aligned}
& \|\eta^i\|^2 - \|\eta^{i+1}\|^2 + 2\Delta t \nu \|\nabla \eta_h^i\|^2 \\
& \leq 2 \left| \left( \int_{t_{i+1}}^{t_i} (I - P_1) \frac{\partial p}{\partial t}(s) ds, \eta^i \right) \right| + 2(\Delta t)^2 \left| \left( \int_{t_{i+1}}^{t_i} \frac{\partial^2 p}{\partial t^2}(s) ds, \eta^i \right) \right| \\
& \quad + (\Delta t)^2 \|y(t_i) \nabla p(t_i)\|^2 + \|\eta^{i+1}\|^2.
\end{aligned}$$

Summing over  $N$  to 0 and using Gronwall's lemma give

$$\begin{aligned}
\|\eta^n\|^2 & \leq \|\eta_{Th}\|^2 + \exp(N) \left\{ \frac{C}{\nu} \left\| \int_{t_{i+1}}^{t_i} (I - P_1) \frac{\partial y}{\partial t}(s) ds \right\|^2 \right. \\
& \quad \left. + \frac{C(\Delta t)^2}{\nu} \left\| \int_{t_{i+1}}^{t_i} \frac{\partial^2 p}{\partial t^2}(s) ds \right\|^2 + (\Delta t)^2 \|y(t_i) \nabla p(t_i)\|^2 \right\}.
\end{aligned}$$

■

**Remark.** As a corollary of the Theorem we can state that the expected order of convergence is  $O(h + k)$ .

Similar to semi-implicit scheme, we can derive the stability and convergence results of discrete adjoint obtained from the control problem with Crank-Nicolson time scheme.

We consider the continuous adjoint equation

$$\begin{aligned}
p_t^* + \nu \Delta p^* + \beta \nabla p^* & = y_d - y^* & \text{in } Q, \\
p^*(t, 0) = p^*(t, 1) & = 0 & \text{on } \Sigma, \\
p^*(T) & = 0 & \text{in } \Omega.
\end{aligned}$$

Then, the weak formulation follows as

$$\begin{cases} \frac{1}{\Delta t} (p_h^i - p_h^{i+1}, w_h) + \nu (\nabla p_h^i, \nabla w_h) + \beta (\nabla p, w_h) = (y_h^i - y_d, w_h), \\ p_h^T = 0, \text{ for any } w_h \in V_h. \end{cases} \quad (4.23)$$

Note that Crank-Nicolson scheme applied to above formulation satisfies the stability result as in Theorem 4.1.4 and convergence follows from [Theorem 11.3.2, [44]].

**Theorem 4.1.10** (*Stability for the Crank-Nicolson scheme*) Let  $p_{T,h}$  be given. The solution to (4.23) is stable and satisfies

$$\|p_h^n\|^2 \leq C(\|p_{T,h}\|^2 + \frac{T}{\nu} \|f\|_{L^2(0,T;\Omega)}^2),$$

where  $C$  is a constant independent of  $h, \Delta t$  and  $\nu$ .

**Theorem 4.1.11** (*Convergence for the Crank-Nicolson scheme*)

Assume that the solution to (4.23) is such that  $\frac{\partial p}{\partial t} \in L^2(0, T; H_0^1(\Omega))$  and  $\frac{\partial^2 p}{\partial t^2} \in L^2(0, T; L^2(\Omega))$ . Then  $p_h^n$  satisfies

$$\begin{aligned} & \|p_h^n - p(t_n)\|^2 \\ & \leq \|(I - P_1)p(t_n)\|^2 + \exp(C^* t_n) \cdot \left\{ \|p_{h,T} - P_1 p_T\|^2 \right. \\ & \quad \left. + \frac{C}{\nu} \left\| \int_0^{t_n} (I - P_1) \frac{\partial p}{\partial t}(s) ds \right\|^2 + \frac{C(\Delta t)^4}{\nu} \left\| \int_0^{t_n} \frac{\partial^3 p}{\partial t^3}(s) ds \right\|^2 \right\}, \end{aligned}$$

where  $C^*$  only depends on  $\nabla y$  and  $\nu$ .

#### 4.1.6.6 Error in the control variable

In this section, we find an error estimate for the control variable. Actually the error analysis of control variable is related to adjoint equation. The following theorem shows this relation.

**Theorem 4.1.12** *The solutions to continuous and discretized control problem satisfy*

$$\|\bar{u} - \bar{u}_h^n\| \leq \frac{1}{\alpha} \|p - p_h^n\| + \|\bar{u} - P_1 \bar{u}\|. \quad (4.24)$$

In order to prove the Theorem 4.1.12, we need some results related to the cost function. We recall the continuous cost function

$$J(y, u) = \frac{1}{2} \|y - y_d\|_Q^2 + \frac{\alpha}{2} \|u\|_Q^2.$$

The reduced cost function can be stated as

$$j(u) = J(S(u), u),$$

where  $S$  is the solution operator as defined in chapter 1. The derivative of the reduced cost function can be stated as

$$j'(u)(\delta u) = (p, \delta u) + \alpha(u, \delta u),$$

where  $p$  corresponds to the adjoint variable. The necessary and sufficient optimality conditions read as

$$j'(\bar{u})(\delta u - \bar{u}) \geq 0 \quad \forall \delta u \in Q, \quad (4.25)$$

and

$$j''(u)(\delta u, \delta u) \geq \alpha \|\delta u\|^2 \quad \forall \delta u \in Q, \quad (4.26)$$

where  $\bar{u}$  is the optimal solution.

We can derive similar results for the discretized problem. We assume that  $S_{hn}$  is the discrete solution operator between control and state variables. We let  $j_{hn}(u_h^n) = J_{hn}(S_{hn}(u_h^n), u_h^n)$ . Then, the optimality conditions give

$$j'_{hn}(\bar{u}_h^n)(\delta u_h^n - \bar{u}_h^n) \geq 0 \quad \forall \delta u_h^n \in V_h \quad (4.27)$$

and

$$j''_{hn}(u_h^n)(\delta u_h^n, \delta u_h^n) \geq \alpha \|\delta u_h^n\|^2 \quad \forall \delta u_h^n \in V_h. \quad (4.28)$$

**Lemma 4.1.13** *The error between the solutions of the continuous and discretized control problem satisfies*

$$\|j'(u)(r) - j'_{hn}(u)(r)\| \leq \|p(u) - p_h^n(u)\| \|r\| \quad \text{for } u, r \in Q.$$

**Proof.** Since

$$j'(u)(r) = (p(u), r) + \alpha(u, r) \text{ and } j'_{hn}(u)(r) = (p_h^n(u), r) + \alpha(u, r)$$

implies directly

$$\|j'(u)(r) - j'_{hn}(u)(r)\| = \|(p(u) - p_h^n(u), r)\| \leq \|p(u) - p_h^n(u)\| \|r\|.$$

■

**Lemma 4.1.14** *Let  $u$  be a given control. The error between the continuous state  $y$  and the discrete state  $y_h^n$  can be estimated as:*

*For semi-implicit scheme*

$$\|y - y_h^n\| \leq C(\Delta t)^{1/2} \|u - q\| + O(h + \Delta t),$$

*where  $q \in Q$  and  $O$  denotes the order.*

*Similarly, for Crank-Nicolson scheme*

$$\|y - y_h^n\| \leq C(\Delta t)^{1/2} \|u - q\| + O(h + (\Delta t)^2).$$

**Proof.**

We take  $u$  instead of  $f$  in the Eq. (3.11) and  $q$  in the place of  $f(t^{i+1})$  in (4.19). Then we have additional terms to Theorem 2.2. Proceeding the same steps gives the desired result. It is obtained similarly for Crank-Nicolson scheme.

■

**Lemma 4.1.15** *Let  $q$  be a given control. The error between the continuous adjoint state  $p$  and the discrete adjoint state  $p_h^n$  can be estimated as:*

For semi-implicit scheme

$$\|p - p_h^n\| \leq C\Delta t \|u - q\| + O(h + \Delta t),$$

where  $q \in Q$  and  $O$  denotes the order and  $C$  is independent of  $h$  and  $\Delta t$ .

Similarly, for Crank-Nicolson scheme

$$\|p - p_h^n\| \leq C\Delta t \|u - q\| + O(h + (\Delta t)^2).$$

**Proof.** The same procedure holds as in the proof of Lemma 4.1.15 ■

We now come to proof of the Theorem 4.1.12. Let  $\bar{u}$  and  $\bar{u}_h^n$  be the optimal solutions to discrete and continuous control problems, respectively. For an arbitrary  $q$  we write

$$\bar{u} - \bar{u}_h^n = \bar{u} - q + q - \bar{u}_h^n.$$

From (4.28)

$$\alpha \|q - \bar{u}_h^n\|^2 \leq j''_{hn}(q)(q - \bar{u}_h^n, q - \bar{u}_h^n) = j'_{hn}(\bar{u})(q_h^n - \bar{u}_h^n) - j'_{hn}(\bar{u}_h^n)(q_h^n - \bar{u}_h^n).$$

From optimality we have

$$j'_{hn}(\bar{u}_h^n)(q_h^n - \bar{u}_h^n) = 0 = j'(\bar{u})(q_h^n - \bar{u}_h^n). \quad (4.29)$$

Then,

$$\begin{aligned} \alpha \|q_h^n - \bar{u}_h^n\|^2 &\leq j'_{hn}(\bar{u})(q_h^n - \bar{u}_h^n) - j'(\bar{u})(q_h^n - \bar{u}_h^n) \\ &\leq \|p(\bar{u}) - p_h^n(\bar{u})\| \|q_h^n - \bar{u}_h^n\|. \end{aligned}$$

Finally,  $\|q_h^n - \bar{u}_h^n\| \leq \frac{1}{\alpha} \|p(\bar{u}) - p_h^n(\bar{u})\|$ . We let  $q = P_1(\bar{u})$  and use Lemma 4.1.13 to get the desired result.

**Corollary 4.1.16** *The solutions to continuous and discretized control problem satisfy the following estimations:*

*For the semi-implicit scheme*

$$\|\bar{u} - \bar{u}_h^n\| \leq O(h + h\Delta t + \Delta t),$$

*and for the Crank-Nicolson scheme*

$$\|\bar{u} - \bar{u}_h^n\| \leq O(h + h\Delta t + (\Delta t)^2).$$

**Proof.** This corollary is a result of the projection  $P_1$  property and Lemma 4.1.15. ■

#### 4.1.7 Error analysis for the control constrained problem

In this section, we provide an error estimate for the control constrained case. Since (4.29) does not hold any more, we can not use the same argument as in the unconstrained problem. We recall that there exists an additional constraint as

$$u_a(t, x) \leq u(t, x) \leq u_b(t, x) \text{ in } Q. \quad (4.30)$$

This condition leads to a variational inequality as

$$j'(\bar{u})(u - \bar{u}) \geq 0 \text{ for all } u \in U_{ad},$$

where  $j(u)$  is represented as

$$\min J(y, u) \leftrightarrow \min j(u).$$

It is known that the inequality above is equivalent to

$$\bar{u} = \Pi_{Q_{ad}}\left(-\frac{1}{\alpha}\bar{p}\right), \quad (4.31)$$

where  $\Pi_{Q_{ad}}(t, x) := \max(u_a, \min(u_b, r(t, x)))$  is the projection into the admissible space  $Q_{ad}$ .

As in the continuous case we can deduce a projection formula as

$$\bar{u}_h^n = \Pi_{Q_{ad}}\left(-\frac{1}{\alpha}\bar{p}_h^n\right).$$

This projection  $\Pi_{Q_{ad}}$  satisfies the regularity properties

$$\left\|\Pi_{Q_{ad}}\left(-\frac{1}{\alpha}\bar{p}\right) - \Pi_{Q_{ad}}\left(-\frac{1}{\alpha}\bar{p}_h^n\right)\right\|_{L(Q)} \leq \frac{1}{\alpha}\|\bar{p} - \bar{p}_h^n\|_{L^2(Q)}. \quad (4.32)$$

**Theorem 4.1.17** *Let  $\bar{u}$  and  $\bar{u}_h^n$  be the solutions to continuous and discrete optimal control problems respectively. Then*

$$\|\bar{u} - \bar{u}_h^n\| \leq \frac{1}{\alpha}\|\bar{p} - \bar{p}_h^n\|,$$

where  $\bar{p}$  and  $\bar{p}_h^n$  are the corresponding continuous and discrete adjoint state variables, respectively.

**Proof.**

This proof is a simple result of (4.31) and (4.32). ■

#### 4.1.8 Numerical examples for the distributed control problems

We carried out some numerical tests for both unconstrained and control constrained control problems of Burgers equation. Because the exact solution of the optimal control problems are unknown, we have used the cost function to show the convergence of the numerical solutions.

**Run 4.1.** (*Distributed unconstrained problem*) As a numerical example we have chosen the following optimal control problem in [13] with the parameters  $\alpha = 0.05$ ,  $\nu = 0.01$ ,  $f = 0$ , with the desired state  $y_d(t, x) = y_0$  and with the initial condition

$$y_0 = \begin{cases} 1 & \text{in } (0, \frac{1}{2}], \\ 0 & \text{otherwise.} \end{cases}$$

We use both direct solver and MINRES to solve control problem. We present the direct solver results in the following table because both solvers give the same result. In Table 1 we

compare the numerical results of Crank-Nicolson (CN) and semi-implicit (SI) schemes for a fixed space mesh  $\Delta x = 2^{-7}$ . Let  $J_{hk}$  be computed value at the corresponding  $\Delta x = h$  and  $\Delta t = k$ . The order of convergence of both schemes are as expected. When  $\Delta t \rightarrow 0$ , the order of the CN scheme is around two, whereas the order of the SI scheme is one, as predicted by the a priori error estimates.

Table 4.1: Unconstrained distributed control problem with a fixed  $\Delta x = 2^{-7}$

$\Delta t$	$\ J_{hk}\ $ CN(SI)	$\ J_{hk} - J_{h(k+1)}\ $ CN(SI)	Observed order CN(SI)
$2^{-4}$	6.153e-2(7.062e-2)	-	-
$2^{-5}$	6.701e-2 (6.892e-2)	5.486e-4(1.706e-3)	-
$2^{-6}$	6.900e-2(6.960e-2)	1.989e-4(6.794e-4)	1.46(1.32)
$2^{-7}$	6.976e-2(6.999e-2)	7.579e-5(3.992e-4)	1.40(0.76)
$2^{-8}$	6.999e-2( 7.019e-2)	2.323e-5(1.916e-4)	1.70(1.05)

Now we fix  $\Delta t$  at  $2^{-7}$  in order to see the order of convergence for space variable. As we expect we have first order convergency in space.

Table 4.2: Unconstrained distributed control problem with a fixed  $\Delta t = 2^{-7}$

$\Delta t$	$\ J_{hk}\ $ CN(SI)	$\ J_{hk} - J_{(h+1)k}\ $ CN(SI)	Observed order CN(SI)
$2^{-3}$	6.983e-2(5.210e-2)	-	-
$2^{-5}$	7.266e-2 (6.390e-2)	2.830e-3(8.880e-3)	-
$2^{-5}$	7.139e-2(6.744e-2)	1.273e-3(3.540e-3)	1.15(1.12)
$2^{-6}$	7.061e-2(6.901e-2)	7.830e-4(1.570e-3)	0.70(1.38)
$2^{-7}$	7.023e-2( 6.999e-2)	3.753e-4(9.840e-4)	1.06(0.67)

The mesh independence concept was discussed in Chapter 3. When we store the iteration numbers corresponding to the a given tolerance we see the mesh independence in Table 4.3. These numbers result from the necessary iteration for convergence of the nonlinear problem. We fix  $\Delta t = 2^{-6}$ . We give the Crank-Nicolson results in Table 4.3.

We present the CPU times for an iterative solver MINRES in Figure 4.1. We compare the CPU times of CN and SI for MINRES with respect to various mesh size. As expected CPU time for CN is much more than for SI. This is a result of that the system matrix for CN scheme is updated at every iteration, whereas it is constant for SI scheme.

Table 4.3: Mesh independence for Run 4.1

$tol/\Delta x$	$2^{-4}$	$2^{-5}$	$2^{-6}$	$2^{-7}$
1e-5	9	9	9	9
1e-6	11	11	11	11
1e-7	13	13	13	13
1e-8	14	14	14	15
1e-9	15	16	16	16
1e-10	17	18	18	18
1e-11	18	19	20	20

The difference of iteration numbers between two consecutive mesh sizes is at most 1 for varying convergence criteria

We present the graphical interpretation for direct solver, which are similar to the results in [13], in Figure 3. We have the same results for MINRES. Optimal state, adjoint state and control solutions are given.

**Run 4.2.** (*Distributed control constrained problem*) We choose the problem in [57]. We consider the same space as in example of unconstrained problem. We let  $\nu = 0.01$ ,  $\alpha = 0.0175$  and  $y_0 = 0$ . As a desired function we choose

We compare the CN and SI for the control constrained problem. Table 4.4 also compares the order of convergence of both schemes.

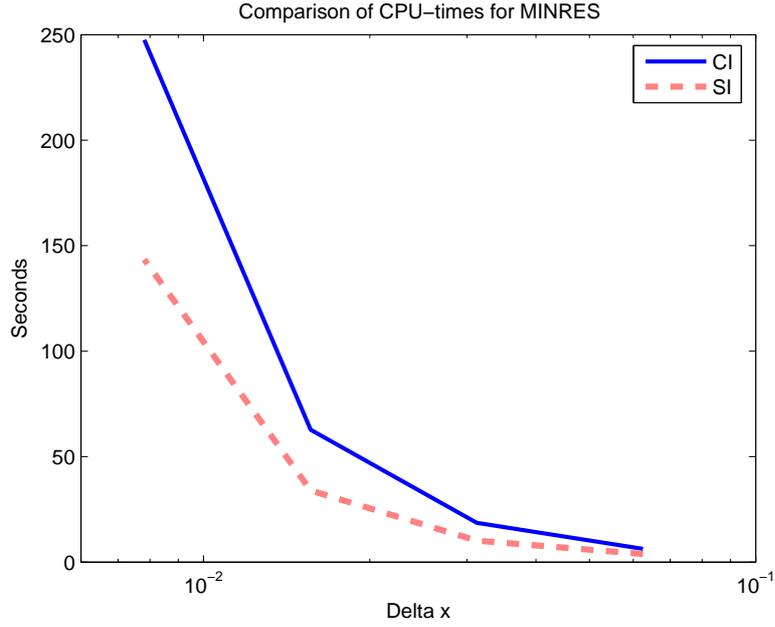


Figure 4.1: The full line and dotted line correspond to Crank-Nicolson and semi-implicit schemes, respectively

Table 4.4: Distributed control constrained problem with a fixed  $\Delta x = 2^{-7}$

$\Delta t$	$\ J_{hk}\ $ CN(SI)	$\ J_{hk} - J_{h(k+1)}\ $ CN(SI)	Observed order CN(SI)
$2^{-4}$	1.212e-1(1.186e-1)	-	-
$2^{-5}$	1.161e-1 (1.149e-1)	5.170e-4(3.706e-4)	-
$2^{-6}$	1.142e-1(1.125e-1)	1.900e-4(2.410e-4)	1.44(0.62)
$2^{-7}$	1.096e-1(1.089e-1)	4.700e-4(3.529e-4)	1.30(0.90)
$2^{-8}$	1.083e-1( 1.067e-1)	1.130e-4(2.209e-5)	1.85(1.03)

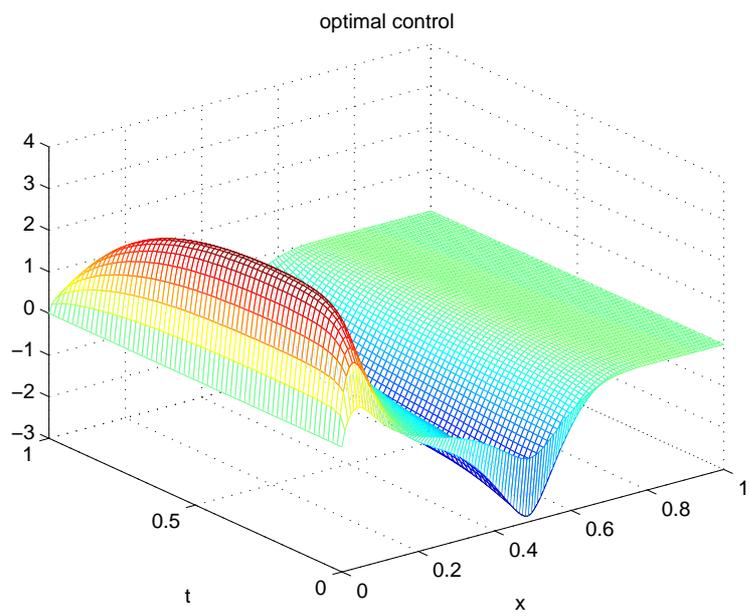
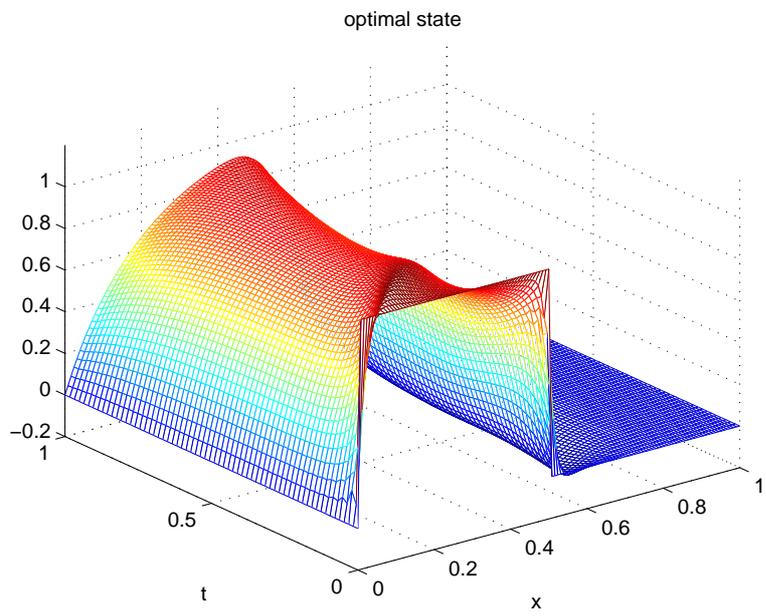


Figure 4.2: Computed  $y$  and  $u$  for  $\Delta t = 2^{-6}, \Delta x = 2^{-7}$

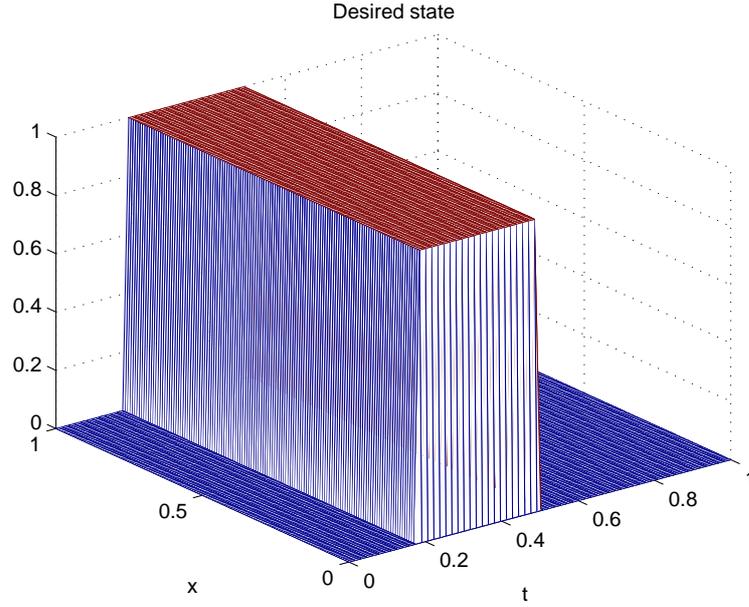


Figure 4.3: Desired state

We now give the observed order for space variable in the Table 4.5. We let  $\Delta t = 2^{-7}$  to see the expected space order which is 1.

Table 4.5: Constrained distributed control problem with a fixed  $\Delta t = 2^{-7}$

$\Delta t$	$\ J_{hk}\ $ CN(SI)	$\ J_{hk} - J_{(h+1)k}\ $ CN(SI)	Observed order CN(SI)
$2^{-3}$	9.635e-2(9.634e-2)	-	-
$2^{-5}$	1.027e-1 (1.013e-1)	2.521e-3(2.605e-3)	-
$2^{-5}$	1.056e-1(1.040e-1)	1.476e-3(1.464e-3)	0.84(0.83)
$2^{-6}$	1.071e-1(1.055e-1)	2.877e-3(2.754e-3)	0.96(0.91)
$2^{-7}$	1.096e-1( 1.081e-1)	6.414e-3(4.988e-3)	1.15(0.85)

The Table 4.6. shows the mesh independence for Crank-Nicolson scheme. Similar results are obtained for semi-implicit method.

We present the state and adjoint variables in the following figures. The results are similar to the results in [57].

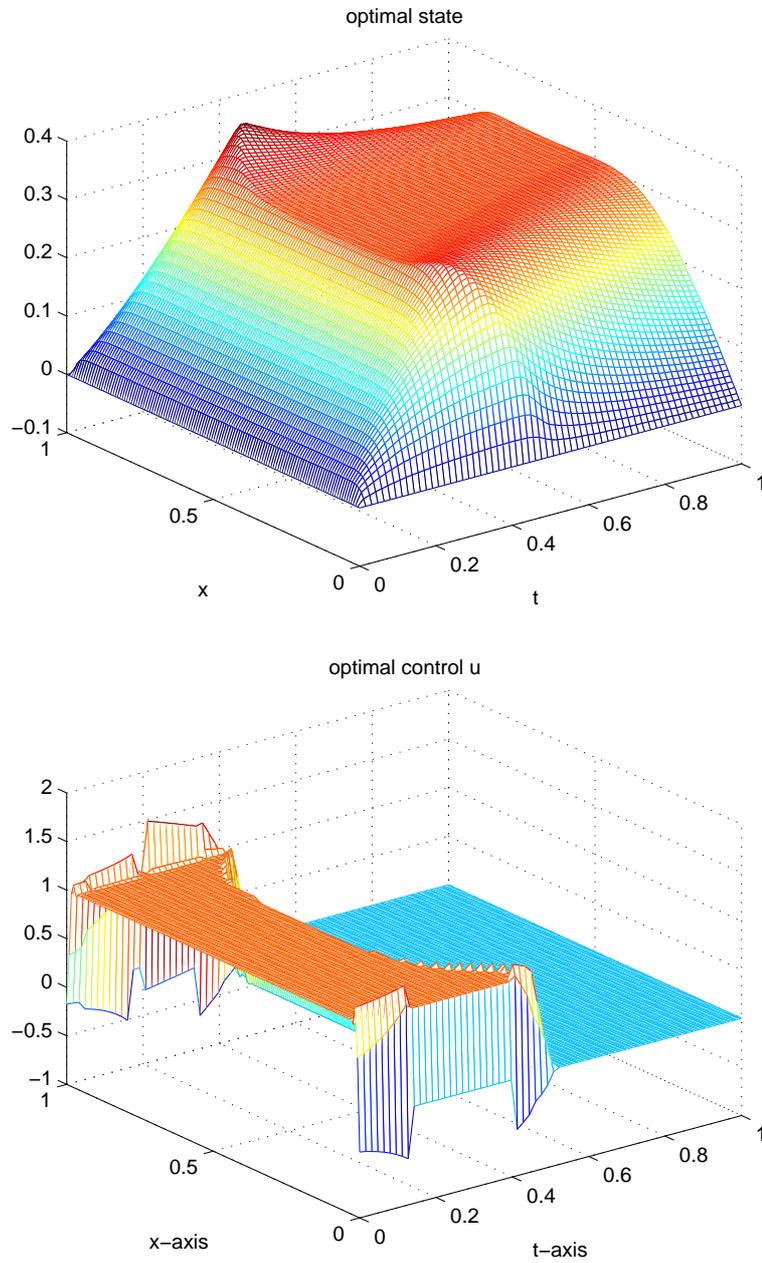


Figure 4.4: Control constrained problem

Table 4.6: Mesh independence for Run 4.2

$\Delta x_{max}$	$2^{-4}$	$2^{-5}$	$2^{-6}$	$2^{-7}$
tol=1e-5	9	6	7	6
tol=1e-6	-	7	7	7
tol=1e-7	-	7	7	7
tol=1e-8	-	7	7	7
tol=1e-9	-	8	8	7
tol=1e-10	-	8	8	8
tol=1e-11	-	9	9	9

## 4.2 Boundary control problem

We consider the unconstrained and control constrained boundary control problems.

### 4.2.1 Space-discretization for the linearized state equation

We use the same finite element discretization as in the distributed control problem. The difference occurs at the control variables, as they are not discretized. We use the vector valued variables defined in the previous subsection. It follows that

$$M\mathbf{y}_t + S\mathbf{y} + C(\bar{\mathbf{y}})\mathbf{y} = q(\bar{\mathbf{y}}) + f_h(u, v), \quad (4.33)$$

where

$$f_h(u, v) := \begin{pmatrix} -u(t) - \sigma_1 y(1, t) \\ 0 \\ \vdots \\ 0 \\ v(t) - \sigma_2 y(nx + 1, t) \end{pmatrix}.$$

Defining the vectors  $\mathbf{v} = (0, \dots, 0, v(t))$  and  $\mathbf{u} = (u(t), 0, \dots, 0)$  give the semi-discrete control problem as

$$\min J_h = \int_0^T \frac{1}{2} (\mathbf{y} - \mathbf{y}_d)^T M (\mathbf{y} - \mathbf{y}_d) dt + \int_0^T \beta_u |\mathbf{u}|^2 + \beta_v |v|^2 dt \quad (4.34)$$

$$\begin{aligned} \text{s.t. } \quad & M\mathbf{y}_t + S\mathbf{y} + C(\bar{\mathbf{y}})\mathbf{y} = q(\bar{\mathbf{y}}) + f_h(u, v), \\ & \mathbf{y}(0) = \mathbf{y}_0. \end{aligned}$$

#### 4.2.2 Crank-Nicolson scheme for the linearized problem

We define  $V := (\mathbf{v}^1, \dots, \mathbf{v}^N)$  for  $N$  time-steps. Similarly we get

$$\mathcal{K}Y + \frac{\Delta t}{2}\tilde{\mathcal{L}}_1U - \frac{\Delta t}{2}\tilde{\mathcal{L}}_2V = Q + \begin{pmatrix} (-M + \frac{\Delta t}{2}S + \frac{\Delta t}{2}C(\bar{\mathbf{y}}^0))\mathbf{y}_0 \\ 0 \\ \vdots \\ 0 \end{pmatrix},$$

with

$$\mathcal{L}_1 := \begin{pmatrix} L_1 & & & & & \\ L_1 & L_1 & & & & \\ & & \ddots & \ddots & & \\ & & & L_1 & L_1 & \\ & & & & L_1 & L_1 \end{pmatrix} \text{ and } \mathcal{L}_2 := \begin{pmatrix} L_2 & & & & & \\ L_2 & L_2 & & & & \\ & & \ddots & \ddots & & \\ & & & L_2 & L_2 & \\ & & & & L_2 & L_2 \end{pmatrix},$$

where

$$L_1 := \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 0 & & \\ \vdots & & \ddots & \\ 0 & & & 0 \end{pmatrix}, \quad L_2 := \begin{pmatrix} 0 & \dots & 0 \\ \vdots & \ddots & \\ & & 0 & 0 \\ 0 & & 0 & 1 \end{pmatrix}.$$

After time integration the fully discrete control problem is obtained by

$$\min_{\mathbf{u}_1, \dots, \mathbf{u}_N} \sum_{i=0}^N \frac{\Delta t_i + \Delta t_{i+1}}{2} \left( \frac{1}{2}(\mathbf{y} - \mathbf{y}_d)^T M(\mathbf{y} - \mathbf{y}_d) + \beta_u |\mathbf{u}|^2 + \beta_v |\mathbf{v}|^2 \right), \quad (4.35)$$

with the discrete state equation

$$\mathcal{K}Y + \frac{\Delta t}{2}\tilde{\mathcal{L}}_1U - \frac{\Delta t}{2}\tilde{\mathcal{L}}_2V = Q + d.$$

Then the discrete control problem can be stated as

$$\min J_h(Y, U, V) = \frac{\Delta t}{2}(Y - Y_d)^T \mathcal{M}_{1/2}(Y - Y_d) + \frac{\beta_u \Delta t}{2} U^T \mathcal{L}_1 U + \frac{\beta_v \Delta t}{2} V^T \mathcal{L}_2 V.$$

In a similar way, the optimality conditions for the Lagrangian can be stated as

$$\nabla_Y L(Y^*, U^*, V^*, P^*) = \Delta t \mathcal{M}_{1/2}(Y^* - Y_d) - \mathcal{K}^T P^* = 0,$$

and,

$$\nabla_P L(Y^*, U^*, V^*, P^*) = -\mathcal{K} Y^* + \Delta t \mathcal{L}_2 V^* - \Delta t \mathcal{L}_1 U^* + Q + d = 0,$$

with the gradient equations

$$\beta_u \Delta t \mathcal{L}_1 U^* - \Delta t \mathcal{L}_1 P^* = 0,$$

and

$$\beta_v \Delta t \mathcal{L}_2 V^* + \Delta t \mathcal{L}_2 P^* = 0.$$

The optimality system can be written as

$$\begin{pmatrix} \Delta t \mathcal{M} & 0 & 0 & -\mathcal{K}^T \\ 0 & \beta_v \Delta t \mathcal{L}_2 & 0 & \frac{\Delta t}{2} \mathcal{L}_2 \\ 0 & 0 & \beta_u \Delta t \mathcal{L}_1 & -\frac{\Delta t}{2} \mathcal{L}_1 \\ -\mathcal{K} & \frac{\Delta t}{2} \mathcal{L}_2 & -\frac{\Delta t}{2} \mathcal{L}_1 & 0 \end{pmatrix} \begin{pmatrix} Y \\ V \\ U \\ P \end{pmatrix} = \begin{pmatrix} \mathcal{M}_{1/2} Y_d \\ 0 \\ 0 \\ Q + d \end{pmatrix}. \quad (4.36)$$

### 4.2.3 Space-discretization for the nonlinear state equation

The semi-discrete control problem follows

$$\min J_h = \int_0^T \frac{1}{2} (\mathbf{y} - \mathbf{y}_d)^T M (\mathbf{y} - \mathbf{y}_d) dt + \int_0^T \beta_u |\mathbf{u}|^2 + \beta_v |\mathbf{v}|^2 dt \quad (4.37)$$

$$\text{s.t. } M \mathbf{y}_t + S \mathbf{y} + q(\mathbf{y}) = f_h(\mathbf{u}, \mathbf{v}),$$

$$\mathbf{y}(0) = \mathbf{y}_0.$$

#### 4.2.4 Semi-implicit scheme

Using semi-implicit time approximation the following scheme can be obtained as:

$$\underbrace{\begin{pmatrix} Z & & & & \\ -M & Z & & & \\ & & \ddots & \ddots & \\ & & & & -M & Z \end{pmatrix}}_{\tilde{\mathcal{K}}} Y + \Delta t \tilde{\mathcal{L}}_1 U - \Delta t \tilde{\mathcal{L}}_2 V = \tilde{Q} + \tilde{d},$$

where  $Z = M + \Delta t A$ ,  $\tilde{\mathcal{L}}_1 = \text{blockdiag}\{L_1, \dots, L_1\}$  and  $\tilde{\mathcal{L}}_2 = \text{blockdiag}\{L_2, \dots, L_2\}$

with

$$\tilde{d} = \begin{pmatrix} -M \mathbf{y}_0 + \Delta t q(\bar{\mathbf{y}}^0) \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

The discrete control problem follows as

$$\min_{\mathbf{u}_1, \dots, \mathbf{u}_N} \sum_{i=0}^{N+1} \frac{\Delta t_i + \Delta t_{i+1}}{2} \left( \frac{1}{2} (\mathbf{y} - \mathbf{y}_d)^T M (\mathbf{y} - \mathbf{y}_d) + \int_0^T \beta_u |\mathbf{u}|^2 + \beta_v |\mathbf{v}|^2 \right). \quad (4.38)$$

Using the optimality conditions, the optimality system follows

$$\begin{pmatrix} \Delta t \tilde{\mathcal{M}} & 0 & 0 & -\tilde{\mathcal{K}}^T \\ 0 & \beta_v \Delta t \tilde{\mathcal{L}}_2 & 0 & \Delta t \tilde{\mathcal{L}}_2 \\ 0 & 0 & \beta_u \Delta t \tilde{\mathcal{L}}_1 & -\Delta t \tilde{\mathcal{L}}_1 \\ -\tilde{\mathcal{K}} & \Delta t \tilde{\mathcal{L}}_2 & -\Delta t \tilde{\mathcal{L}}_1 & 0 \end{pmatrix} \begin{pmatrix} Y \\ V \\ U \\ P \end{pmatrix} = \begin{pmatrix} M Y_d \\ 0 \\ 0 \\ \tilde{Q} + \tilde{d} \end{pmatrix}. \quad (4.39)$$

#### 4.2.5 Implementation

As we discussed in the previous subsection the system matrices arising from Crank-Nicolson and semi-implicit time approximation schemes for boundary control problem correspond to a saddle point system. Indeed, for the discrete problem we let

We can choose  $E := \begin{pmatrix} \mathcal{M} & 0 & 0 \\ 0 & \beta_v \Delta t \mathcal{L}_1 & 0 \\ 0 & 0 & \beta_v \Delta t \mathcal{L}_2 \end{pmatrix}$ . Also defining

$$x := \begin{pmatrix} Y \\ V \\ U \\ P \end{pmatrix}, \quad L := \begin{pmatrix} -\mathcal{K} & \Delta t \mathcal{L}_1 & \Delta t \mathcal{L}_2 \end{pmatrix} \text{ and } b := \begin{pmatrix} \mathcal{M}_{1/2} Y_d \\ 0 \\ 0 \\ Q + d \end{pmatrix}.$$

It follows that

$$\underbrace{\begin{pmatrix} E & L^T \\ L & 0 \end{pmatrix}}_{\mathcal{A}} x = b.$$

#### 4.2.5.1 Direct solver

We present the solution algorithm for Crank-Nicolson scheme, it is similar for the semi-implicit scheme.

*(All-at-once method with the Crank-Nicolson scheme)*

1. Given  $U_0, V_0, Y_0$ , and  $tol > 0$ . Set  $k = 0$
2. Set  $done = inf$
3. While  $done > tol$ 
  - 3.1. Set  $k = k + 1$
  - 3.2. Compute  $\mathcal{K}$
  - 3.3. By using LU decomposition solve

$$\begin{pmatrix} \Delta t \mathcal{M} & 0 & 0 & -\mathcal{K}^T \\ 0 & \beta_v \Delta t \mathcal{L}_2 & 0 & \frac{\Delta t}{2} \mathcal{L}_2 \\ 0 & 0 & \beta_u \Delta t \mathcal{L}_1 & -\frac{\Delta t}{2} \mathcal{L}_1 \\ -\mathcal{K} & \frac{\Delta t}{2} \mathcal{L}_2 & -\frac{\Delta t}{2} \mathcal{L}_1 & 0 \end{pmatrix} \begin{pmatrix} Y \\ V \\ U \\ P \end{pmatrix} = \begin{pmatrix} \mathcal{M}_{1/2} Y_d \\ 0 \\ 0 \\ Q + d \end{pmatrix}$$

- 3.4. Set  $done = \|Y_{k+1} - Y_k\| + \|P_{k+1} - P_k\| + \|U_{k+1} - U_k\|$

4. End while.

#### 4.2.5.2 Iterative solver

We propose the following preconditioner

$$\mathcal{P} = \begin{pmatrix} \Delta t \mathcal{M} & 0 & 0 & 0 \\ 0 & \beta_v \Delta t \bar{\mathcal{L}}_2 & 0 & 0 \\ 0 & 0 & \beta_v \Delta t \bar{\mathcal{L}}_1 & 0 \\ 0 & 0 & 0 & S \end{pmatrix}$$

with  $S^{-1} := \mathcal{K}^{-T} \mathcal{M} \mathcal{K}^{-1}$ , and

$$\bar{\mathcal{L}}_1 := \begin{pmatrix} \bar{L}_1 & & & & & \\ \bar{L}_1 & \bar{L}_1 & & & & \\ & & \ddots & \ddots & & \\ & & & \bar{L}_1 & \bar{L}_1 & \\ & & & & \bar{L}_1 & \bar{L}_1 \end{pmatrix} \text{ and } \bar{\mathcal{L}}_2 := \begin{pmatrix} \bar{L}_2 & & & & & \\ \bar{L}_2 & \bar{L}_2 & & & & \\ & & \ddots & \ddots & & \\ & & & \bar{L}_2 & \bar{L}_2 & \\ & & & & \bar{L}_2 & \bar{L}_2 \end{pmatrix},$$

where

$$\bar{L}_1 := \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & \sigma & & \\ \vdots & & \ddots & \\ 0 & & & \sigma \end{pmatrix}, \bar{L}_2 := \begin{pmatrix} \sigma & \dots & 0 \\ \vdots & \ddots & \\ & & \sigma & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

We note that we choose  $\sigma$  as a very small number in order to preserve consistency.

#### 4.2.6 Control constrained problem

We can obtain the optimality conditions in a similar way. We introduce the following parameters

$$\mu_a := (\beta_u \Delta t \mathcal{L}_1 U^* + \Delta t \mathcal{L}_1 P^*)^+ \text{ and } \mu_b := (\beta_u \Delta t \mathcal{L}_1 U^* + \Delta t \mathcal{L}_1 P^*)^-$$

$$\eta_a := (\beta_v \Delta t \mathcal{L}_2 V^* + \Delta t \mathcal{L}_2 P^*)^+ \text{ and } \eta_b := (\beta_v \Delta t \mathcal{L}_2 V^* + \Delta t \mathcal{L}_2 P^*)^-$$

with  $\eta = \eta_a - \eta_b$ . Then

Then the implementation of the constrained problem can be given as

***Inequality constrained problem.***

1. Solve

$$\begin{pmatrix} \mathcal{M} & 0 & 0 & -\mathcal{K}^T \\ 0 & \beta_v \Delta t \mathcal{L}_2 & 0 & \frac{\Delta t}{2} \chi_{\tilde{I}} \mathcal{M} \\ 0 & 0 & \beta_u \Delta t \mathcal{L}_1 & \frac{\Delta t}{2} \chi_I \mathcal{M} \\ -\mathcal{K} & \frac{\Delta t}{2} \mathcal{L}_2 & \frac{\Delta t}{2} \mathcal{L}_1 & 0 \end{pmatrix} \begin{pmatrix} Y \\ V \\ U \\ P \end{pmatrix} = \begin{pmatrix} \mathcal{M}_{1/2} Y_d \\ \beta_v \Delta t \mathcal{L}_2 (\chi_{\tilde{A}_-} V_a + \chi_{\tilde{A}_+} V_b) \\ \beta_u \Delta t \mathcal{L}_1 (\chi_{A_-} U_a + \chi_{A_+} U_b) \\ Q + d \end{pmatrix}$$

2. Set  $A_+ = \{x \in Q : -\beta_u \Delta t \mathcal{L}_1 U_a - \frac{\Delta t}{2} \mathcal{L}_1 P < 0\}$

3. Set  $A_- = \{x \in Q : -\beta_u \Delta t \mathcal{L}_1 U_b - \frac{\Delta t}{2} \mathcal{L}_1 P > 0\}$

4. Set  $\tilde{A}_+ = \{x \in Q : -\beta_v \Delta t \mathcal{L}_2 V_a - \frac{\Delta t}{2} \mathcal{L}_2 P < 0\}$

5. Set  $\tilde{A}_- = \{x \in Q : -\beta_v \Delta t \mathcal{L}_2 V_b - \frac{\Delta t}{2} \mathcal{L}_2 P > 0\}$

6. Set  $I = Q \setminus (A_+ \cup A_-)$  and  $\tilde{I} = Q \setminus (\tilde{A}_+ \cup \tilde{A}_-)$

**4.2.7 Numerical examples for the boundary control problem**

**Run 4.3.** (*Unconstrained problem*) Let  $Q = (0, 1) \times (0, 1)$ . We consider a Neumann-type boundary control problem with  $\beta_u = 0.01, \beta_v = 0.01, \sigma_0 = \sigma_1 = 0$ . The viscosity parameter is  $\nu = 0.1$ . The initial condition is taken as  $y_0(\cdot, 0) = x^2(1-x)^2$  and the desired state is  $y_d(x, t) = y_0(\cdot, 0)$ .

Let the desired state  $y_d = 0.035$ .

We compare the numerical results of Crank-Nicolson (CN) and semi-implicit (SI) schemes for a fixed space mesh  $\Delta x = 2^{-7}$  and with fixed  $\Delta t = 2^{-7}$ .

Table 4.7: Mesh independence for Run 4.3

$tol/\Delta x_{max}$	$2^{-4}$	$2^{-5}$	$2^{-6}$	$2^{-7}$
1e-5	2	2	2	2
1e-6	2	2	2	2
1e-7	2	2	2	2
1e-8	2	2	2	2
1e-9	2	2	2	2
1e-10	3	2	2	2
1e-11	3	3	3	3

We give the inner iteration number of MINRES with Crank-Nicolson scheme with respect to given mesh sizes in the Table 4.7.

Table 4.8: Inner iteration numbers for MINRES of Run 4.3

$\Delta x$	$2^{-4}$	$2^{-5}$	$2^{-6}$	$2^{-7}$
# of iteration	36	35	34	34

We present the graphical interpretation, which are similar to the results in [67], in Figure 4.5. Optimal state and control solutions are also presented.

**Run 4.4** (*Control constrained problem*) We solve the boundary control problem in [70], *Run 8.1, pp.24*. The same space-time domain is used as in above example. We consider a Robin-type boundary control problem with  $\beta_u = 0.05, \beta_v = 0.01, \sigma_0 = -0.1, \sigma_1 = 0$ . The viscosity parameter is  $\nu = 0.05$ . The initial condition is given by

$$y_0(\cdot, 0) = \begin{cases} 1 & \text{in } (0, \frac{1}{2}], \\ 0 & \text{otherwise.} \end{cases}$$

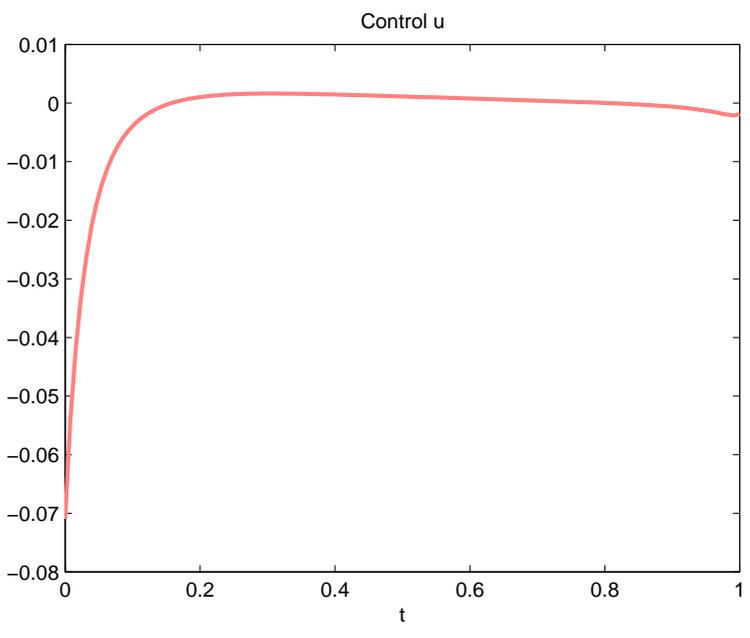
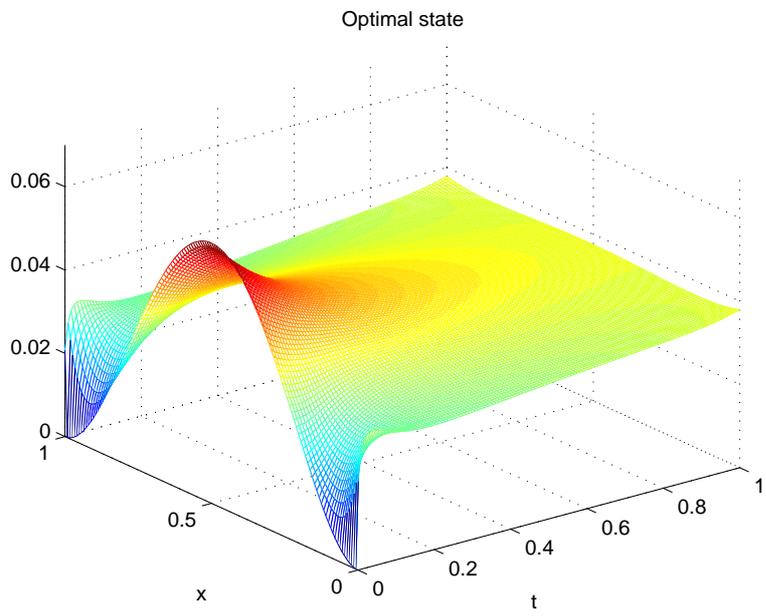


Figure 4.5: Unconstrained problem.

The desired state is  $y_Q(x, t) = y_0(\cdot, 0)$ . The bounds for the unilaterally constraint pointwise control constraints are:

$$u_a(t) = \begin{cases} -0.2 & \text{in } [0, 0.5], \\ -0.1 + 5(t - 0.52) & \text{in } [0.5, 0.52], \\ -0.1 & \text{in } [0.52, 1]. \end{cases}$$

and

$$u_b = 0, v_a = -0.25, v_b = 0.$$

Due to the less regularity in boundary control problem comparing to distributed control problem, direct solver does not converge for the mesh size bigger than  $\Delta x = 2^{-6}$ . We present the MINRES with Crank-Nicolson results. First we cover the iteration numbers in Table 4.9. As discussed before the mesh independence can be seen from the table.

Table 4.9: Mesh independence for Run 4.4

$tol/\Delta x_{max}$	$2^{-4}$	$2^{-5}$	$2^{-6}$	$2^{-7}$
1e-5	6	5	5	5
1e-6	7	6	6	6
1e-7	8	6	6	7
1e-8	9	7	7	8
1e-9	9	8	7	8
1e-10	10	9	8	8
1e-11	10	9	8	8

We also point out the inner iteration numbers for MINRES solver. Because of nonlinearity MINRES performs unless the convergence criteria is satisfied. We give the inner number of iterations in the Table 4.10. We remark that for a given mesh size, until convergence criteria is satisfied for the nonlinear problem, the inner iteration number is the same MINRES.

Table 4.10: Inner iteration numbers for MINRES of Run 4.4

$\Delta x$	$2^{-4}$	$2^{-5}$	$2^{-6}$	$2^{-7}$
# of iteration	70	64	65	56

The numerical solutions are presented in Figure 4.6. When we compare the obtained results of [70] which are very similar.

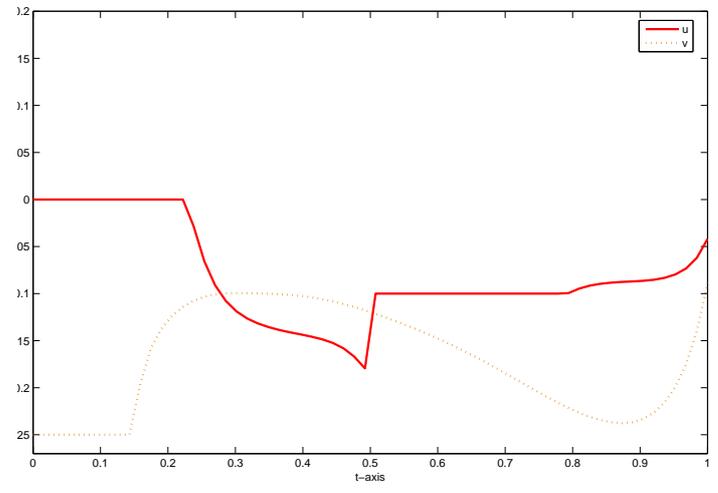
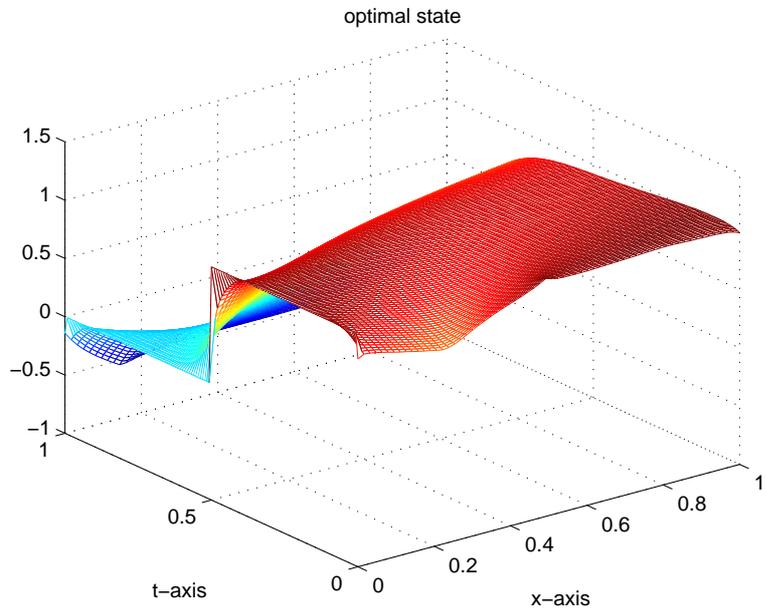


Figure 4.6: Run 4.4. The full line and dotted line correspond to control  $u$  and  $v$ , respectively

## CHAPTER 5

### CONCLUSION AND FUTURE WORKS

In this thesis, we have discussed optimal control problems of unsteady Burgers equations using two both *optimize-then-discretize* and *discretize-then-optimize* approaches. We first covered some related functional preliminaries and existence and uniqueness results for Burgers equation in Chapter 2. We summarized well-known results for both distributed and boundary control problems of Burgers equation. We obtained optimality systems for both unconstrained and control constrained problems. In order to solve optimization problem, a classical method, gradient method, was given. Implementation of control constraints is done by using active set strategy.

The main issue of the work at hand was the application of all-at-once type method to control problems of unsteady Burgers equation in Chapter 3 and 4. In Chapter 3, one-step method was used after applying *optimize-then-discretize*. First the nonlinear problem control problem is linearized and then first order optimality conditions are obtained. Instead of solving a parabolic problem, the system of equations were transformed to an elliptic system. Both distributed and boundary control problems were investigated. Then, solution algorithm were constructed by space-time discretization which pretends time as a space variable. Using an efficient simulation environment, COMSOL Multiphysics, the numerical results were obtained.

We followed *discretize-then-optimize* approach in Chapter 4. It is the first time that by following *discretize-then-optimize* approach, all-at-once method for control problems of unsteady Burgers equation was investigated. We focused on the discretization issue. Standard Galerkin method was applied to control problem for space discretization. As for time approach, we considered two different methods: Crank-Nicolson and semi implicit time schemes. Our aim was to obtain a problem  $Ax = b$ , where  $A$  is a symmetric matrix. To get a symmetric system

we had to linearize the control problem when using Crank-Nicolson scheme. After obtaining the fully discrete problem, we transformed the systems of equations arising from time iterations into a matrix formulation. By pretending the state and control variables as independent optimization variables, we obtained the solution algorithms. Moreover, we provided an a priori error estimation for the distributed control problem. We verified the expected convergence orders for space and time approximations.

Distributed control problem with *optimize-then-discretize* approach was developed in paper [71]. We submitted a paper concerning boundary control problem of Burgers equation. We have two more papers in preparation concerning all-at-once approach.

As for future work, All-at-once type method with discontinuous Galerkin methods for space and time in order to solve control problems of Burgers equation will be considered. Error analysis for boundary control problem may be handled.

Efficient solution of optimal control problems with two dimensional Burgers equation using the all-at-once approach is also in our agenda.

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