SOLVING OPTIMAL CONTROL TIME-DEPENDENT DIFFUSION-CONVECTION-REACTION EQUATIONS BY SPACE TIME DISCRETIZATION

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

BY

Zahire Seymen

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

FEBRUARY 2013

Approval of the thesis:

SOLVING OPTIMAL CONTROL TIME-DEPENDENT DIFFUSION-CONVECTION-REACTION EQUATIONS BY SPACE TIME DISCRETIZATION

submitted by **Zahire Seymen** in partial fulfillment of the requirements for the degree of **Doctor of Philosophy in Mathematics Department, Middle East Technical University** by,

Prof. Dr. Canan Özgen
Dean, Graduate School of **Natural and Applied Sciences** ________________

Prof. Dr. Mustafa Korkmaz
Head of Department, **Mathematics** ________________

Prof. Dr. Bülent Karasözen
Supervisor, **Mathematics, METU** ________________

Examining Committee Members:

Prof. Dr. Münevver Tezer
Department of Mathematics, METU ________________

Prof. Dr. Bülent Karasözen
Department of Mathematics, METU ________________

Prof. Dr. Gerhard-Wilhelm Weber
Department of Mathematics, METU ________________

Prof. Dr. Ömer Akın
Department of Mathematics,
TOBB Economics and Technology University ________________

Doç. Dr. Songül Kaya Merdan
Institute of Applied Mathematics, METU ________________

Date: ________________

I hereby declare that all information in this document has been obtained and presented in accordance with academic rules and ethical conduct. I also declare that, as required by these rules and conduct, I have fully cited and referenced all material and results that are not original to this work.

Name, Last Name: Zahire Seymen

Signature :

ABSTRACT

SOLVING OPTIMAL CONTROL TIME-DEPENDENT DIFFUSION-CONVECTION-REACTION EQUATIONS BY SPACE TIME DISCRETIZATION

Seymen, Zahire
Ph.D., Department of Mathematics
Supervisor : Prof. Dr. Bülent Karasözen

February 2013, 91 pages

Optimal control problems (OCPs) governed by convection dominated diffusion-convection-reaction equations arise in many science and engineering applications such as shape optimization of the technological devices, identification of parameters in environmental processes and flow control problems. A characteristic feature of convection dominated optimization problems is the presence of sharp layers. In this case, the Galerkin finite element method performs poorly and leads to oscillatory solutions. Hence, these problems require stabilization techniques to resolve boundary and interior layers accurately. The Streamline Upwind Petrov-Galerkin (SUPG) method is one of the most popular stabilization technique for solving convection dominated OCPs.

The focus of this thesis is the application and analysis of the SUPG method for distributed and boundary OCPs governed by evolutionary diffusion-convection-reaction equations. There are two approaches for solving these problems: *optimize-then-discretize* and *discretize-then-optimize*. For the *optimize-then-discretize* method, the time-dependent OCPs is transformed to a biharmonic equation, where space and time are treated equally. The resulting optimality system is solved by the finite element package COMSOL. For the *discretize-then-optimize* approach, we have used the so called *all-*

at-once method, where the fully discrete optimality system is solved as a saddle point problem at once for all time steps. A priori error bounds are derived for the state, adjoint, and controls by applying linear finite element discretization with SUPG method in space and using backward Euler, Crank-Nicolson and semi-implicit methods in time. The stabilization parameter is chosen for the convection dominated problem so that the error bounds are balanced to obtain L^2 error estimates. Numerical examples with and without control constraints for distributed and boundary control problems confirm the effectiveness of both approaches and confirm a priori error estimates for the *discretize-then-optimize* approach.

Keywords: Optimal control, diffusion-convection-reaction equation, Streamline Upwind Petrov-Galerkin method, COMSOL Multipysics, all-at-once method

ÖZ

ZAMANA BAĞLI DİFÜZYON-KONVEKSİYON-REAKSİYON DENKLEMLERİNİN ENİYİLEMELİ KONTROL PROBLEMLERİNİN UZAY-ZAMAN EŞZAMANLI AYRIKLAŞTIRILMASI İLE ÇÖZÜMÜ

Seymen, Zahire
Doktora, Matematik Bölümü
Tez Yöneticisi : Prof. Dr. Bülent Karasözen

Şubat 2013, 91 sayfa

Teknolojik sistemlerin eniyileme yöntemi ile kontrolü, çevresel süreç içindeki parametrelerin tahmini, akışkan kontrol problemleri gibi çok sayıda problem difüzyon, konveksiyon, reaksiyon terimleri içeren kısmi türevli denklem sistemlerinden oluşan eniyileme problemleri şeklindedir. Konveksiyon terimlerinin difüzyon terimlerinden çok büyük olduğu durumlarda, bu tür denklemlerin çözümleri, çözümün yüksek eğime sahip olduğu bölgelerde katmanlar oluşturmaktadır. Galerkin sonlu elemanlar yönteminin bu tür problemler için uygun olmadığı ve sayısal çözümlerin salınımlar oluşturduğu bilinmektedir. Sınırda ve iç katmanlarda oluşan katmanları azaltmak için farklı stabilizasyon yöntemleri kullanılmakta olup, bunların arasında en çok bilineni Streamline Upwind Petrov Galerkin (SUPG) yöntemidir.

Bu tez, konveksiyon ağırlıklı dağıtık ve sınır değer eniyileme kontrol problemlerinin SUPG ile çözümünü ve analizini içermektedir. Kısmı türev denklemlerini içeren eniyileme kontrol problemlerinin çözümünde genellikle iki farklı yaklaşım kullanılmaktadır: doğrudan ayrıklaş-
tırmasıyla elde edilen ve eniyileme sisteminin çözümü elde edildikten sonra ayrıklaştırmasıyla elde edilen sistemin çözümü. Bu çalışmanın ilk bölümünde, eniyileme koşullarının elde edildikten sonra

sayısal ayrıklaştırma yaklaşımı için zamana bağlı eniyileme kontrol problemi ikili harmonik bir denkleme dönüştürülmüş ve COMSOL adlı sonlu elemanlar paketi ile çözülmüştür. Çalışmanın ikinci bölümünde, sayısal ayrıklaştırma yaklaşımı için elde edilen problemin çözümü için *hepbirlikte çözüm* olarak adlandırılan eniyileme problemi bir eğer nokta problemi halinde çözülmüştür. Zaman değişkeninde geriye dönük backward Euler, Crank-Nicolson, yarı kapalı yöntemlerle ayrıklaştırılan eniyileme sistemi, uzay değişkeninde doğrusal sonlu elemanlar ve SUPG kararlılığı kullanılarak ayrıklaştırılmış, önceden hata analiz leri geliştirilmiştir. Kararlılık parametresi eniyilemeli hata tahmini elde edilecek şekilde seçilmiştir. Kontrol kısıtlamalı ve kısıtsamasız problemler için çeşitli sayısal örneklerde elde edilen sonuçlar, her iki yaklaşımın etkinliğini göstermekte olup, ayrıklaştırma sonrası eniyileme yaklaşımı için elde edilen sonuçlar, hata tahminlerini doğrulamaktadır.

Anahtar Kelimeler: Optimal kontrol, zamana bağlı konveksiyon-reaksiyon-difüzyon denklemi, Streamline Upwind Petrov-Galerkin yöntemi, COMSOL, tek adımlı çözüm yöntemi

To my family

ACKNOWLEDGMENTS

I would like to express my gratitude to people who contributed to this thesis.

First of all, I would like to thank to my supervisor Prof. Dr. Bülent Karasözen for his unlimited help, invaluable guidance and crucial contribution not only to this thesis but also to all my academic studies. He has been a constant source of support to proceed and complete my PhD thesis.

I am also grateful to the personnel of Turkish Petroleum Corporation which supports me and encourages me to complete my study.

I gratefully acknowledge the financial support of Turkish Scientific and Technical Research Council (TÜBİTAK) which had been given to me during the first four years of PhD education.

I am also thankful to the members of my thesis defence committee for their guidance and useful comments. I especially acknowledge Prof. Dr. Gerhard-Wilhelm Weber for his kindness and contributions while revising my thesis.

I would like to give special thanks to Prof.Dr. R.H.W. Hoppe for providing me an opportunity to study in the University of Houston.

I am very thankful to Fikriye N. Yılmaz, Tuğba Akman and Hamdullah Yücel for their useful comments and support.

Finally, I offer my special thanks to my big family. Firstly, I thank to Mustafa Kanar, my dad and Sevim Kanar, my mom who brought me up and supported me whenever I needed them. Then I would like to acknowledge Mehmet Kanar, my brother, Nevin Yazıcı, Songül Erevik, my sisters for their invaluable support. Moreover I would like to thank to Mahmut Erevik, my sister's husband, who has encouraged me from the first day of my doctorate study. Last but not least, I gratefully acknowledge to Şükrü Seymen, my husband, who has provided me love, support, encourage and motivation during my PhD education.

TABLE OF CONTENTS

LIST OF TABLES

TABLES

LIST OF FIGURES

FIGURES

CHAPTER 1

INTRODUCTION

Recently, the optimal control problems (OCPs) that are governed by elliptic or time-dependent partial differential equations (PDEs) have been extensively studied [1, 38, 53, 54, 58, 66]. Among them OCPs governed by the diffusion-convection-reaction equations arise in environmental modeling, petroleum reservoir simulation and in many other applications. Extensive research has been carried out on various theoretical and numerical aspects of these problems [3, 4, 9, 13, 21, 23, 27, 28, 40, 45, 50, 52, 90]. In applications, the size of the diffusion term is smaller by several orders of magnitude than the norm of the convection term. In convection dominated problems, interior and/or boundary layers generally occur on a small region where the derivatives of the solution are large. Hence, the solution procedure becomes hard to tackle to the steep gradients caused by these sharp layers. The accurate simulation of these problems requires numerical methods which are able to compute sharp layers and prevent the occurrence of spurious solutions. The standard Galerkin finite element method which is used to approximate the solution of convection dominated problems leads to strong oscillatory solutions if the mesh size h is large when compared to the ratio $\epsilon/\|\beta\|$ where ϵ, β are the diffusion and convection terms, respectively. In order to eliminate the oscillations around the boundary and/or interior layers and to obtain accurate solutions, several stabilization techniques have been proposed and analyzed, including the streamline diffusion finite element method [34, 46], and symmetric stabilization method [9, 12]. Among them, the streamline upwind/Petrov Galerkin(SUPG) method, is one of the most well known stabilization technique in the literature [10, 34, 46].

In the OCPs, there is a cost functional $J(y, u)$ which is a function of the state variable y, and the control variable u. The aim of the OCPs minimize the cost functional by approximating the state variable to a given desired state y_d as well as possible by using distributed or boundary controls. In this thesis, we consider the time-dependent convection dominated diffusion-convection-reaction equation as a constraint of the optimization problem. Moreover, the problems might include constraints on the control given in a form of the box constraints. The OCPs governed by diffusion-convection-reaction equations cause additional challenges due to one more diffusion-convection-reaction equation with an opposite convection term, which is called the adjoint equation. In this sense, these problems have boundary and/or interior layers generated not only in the state PDE but also in the adjoint PDE and so the spurious oscillations are propagated along upwind and downwind directions due to this coupled systems. Hence, the convergence properties for SUPG method applied to diffusion-convection-reaction control problems can be different from the convergence properties of the SUPG method used to solve a single PDE.

In case of steady-state convection dominated OCPs, various stabilization methods are proposed [3, 4, 9, 21, 23, 40, 45, 52, 90]. The discretized optimization problems governed by the elliptic diffusion-convection-reaction equation were studied using the local projection approach [4, 52]. The variational discretization and the edge stabilization Galerkin methods were combined in [45, 90]. Instead of stabilizing the state and adjoint equations separately, stabilization of the Lagrangian was introduced in [23]. In [3, 21, 40], the SUPG method was applied to the convection dominated stationary control problems. Heinkenschloss and co-workers have emphasized that the solutions of the elliptic problems by the SUPG method is hard to tackle numerically when compared to the solution of a single PDE in [21, 40]. In these studies, error between the exact and SUPG solution is measured on a region which is far away from the interior and/or boundary layers. In order to obtain a stable numerical solution, SUPG method is applied by adding a term to the state equation. It is noted in [21] that the added term vanishes at the exact solution. Thus, SUPG method is considered as a strongly consistent stabilization method [84].

In contrast to the steady-state convection dominated optimization problems, there are few papers dealing with the control problems governed by time-dependent PDEs. Dirichlet boundary OCPs of evolutionary equations were studied in [50]. The characteristic finite-element method used in [27, 28] and Crank-Nicholson method with symmetric stabilization was applied in [13] for distributed control problems. To the best of our knowledge, there is no study dealing with the OCPs governed by time dependent PDEs in terms of SUPG method. And in this thesis, we study the effect of the SUPG method applied to the OCPs governed by convection dominated diffusion-convection-reaction equation.

There are two approaches for the numerical solution of the OCPs: *optimize-then-discretize* (OD) and *discretize-then-optimize* (DO). In the OD approach, one first derives the optimality conditions which consist of state, adjoint and gradient equations and then discretizes each equation using an appropriate discretization scheme. In the DO approach, we first discretize the state equation and the cost functional. Then, we construct the finite dimensional Lagrangian and derive the finite dimensional optimization problem. Actually, the time-dependent diffusion-convection-reaction equation is not self-adjoint. As a result, OD approach and DO approach will generally lead to the different discretization scheme for solving optimality system involving the state and the adjoint equation which are discretized by pure Galerkin method. In general, both approaches do not commute and lead to different discrete problems. For the residual based stabilization methods [3, 21, 23, 40] and the SUPG method [21, 40, 46], OD approach and DO approach lead to different discrete problems too.

The main objective of this thesis is the analysis and application of the SUPG method for time-dependent convection dominated OCPs. Actually, the performance of the SUPG method is mostly proportional to the choice of the stabilization parameter. In [33], different methods are studied to derive the error estimates for the SUPG method with backward Euler and Crank-Nicolson scheme applied to a single evolutionary diffusion-convection-reaction equation. By choosing the stabilization parameter depending on the length of the time step size k, we derive the error estimate for the SUPG method with backward Euler and semi-implicit scheme. The error estimate for the SUPG method with Crank-Nicolson scheme are derived due to the choice of the parameter proportional to the mesh size h as for the steady-state case. Hence, we have illustrated the efficiency of the error estimates with numerical examples. The rest of the thesis is organized as follows:

In Chapter 2, we consider both approaches, i.e., OD and DO to give the optimality systems of OCPs. Firstly, we give the related functional preliminaries and the existence and uniqueness results for diffusion-convection-reaction equation. Then, we introduce the distributed and boundary OCPs and summarize the well-known results for these problems. In the rest of Chapter 2, we give optimality systems for the OD approach by discretizing the state, the adjoint and the gradient equation. We apply the SUPG method to both of the coupled system involving the original state equation as well as the adjoint PDE which is also convection dominated diffusion-convection-reaction equation with negative convection term. For time discretization, Θ scheme and semi-implicit scheme are used. In the DO approach, we first discretize the cost functional and state equation using a standard finite element method with SUPG in space, Θ-scheme and semi-implicit scheme in time. Then, we derive the Lagrangian and obtain the optimality system of the finite dimensional optimization problem by taking the derivatives of Lagrangian with respect to $y,\ u,\ p$.

In Chapter 3, we consider one-shot approach to solve the state, adjoint and gradient equation at once after converting the optimality system into a biharmonic equation in the space-time domain. The transformation of the optimality system of linear parabolic OCPs with pointwise control constraints into a biharmonic PDE were studied in [61, 64, 62, 65]. We solve the evolutionary convection dominated distributed and boundary OCPs as an elliptic PDEs where space and time variables are treated equally. Moreover, we show the existence of a solution of OCPs which are transformed into biharmonic PDEs. For the distributed optimal control of the unsteady Burgers equation, the same approach was used in [91]. For the numerical solution of the OCPs, we use the equation-based modeling and simulation environment COMSOL Multiphysics.

In Chapter 4, we use *all-at-once method* to compute the solution of the distributed and boundary OCPs with DO approach which results in a symmetric optimality system. Recently, all-at-once methods were applied for OCPs governed by linear elliptic problems in [72, 73, 74] and for parabolic problems in [78, 79]. These methods solve the state, control and adjoint equations explicitly for all time steps at the same time by treating the state and control as independent optimization variables. The linear system arising from the optimality system leads to a saddle-point system. The saddle point system can be solved by employing a direct solver or an iterative solver. In general, iterative solvers can be applied with a preconditioner chosen to speed up the convergence of the method. There have been much effort spent for the solutions of saddle point systems [25, 55, 56, 57] and related to all-at-once preconditioning of linear control problems [73, 74, 72, 78, 80]. In this thesis, as an iterative solver, we choose the minimal residual method (MINRES) of Paige and Saunders [67] and appropriate symmetric and positive definite block-diagonal preconditioner for MINRES. By using backward Euler, Crank-Nicolson, and semi-implicit schemes as a time discretization, the effect of the stabilization parameter for the time-dependent OCP is discussed in detail. Moreover, we derive a priori error estimates for the SUPG method with these time integrators applied to the distributed OCPs. Due to the stabilization parameter which depend on the length of the time step or mesh size, there are different approaches in the a priori error analysis. The error bounds of these estimates are balanced to obtain L^2 error estimate by choosing the optimal scaling of the mesh size h and time step size k. Numerical result for problems with and without control constraints confirm the predicted a priori error estimates.

CHAPTER 2

OPTIMALITY SYSTEMS FOR DIFFUSION-CONVECTION-REACTION EQUATION

In this chapter, we give the precise formulation of the optimization problems and cover some of their theoretical results. We consider two approaches DO and OD to solve the distributed and boundary OCPs.

In Section 2.1, we give some basic notations. Then, in Section 2.2, we formulate our distributed control problem with and without control constraints. In the rest of the section, we give the existence and uniqueness of solutions for DO and OD approaches. For both cases, we use SUPG stabilized spatial discretization, Θ scheme and semi-implicit scheme as an temporal discretization. Then, we obtain the optimality systems. In Section 2.3, we consider the boundary OCPs with and without control constraints. Similarly, we first give the existence and uniqueness of solutions and then consider the approaches mentioned above with the same discretization techniques in space and time.

2.1 Basic notations

Throughout this thesis, Ω denotes a bounded domain in $\mathbb{R}^m$ for $\{m \in 1, 2\}$, with Lipschitz boundary $\partial\Omega$ [39]. Furthermore, we denote by $I := (0, T)$ a bounded time interval with $0 < T < \infty$. And we define $Q = I \times \Omega,\ \Sigma = I \times \partial\Omega$. We employ the usual notion for Lebesgue spaces $L^p(D)$ and sobolev spaces $W^{m,p}(D)$ with $1 \leq p \leq \infty,\ m \in \mathbb{N}^n$, see [51, 84, 86]
We use the same notations as in [84], consider the set of measurable functions w such that

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

and, when $p = \infty$,

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

The associated norm of $L^p(\Omega)$ is the following:

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

and, when $p = \infty$,

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

Considering the classical Sobolev space $W^{k,p}(\Omega)$, k is non-negative integer and $1 \le p \le \infty$, on a domain $\Omega \subset \mathbb{R}^n$

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

with the norm

$$\|w\|_{k,p,\Omega} := \Big(\sum_{|\sigma|\le k} \big\| D^\sigma w \big\|^p_{L^p(\Omega)} \Big)^{1/p}.$$

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 $H^1_0(\Omega)$.

For the time-dependent norms

$$L^q(I; W^{k,p}(\Omega)) := \Big\{ w : I \to W^{k,p}(\Omega) |\ w \text{ is measurable}$$
$$\text{and satisfies } \int_0^T \|w(t)\|^q_{k,p,\Omega} dt < \infty \Big\}$$

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

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

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

$$H^1(I; V) := \Big\{ w \in L^2(I; V) |\ \frac{\partial w}{\partial t} \in L^2(I; V) \Big\}.$$

Throughout this thesis, we use the following notation for norms and inner products. The scalar product $(\cdot,\cdot)_{L^2(\Omega)}$ is considered as $(\cdot,\cdot)_{0,\Omega}$ or simply $(\cdot,\cdot)$ and the norm in $L^2(\Omega)$ is denoted by $\|\cdot\|_{0,\Omega}$ or simply $\|\cdot\|$. Similarly, $\|\cdot\|_k$ is the norm in the sobolev space $H^k(\Omega)$ for $k \ge 0$ and the scalar product

$$(w, v)_{k,\Omega} := \sum_{|\sigma|\le k} (D^\sigma w, D^\sigma v).$$

2.2 Distributed optimal control problem

We consider the following time-dependent distributed OCPs governed by the diffusion-convection-reaction equation

$$\min \ J(y,u) = \frac{1}{2} \|y - y_d\|^2_Q + \frac{\alpha}{2} \|u\|^2_Q , \tag{2.1a}$$

subject to

$$\begin{aligned} y_t - \epsilon\Delta y + \beta\cdot\nabla y + \sigma y &= f + u, && \text{in } Q, \\ y &= 0, && \text{on } \Sigma, \\ y(\cdot,0) &= y_0, && \text{in } \Omega, \end{aligned} \tag{2.1b}$$

with control constraints

$$u \in U_{ad} \subset L^2(Q), \tag{2.1c}$$

where

$$U_{ad} = \{ u \in L^2(Q) : u_a \le u \le u_b, \ \text{a.e. in } Q\}$$

given the domain $\Omega \in \mathbb{R}^n$ for $n = 1, 2, ...,$ with $u_a,\ u_b, \in L^2(Q)$ and $u_a \leq u_b$ almost everywhere (a.e.) in Q. The regularization parameter is $\alpha > 0$, y and u denote the state and control variables, $y_d(x)$ is the desired state. Let $H = L^2(\Omega)$ and $V = H_0^1(\Omega)$ be Hilbert spaces. We make use of the following Hilbert space

$$X := W(I) = \{\varphi \in L^2(I; V);\ \varphi_t \in L^2(I; V^*)\},$$

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

$$(\varphi, \psi)_1 = (\varphi', \psi'), \quad \text{for all } \varphi, \psi \in V.$$

It is well known that the standard Galerkin finite element method applied to the state equation (2.1b) leads to strongly oscillatory solutions for mesh sizes that are larger than the ratio of diffusion and convection. To produce better approximations to the solutions of (2.1b) for moderately sized meshes, several well-established techniques have been proposed and analyzed [30, 59, 75, 84, 93]. There are methods to stabilize this phenomenon such that the streamline diffusion finite element method [36, 46, 84], the discontinuous Galerkin method [35], edge stabilization [11] and local projection stabilization methods [5, 68]. The streamline upwind/Petrov Galerkin method (SUPG) stabilized finite element method [34, 46] is the most used stabilization methods for convection dominated partial differential equations (PDEs).

In this thesis, we focus on the SUPG method [46]. By applying SUPG method, we add a term to weak form of (2.1b). With this term, the modified weak form has better stability properties than unstabilized case.

There are two approaches to solve the optimal control problem. In the first approach OD, we first derive the optimality conditions which consist of the state equation (2.1b), the adjoint equation

$$\begin{aligned} -p_t - \epsilon\Delta p - \beta\cdot\nabla p + \sigma p &= -(y - y_d), && \text{in } Q, \\ p &= 0, && \text{on } \Sigma, \\ p(\cdot, T) &= 0, && \text{in } \Omega, \end{aligned} \tag{2.2}$$

with the gradient equations

$$\alpha u - p = 0 \quad \text{in } Q. \tag{2.3}$$

In case of pointwise control constraints, the gradient condition is

$$\alpha u - p + \mu_b - \mu_a = 0, \quad \text{in } Q \tag{2.4}$$

with an additional complementary slackness condition

$$\begin{aligned} (\mu_a, u_a - u)_{L_2(Q)} = 0\ ,\ u \geq u_a\ ,\ \mu_a \geq 0, && \text{a.e. in Q}, \\ (\mu_b, u - u_b)_{L_2(Q)} = 0\ ,\ u \leq u_b\ ,\ \mu_b \geq 0 && \text{a.e. in Q}. \end{aligned}$$

Then, we discretize each equation (2.1b), (2.2), (2.3) or (2.4) by using conforming finite elements. We also use SUPG method to discretize the adjoint equation (2.2) which is also a diffusion-convection-reaction equation. By this way, we obtain 'strongly consistent' optimality system. However, there is no finite dimensional optimization problem because of the nonsymmetric linear system obtained by this optimality system (2.1b), (2.2), (2.3) or (2.4). The other approach for solution of (2.1) is DO in which we discretize the state equation (2.1b) using SUPG and the objective function. By defining the Lagrangian and taking derivative of Lagrangian with respect to y, u, p, we obtain the discrete adjoint equation, discrete gradient equation and discretized state equation respectively. The discrete adjoint equation and discrete gradient equation are considered as a discretization of (2.2) and (2.3) or (2.4), respectively. Although the discrete adjoint equation has a stabilizing effect due to the contribution of the stabilization term added to the state eqaution (2.1b), the discrete adjoint equation is not a strongly consistent stabilization method for (2.2). In the rest of the section, we discuss the existence and uniqueness of solutions, and present details of DO, OD approaches and optimality systems obtained by these approaches.

2.2.1 Existence and uniqueness of solutions

In this section, we consider the existence and uniqueness of distributed OCPs as stated in the texts [29, 51, 82]. Let first pose the state equation of time-dependent distributed control problem (2.1b) is a weak form for a given control $u \in U_{ad},\ y \in X,\ f \in L^2(Q)$, and $y_0 \in L^2(\Omega)$

$$\begin{aligned} (y_t, v) + a(y, v) + b(u, v) &= \langle f, v\rangle, \quad \forall v \in V, \\ y(0) &= y_0, \end{aligned} \tag{2.5}$$

where

$$\begin{aligned} a(y, v) &= \int_\Omega \epsilon \nabla y \nabla v + \beta \cdot \nabla y v + \sigma y v dx, \\ b(u, v) &= -\int_\Omega u v dx, \\ \langle f, v\rangle &= \int_\Omega f v dx. \end{aligned}$$

The bilinear form a is continuous and moreover, weakly coercive in V [84], i.e., there exist two constants $\xi > 0$ and $\lambda \geq 0$ such that

$$a(v, v) + \lambda \|v\|^2 \geq \xi \|v\|_1^2 \qquad \forall v \in V. \tag{2.6}$$

The bilinear form $a(\cdot, \cdot)$ is coercive if $\lambda = 0$.
Now we consider the solution of the OCPs

$$\min \ \ J(y, u) = \frac{1}{2} \|y - y_d\|_Q^2 + \frac{\alpha}{2} \|u\|_Q^2, \tag{2.7a}$$

subject to

$$\begin{aligned} (y_t, v) + a(y, v) + b(u, v) &= \langle f, v\rangle, \quad \forall v \in V, \\ y(0) &= y_0. \end{aligned} \tag{2.7b}$$

Theorem 2.2.1 *Let us assume that the bilinear form $a(\cdot, \cdot)$ is continuous in $V \times V$ and that (2.6) is satisfied with $\lambda = 0$. Given $f, y_d \in L^2(Q)$, $y_0 \in H$, $\epsilon > 0$, β, and σ are fixed. Then the OCP (2.7) has a unique solution $(y, u) \in X \times U_{ad}$.*

Proof. The proof can be found Lions [51], Wloka [86] and Tröltzsch [82]. ■
As in [51], we can define the Lagrangian to provide necessary and sufficient optimality conditions

$$L(y, u, p) = \tfrac{1}{2} \|y - y_d\|_Q^2 + \tfrac{\alpha}{2} \|u\|_Q^2 + (y_t, p) + a(y, p) + b(u, p) - \langle f, p\rangle. \tag{2.8}$$

Taking derivative of Lagrangian with respect to $y,\ u,\ p$ respectively, we obtain the following necessary and sufficient optimality conditions:

$$(-p_t, \psi) + a(\psi, p) = -\langle y - y_d, \psi\rangle, \qquad \forall \psi \in V,\ p \in X, \tag{2.9a}$$

$$b(w, p) + \alpha\langle u, w\rangle = 0, \qquad \forall w \in U_{ad}, \tag{2.9b}$$

$$(y_t, v) + a(y, v) + b(y, v) = \langle f, v\rangle, \qquad \forall v \in V, \tag{2.9c}$$

where (2.9a) is the weak form of the adjoint equation (2.2), (2.9b) is the weak form of gradient equation (2.3) and (2.9c) is the weak form of state equation (2.1b). We also note that for the control constraint problem, we add the term $\mu_b(u-u_b)+\mu_a(u_a-u)$ to (2.8); then the term $\mu_b-\mu_a$ is added to (2.9b) which is the weak form of the gradient equation (2.4).
Moreover, we need more regular $y,\ u,\ p$ solutions than shown in Theorem 2.2.1 for convergence theory of SUPG. Thm. 2.4,2.5 in [39] and Thm. 2.2 in [21] show that the unique solution of (2.7) and the associated adjoint admit more regular solutions.

2.2.2 Discretize-then-optimize approach

2.2.2.1 Spatial discretization using SUPG method

In this section, we consider the approach DO to solve the optimization problem. For this scenario, we discretize the functional (2.1a) and the state equation (2.1b) by using a standard finite element approach in space.
As in [21], we consider the following finite element spaces to discretize the state and the control:

$$\begin{aligned} V_h &= \{v_h \in V : v_h|_T \in P_k(T) \text{ for all } T \in \mathfrak{T}_h\}, \quad k \geq 1, \\ U_h &= \{w_h \in L^2(\Omega) : w_h|_T \in P_m(T) \text{ for all } T \in \mathfrak{T}_h\}, \quad m \geq 0, \end{aligned} \tag{2.10}$$

where $\{\mathfrak{T}_h\}_{h>0}$ be a family of quasi-uniform triangulations of Ω [19].

When we use the standard Galerkin method to discretize the state equation (2.1b) which is a convection dominated problem, there is a strongly oscillatory solution. In this thesis, we analyze the stabilized solution of the problem. For the stabilization method, we use SUPG method [21, 46] with the stabilization parameter τ. We use the notation s as a superscript or underscript to indicate that the stabilization method is applied to state equation. This leads to the following bilinear forms applied to $y_h \in X_h = H^1(I; V_h)$

$$(y_{h,t}, v_h) + \sum_{K\in\mathfrak{T}_h} \tau(y_{h,t}, \beta\cdot\nabla v_h)_K + a_h^s(y_h, v_h) + b_h^s(u_h, v_h) = \langle f, v_h\rangle_h^s, \forall v_h \in V_h, \tag{2.11}$$

$$a_h^s(y, v_h) = a(y, v_h) + \sum_{K\in\mathfrak{T}_h} \tau\langle -\epsilon\Delta y + \beta\cdot\nabla y + \sigma y, \beta\cdot\nabla v_h\rangle_K, \tag{2.12a}$$

$$b_h^s(u, v_h) = b(y, v_h) - \sum_{K\in\mathfrak{T}_h} \tau\langle u, \beta\cdot\nabla v_h\rangle_K, \tag{2.12b}$$

$$\langle f, v_h\rangle_h^s = \langle f, v_h\rangle + \sum_{K\in\mathfrak{T}_h} \tau\langle f, \beta\cdot\nabla v_h\rangle_K. \tag{2.12c}$$

We can clearly see that if we extract the stabilizing term from (2.12), we obtain an approximation $y_h \in X_h$ of the solution y of the state equation (2.1b) for the unstabilized case.
Then our optimization problem becomes

$$\min \quad J(y,u) = \frac{1}{2}\,\|y_h - y_d\|_Q^2 \; + \frac{\alpha}{2}\,\|u_h\|_Q^2 \tag{2.13a}$$

subject to

$$(y_{h,t}, v_h) + \sum_{K\in\mathfrak{T}_h} \tau(y_{h,t}, \beta\cdot\nabla v_h)_K + a_h^s(y_h, v_h) + b_h^s(u_h, v_h) = \langle f, v_h\rangle_h^s, \forall v_h \in V_h, \tag{2.13b}$$

$$y_h(0) = y_{0,h}. \tag{2.13c}$$

The Lagrangian for the discretized problem (2.13) is given by

$$L^s(y,u,p) = \frac{1}{2}\|y_h - y_d\|_Q^2 + \frac{\alpha}{2}\|u_h\|_Q^2 + (y_{h,t}, p_h) + \sum_{K\in\mathfrak{T}_h} \tau(y_{h,t}, \beta\cdot\nabla p_h)_K \qquad (2.14)$$
$$+a_h^s(y_h,p_h) + b_h^s(u_h,p_h) - \langle f, p_h\rangle_h^s,$$

where $y_h, p_h \in X_h$ and $u_h \in U_{ad}^h := \{u_h \in L^2(I;U_h) : u_a \le u_h \le u_b$ a.e., in $Q\}$. Setting partial derivative of L^s (2.14) to zero, we obtain the following necessary and sufficient optimality conditions for the discretized problem (2.13):

$$-(p_{h,t},\psi_h) - \sum_{K\in\mathfrak{T}_h} \tau(p_{h,t},\beta\cdot\nabla\psi_h)_K + a_h^s(\psi_h,p_h) = -\langle y_h - y_d, \psi_h\rangle, \qquad \forall \psi_h \in V_h, \qquad (2.15a)$$

$$b_h^s(w_h,p_h) + \alpha\langle u_h, w_h\rangle = 0, \qquad \forall w_h \in U_h, \qquad (2.15b)$$

$$(y_{h,t},v_h) + \sum_{K\in\mathfrak{T}_h} \tau(y_{h,t},\beta\cdot\nabla v_h)_K + a_h^s(y_h,v_h) + b_h^s(u_h,v_h) = \langle f, v_h\rangle_h^s. \qquad \forall v_h \in V_h, \qquad (2.15c)$$

Corollary 2.2.2 *Assume that the bilinear form $a_h^s(\cdot,\cdot)$ is continuous and coercive in $V_h \times V_h$. Given $f, y_d \in L^2(Q)$, $y_{0,h} \in H$, $\epsilon > 0$, β, and σ are fixed. The semi discrete optimal control problem (2.13) has a unique solution $(y_h, u_h) \in X_h \times U_h^{ad}$. The functions $(y_h,u_h) \in X_h \times U_h^{ad}$ solve (2.13) if and only if $(y_h,u_h,p_h) \in X_h \times U_h^{ad} \times X_h$ is a unique solution of the optimality system (2.15).*

Proof. The proof can be found [51, 84]. ■

As in [21], we use the discrete adjoint equation (2.15a) and the discrete gradient equation (2.15b), which means that these are obtained from the discretized OCP. In the next section, we discretize the adjoint equation (2.2) by SUPG method and gradient equation (2.3) to obtain discretized adjoint equation and discretized gradient equation respectively.

We note that since the optimal control u and the optimal state y satisfy (2.15c), the discretized state equation (2.15c) is strongly consistent. The optimal state y and the corresponding adjoint p do not satisfy (2.15a) which means that the discrete adjoint equation (2.15a) is not strongly consistent. Similarly, the discrete gradient equation (2.15b) is not strongly consistent, too.

We discretize the state, adjoint and control using the same finite element basis functions φ_i in the DO. The approximation of y and u is the following form

$$y_h(x,t) = \sum_{j=1}^{n+1}\sum_{k=1}^{l} y_k^j(t)\varphi_j^k(x), \quad u_h(x,t) = \sum_{j=1}^{n+1}\sum_{k=1}^{l} u_k^j(t)\varphi_j^k(x), \qquad (2.16)$$

set

$$\vec{y(t)} = (y_1^1(t), y_2^1(t), ..., y_l^1(t), ..., y_1^{n+1}(t), y_2^{n+1}(t), ..., y_l^{n+1}(t))^T$$
$$\vec{u(t)} = (u_1^1(t), u_2^1(t), ..., u_l^1(t), ..., u_1^{n+1}(t), u_2^{n+1}(t), ..., u_l^{n+1}(t))^T, \qquad (2.17)$$

where $n+1$ is the number of triangles and l is local dimension. If we insert (2.16) into (2.13), we obtain the following form of the semi discretization of the OCP

$$\min \quad J_h(\vec{y},\vec{u}) = \int_0^T \frac{1}{2}(\vec{y}-\vec{y}_d)^T M(\vec{y}-\vec{y}_d)dt + \int_0^T \frac{\alpha}{2}\vec{u}^T M\vec{u}dt \qquad (2.18a)$$

subject to

$$\begin{aligned} M^s\vec{y}_t + \tilde{K}^s\vec{y} - M^s\vec{u} &= f^s, \\ \vec{y}(0) &= \vec{y}_0. \end{aligned} \qquad (2.18b)$$

Also note that if we extract the stabilization term from (2.18b), we get the following unstabilized semi discretization of the state equation:

$$\begin{aligned} M\vec{y}_t + \tilde{K}\vec{y} - M\vec{u} &= f_h, \\ \vec{y}(0) &= \vec{y_0}, \end{aligned} \tag{2.18c}$$

where

$$M^s = M + \tau N; \;\; \tilde{K}^s = \tilde{K} + \tau(\beta^T\beta K + \sigma\beta N); \;\; \tilde{K} = \epsilon K + \beta N + \sigma M; \;\; f^s = f_h + \tau\beta {f_h}^s$$

$$\begin{aligned} M &= \int_{R_i} \varphi_j(x)\varphi_i(x)dx, \\ K &= \int_{R_i} \nabla\varphi_j(x)\nabla\varphi_i(x)dx, \\ N &= \int_{R_i} \nabla\varphi_j(x)\varphi_i(x)dx, \\ f_h &= \int_{R_i} f(x,t)\varphi_i(x)dx, \\ {f_h}^s &= \int_{R_i} f(x,t)\nabla\varphi_i(x)dx, \end{aligned} \tag{2.19}$$

where R_i is the region over the i-th element, M is the mass matrix, $\tilde{K}$ is the stiffness matrix and f_h is the vector coming from right hand side for the unstabilized case. When we apply SUPG method, we have a new mass matrix M^s, a new stiffness matrix $\tilde{K}^s$ and ${f_h}^s$.

2.2.2.2 Time discretization using Θ scheme

In this section, we use SUPG stabilized semi discretization (2.18b) and Θ scheme for time discretization so that we obtain the fully discretized system. The approximation of the state y and the control u is given in (2.16) on the interval (0,1) with n uniform subdivisions. We use the following notations:

$$\mathbf{y} := y(\vec{t}) \;\; , \mathbf{u} := u(\vec{t}).$$

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

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

and for given time interval $(0, T)$ with N uniform subdivions $0 = t_0 < t_1 < ... < t_{N+1} = T$. Then using a standard finite element approach in space and a trapezoidal rule, the cost functional (2.1a) becomes

$$J_h(Y, U) = \frac{\Delta t}{2}(Y - Y_d)^T \mathcal{M}_{1/2}(Y - Y_d) + \frac{\alpha\Delta t}{2} U^T \mathcal{M}_{1/2} U \tag{2.20}$$

with the matrix

$$\mathcal{M}_{1/2} = \begin{pmatrix} \frac{1}{2}M & 0 & 0 & 0 \\ 0 & M & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \frac{1}{2}M \end{pmatrix} \in \mathbb{R}^{(n+1)\times N,(n+1)\times N}. \tag{2.21}$$

where M is mass matrix defined in (2.19) and

$$Y = (\mathbf{y^1}, ..., \mathbf{y^{N+1}}) \text{ and } U = (\mathbf{u^0}, ..., \mathbf{u^{N+1}}),$$

where $\mathbf{y^i}$ and $\mathbf{u^i}$ correspond to vector valued functions at the time step i.
When we apply Θ scheme [84] to (2.18b)

$$\begin{aligned} M^s(\mathbf{y}^{i+1} - \mathbf{y}^i) \;\; &+ \;\; \Delta t\tilde{K}^s(\Theta\mathbf{y}^{i+1} + (1-\Theta)\mathbf{y}^i) - \Delta t M^s(\Theta\mathbf{u}^{i+1} + (1-\Theta)\mathbf{u}^i) \\ &= \;\; \Delta t(\Theta f^s(t_{i+1}) + (1-\Theta)f^s(t_i)), \;\; (i = 0, ..., N), \end{aligned} \tag{2.22}$$

where $M^s,\ \tilde{K}^s,\ f^s$ are given in (2.19).
By defining

$$F_1^s = (M^s + \Delta t\Theta\tilde{K}^s),\quad F_0^s = (-M^s + \Delta t(1-\Theta)\tilde{K}^s), \tag{2.23}$$

we obtain the following fully discrete system in matrix form

$$E_s Y - \Delta t Z_s U = F_s \tag{2.24}$$

where

$$E_s = \begin{pmatrix} F_1^s & 0 & 0 & 0 \\ F_0^s & F_1^s & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & F_0^s & F_1^s \end{pmatrix}, Z_s = \begin{pmatrix} \Theta M^s & 0 & 0 & 0 & 0 \\ (1-\Theta)M^s & \Theta M^s & 0 & 0 & 0 \\ 0 & \ddots & \ddots & 0 & 0 \\ 0 & 0 & (1-\Theta)M^s & \Theta M^s & 0 \\ 0 & 0 & 0 & (1-\Theta)M^s & \Theta M^s \end{pmatrix} \tag{2.25}$$

and

$$F_s = \begin{pmatrix} -F_0^s \mathbf{y}^0 + \Delta t(\Theta f^s(t_1) + (1-\Theta)f^s(t_0)) \\ \vdots \\ \Delta t(\Theta f^s(t_{N+1}) + (1-\Theta)f^s(t_N)) \end{pmatrix}. \tag{2.26}$$

We introduce Lagrangian function L with the Lagrange multiplier P [83] to obtain the optimality system containing the first order optimality conditions:

$$L(Y,U,P) := J_h(Y,U) + P^T\big(- E_s Y + \Delta t Z_s U + F_s\big). \tag{2.27}$$

In this sense by inserting (2.20) to (2.27), taking derivative of L with respect to to y and u and with the equation (2.24), we obtain the following optimality conditions

$$\nabla_Y L(Y^*,U^*,P^*) = \Delta t\mathcal{M}_{1/2}(Y^* - Y_d) - E_s^T P^* = 0, \tag{2.28a}$$
$$\nabla_P L(Y^*,U^*,P^*) = -E_s Y^* + \Delta t Z_s U^* + F_s = 0, \tag{2.28b}$$
$$\nabla_U L(Y^*,U^*,P^*) = \alpha\Delta t\mathcal{M}_{1/2}U^* + \Delta t Z_s^T P^* = 0, \tag{2.28c}$$

where (2.28a), (2.28b), (2.28c) give the discrete adjoint equation, the discretized state equation and the discrete gradient equation, respectively. Both of the discrete adjoint equation and the discrete gradient equation have a stabilizing effect coming from the stabilization term added to state equation. However, the discrete adjoint equation and the discrete gradient equation are not strongly consistent for (2.2) and (2.3), respectively. Although the optimality system (2.28) is not strongly consistent, there is finite-dimensional problem and the following symmetric indefinite linear system:

$$\begin{pmatrix} \Delta t\mathcal{M}_{1/2} & 0 & -E_s^T \\ 0 & \alpha\Delta t\mathcal{M}_{1/2} & \Delta t Z_s^T \\ -E_s & \Delta t Z_s & 0 \end{pmatrix}\begin{pmatrix} Y \\ U \\ P \end{pmatrix} = \begin{pmatrix} \Delta t\mathcal{M}_{1/2}Y_d \\ 0 \\ -F_s \end{pmatrix}. \tag{2.29}$$

The above system is solved for $\Theta = \frac{1}{2}$ and $\Theta = 1$ which are called *Crank-Nicolson method* and *backward Euler method* respectively.

For the unstabilized case with Θ scheme:
We take $F_1 = (M + \Delta t\Theta\tilde{K})$ and $F_0 = (-M + \Delta t(1-\Theta)\tilde{K})$ instead of F_1^s and F_0^s given in (2.23), where $M, \tilde{K}$ are given in (2.19). We can define the new matrix E for the unstabilized case by inserting F_1, F_0 instead of F_1^s, F_0^s in the matrix E_s (2.25)and a new matrix Z by inserting M instead of M^s in the matrix

form Z_s (2.25). We obtain a new vector F by inserting F_0, f instead of F_0^s and f^s in the vector form (2.29). Moreover, the fully discrete system for the unstabilized case becomes

$$EY - \Delta t Z U = F. \tag{2.30}$$

Then, by following the same steps, we obtain the symmetric indefinite linear system for unstabilized case:

$$\begin{pmatrix} \Delta t \mathcal{M}_{1/2} & 0 & -E^T \\ 0 & \alpha \Delta t \mathcal{M}_{1/2} & \Delta t Z^T \\ -E & \Delta t Z & 0 \end{pmatrix} \begin{pmatrix} Y \\ U \\ P \end{pmatrix} = \begin{pmatrix} \Delta t \mathcal{M}_{1/2} Y_d \\ 0 \\ -F \end{pmatrix}. \tag{2.31}$$

2.2.2.3 Time discretization using semi-implicit scheme

Similar to Θ scheme, in this section we apply semi implicit scheme to SUPG stabilized semi discrete problem (2.18b). By using semi implicit scheme, we can avoid stability restrictions without resorting to the fully implicit approximation. In this sense, we evaluate the diffusion term, $-\epsilon\Delta$ at the time level t_{n+1}, whereas the remaining parts, convection and reaction terms, are considered at the time level t_n. Then this scheme:

$$\begin{aligned} M^s(\mathbf{y}^{i+1} - \mathbf{y}^i) \quad &+ \quad \Delta t \epsilon K \mathbf{y}^{i+1} + (\Delta t \beta N + \sigma M + \tau(\beta^T \beta K + \sigma \beta N))\mathbf{y}^i - \Delta t M^s \mathbf{u}^{i+1} \\ &= \quad \Delta t f^s(t_{i+1}), \quad (i = 0, ..., N), \end{aligned} \tag{2.32}$$

where $M^s,\ K,\ N,\ M,\ f^s$ are given in (2.19) and τ is the stabilization parameter.
Then we define

$$\tilde{F}_1^s = (M^s + \Delta t \epsilon K), \tilde{F}_0^s = (-M^s + \Delta t(\beta N + \sigma M + \tau(\beta^T \beta K + \sigma \beta N))). \tag{2.33}$$

The fully discrete system in the matrix form

$$\tilde{E}_s Y - \Delta t \tilde{Z}_s U = \tilde{F}_s, \tag{2.34}$$

where

$$\tilde{E}_s = \begin{pmatrix} \tilde{F}_1^s & 0 & 0 & 0 \\ \tilde{F}_0^s & \tilde{F}_1^s & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & \tilde{F}_0^s & \tilde{F}_1^s \end{pmatrix}, \quad \tilde{Z}_s = \begin{pmatrix} M^s & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & M^s \end{pmatrix} \tag{2.35}$$

and

$$\tilde{F}_s = \begin{pmatrix} -\tilde{F}_0^s \mathbf{y}^0 + \Delta t f^s(t_1) \\ \vdots \\ \Delta t f^s(t_{N+1})) \end{pmatrix}, \tag{2.36}$$

then by following the same procedure as in the previous section, we obtain the saddle point system

$$\begin{pmatrix} \Delta t \mathcal{M}_{1/2} & 0 & -\tilde{E}_s^T \\ 0 & \alpha \Delta t \mathcal{M}_{1/2} & \Delta t \tilde{Z}_s^T \\ -\tilde{E}_s & \Delta t \tilde{Z}_s & 0 \end{pmatrix} \begin{pmatrix} Y \\ U \\ P \end{pmatrix} = \begin{pmatrix} \Delta t \mathcal{M}_{1/2} Y_d \\ 0 \\ -\tilde{F}_s \end{pmatrix}. \tag{2.37}$$

For the unstabilized case with semi-implicit scheme:
We take

$$\tilde{F}_1 = (M + \Delta t \epsilon K), \tilde{F}_0 = (-M + \Delta t(\beta N + \sigma M)). \tag{2.38}$$

The block matrices are defined as

$$\tilde{E} = \begin{pmatrix} \tilde{F}_1 & 0 & 0 & 0 \\ \tilde{F}_0 & \tilde{F}_1 & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & \tilde{F}_0 & \tilde{F}_1 \end{pmatrix}, \tilde{Z} = \begin{pmatrix} M & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & M \end{pmatrix} \tag{2.39}$$

and

$$\tilde{F} = \begin{pmatrix} -\tilde{F}_0 \mathbf{y}^0 + \Delta t f(t_1) \\ \vdots \\ \Delta t f(t_N)) \end{pmatrix} \tag{2.40}$$

and the indefinite linear system

$$\begin{pmatrix} \Delta t \mathcal{M}_{1/2} & 0 & -\tilde{E}^T \\ 0 & \alpha \Delta t \mathcal{M}_{1/2} & \Delta t \tilde{Z}^T \\ -\tilde{E} & \Delta t \tilde{Z} & 0 \end{pmatrix} \begin{pmatrix} Y \\ U \\ P \end{pmatrix} = \begin{pmatrix} \Delta t \mathcal{M}_{1/2} Y_d \\ 0 \\ -\tilde{F} \end{pmatrix} \tag{2.41}$$

2.2.2.4 Control constrained problem

When we consider the OCP (2.1), it is desirable to impose the control constraints. In this sense, with the box constraints defined in (2.1c), we define the following optimality condition:

$$(U - U^*)^T \nabla_U L(Y^*, U^*, P^*) = (U - U^*)^T (\alpha \Delta t \mathcal{M}_{1/2} U^* + \Delta t Z_s^T P^*) \geq 0, \tag{2.42}$$

where ∇_U given in (2.28c). In this section, we consider the Θ scheme for time discretization. The idea is the same as in the case of the semi-implicit scheme.

The following Lagrange multipliers μ_a and μ_b for the inequality constraints on the control variable defined as

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

So, we introduce the following augmented Lagrange function [83]:

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

We consider an extension of theorem in [83] about the optimality conditions to N time-steps.

Theorem 2.2.3 *For an optimal solution (y^*, u^*), there exists Lagrange multipliers p, μ_a, and μ_b such that*

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

The OCPs with additional constraints can be solved by interior point methods and active-set strategies. We follow [7] to solve control constraint problem by using the active set method determined by

$$\begin{aligned} A_+ : &= \{i \in \{1, \dots, N\} : (U^* - \mu)_i > (U_b)_i\}, \\ A_- : &= \{i \in \{1, \dots, N\} : (U^* - \mu)_i < (U_a)_i\}, \\ I : &= \{1, 2, \dots, N\} \backslash (A_+ \cup A_-). \end{aligned}$$

With additional control constraints, the optimality conditions given for the unconstrained OCP (2.18) is redefined by

$$\nabla_Y L(Y^*, U^*, P^*) = \Delta t \mathcal{M}_{1/2}(Y^* - Y_d) - E_s^T P^* = 0, \tag{2.43a}$$

$$\nabla_P L(Y^*, U^*, P^*) = -E_s Y^* + \Delta t Z_s U^* + F_s = 0, \tag{2.43b}$$

$$\nabla_U L(Y^*, U^*, P^*) = \alpha \Delta t \mathcal{M}_{1/2} U^* + \Delta t \chi_I Z_s^T P^* = \alpha \Delta t \mathcal{M}_{1/2}(\chi_{A_-} U_a + \chi_{A_+} U_b), \tag{2.43c}$$

where χ denotes the characteristic function of the given set.
By setting

$$\begin{aligned} A_+ &= \{x \in Q : -\alpha \Delta t \mathcal{M}_{1/2} U_a - \Delta t Z_s^T P < 0\}, \\ A_- &= \{x \in Q : -\alpha \Delta t \mathcal{M}_{1/2} U_b - \Delta t Z_s^T P > 0\}, \\ I &= Q \backslash (A_+ \cup A_-), \end{aligned}$$

we solve the following saddle point system for the control constrained OCP.

$$\begin{pmatrix} \Delta t \mathcal{M}_{1/2} & 0 & -E_s^T \\ 0 & \alpha \Delta t \mathcal{M}_{1/2} & \Delta t \chi_I Z_s^T \\ -E_s & \Delta t Z_s & 0 \end{pmatrix} \begin{pmatrix} Y \\ U \\ P \end{pmatrix} = \begin{pmatrix} \Delta t \mathcal{M}_{1/2} Y_d \\ \alpha \Delta t \mathcal{M}_{1/2}(\chi_{A_-} U_a + \chi_{A_+} U_b), \\ -F_s \end{pmatrix}. \tag{2.44}$$

A detailed discussion of active-set methods can be found in [7, 83].

2.2.3 Optimize-then-discretize approach

2.2.3.1 Space discretization with SUPG

In this section, we directly discretize each equation in (2.9) to obtain approximate solution of the OCP. As we mentioned, this prodecure is called as OD approach. We use the same space X_h defined in (2.10) for state and adjoint equation and U_{ad}^h for control equation. When we discretize the adjoint equation (2.2), we again use SUPG method for the convection dominated adjoint equation. Then the discretized adjoint equation with SUPG method is as follows:

$$(-p_{h,t}, \psi_h) + \sum_{K \in \mathfrak{T}_h} \tau(-p_{h,t}, -\beta \cdot \nabla \psi_h)_K + a_h^a(\psi_h, p_h) = -\langle y_h - y_d, \psi_h \rangle_h^a, \quad \forall \psi_h \in V_h, \ p_h \in X_h, \tag{2.45a}$$

where

$$a_h^a(\psi_h, p_h) = a(\psi_h, p_h) + \sum_{K \in \mathfrak{T}_h} \tau \langle -\epsilon \Delta p_h - \beta \cdot \nabla p_h + \sigma p_h, -\beta \cdot \nabla \psi_h \rangle_K, \tag{2.45b}$$

$$\langle y_h - y_d, \psi_h \rangle_h^a = \langle y_h - y_d, \psi_h \rangle + \sum_{K \in \mathfrak{T}_h} \tau \langle y_h - y_d, -\beta \cdot \nabla \psi_h \rangle_K. \tag{2.45c}$$

After discretization of the gradient equation (2.9b), we have

$$b(w_h, p_h) + \alpha \langle u_h, w_h \rangle = 0 \ \ \forall w_h \in U_h. \tag{2.45d}$$

and the discrete state equation is the same as in (2.15c).
We note that the discretized state, adjoint and gradient equations are strongly consistent which means that the solution $y, \ u, \ p$ of (2.9) also satisfy (2.45). However, the system (2.45) is non-symmetric and so there is no finite-dimensional optimization problem of the optimality system.

For the finite element representation of this approach, we use the same approximation of y and u in (2.16) and the approximation of p

$$p_h(x,t) = \sum_{j=1}^{n+1} \sum_{k=1}^{l} p_k^j(t) \varphi_j^k(x), \tag{2.46}$$

by setting

$$\vec{p(t)} = (p_1^1(t), p_2^1(t), ..., p_l^1(t), ..., p_1^{n+1}(t), p_2^{n+1}(t), ..., p_l^{n+1}(t))^T$$

and we have the following semi discretization of the adjoint equation

$$\begin{aligned} M^a \vec{p}_t + \tilde{K}^a \vec{p} - \tilde{M}^a \vec{y} &= -\tilde{M}^a \vec{y_d}, \\ \vec{y}(0) &= \vec{y_0}, \end{aligned} \tag{2.47}$$

where

$$M^a = -M + \tau N; \;\; \tilde{K}^a = \epsilon K - \beta N + \sigma M + \tau(\beta^T \beta K - \sigma \beta N); \;\; \tilde{M}^a = (M - \tau \beta N), \tag{2.48}$$

The semi discretization of the gradient equation is

$$\alpha M \vec{u} - M \vec{p} = 0, \tag{2.49}$$

and the semi discretization of state equation is the same as in (2.18b), where the matrices $M,\ K,\ N$ are defined in (2.19). We note that the superscript a is used for the discretization of the adjoint equation with SUPG.

2.2.3.2 Time discretization with Θ scheme

As in the previous section, we obtain the fully discrete matrix form (2.24) of the stabilized semi discrete state equation (2.18b). The matrix form of state equation is the same as the one obtained by OD approach. Hence, we compute the fully discrete form of the adjoint equation by applying Θ-scheme to the stabilized semi discrete adjoint equation (2.47).
Let us define $P = (\mathbf{p^1}, ..., \mathbf{p^{N+1}})$ where $\mathbf{p^i}$ correspond to vector valued functions at the time step i.
When we apply Θ scheme [84] to (2.47), we get

$$\begin{aligned} M^a(\mathbf{p}^{i+1} - \mathbf{p}^i) \;\; + &\;\; \Delta t \tilde{K}^a(\Theta \mathbf{p}^i + (1-\Theta)\mathbf{p}^{i+1}) + \Delta t \tilde{M}^a(\Theta \mathbf{y}^i + (1-\Theta)\mathbf{y}^{i+1}) \\ = &\;\; \Delta t \tilde{M}^a(\Theta \mathbf{y_d}^i + (1-\Theta)\mathbf{y_d}^{i+1}), \quad (i = N, ..., 0). \end{aligned} \tag{2.50}$$

By defining

$$F_1^a = (M^a + \Delta t \Theta \tilde{K}^a), \;\; F_0^a = (-M^a + \Delta t(1-\Theta)\tilde{K}^a), \tag{2.51}$$

we obtain the following full discrete system in matrix form

$$E_a P + \Delta t Z_a Y = \Delta t Z_a Y_d, \tag{2.52}$$

where

$$E_a = \begin{pmatrix} F_1^a & 0 & 0 & 0 \\ F_0^a & F_1^a & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & F_0^a & F_1^a \end{pmatrix}, Z_a = \begin{pmatrix} \Theta\tilde{M}^a & 0 & 0 & 0 & 0 \\ (1-\Theta)\tilde{M}^a & \Theta\tilde{M}^a & 0 & 0 & 0 \\ 0 & \ddots & \ddots & & \\ 0 & 0 & (1-\Theta)\tilde{M}^a & \Theta\tilde{M}^a & 0 \\ 0 & 0 & 0 & (1-\Theta)\tilde{M}^a & \Theta\tilde{M}^a \end{pmatrix} \tag{2.53}$$

Now we define following non-symmetric linear system

$$\begin{pmatrix} \Delta t Z_a & 0 & E_a^T \\ 0 & \alpha\Delta t \mathcal{M}_{1/2} & -\Delta t Z^T \\ E_s & -\Delta t Z_s & 0 \end{pmatrix} \begin{pmatrix} Y \\ U \\ P \end{pmatrix} = \begin{pmatrix} \Delta t Z_a Y_d \\ 0 \\ F_s \end{pmatrix}, \tag{2.54}$$

where Z is the matrix including M instead of M^s.
Clearly we can see that the optimality system (2.29) obtained from DO approach and the optimality system (2.56) obtained from OD approach don't commute, that is, these approaches lead to different discrete equations.

2.2.3.3 Time discretization with semi-implicit scheme

We compute the fully discrete form of adjoint equation by applying semi-implicit scheme to the stabilized semi discrete adjoint equation (2.47). Let us note that we obtain the full discretized state equation with semi-implicit scheme (2.32) and then the fully discrete matrix system (2.34); so we use this system as a fully discretized state equation:

$$\begin{aligned} M^a(\mathbf{p}^{i+1} - \mathbf{p}^i) \quad + & \quad \Delta t \epsilon K \mathbf{p}^i + (-\Delta t \beta N + \sigma M + \tau(\beta^T \beta K - \sigma \beta N))\mathbf{p}^{i+1} + \Delta t \tilde{M}^a \mathbf{y}^i \\ = & \quad +\Delta t \tilde{M}^a \mathbf{y_d}^i, \quad (i = N, ..., 0), \end{aligned} \tag{2.55}$$

where K is given in (2.19), M^a K^a, $\tilde{M}^a$ are given in (2.48) and τ is the stabilization parameter.
In a similar way, when we define

$$\tilde{F}_1^a = (M^a + \Delta t \epsilon K), \tilde{F}_0^a = (-M^a + \Delta t(-\beta N + \sigma M + \tau(\beta^T \beta K - \sigma \beta N))), \tag{2.56}$$

we obtain the full discrete system in matrix form

$$\tilde{E}_a P + \Delta t \tilde{Z}_a Y = \Delta t \tilde{Z}_a Y_d, \tag{2.57}$$

where

$$\tilde{E}_a = \begin{pmatrix} \tilde{F}_1^a & 0 & 0 & 0 \\ \tilde{F}_0^a & \tilde{F}_1^a & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & \tilde{F}_0^a & \tilde{F}_1^a \end{pmatrix}, \tilde{Z}_a = \begin{pmatrix} \tilde{M}^a & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \tilde{M}^a \end{pmatrix} \tag{2.58}$$

and

$$\mathcal{M} = \begin{pmatrix} M & 0 & 0 & 0 \\ 0 & M & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & M \end{pmatrix} \in \mathbb{R}^{(n+1)\times N,(n+1)\times N}. \tag{2.59}$$

Then, by following a procedure similar to the one in the previous section, we obtain the non-symmetric saddle point system which is different from the symmetric system obtained by the semi-implicit scheme in DO approach (2.37).

$$\begin{pmatrix} \Delta t \tilde{Z}_a & 0 & \tilde{E}_a^T \\ 0 & \alpha\Delta t \mathcal{M}_{1/2} & -\Delta t \mathcal{M} \\ \tilde{E}_s & -\Delta t \tilde{Z}_s & 0 \end{pmatrix} \begin{pmatrix} Y \\ U \\ P \end{pmatrix} = \begin{pmatrix} \Delta t \tilde{Z}_a Y_d \\ 0 \\ \tilde{F}_s \end{pmatrix}. \tag{2.60}$$

2.2.3.4 Control constrained problem

In the DO approach, we give brief information about the active set method used for the control constrained problem. Therefore, we only give the optimality system of OCP (2.1) with control constraints (2.1c). Let us use the semi implicit scheme for time discretization; then we have the following linear system:

$$\begin{pmatrix} \Delta t\tilde{Z}_a & 0 & \tilde{E}_a^T \\ 0 & \alpha\Delta t\mathcal{M}_{1/2} & -\Delta t\chi_I\mathcal{M} \\ \tilde{E}_s & -\Delta t\tilde{Z}_s & 0 \end{pmatrix}\begin{pmatrix} Y \\ U \\ P \end{pmatrix} = \begin{pmatrix} \Delta t\tilde{Z}_a Y_d \\ \alpha\Delta t\mathcal{M}_{1/2}(\chi_{A_-}U_a + \chi_{A_+}U_b), \\ \tilde{F}_s \end{pmatrix}. \tag{2.61}$$

2.3 Boundary optimal control problem

We consider the following time dependent boundary OCP governed by the diffusion-convection-reaction equation with and without control constraints. We consider Robin type boundary conditions:

$$\min \quad J(y,u) = \frac{1}{2}\,\|y-y_d\|_Q^2 \;+\; \frac{\alpha}{2}\,\|u\|_\Sigma^2 \tag{2.62a}$$

subject to

$$\begin{aligned} y_t - \epsilon\Delta y + \beta\nabla y + \sigma y &= f, \quad \text{in } Q, \\ \epsilon\nabla y + \gamma y &= u, \quad \text{in } \Sigma, \\ y(\cdot,0) &= y_0, \quad \text{in } \Omega, \end{aligned} \tag{2.62b}$$

and

$$u \in \tilde{U}_{ad} \subset L^2(\Sigma), \tag{2.63}$$

where

$$\tilde{U}_{ad} = \{u \in L^\infty(\Sigma) : \tilde{u}_a \le u \le \tilde{u}_b,\ a.e., \ \text{ in } I\},$$

with $\tilde{u}_a,\ \tilde{u}_b \in L^\infty(\Sigma)$ and $u_a \le u_b$ almost everywhere in Σ.
Here the domain $\Omega \in \mathbb{R}^n$ for $\{n = 1,2\}$, and $\epsilon,\beta,\sigma > 0$ are diffusion, convection and reaction coefficients, respectively. Given the desired state $y_d \in L^2(Q)$, u denote the control variable and α is regularization parameter, and $\gamma \in L^\infty(\Sigma)$, and $f \in L^2(Q), y_0 \in L^2(\Omega)$ are the forcing function and the initial state respectively. We make use of the following Hilbert space Y:

$$Y := \{\varphi \in L^2(I;H^1(\Omega));\ \varphi_t \in L^2(I;H^1(\Omega)^*)\},$$

where $H^1(\Omega)^*$ denotes the dual space of $H^1(\Omega)$.
Using the approach OD, we obtain the following optimality conditions, the adjoint equation:

$$\begin{aligned} -p_t - \epsilon\Delta p - \beta\nabla y + \sigma p &= -(y-y_d), \quad \text{in } Q, \\ \epsilon\nabla p + (\gamma+\beta)p &= 0, \quad \text{in } \Sigma, \\ p(\cdot,T) &= 0, \quad \text{in } \Omega, \end{aligned} \tag{2.64}$$

with the gradient equations

$$\alpha u - p \;=\; 0, \quad \text{in } \Sigma. \tag{2.65}$$

In case of pointwise control constraints, we get the gradient condition

$$\alpha u - p + \mu_b - \mu_a \;=\; 0, \quad \text{in } \Sigma. \tag{2.66}$$

By a similar way as in previous section, we get, 'strongly consistent' optimality system obtained by discretizing each equation (2.63b), (2.65), (2.66) and (2.67) with the use of discretization schemes. We also apply DO approach, too.

2.3.1 Existence and uniqueness of solutions

We define the weak form for the state equation (2.63b) of time dependent boundary control problem. Let us take $u \in \tilde{U}_{ad}, \; y \in Y, \; f \in L^2(Q), \; y_0 \in L^2(\Omega)$:

$$\begin{aligned} (y_t, v) + \tilde{a}(y, v) + \tilde{b}(u, v) &= \langle f, v\rangle, \quad \forall v \in H^1(\Omega), \\ y(0) &= y_0, \end{aligned} \tag{2.67}$$

where

$$\tilde{a}(y, v) = a(y, v) + \int_{\partial\Omega} \vec{n} \cdot \gamma y v ds,$$

$$\tilde{b}(u, v) = -\int_{\partial\Omega} \vec{n} \cdot u v ds,$$

where a, $\langle f, v\rangle$ is defined in (2.5) and the bilinear form $\tilde{a}$ is continuous and satisfies the coercivity (2.6) with $\lambda = 0$. Now, we consider the solution of the OCP

$$\min \quad J(y, u) = \frac{1}{2} \|y - y_d\|_Q^2 + \frac{\alpha}{2} \|u\|_\Sigma^2 \tag{2.68a}$$

subject to

$$\begin{aligned} (y_t, v) + \tilde{a}(y, v) + \tilde{b}(u, v) &= \langle f, v\rangle, \quad \forall v \in H^1(\Omega) \\ y(0) &= y_0. \end{aligned} \tag{2.68b}$$

Theorem 2.3.1 *Let us assume that the bilinear form $\tilde{a}(\cdot,\cdot)$ is continuous in $H^1(\Omega) \times H^1(\Omega)$ and that (2.6) is satisfied with $\lambda = 0$. Furthermore, let me given $f, y_d \in L^2(Q)$, $y_0 \in H$, and $\epsilon > 0$, β, σ, γ are fixed. Then the OCP (2.69) has a unique solution $(y, u) \in Y \times \tilde{U}_{ad}$.*

Proof. The proof can be found in the study of Lions [51], Wloka [86] and Tröltzsch [82]. ∎

Let define the Lagrangian to provide necessary and sufficient optimality conditions

$$\tilde{L}(y, u, p) = \tfrac{1}{2} \|y - y_d\|_Q^2 + \tfrac{\alpha}{2} \|u\|_\Sigma^2 + (y_t, p) + \tilde{a}(y, p) + \tilde{b}(u, p) - \langle f, p\rangle, \tag{2.69}$$

by taking derivative of $\tilde{L}$ with respect to $y, \; u, \; p$ respectively,

$$(-p_t, \psi) + \tilde{a}(\psi, p) = -\langle y - y_d, \psi\rangle, \qquad \forall \psi \in H^1(\Omega), \tag{2.70a}$$

$$\tilde{b}(w, p) + \alpha\langle u, w\rangle_\Sigma = 0, \qquad \forall w \in \tilde{U}_{ad}, \tag{2.70b}$$

$$(y_t, v) + \tilde{a}(y, v) + \tilde{b}(u, v) = \langle f, v\rangle, \qquad \forall v \in H^1(\Omega), \tag{2.70c}$$

where (2.71a) is the weak form of the adjoint equation (2.65), (2.71b) is the weak form of gradient equation (2.66) and (2.71c) is the weak form of state equation (2.63b). For the control constraint problem, by adding the term $\mu_b(u - u_b) + \mu_a(u_a - u)$ to (2.70), the term $\mu_b - \mu_a$ is added to (2.71b) which is the weak form of the gradient equation (2.67).

2.3.2 Discretize-then-optimize approach

2.3.2.1 SUPG stabilized semi discretization in space

In the sense of DO approach, we use the similar finite element space to (2.10) such that $\tilde{V}_h$ for the state and $\tilde{U}_h$ for the control variable. The only difference is that we take $H^1(\Omega), \; \tilde{U}_{ad}$ instead of $V, \; U_{ad}$

respectively. Similar to (2.12), by discretizing (2.63b) by using the standard Galerkin method with SUPG, we obtain

$$(y_{h,t}, v_h) + \sum_{K\in\mathfrak{T}_h} \tau(y_{h,t},\beta\cdot\nabla v_h)_K + \tilde{a}_h^s(y_h, v_h) + \tilde{b}_h^s(u_h, v_h) = \langle f, v_h\rangle_h^s, \forall v_h \in \tilde{V}_h, \tag{2.71}$$

$$\tilde{a}_h^s(y, v_h) = a_h^s(y, v) + \int_{\partial\Omega} \vec{n}\cdot\gamma y v ds, \tag{2.72a}$$

$$\tilde{b}_h^s(u, v_h) = \tilde{b}(u, v_h), \tag{2.72b}$$

where a_h^s, $\langle f, v_h\rangle_h^s$ is defined in (2.12) and $y_h \in Y_h := H^1(I; \tilde{V}_h)$, $u_h \in \tilde{U}_{ad}^h$. Then, the semi discretized boundary OCPS is given as:

$$\min \quad J(y, u) = \frac{1}{2}\|y_h - y_d\|_Q^2 + \frac{\alpha}{2}\|u_h\|_\Sigma^2 \tag{2.73a}$$

subject to

$$(y_{h,t}, v_h) + \sum_{K\in\mathfrak{T}_h} \tau(y_{h,t},\beta\cdot\nabla v_h)_K + \tilde{a}_h^s(y_h, v_h) + \tilde{b}_h^s(u_h, v_h) = \langle f, v_h\rangle_h^s, \forall v_h \in V_h \tag{2.73b}$$

$$y_h(0) = y_{0,h}.$$

The Lagrangian for the discretized boundary control problem (2.74) is given by

$$\tilde{L}^s(y, u, p) = \frac{1}{2}\|y_h - y_d\|_Q^2 + \frac{\alpha}{2}\|u_h\|_\Sigma^2 + (y_{h,t}, p_h) + \sum_{K\in\mathfrak{T}_h} \tau(y_{h,t},\beta\cdot\nabla p_h)_K \tag{2.74}$$
$$+ \tilde{a}_h^s(y_h, p_h) + \tilde{b}_h^s(u_h, p_h) - \langle f, p_h\rangle_h^s,$$

where $y_h, p_h \in Y_h$ and $u_h \in \tilde{U}_{ad}^h$.
By setting the derivatives of $\tilde{L}^s$ (2.75) with respect to the state, adjoint and control variable, we get the following discrete adjoint equation and discrete gradient equation, which are not strongly consistent:

$$-(p_{h,t}, \psi_h) - \sum_{K\in\mathfrak{T}_h} \tau(p_{h,t},\beta\cdot\nabla\psi_h)_K + \tilde{a}_h^s(\psi_h, p_h) = -\langle y_h - y_d, \psi_h\rangle, \qquad \forall\psi_h \in V_h, \tag{2.75a}$$

$$\tilde{b}_h^s(w_h, p_h) + \alpha\langle u_h, w_h\rangle_\Sigma = 0, \qquad \forall w_h \in U_h, \tag{2.75b}$$

$$(y_{h,t}, v_h) + \sum_{K\in\mathfrak{T}_h} \tau(y_{h,t},\beta\cdot\nabla v_h)_K + \tilde{a}_h^s(y_h, v_h) + \tilde{b}_h^s(u_h, v_h) = \langle f, v_h\rangle_h^s, \qquad \forall v_h \in V_h, \tag{2.75c}$$

now, using the approximation (2.16) we have

$$\min \quad J_h(\vec{y}, \vec{u}) = \int_0^T \frac{1}{2}(\vec{y} - \vec{y}_d)^T M(\vec{y} - \vec{y}_d)dt + \int_0^T \frac{\alpha}{2}\vec{u}^T M_b\vec{u}dt \tag{2.76a}$$

subject to

$$\begin{aligned} M^s\vec{y}_t + \tilde{K}_b^s\vec{y} - N_b\vec{u} &= f^s, \\ \vec{y}(0) &= \vec{y}_0. \end{aligned} \tag{2.76b}$$

We also note that if we extract the stabilization term from (2.77b), we get the following unstabilized semi discretization of the state equation:

$$\begin{aligned} M\vec{y}_t + \tilde{K}_b\vec{y} - N_b\vec{u} &= f_h, \\ \vec{y}(0) &= \vec{y}_0. \end{aligned} \tag{2.76c}$$

Let us use the matrices defined in (2.19) except M_b which is the boundary mass matrix and N_b which corresponds to entries arising from terms within the integrals $\int_{\partial\Omega} u tr(v)ds$ and $\int_{\partial\Omega} y tr(v)ds$ where u is the boundary control, y is the state equation coming from Robin type boundary condition and $tr(v)$ denotes the trace function acting on a member of the Galerkin test space .
Moreover, we add a term to the stiffness matrix because of the Neumann boundary conditions such that

$$\tilde{K}_b^s = \tilde{K}^s + \gamma N_b; \; \tilde{K}_b = \tilde{K} + \gamma N_b. \tag{2.77}$$

2.3.2.2 Time discretization with Θ scheme and semi-implicit scheme

In this section, we apply both Θ scheme and semi implicit scheme respectively. First, we apply trapezoidal rule to the cost functional (2.76a)

$$J_h(Y,U) = \frac{\Delta t}{2}(Y - Y_d)^T \mathcal{M}_{1/2}(Y - Y_d) + \frac{\alpha\Delta t}{2} U^T \mathcal{M}_{1/2,b} U, \tag{2.78}$$

where the matrix

$$\mathcal{M}_{1/2,b} = \begin{pmatrix} \frac{1}{2}M_b & 0 & 0 & 0 \\ 0 & M_b & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \frac{1}{2}M_b \end{pmatrix} \in \mathbb{R}^{(n+1)\times N,(n+1)\times N}. \tag{2.79}$$

When we apply Θ scheme similar to the distributed case (2.22), and define

$$F_1^{s,b} = (M^s + \Delta t\Theta\tilde{K}_b^s), \;\; F_0^{s,b} = (-M^s + \Delta t(1-\Theta)\tilde{K}_b^s), \tag{2.80}$$

then, we obtain the following fully discrete system in matrix form:

$$E_{s,b}Y - \Delta t Z_{s,b} U = F_{s,b}, \tag{2.81}$$

where

$$E_{s,b} = \begin{pmatrix} F_1^{s,b} & 0 & 0 & 0 \\ F_0^{s,b} & F_1^{s,b} & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & F_0^{s,b} & F_1^{s,b} \end{pmatrix}, Z_{s,b} = \begin{pmatrix} \Theta N_b & 0 & 0 & 0 & 0 \\ (1-\Theta)N_b & \Theta N_b & 0 & 0 & 0 \\ 0 & \ddots & \ddots & 0 & 0 \\ 0 & 0 & (1-\Theta)N_b & \Theta N_b & 0 \\ 0 & 0 & 0 & (1-\Theta)N_b & \Theta N_b \end{pmatrix} \tag{2.82}$$

and

$$F_{s,b} = \begin{pmatrix} -F_0^{s,b}\mathbf{y}^0 + \Delta t(\Theta f^s(t_1) + (1-\Theta)f^s(t_0)) \\ \vdots \\ \Delta t(\Theta f^s(t_{N+1}) + (1-\Theta)f^s(t_N)) \end{pmatrix}. \tag{2.83}$$

Similar to the previous section, by defining the Lagrangian function and taking derivatives of the Lagrangian with respect to $y, \; u, \; p$, we obtain the following symmetric linear system

$$\begin{pmatrix} \Delta t\mathcal{M}_{1/2} & 0 & -E_{s,b}^T \\ 0 & \alpha\Delta t\mathcal{M}_{1/2,b} & \Delta t Z_{s,b}^T \\ -E_{s,b} & \Delta t Z_{s,b} & 0 \end{pmatrix}\begin{pmatrix} Y \\ U \\ P \end{pmatrix} = \begin{pmatrix} \Delta t\mathcal{M}_{1/2}Y_d \\ 0 \\ -F_{s,b} \end{pmatrix}. \tag{2.84}$$

For semi-implicit scheme, by using similar argument to (2.32), we obtain the following optimality system:

$$\begin{pmatrix} \Delta t\mathcal{M}_{1/2} & 0 & -\tilde{E}_{s,b}^T \\ 0 & \alpha\Delta t\mathcal{M}_{1/2,b} & \Delta t \tilde{Z}_{s,b}^T \\ -\tilde{E}_{s,b} & \Delta t \tilde{Z}_{s,b} & 0 \end{pmatrix}\begin{pmatrix} Y \\ U \\ P \end{pmatrix} = \begin{pmatrix} \Delta t\mathcal{M}_{1/2}Y_d \\ 0 \\ -\tilde{F}_{s,b} \end{pmatrix}. \tag{2.85}$$

Here,

$$\tilde{F}_1^{s,b} = (M^s + \Delta t\epsilon K), \tilde{F}_0^{s,b} = (-M^s + \Delta t(\beta N + \sigma M + \gamma N_b + \tau(\beta^T\beta K + \sigma\beta N))), \tag{2.86}$$

$$\tilde{E}_{s,b} = \begin{pmatrix} \tilde{F}_1^{s,b} & 0 & 0 & 0 \\ \tilde{F}_0^{s,b} & \tilde{F}_1^{s,b} & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & \tilde{F}_0^{s,b} & \tilde{F}_1^{s,b} \end{pmatrix}, \tilde{Z}_{s,b} = \begin{pmatrix} N_b & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & N_b \end{pmatrix} \tag{2.87}$$

and

$$\tilde{F}_{s,b} = \begin{pmatrix} -\tilde{F}_0^{s,b}\mathbf{y}^0 + \Delta t f^s(t_1) \\ \vdots \\ \Delta t f^s(t_{N+1})) \end{pmatrix}. \tag{2.88}$$

2.3.3 Optimize-then-discretize approach

2.3.3.1 SUPG stabilized in space and time discretization

In this section, we give both of the space and time discretization. We don't need to the give details of the steps which are similar to the distributed case. In the OD approach, we discretize each equation in (2.70) to obtain an approximate solution of the boundary OCP. We use the SUPG method to get the following strongly consistent discretized adjoint equation

$$(-p_{h,t}, \psi_h) + \sum_{K\in\mathfrak{T}_h} \tau(-p_{h,t}, -\beta\cdot\nabla\psi_h)_K + \tilde{a}_h^a(\psi_h, p_h) = -\langle y_h - y_d, \psi_h\rangle_h^a, \quad \forall v_h \in V_h, \tag{2.89a}$$

where

$$\tilde{a}_h^a(\psi_h, p_h) = a_h^a(\psi_h, p_h) + \int_{\partial\Omega} \vec{n}\cdot(\gamma+\beta) yv ds, \tag{2.89b}$$

where a_h^a, $\langle y_h - y_d, \psi_h\rangle_h^a$ is defined in (2.45). The strongly consistent discretized gradient equation is obtained by discretization of the gradient equation (2.70b):

$$\tilde{b}(w_h, p_h) + \alpha\langle u_h, w_h\rangle_\Sigma = 0 \ \ \forall w_h \in U_h. \tag{2.89c}$$

The discretization of the state equation is same as (2.75c).
Then, by using Θ scheme, we have

$$\begin{pmatrix} \Delta t Z_{a,b} & 0 & E_{a,b}^T \\ 0 & \alpha\Delta t \mathcal{M}_{1/2,b} & -\Delta t Z^T \\ E_{s,b} & -\Delta t Z_{s,b} & 0 \end{pmatrix}\begin{pmatrix} Y \\ U \\ P \end{pmatrix} = \begin{pmatrix} \Delta t Z_{a,b} Y_d \\ 0 \\ F_{s,b} \end{pmatrix}, \tag{2.90}$$

where $E_{a,b}$ have the diagonal entries $F_1^{a,b} = (M^a + \Delta t\Theta\tilde{K}_b^a)$ and subdiagonal entries $F_0^{a,b} = (-M^a + \Delta t(1-\Theta)\tilde{K}_b^a)$ with $\tilde{K}_b^a = (\tilde{K}^a + (\gamma+\beta)N_b)$. Here, $Z_{a,b} = Z_a$ is given in (2.53), $E_{s,b}$, $Z_{s,b}$ are introduced in (2.82), $F_{s,b}$ defined in (2.83)
For the semi-implicit scheme, we have

$$\begin{pmatrix} \Delta t \tilde{Z}_{a,b} & 0 & \tilde{E}_{a,b}^T \\ 0 & \alpha\Delta t \mathcal{M}_{1/2,b} & -\Delta t Z^T \\ \tilde{E}_{s,b} & -\Delta t \tilde{Z}_{s,b} & 0 \end{pmatrix}\begin{pmatrix} Y \\ U \\ P \end{pmatrix} = \begin{pmatrix} \Delta t \tilde{Z}_{a,b} Y_d \\ 0 \\ \tilde{F}_{s,b} \end{pmatrix}, \tag{2.91}$$

where $\tilde{E}_{s,b}$, $\tilde{Z}_{s,b}$ are given in (2.87), $\tilde{F}_{s,b}$ given in (2.88). Here, $\tilde{Z}_{a,b} = \tilde{Z}_a$ is given in (2.58),$\tilde{E}_{a,b}$ have the diagonal entries $\tilde{F}_1^{a,b} = (M^a + \Delta t\epsilon K)$ and subdiagonal entries $\tilde{F}_0^{a,b} = (-M^a + \Delta t(-\beta N + \sigma M + (\gamma+\beta)N_b + \tau(\beta^T\beta K - \sigma\beta N)))$. where K is given in (2.19), M^a K^a, $\tilde{M}^a$ are given in (2.48) and τ is the stabilization parameter.

2.3.4 Control constrained problem

When we consider the boundary control problem (2.62) with control constraints (2.63), we follow the same way as we considered in the case of the distributed OCPs. We present the active set method introduced in the previous section. In this section, we give the optimality systems for DO and OD approach together.
For DO approach and the Θ scheme, we have the following optimality system:

$$\begin{pmatrix} \Delta t\mathcal{M}_{1/2} & 0 & -E^T_{s,b} \\ 0 & \alpha\Delta t\mathcal{M}_{1/2,b} & \Delta t\chi_{\tilde{I}}Z^T_{s,b} \\ -E_{s,b} & \Delta t Z_{s,b} & 0 \end{pmatrix}\begin{pmatrix} Y \\ U \\ P \end{pmatrix} = \begin{pmatrix} \Delta t\mathcal{M}_{1/2}Y_d \\ \alpha\Delta t\mathcal{M}_{1/2,b}(\chi_{\tilde{A}_-}\tilde{U}_a + \chi_{\tilde{A}_+}\tilde{U}_b) \\ -F_{s,b} \end{pmatrix}, \tag{2.92}$$

where $E_{s,b},\ Z_{s,b},\ F_{s,b}$ are as in (2.82) and (2.83). Moreover, $\mathcal{M}_{1/2,b}$ is defined in (2.79) for boundary OCPs.
By setting for boundary OCPs,

$$\begin{aligned} \tilde{A}_+ &= \{x \in \Sigma : -\alpha\Delta t\mathcal{M}_{1/2,b}\tilde{U}_a - \Delta t Z^T_{s,b}P < 0\} \\ \tilde{A}_- &= \{x \in \Sigma : -\alpha\Delta t\mathcal{M}_{1/2,b}\tilde{U}_b - \Delta t Z^T_{s,b}P > 0\} \\ \tilde{I} &= \Sigma\backslash(\tilde{A}_+ \cup \tilde{A}_-). \end{aligned}$$

with χ denotes the characteristic function of the given set.
Now, the optimality system for OD approach with semi-implicit scheme is following as:

$$\begin{pmatrix} \Delta t\tilde{Z}_{a,b} & 0 & \tilde{E}^T_{a,b} \\ 0 & \alpha\Delta t\mathcal{M}_{1/2,b} & -\Delta t\chi_{\tilde{I}}Z^T \\ \tilde{E}_{s,b} & -\Delta t\tilde{Z}_{s,b} & 0 \end{pmatrix}\begin{pmatrix} Y \\ U \\ P \end{pmatrix} = \begin{pmatrix} \Delta t\tilde{Z}_{a,b}Y_d \\ \alpha\Delta t\mathcal{M}_{1/2,b}(\chi_{\tilde{A}_-}\tilde{U}_a + \chi_{\tilde{A}_+}\tilde{U}_b) \\ \tilde{F}_{s,b} \end{pmatrix}, \tag{2.93}$$

where $\tilde{E}_{a,b},\ \tilde{Z}_{a,b},\ \tilde{F}_{a,b}$ are given (2.91).

In this chapter, we have the optimality systems for both OD and DO approaches. In both cases, we apply SUPG finite element method in space discretization, Θ scheme and semi-implicit scheme in time discretization. We can see that the optimality systems of these approaches lead to the different discrete solution. In the DO approach, we get the finite-dimensional optimization problem whereas, there is no finite-dimensional optimization problem in the DO approach. In the following Chapter 3, we follow the OD approach and the software Comsol Multiphsics is used to solve OCPS.

CHAPTER 3

OPTIMIZE-THEN-DISCRETIZE

In this chapter, we use the OD approach to solve the optimality system involving the state and the adjoint equations. In this approach, firstly 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. In this sense, we consider two strategies. One of these strategies is the classical approach of sequentially solving state and adjoint equations, the other is to interpret the time as an additional space dimension, i.e., to solve the whole optimality system in the space-time cylinder by finite elements. These two approaches for linear parabolic control problems are implemented in [61, 62, 63, 64] and for the optimal control of Burgers equation [91]. As in [14], we need to show that the optimality system of the parabolic PDE constraints are elliptic, i.e., they are equivalent to biharmonic equation which satisfy the condition of V-ellipticity. Then, we can solve this elliptic system by using the space time meshes, adaptive and nonadaptive solvers, e.t.c; also [42].

Actually, some software packages define the systems of PDEs symbolically, i.e., the equations are considered as differential operators instead of coefficients. Hence, predefined functions and operators are obtained by these packages. As in [65], in our computations, we use an integrated modeling and simulation environment COMSOL multiphysics, which provide us a few specialized programs build-in tools as adaptivity and multigrid solvers.

In Section 3.1, we are concerned with the distributed optimal control of convection dominated diffusion-convection-reaction equation with and without inequality constraints. Firstly, we show that the optimality system is equivalent to V-elliptic equation; in this sense we obtain the biharmonic equation. Then an iterative approach and the algorithm of the gradient method are introduced. Moreover the variational formulation of the optimality system and its stabilization is covered. In the end of the section, we give the implementation and numerical examples of these approaches. In Section 3.2, we obtain the biharmonic equation for the boundary optimal control of convection dominated diffusion-convection-reaction equation with and without inequality constraints. Moreover, we give the variational formulation of the optimality system and its stabilization. Finally, the implementation and numerical results are presented.

3.1 Distributed optimal control problem

In this section, we consider the distributed optimal control problem (OCP) (2.1) and its optimality system (2.2), (2.3). This optimality system is computed using one of the two approaches [61, 62, 63, 64].

- The *classical iterative approach*: the optimality system is solved iteratively using the gradient method. The control variable u is first initialized and the state equation and the adjoint equation is found for y forwards and p backwards until convergence, respectively

- The *one-shot approach*: the optimality system in the whole space-time cylinder is resolved as an elliptic (biharmonic) equation by considering the time as an additional space variable.

3.1.1 Transformation of the optimality system into elliptic pde: One shot approach

In this approach, we have to show how the time-dependent diffusion-convection-reaction equation can be interpreted as an elliptic (biharmonic) equation in the time and space variables. The time is defined as an additional space dimension. In this sense, we consider the space-time domain Q where space and time are treated in the same manner. The transformation of the optimality system with the state and the adjoint equation is described in detail in [63] for parabolic equations having only diffusion and reaction terms with Neumann boundary conditions. It was shown that the optimality system for parabolic optimal control problems is equivalent to a biharmonic $H_{2,1}$ elliptic pde. Linear parabolic problems without inequality constraints, with control and state constraints are solved using the one-shot approach in [61, 64]. This approach was then extended to the optimal control of Burgers equation in [91].

In the following, we will use this approach for distributed OCP problems with the diffusion-convection-reaction equation. The state equation (2.1b) is homogenized as in [63] by setting $\tilde{y} = y - y_d$, $\tilde{u} = u$:

$$\begin{aligned} \tilde{y}_t - \epsilon\Delta\tilde{y} + \beta\cdot\nabla\tilde{y} + \sigma\tilde{y} &= \tilde{u} - f - (\frac{d}{dt}y_d - \epsilon\Delta y_d + \beta\cdot\nabla y_d + \sigma y_d), \quad \text{in } Q, \\ \tilde{y} &= -y_d, \quad \text{on } \Sigma, \\ \tilde{y}(\cdot,0) &= y_0 - y_d(0), \quad \text{in } \Omega. \end{aligned} \tag{3.1}$$

We assume the existence of a function $\tilde{f}$ fulfilling the initial and boundary conditions of (3.1). After defining $y := \tilde{y} + \tilde{f}$ and renaming $u = \tilde{u}$, we obtain

$$\begin{aligned} y_t - \epsilon\Delta y + \beta\cdot\nabla y + \sigma y &= u - f - (\tfrac{d}{dt}y_d - \epsilon\Delta y_d + \beta\cdot\nabla y_d + \sigma y_d) \\ &+ \tfrac{d}{dt}\tilde{f} - \epsilon\Delta\tilde{f} + \beta\cdot\nabla\tilde{f} + \sigma\tilde{f}, \qquad \text{in } Q, \\ y &= 0, \qquad \text{on } \Sigma, \\ y(\cdot,0) &= 0, \qquad \text{in } \Omega. \end{aligned}$$

By resetting

$$f = -(\frac{d}{dt}y_d - \epsilon\Delta y_d + \beta\cdot\nabla y_d + \sigma y_d) - f + \frac{d}{dt}\tilde{f} - \epsilon\Delta\tilde{f} + \beta\cdot\nabla\tilde{f} + \sigma\tilde{f},$$

we obtain the homogenized state equation

$$\begin{aligned} y_t - \epsilon\Delta y + \beta\cdot\nabla y + \sigma y &= u + f, \quad \text{in } Q, \\ y &= 0, \quad \text{on } \Sigma, \\ y(0) &= 0 \quad \text{in } \Omega. \end{aligned} \tag{3.2}$$

Then the adjoint system becomes

$$\begin{aligned} -p_t - \epsilon\Delta p - \beta\cdot\nabla p + \sigma p &= y, \quad \text{in } Q, \\ p &= 0, \quad \text{on } \Sigma, \\ p(T) &= 0 \quad \text{in } \Omega. \end{aligned} \tag{3.3}$$

In [65], it was shown that the optimality system for the distributed control problem of parabolic type PDE equation can be transformed to a biharmonic elliptic pde. Also the existence, uniqueness and regularity of the state equation is given in [65]. In the same manner, we will show that the optimality system (3.2), (3.3) is equivalent to an elliptic pde. For the weak formulations of the optimality systems, we give the following definitions of Hilbert spaces which are also used in [65].

Definition 3.1.1 *The set*

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

is a Hilbert space with the inner product

$$(y_1,y_2)_{H^{2,1}(Q)} := \int\int_Q y_1y_2 + \frac{d}{dt}y_1\frac{d}{dt}y_2 + \nabla y_1\nabla y_2 + \sum_{i,j=1}^{N}\left(\frac{\partial^2 y_1}{\partial x_i\partial x_j}\frac{\partial^2 y_2}{\partial x_i\partial x_j}\right)dxdt,$$

and the natural norm

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

For the distributed OCP with the homogenous Dirichlet boundary conditions, now we introduce another Hilbert space.

Definition 3.1.2 *The set*

$$\bar{H}^{2,1}(Q) := \left\{y \in H^{2,1}(Q) : y = 0 \; on \; \Gamma \; and \; y(T) = 0\right\}$$

is a closed subspace of $H^{2,1}(Q)$ *and it is also a Hilbert space with the inner product*

$$(y_1,y_2)_{\bar{H}^{2,1}(Q)} := \int\int_Q\left(y_1y_2 + \frac{\partial y_1}{\partial t}\frac{\partial y_2}{\partial t} + \nabla y_1\nabla y_2 + \Delta y_1\Delta y_2\right)dxdt$$

and the natural norm

$$||y||_{\bar{H}^{2,1}(Q)} = \left(||y||^2 + \left\|\frac{\partial y}{\partial t}\right\|^2 + ||\nabla y||^2 + ||\Delta y||^2\right)^{1/2}.$$

We note that for $u \in H^{2,1}(Q)$ the functions $u(0) := u(0,\cdot)$, $u(T) := u(T,\cdot)$ both are well defined in $L^2(Q)$, because $H^1(I)$ is continuously embedded in $C(I)$.

Theorem 3.1.3 *Let* (u,y,p) *be smooth function of the control problem (3.2)-(3.3) with* $y,p \in \bar{H}^{2,1}(Q)$ *and* $u \in L^2(0,T)$. *Then p satisfies the following pde*

$$-p_{tt} + \epsilon^2\Delta^2 p - (2\sigma\epsilon + \beta^T\beta)\Delta p - 2\beta\cdot\frac{d}{dt}(\nabla p) + (\sigma^2 + \frac{1}{\alpha})p = f, in \; Q, \tag{3.4a}$$

with the boundary conditions

$$-\epsilon\Delta p - \beta\cdot\nabla p = 0, on \; \Sigma, \tag{3.4b}$$

$$p = 0, \; on \; \Sigma, \tag{3.4c}$$

$$-p_t(\cdot,0) - \epsilon\Delta p(\cdot,0) - \beta\cdot\nabla p(\cdot,0) + \sigma p(\cdot,0) = 0, in \; \Omega, \tag{3.4d}$$

$$p(\cdot,T) = 0, in \; \Omega. \tag{3.4e}$$

Proof. We follow the procedure in [63]. Let us assume that all functions are smooth enough for the following operations.
Taking derivative of $-p_t - \epsilon\Delta p - \beta\cdot\nabla p + \sigma p = y$ with respect to t gives

$$-\frac{d^2}{dt^2}p - \epsilon\frac{d}{dt}\Delta p - \beta\cdot\frac{d}{dt}(\nabla p)_t + \sigma\frac{d}{dt}p = \frac{d}{dt}t.$$

Now replacing y_t into state equation

$$-\frac{d^2}{dt^2}p - \epsilon\frac{d}{dt}\Delta p - \beta\cdot\frac{d}{dt}(\nabla p)_t + \sigma\frac{d}{dt}p - \epsilon\Delta y + \beta\cdot\nabla y + \sigma y = -\frac{1}{\alpha}p + f.$$

We use again the adjoint equation to replace y in the above equation

$$\begin{aligned} - \quad & \frac{d^2}{dt^2}p - \epsilon\frac{d}{dt}\Delta p - \beta\cdot\frac{d}{dt}(\nabla p)_t + \sigma\frac{d}{dt}p - \epsilon\Delta(-p_t - \epsilon\Delta p - \beta\cdot\nabla p + \sigma p) \\ + \quad & \beta\cdot\nabla(-p_t - \epsilon\Delta p - \beta\cdot\nabla p + \sigma p) + \sigma(-p_t - \epsilon\Delta p - \beta\cdot\nabla p + \sigma p) = -\frac{1}{\alpha}p + f. \end{aligned}$$

Rearranging the equation above, we obtain

$$-p_{tt} + \epsilon^2\Delta^2 p - (2\sigma\epsilon + \beta^T\beta)\Delta p - 2\beta\cdot\frac{d}{dt}(\nabla p) + (\sigma^2 + \frac{1}{\alpha})p = f,$$

where all third-order and first-order terms of p disappear. Then we evaluate $y = -p_t - \epsilon\Delta p - \beta\cdot\nabla p + \sigma p$ on the boundary and obtain the boundary conditions (3.4b) and (3.4c) which are the original homogenous Dirichlet boundary condition of adjoint equation. And we get the last two conditions (3.4d) and (3.4e) by evaluating $p(\cdot, T) = 0$ and $y(0) = 0$. By the same technique, we can derive analogous equations for y and u. ∎

We continue with the bilinear form and give the ellipticity and boundness of the bilinear form.

Lemma 3.1.4 *The solution p of the equation (3.4) satisfies the non-symmetric bilinear form*

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

where

$$\begin{aligned} \boldsymbol{a}[p, w] \quad = \quad & \iint_Q \frac{d}{dt}p\frac{d}{dt}w + \epsilon^2\Delta p\Delta w + (2\sigma\epsilon + \beta^T\beta)\nabla p\nabla w + 2\beta\cdot(\nabla p)\frac{d}{dt}w + (\sigma^2 + \frac{1}{\alpha})pw\, dxdt \\ + \quad & \int_\Omega \epsilon\nabla p(x,0)\nabla w(x,0) + \beta\cdot\nabla p(x,0)w(x,0) + \sigma p(x,0)w(x,0)\, dx \\ + \quad & \iint_\Sigma \epsilon\beta\cdot\vec{n}\cdot\nabla p\nabla w\, dsdt. \end{aligned} \tag{3.5}$$

Proof. Let us test (3.4a) by a function from $w \in \bar{H}^{2,1}(Q)$ such that

$$-\iint_Q -p_{tt}w + \epsilon^2\Delta^2 pw - (2\sigma\epsilon + \beta^T\beta)\Delta pw - 2\beta\cdot\frac{d}{dt}(\nabla p)w + (\sigma^2 + \frac{1}{\alpha})pw = \iint_Q fwdxdt.$$

Integration by parts yields

$\iint_Q -p_{tt}w + \epsilon^2\Delta^2 pw - (2\sigma\epsilon + \beta^T\beta)\Delta pw - 2\beta\cdot\frac{d}{dt}(\nabla p)w + (\sigma^2 + \frac{1}{\alpha})pw$

$= \iint_Q \frac{d}{dt}p\frac{d}{dt}w + \epsilon^2\Delta p\Delta w + (2\sigma\epsilon + \beta^T\beta)\nabla p\nabla w + 2\beta\cdot(\nabla p)\frac{d}{dt}w\, dxdt$

$+ \iint_Q(\sigma^2 + \frac{1}{\alpha})pwdxdt - \int_\Omega \frac{d}{dt}pw|_0^T dx - \int_\Omega 2\beta\cdot\nabla pw|_0^T dx + \iint_Q(2\sigma\epsilon + \beta^T\beta)\nabla p\nabla wdxdt$

$-\iint_\Sigma (2\sigma\epsilon + \beta^T\beta)\vec{n}\cdot\nabla p w ds dt - \epsilon^2 \iint_\Sigma \vec{n}\cdot(\nabla(\Delta p))w ds dt + \vec{n}\cdot((\Delta p)\nabla w) ds dt.$

The integrals

$$\iint_\Sigma (2\sigma\epsilon + \beta^T\beta)\vec{n}\cdot\nabla p w ds dt = 0$$

and

$$\epsilon^2 \iint_\Sigma \vec{n}\cdot(\nabla(\Delta p))w ds dt = 0$$

vanish on the boundary Σ because $w = 0$ for all $w \in \bar{H}^{2,1}(Q)$.

Using the boundary condition (3.4b) we get
$-\epsilon^2 \iint_\Sigma \vec{n}\cdot((\Delta p)\nabla w) ds dt = \iint_\Sigma \epsilon\beta\cdot\vec{n}\cdot\nabla p\nabla w \, ds dt,$

After integrating by parts of (3.4d), and $w(x,T) = 0$, we obtain

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

$-\int_\Omega 2\beta\cdot\nabla pw|_0^T dx = \int_\Omega 2\beta\cdot\nabla p(x,0)w(x,0)dx.$

The right-hand side

$$\iint_Q fw =: F(w)$$

is a functional from $(\bar{H}^{2,1}(Q))^*$. ■

Lemma 3.1.5 *The bilinear form (3.5) is $\bar{H}^{2,1}$-elliptic, i.e., there is a constant $c > 0$ such that*

$$\boldsymbol{a}[v,v] \geq c\|v\|^2_{\bar{H}^{2,1}(Q)}$$

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

Proof. We choose $v \in \bar{H}^{2,1}(Q)$ and estimate $\mathbf{a}[v,v]$:

$$\begin{aligned} \mathbf{a}[v,v] &= \iint_Q (\frac{d}{dt}v)^2 + \epsilon^2(\Delta v)^2 + (2\sigma\epsilon + \beta^T\beta)(\nabla v)^2 + 2\beta\cdot(\nabla v)\frac{d}{dt}v + (\sigma^2 + \frac{1}{\alpha})v^2 \, dxdt \\ &+ \int_\Omega \epsilon(\nabla v(x,0))^2 + \beta\cdot\nabla v(x,0)v(x,0) + \sigma(v(x,0))^2 \, dx + \iint_\Sigma \epsilon\beta\cdot\vec{n}\cdot(\nabla v)^2 \, ds dt \end{aligned}$$

Let us note that $\epsilon > 0,\ \beta < 0,\ \sigma > 0, \iint_\Sigma \epsilon\beta\cdot\vec{n}\cdot(\nabla v)^2 \, ds dt \geq 0$. Since β is divergence free, we get $\int_\Omega \beta\cdot\nabla v(x,0)v(x,0) = -\int_\Omega div\beta \, v(x,0)^2 = 0$. For the ellipticity, we assume

$$\iint_Q 2\beta\cdot(\nabla v)\frac{d}{dt}v \geq 0.$$

By using these assumptions, we have

$$\begin{aligned} \mathbf{a}[v,v] &= \geq \min\left\{1, \epsilon^2, (2\sigma\epsilon + \beta^T\beta), (\sigma^2 + \frac{1}{\alpha})\right\} \iint_Q (\frac{d}{dt}v)^2 + (\Delta v)^2 + (\nabla v)^2 + v^2 \, dxdt \\ &= c\|v\|^2_{\bar{H}^{2,1}(Q)} \\ &\geq c\|v\|^2_{H^{2,1}(Q)}. \end{aligned}$$

■

Lemma 3.1.6 *The bilinear form $a[v, w]$ is bounded in $\bar{H}^{2,1}(Q)$, i.e.,*

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

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

Proof. Let $c > 0$ be a generic constant. We have by $v, w \in H^{2,1}(Q)$

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

In the same way, we obtain

$$\beta(\nabla p(x,0), w(x,0))_{L^2(\Omega)} \leq c\,\|p\|_{H^{2,1}(Q)}\,\|w\|_{H^{2,1}(Q)}\,,$$

$$\sigma(p(x,0), w(x,0))_{L^2(\Omega)} \leq c\,\|p\|_{H^{2,1}(Q)}\,\|w\|_{H^{2,1}(Q)}\,,$$

Using the inner product in $H^{2,1}(Q)$, $\|w_t\|_{L^2(Q)}$ can be bounded, so that

$$2\beta(\nabla p, w_t)_{L^2(Q)} \leq c\,\|\nabla p\|_{L^2(Q)}\,\|w_t\|_{L^2(Q)} \leq c\,\|p\|_{H^{2,1}(Q)}\,\|w\|_{H^{2,1}(Q)}\,.$$

and we receive

$$\epsilon\beta(\vec{n}\cdot\nabla p, \nabla w)_{L^2(\Sigma)} \leq c\,\|\nabla p\|_{L^2(Q)}\,\|\nabla w\|_{L^2(Q)} \leq c\,\|p\|_{H^{2,1}(Q)}\,\|w\|_{H^{2,1}(Q)}\,.$$

After all these preparations, we can show that the bilinear form is bounded

$$\begin{aligned} |\mathbf{a}[p, w]| &\leq \left|\int\int_Q \frac{d}{dt}p\frac{d}{dt}w + \epsilon^2\Delta p\Delta w + (2\sigma\epsilon + \beta^T\beta)\nabla p\nabla w + 2\beta\cdot(\nabla p)\frac{d}{dt}w + (\sigma^2 + \frac{1}{\alpha})pw\,dxdt\right| \\ &+ \left|\int_\Omega \epsilon\nabla p(x,0)\nabla w(x,0) + \beta\cdot\nabla p(x,0)w(x,0) + \sigma p(x,0)w(x,0)dx\right| \\ &+ \left|\int\int_\Sigma \epsilon\beta\cdot\vec{n}\cdot\nabla p\nabla w\,dsdt\right| \\ &\leq \left|\epsilon(\nabla p(x,0), \nabla w(x,0))_{L^2(\Omega)}\right| + \left|\beta(\nabla p(x,0), w(x,0))_{L^2(\Omega)}\right| + \left|\sigma(p(x,0), w(x,0))_{L^2(\Omega)}\right| \\ &+ \left|\int\int_\Sigma \epsilon\beta\cdot\vec{n}\cdot\nabla p\nabla w\,dsdt\right| + \max\left\{1, \epsilon^2, (2\sigma\epsilon + \beta^T\beta), (\sigma^2 + \frac{1}{\alpha})\right\}\left|(v, w)_{\hat{H}^{2,1}(Q)}\right| \\ &\leq c_Q\,\|p\|_{H^{2,1}(Q)}\,\|w\|_{H^{2,1}(Q)} + c_{max}\,\|p\|_{\hat{H}^{2,1}(Q)}\,\|w\|_{\hat{H}^{2,1}(Q)} \\ &\leq c\,\|p\|_{H^{2,1}(Q)}\,\|w\|_{H^{2,1}(Q)}\,. \end{aligned}$$

■ Using the Lemma 3.1.5, Lemma 3.1.6 and the Lax-Milgram Theorem [51] we can state the Main Theorem:

Theorem 3.1.7 *For all $F \in (\bar{H}^{2,1}(Q))^*$ the bilinear equation*

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

has a unique solution $p \in \bar{H}^{2,1}(Q)$. There is a constant $c > 0$ such that

$$\|p\|_{H^{2,1}(Q)} \leq c\,\|F\|_{\bar{H}^{2,1}(Q)^*}$$

We consider now the regularization of inequality constrained OCP. After the non-differentiable optimality system is described in terms of projections, we introduce a regularized projection formula and prove convergence of the solutions following the approach in [62].

Definition 3.1.8 *Let a,b,z $\in \mathbb{R}$ be given real numbers. We define the projection*

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

Let use state the following helpful properties of the projection given in [65], without proof

Lemma 3.1.9 *The projection $\mathbb{P}_{[a,b]}\{z\}$ satisfies*

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

(ii) $\mathbb{P}_{[a,b]}\{z\}$ *is strongly monotone increasing:*
by $z_1 < z_2$ *follows* $\mathbb{P}_{[a,b]}\{z_1\} \le \mathbb{P}_{[a,b]}\{z_2\}$*, and* $\mathbb{P}_{[a,b]}\{z_1\} = \mathbb{P}_{[a,b]}\{z_2\}$ *iff* $z_1 = z_2$,

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

Now we consider the homogenized version of the inequality constrained problem which has the state equation (3.2), the adjoint equation (3.3) and from variational equality

$$u^* = \mathbb{P}_{[u_a,u_b]}\{-\frac{1}{\alpha}p\}.$$

Similar to Theorem 3.1.3, we find the biharmonic equation

$$\begin{aligned}
-p_{tt} + \epsilon^2\Delta^2 p - (2\sigma\epsilon + \beta^T\beta)\Delta p - 2\beta \cdot \tfrac{d}{dt}(\nabla p) + \sigma^2 p - \mathbb{P}_{[u_a,u_b]}\{-\tfrac{1}{\alpha}p\} &= f, && \text{in } Q,\\
-\epsilon\Delta p - \beta\cdot\nabla p &= 0, && \text{on } \Sigma,\\
p &= 0, && \text{on } \Sigma,\\
-p_t - \epsilon\Delta p - \beta\cdot\nabla p + \sigma p &= 0, && \text{in } \Omega_0,\\
p(\cdot,T) &= 0 && \text{in } \Omega_T.
\end{aligned} \tag{3.6}$$

We identify $-\mathbb{P}_{[u_a,u_b]}\{-\frac{1}{\alpha}\}v(\cdot\}$ with an element from $\bar{H}^{2,1}(Q)^*$. By the same technique as in Lemma 3.1.4, we can show that equation (3.6) can be written in weak formulation as follows.

Corollary 3.1.10 *We define the operators as* $A = A_1 + A_2$*, where*

$$\langle A_1 v, w\rangle = a[v,w], \quad \langle A_2 v, w\rangle = \iint_Q \mathbb{P}_{[u_a,u_b]}\{-\frac{1}{\alpha}v(x,t)\}w(x,t)dxdt.$$

Then, biharmonic form (3.6) is equivalent to

$$Ap = F,$$

where $F \in (\bar{H}^{2,1}(Q)^*)$.

Lemma 3.1.11 *The operator A defined in Corollary 3.1.10 is strongly monotone, coercive, and hemicontinuous.*

Proof. We make use the results of Lemma 3.1.4 and Lemma 3.1.5. Let us first show that A is strongly monotone. From Lemma 3.1.5 we have

$$\langle A_1(v_1 - v_2), v_1 - v_2 \rangle = a[v_1 - v_2, v_1 - v_2] \geq c \, \|v\|^2_{H^{1,2}(Q)} .$$

By monotonicity of $\mathbb{P}_{[u_a,u_b]}\{v\}$ in v we have $(\mathbb{P}_{[-u_b,-u_a]}\{\frac{1}{\alpha}v_1\} - \mathbb{P}_{[-u_b,-u_a]}\{\frac{1}{\alpha}v_2\})(v_1 - v_2) \geq 0$ for all v_1, v_2 and all (x, t), hence,

$$\iint_Q (\mathbb{P}_{[-u_b,-u_a]}\{\frac{1}{\alpha}v_1(x,t)\} - \mathbb{P}_{[-u_b,-u_a]}\{\frac{1}{\alpha}v_2(x,t)\})(v_1(x,t) - v_2(x,t))dxdt \geq 0.$$

We have to estimate $\langle A_2 v, v\rangle$ to prove the coercivity. First we observe that

$$\mathbb{P}_{[-u_b,-u_a]}\{v\}v = \begin{cases} -u_a v, & \text{on } Q_a := \{x,t \in Q \; v > -u_a\} \\ -u_b v, & \text{on } Q_b := \{x,t \in Q \; v < -u_b\} \\ v^2 \text{ on } Q\backslash\{Q_a \cup Q_b\}. \end{cases}$$

Hence,

$$\begin{aligned}
\iint_Q \quad & (\mathbb{P}_{[-u_b,-u_a]}\{\frac{1}{\alpha}v(x,t)\}v(x,t)dxdt = \iint_{Q_a} (\mathbb{P}_{[-u_b,-u_a]}\{\frac{1}{\alpha}v(x,t)\}v(x,t)dxdt \\
+ \iint_{Q_b} \quad & (\mathbb{P}_{[-u_b,-u_a]}\{\frac{1}{\alpha}v(x,t)\}v(x,t)dxdt + \iint_{Q\backslash Q_a \cup Q_b} (\mathbb{P}_{[-u_b,-u_a]}\{\frac{1}{\alpha}v(x,t)\}v(x,t)dxdt \\
= \quad & - \iint_{Q_a} u_a(x,t)v(x,t)dxdt - \iint_{Q_b} u_b(x,t)v(x,t)dxdt + \iint_{Q\backslash Q_a \cup Q_b} v^2(x,t)dxdt \\
\geq \quad & - \iint_{Q_a} u_a(x,t)v(x,t)dxdt - \iint_{Q_b} u_b(x,t)v(x,t)dxdt
\end{aligned}$$

for all $v \in H^{2,1}(Q)$. By the Lemma 3.1.5 we have

$$\begin{aligned}
&\langle Av, v\rangle = \langle A_1 v, v\rangle + \langle A_2 v, v\rangle \\
&= a[v, v] + \textstyle\iint_Q (\mathbb{P}_{[-u_b,-u_a]}\{\frac{1}{\alpha}v(x,t)\}v(x,t)dxdt \\
&\geq c \, \|v\|_{H^{2,1}(Q)} - \textstyle\iint_{Q_a} u_a(x,t)v(x,t)dxdt - \iint_{Q_b} u_b(x,t)v(x,t)dxdt \\
&= c \, \|v\|_{H^{2,1}(Q)} - \|u_a v\|_{L^1(Q_a)} - \|u_b v\|_{L^2(Q_b)} \\
&\geq c \, \|v\|_{H^{2,1}(Q)} - \|u_a\|_{L^2(Q_a)} \|v\|_{L^2(Q_a)} - \|u_b\|_{L^2(Q_b)} \|v\|_{L^2(Q_b)} \\
&\geq c \, \|v\|_{H^{2,1}(Q)} - (\|u_a\|_{L^2(Q_a)} + \|u_b\|_{L^2(Q_b)}) \|v\|_{L^2(Q)} \\
&\geq c \, \|v\|_{H^{2,1}(Q)} - (\|u_a\|_{L^2(Q_a)} + \|u_b\|_{L^2(Q_b)}) \|v\|_{H^{2,1}(Q)},
\end{aligned}$$

which results in

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

with $c_{a,b} = \|u_a\|_{L^2(Q_a)} + \|u_b\|_{L^2(Q_b)}$.

Therefore we obtain

$$\frac{\langle Av, v\rangle}{\|v\|_{H^{2,1}(Q)}} \to \infty \quad \text{if } \|v\|_{H^{2,1}(Q)} \to \infty.$$

It remains to be validated that A is hemi-continuous. By linearity, A_1 is hemi-continuous. We have to show that $\phi(s) = \langle A(v + sw), u\rangle$ is continuous on $[0, 1]$ for all $u, v, w \in H^{2,1}(Q)$. By $\langle A(v + tw), u\rangle = \iint_Q \mathbb{P}_{[u_a,u_b]}\{v(x,t) + sw(x,t)\}u(x,t)dxdt$ and by the continuity of the projection, this follows immediately; hence $A = A_1 + A_2$ is hemi-continuous. Now we are able to use the Main Theorem to show the existence of a unique solution of (3.6). ■

Theorem 3.1.12 *The biharmonic equation (3.6) has a unique solution $p \in \bar{H}^{2,1}(Q)$ for all $F \in (\bar{H}^{2,1}(Q))^*$.*

Proof. This follows by applying Theorem 4.1 in [83] to

$$Ap = F,$$

where A is defined in Corollary 3.1.10. ■

3.1.2 Iterative approach

In this approach, we solved optimality system iteratively and we mention about the gradient method which is used as an iterative method for solving optimal control problems iteratively. We can define the solution operator $G : L^2(Q) \to H$. With the help of the solution operator G, we can express $y = y(u)$ and eliminate y from the objective function. For minimizing the functional $J(G(u), u)$ by the gradient method which is described in [61], we have to evaluate the derivative

$$\begin{aligned}\left\langle \frac{d}{du} J(G(u), u), h \right\rangle &= \langle G(u) - y_d, Gh \rangle + k \langle u, h \rangle \\ &= \langle G^*(G(u) - y_d), h \rangle + k \langle u, h \rangle,\end{aligned}$$

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

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

Finally, $p := G^*(G(u) - y_d) = G^*(y - y_d)$ is the adjoint state.

By using the algorithm of gradient method defined in [63], we provide a mathematically correct formulation of the optimality conditions

3.1.3 Variational formulation of the optimality system and its stabilization

For convection dominated problems standard finite element discretization applied to the equation (2.1b) lead to strongly oscillatating solution unless the mesh size h is sufficiently small with respect to the ratio between ϵ and $\|\beta\|$. There are several methods known to improve the approximation properties of the pure Galerkin discretization and to reduce the oscillatory behavior; see, e.g., [4, 84]. The *Streamline Diffusion Stabilization Technique* (SUPG) stabilizes oscillations and instabilities due to the numerical method. The SUPG is an example of a Petrov-Galerkin method, where the test-function space differs from the solution space. The modified test functions give rise to additional terms in the weak formulation of the problem. The contribution of streamline-diffusion to the diffusion-convection-reaction equation is given by

$$\tau(\beta \cdot \nabla \hat{y})(-\epsilon \Delta y + \beta \cdot \nabla y + \sigma y - f - u),$$

where the 'hat' symbol denotes the corresponding test function.

There exist several approaches for the choice of the stabilization parameter [4, 21]. For the SUPG, the stabilization parameter τ is chosen as

$$\tau = \begin{cases} c \ \frac{h}{\|\beta\|}, & \text{if} \quad Pe \geq 1, \\ 0, & \text{otherwise,} \end{cases} \tag{3.7}$$

where $c \in (0, 1)$ and with the Peclet number $Pe = \frac{h\|\beta\|}{\epsilon}$. The Peclet number measures the relative importance of the convective effects compared to the diffusive effects. Here $Pe >> 1$ indicates that the convective effects dominate over the diffusive effects. In this section, we took $c = 0.1$ for numerical computations.

In COMSOL Multiphysics, when the state and adjoint equation are solved by the gradient method iteratively, the diffusion-convection-reaction equations are discretized in time by the backward Euler method. This will result in the following discrete equations [30]:

$$\begin{aligned} (y^h_{n+1}, v^h) + \Delta t(\epsilon(\nabla y_{n+1}, \nabla v^h) + (\beta \cdot \nabla y_{n+1} + \sigma y_{n+1}, v^h)) &= (y_n, v^h) + \Delta t(f_{n+1} + u_{n+1}, v^h)), \\ & \qquad (n = 0, 1, ..., N), \\ -p_{n-1} + \Delta t(\epsilon(\nabla p_{n-1}, v^h) - (\beta \cdot \nabla p_{n-1} + \sigma p_{n-1}, v^h)) &= p_n + \Delta t((y_n - y_d), v^h)), \\ & \qquad (n = N, N-1, ..., 1). \end{aligned}$$

The SUPG method consists of adding consistent diffusion terms in the state and adjoint equations with the parameter τ_k depending on the mesh cells:

$$\begin{aligned} (y^h_{n+1}, v^h) &+ \Delta t[\epsilon(\nabla y_{n+1}, \nabla v^h) + (\beta \cdot \nabla y_{n+1} + \sigma y_{n+1}, v^h)] \\ &+ \Delta t \sum_{K \in \Omega_h} \tau_K(-\epsilon \Delta y_{n+1} + \beta \cdot \nabla y_{n+1} + \sigma y_{n+1}, \beta \cdot \nabla v^h)_K \\ &= (y_n, v^h) + \Delta t \sum_{K \in \Omega_h} \tau_K(-\epsilon \Delta y_n + \beta \cdot \nabla y_n + \sigma y_n, \beta \cdot \nabla v^h)_K \\ &+ \Delta t(f_{n+1} + u_{n+1}, v^h)) + \Delta t \sum_{K \in \Omega_h} \tau_K((f_{n+1} + u_{n+1}), \beta \cdot \nabla v^h)_K \\ & \qquad (n = 0, 1, ..., N), \end{aligned}$$

$$\begin{aligned} -(p^h_{n-1}, v^h) &+ \Delta t[\epsilon(\nabla p_{n-1}, \nabla v^h) - (\beta \cdot \nabla p_{n-1} + \sigma p_{n-1}, v^h)] \\ &+ \Delta t \sum_{K \in \Omega_h} \tau_K(-\epsilon \Delta p_{n-1} - \beta \cdot \nabla p_{n-1} + \sigma p_{n-1}, \beta \cdot \nabla v^h)_K \\ &= (p_n, v^h) + \Delta t \sum_{K \in \Omega_h} \tau_K(-\epsilon \Delta p_n - \beta \cdot \nabla p_n + \sigma p_n, \beta \cdot \nabla v^h)_K \\ &+ \Delta t((y_n - y_d), v^h)) + \Delta t \sum_{K \in \Omega_h} \tau_K((y_n - y_d), \beta \cdot \nabla v^h)_K, \\ & \qquad (n = N, N-1, ..., 1). \end{aligned}$$

3.1.4 Implementation and Numerical Examples

In this section, we will provide the details of the implementation of numerical realization of the one-shot method in COMSOL Multiphysics for time-dependent convection dominated OCPs. We consider unconstrained and control constrained OCPs for the diffusion-convection-reaction equation in one space dimension by comparing the numerical results for the one-shot approach and the classical gradient method with stabilized and unstabilized solutions. We illustrate the applicability of the one-shot approach using COMSOL Multiphysics for a convection dominated problem in two space dimensions.

Example 3.1.1 (one-dimensional unconstrained problem):

We consider the equation (1) with $\epsilon = 10^{-5}, \beta = -1,\ \sigma = 1,\ \alpha = 0.01$ and with the constant forcing term $f = 1$. The desired state $y_d(x,t) = y_0(\cdot, 0)$ is

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

There exists two different solvers in COMSOL Multiphysics; **adaption**, which solves the elliptic pde using adaptive mesh refinement, and the **femnlin** without adaptation. 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. The subindex h indicates the computed state and control variables with step sizes h. SUPG is implemented in COMSOL Multiphysics for the adaptive and non-adaptive solvers as

```
fem.equ.weak={{'-h*(yx_test)/10*(yx+y-1-u)'
              '-h*(px_test)/10*(px+p-y+yd(x,time))' }};
```

The exact solution of the optimal control problem above is not known. Therefore, the evolution of the values of the cost function $\|J(y_h, u_h)\|$ is shown for a sequence of uniformly refined meshes tending to zero. The numerical results for the nonadaptive and adaptive elliptic solvers with and without the stabilization are given in Table 3.1 and in Figure 3.1 for $h = 2^{-3}\sqrt{2}$. Figure 3.1 shows that the

Table 3.1: One-shot approach for the unconstrained control problem

$h/\sqrt{2}$	non-adaptive solver $\|J(y_h,u_h)\|_Q$ without stabilization	$\|J(y_h,u_h)\|_Q$ with stabilization	adaptive solver $\|J(y_h,u_h)\|_Q$ without stabilization	$\|J(y_h,u_h)\|_Q$ with stabilization
2^{-2}	0.0559	0.0621	0.0703	0.0470
2^{-3}	0.0778	0.0525	0.1520	0.0442
2^{-4}	0.0978	0.0471	0.0906	0.0421
2^{-5}	0.0686	0.0448	0.0661	0.0418
2^{-6}	0.1400	0.0434	0.0422	0.0419
2^{-7}	0.0565	0.0428	out of memory	out of memory

stabilized problem has slight oscillatory solutions only in a thin region on boundary layer, whereas the unstabilized solutions exhibit strong oscillations in a larger region near the boundary layer.

An important feature of the solution of OCPs is the mesh-independence. Mesh-independence asserts that the convergence behavior of the iteration is the same for the discrete problem as for the infinite dimensional problem. The number of iterations to reach a specified tolerance is therefore independent of the mesh size. Mesh-independence of augmented Lagrangian-SQP methods for Burgers equation in [88] was proved and observed numerically. Similarly, the mesh-independence was confirmed for the one-shot approach for Burger's equation in [91]. Mesh-independence for OCP's with PDEs was also shown for the semi-smooth Newton method [44]. Different values of tolerances were used to stop the solver ***femnlin***. The relative tolerances were based on a weighted Euclidean norm for the estimated relative error. The iterations were stopped when the relative tolerance exceeded the relative error computed as the weighted Euclidean norm.

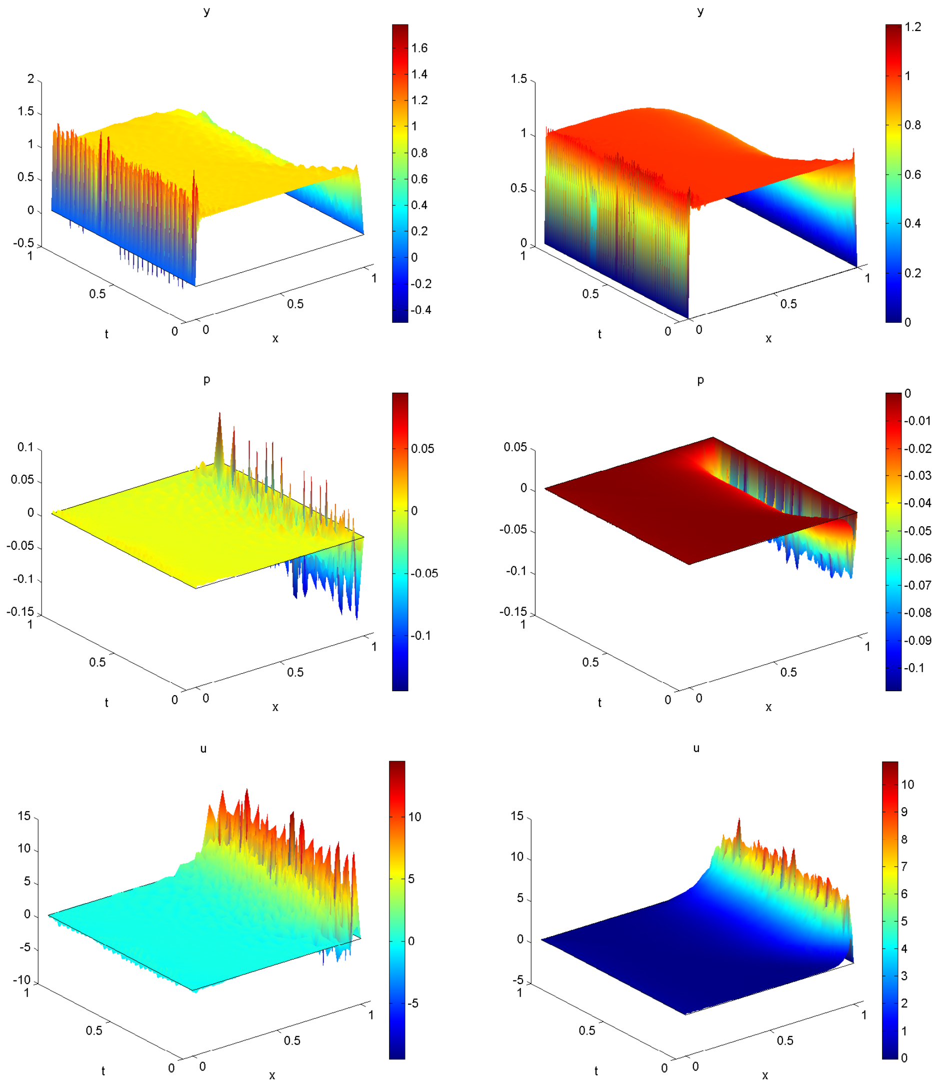


Figure 3.1: One-shot-approach for the unconstrained problem: unstabilized (left), stabilized (right), optimal state (top), optimal adjoint state (middle), optimal control (bottom)

Table 3.2: Mesh independence for the unconstrained problem

$h/\sqrt{2}$	2^{-3}	2^{-4}	2^{-5}	2^{-6}	2^{-7}
$tol = 1e^{-2}$	2	2	2	2	2
$tol = 1e^{-4}$	2	2	2	2	2
$tol = 1e^{-6}$	2	2	2	2	2
$tol = 1e^{-8}$	2	2	2	2	2
$tol = 1e^{-10}$	2	2	2	2	2

Table 3.3: Gradient method for the unconstrained problem

$h/\sqrt{2}$	$\|J(y_h, u_h)\|_Q$ without stabilization	# iterations	$\|J(y_h, u_h)\|_Q$ with stabilization	# iterations
2^{-2}	0.1227	29	0.1266	34
2^{-3}	0.0681	34	0.0702	82
2^{-4}	0.0535	80	0.0551	66
2^{-5}	0.0529	59	0.0480	112
2^{-6}	0.0578	27	0.0452	104
2^{-7}	0.0557	34	0.0438	104

The mesh-independence of the stabilized OCP is observed numerically for all mesh size and tolerances in Table 3.2. The optimality system (2.1b), (2.2)-(2.4) can be solved for the coupled systems of PDEs for each unknown separately by the gradient method in COMSOL Multiphysics. Here, in order to solve the state and adjoint equations by the gradient method iteratively, the diffusion-convection-reaction equations are discretized in time by the backward Euler method [30]. The SUPG method consists of adding consistent diffusion terms in the state and the adjoint equations with the parameter τ_k depending on the mesh cells (see [30]).

The time dependent pde solver to solve state y is

```
fem.sol =
femtime(fem,'solcomp',{'y'},'outcomp',{'y','p','u','uold'},...
                 'u',fem.sol,'tlist',[0,1]}
```

Similarly, the adjoint equation (2.2) and the gradient equations (2.3)-(2.4) are solved by redefining the boundary conditions and the coefficients for p and u.

The SUPG is implemented in the gradient method y and p as

```
fem.equ.weak={{'-h*(yx_test)/10*(yx+y-f-u)' '0' '0' '0'}  };
fem.equ.weak={{'0' '-h*(px_test)/10*(px+p-y+yd(x))' '0' '0' }  };
```

Stabilization requires in for the gradient method more iterations, but the cost function smaller than for the unstabilized solutions (see Table 3.3). The results obtained by the gradient method and by the one-shot approach without adaptation are similar to those given in Figure 3.1.

Table 3.4: One-shot approach for the control constrained problem

	femnlin		**adaption**	
$h/\sqrt{2}$	$\|\|J(y_h,u_h)\|\|_Q$ without stabilization	$\|\|J(y_h,u_h)\|\|_Q$ with stabilization	$\|\|J(y_h,u_h)\|\|_Q$ without stabilization	$\|\|J(y_h,u_h)\|\|_Q$ with stabilization
2^{-2}	0.0247	0.0109	0.0341	0.0117
2^{-3}	0.0330	0.0115	0.0332	0.0120
2^{-4}	0.0317	0.0118	0.0237	0.0122
2^{-5}	0.0281	0.0121	0.0183	0.0123
2^{-6}	0.0234	0.0122	0.0136	out of memory
2^{-7}	0.0179	0.0123	out of memory	out of memory

The control constraints are are handled by the projection method [62] which correspond to the implementation of the active set strategy as a semi-smooth Newton method [43]. It can be shown that complementary slackness conditions

$$\begin{aligned} (\mu_a^*, u_a - u^*)_{L_2(Q)} &= 0\ ,\ u^* \geq u_a\ ,\ \mu_a^* \geq 0, && \text{a.e., in Q,} \\ (\mu_b^*, u^* - u_b)_{L_2(Q)} &= 0\ ,\ u^* \leq u_b\ ,\ \mu_b^* \geq 0, && \text{a.e., in Q,} \end{aligned}$$

are equivalent to

$$\mu_a = \max(0, \mu_a - \mu_b + c(u_a - u)),\ \mu_b = \max(0, \mu_b - \mu_a + c(u - u_b))$$

for any $c > 0$. By choosing $c = \alpha$ and using the gradient equation $\alpha u^* + p + \mu_b - \mu_a = 0$, we obtain

$$\mu_a = \max(0, p + \alpha u_a), \mu_b = \max(0, -p - \alpha u_b), \qquad \text{a.e., in Q.}$$

Example 3.1.2 (one-dimensional control constrained problem):

The parameters of the differential equation (2.1b) and the forcing function are the same as in Example 3.1.1. We have the regularization parameter as $\alpha = 0.05$ and we consider unilateral control constraints with $u_a = 0$ and $u_b = 0.3$. The desired state is given as $y_d = y_0$ with the initial state $y_0(\cdot, 0) = -2x(x-1)$.

The numerical results of the one-shot approach are given in the Table 3.4 and in Figure 3.2 for $h = 2^{-3}\sqrt{2}$. Table 3.5 shows again the mesh-independence for the control constrained problem similar to the unconstrained case.

Example 3.1.3 (two-dimensional control constrained problem):

We consider equation (2.1b) with the parameters $\epsilon = 10^{-5}$, $\beta = (-1, -2)$, $\sigma = 1$, with the forcing function $f = 1$, the desired state $y_d = 1$, $\alpha = 0.1$, initial condition $y_0 = 0$ and with the bounds for the control constraints $u_a = 0.5, u_b = 10, T = 1$. The same was used in [4] as the test example for the stationary OCP problem for the diffusion-convection-reaction equation (2.1b).

SUPG is implemented in one-shot approach as

Table 3.5: Mesh independence for the control constrained problem

$h/\sqrt{2}$	2^{-3}	2^{-4}	2^{-5}	2^{-6}	2^{-7}
$tol = 1e^{-2}$	3	3	3	3	3
$tol = 1e^{-4}$	3	4	4	4	4
$tol = 1e^{-6}$	4	4	4	4	4
$tol = 1e^{-8}$	4	5	5	5	5
$tol = 1e^{-10}$	5	5	5	5	5

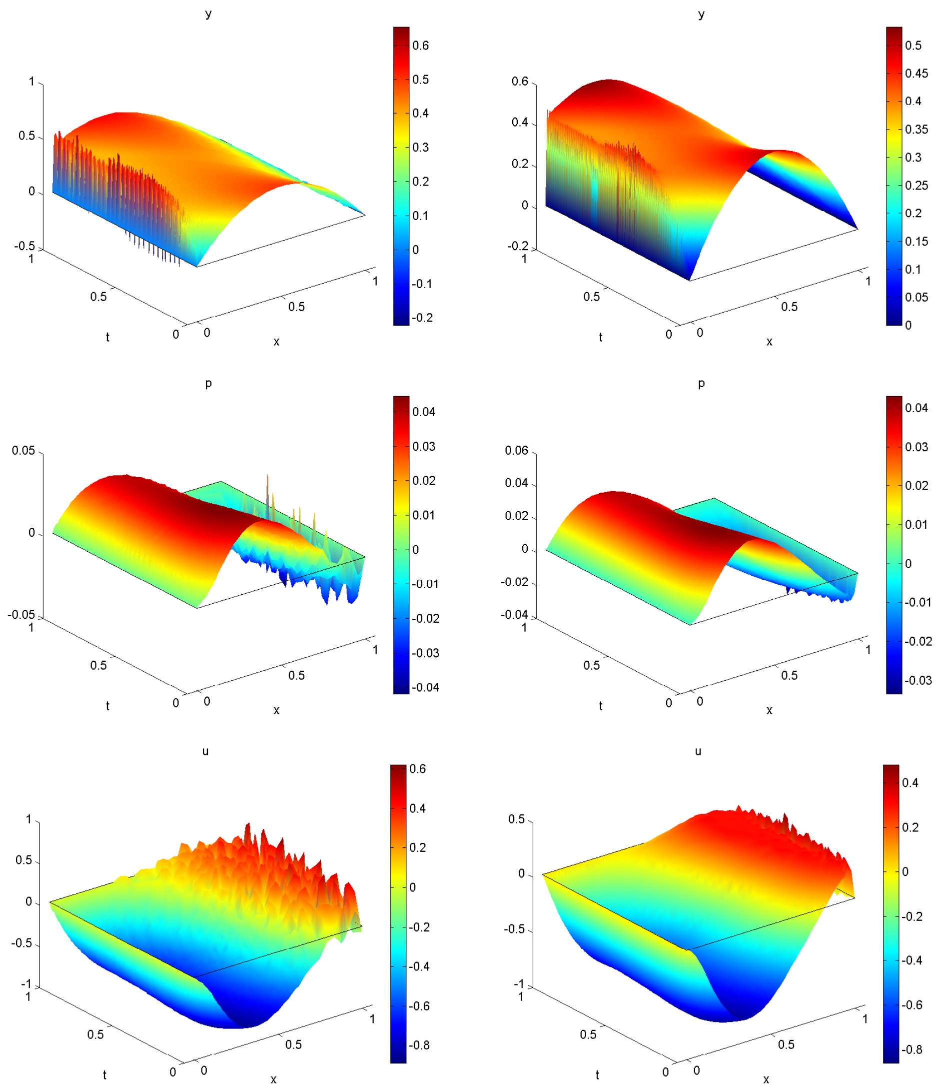


Figure 3.2: One-shot-approach for the control constrained problem: unstabilized (left), stabilized (right), optimal state (top), optimal adjoint state (middle), optimal control (bottom)

Table 3.6: Gradient method for the control constrained problem

$h/\sqrt{2}$	$\|J(y_h, u_h)\|_Q$ without stabilization	# iterations	$\|J(y_h, u_h)\|_Q$ with stabilization	# iterations
2^{-2}	0.0156	32	0.0115	26
2^{-3}	0.0178	14	0.0128	28
2^{-4}	0.0189	22	0.0135	28
2^{-5}	0.0204	31	0.0132	33
2^{-6}	0.0193	20	0.0129	32
2^{-7}	0.0200	24	0.0127	32

Table 3.7: One-shot approach for the 2D control constrained problem

	femnlin		**adaption**	
$h/\sqrt{2}$	$\|J(y_h, u_h)\|_Q$ without stabilization	$\|J(y_h, u_h)\|_Q$ with stabilization	$\|J(y_h, u_h)\|_Q$ without stabilization	$\|J(y_h, u_h)\|_Q$ with stabilization
2^{-1}	0.1802	0.3799	0.2683	0.3617
2^{-2}	0.3372	0.3487	0.3489	0.3245
2^{-3}	0.3206	0.3348	0.3317	0.3072

```
fem.equ.weak={{'-h*(yx1_test+yx2_test)/10*sqrt(5)*(yx1+yx2)'\\
'-h*(px1_test+px2_test)/10*sqrt(5)*(px1+px2)' '0' '0'}  };
```

for the gradient method

```
fem.equ.weak={{'-h*(yx1_test+yx2_test)/10*sqrt(5)*(yx1+yx2)' '0' '0'
'0' '0' '0'}  }; fem.equ.weak={{'0'
'-h*(px1_test+px2_test)/10*sqrt(5)*(px1+px2)' '0' '0' '0' '0'}  };
```

In Table 3.8, we compute the values of the cost function $\|J(y_h, u_h)\|$ and the convergence of the gradient method controlled by the difference of the current value of J and the average of the last and first values of J as in [61]. Moreover the error bound in terms of cost functional can be measured by following the approach in [58] and found the convergence error $O(h + \Delta t)$. For the gradient method, the number of the iterations for the stabilized and unstabilized solutions do not differ much and they are less than for one-dimensional problems. Figure 3.3 shows the computed optimal control u_h, the computed optimal state y_h and the associated optimal adjoint state p_h for the one-shot approach with adaptation for $h = \Delta x_{\max} = 2^{-3}$, $\Delta t_{\max} = 0.01$. Compared with the one-dimensional problem, the unstabilized solutions exhibit strong oscillations almost in the entire space domain, whereas the oscillations of stabilized solutions are located near the boundaries. They also show a different behavior with increasing time; the oscillations are vanishing with time for the control and the adjoint variable. They are distributed in a constant region for the state variable for all times. we want to mention that for the convection dominated stationary OPC problem in [4], the solutions of the stabilized and unstabilized problems behave similarly.

Table 3.8: Gradient method for the control constrained problem with and without stabilization

$h/\sqrt{2}$	$\|J(y_h,u_h)\|_Q$	iteration #	$\|J(y_h,u_h)\|_Q$	iteration #
	without stabilization		with stabilization	
2^{-1}	0.31705	26	0.34671	27
2^{-2}	0.25627	24	0.32825	27
2^{-3}	0.27519	26	0.31032	27
2^{-4}	0.28663	27	0.30046	27
2^{-5}	0.28848	23	0.29581	27
2^{-6}	0.28503	16	0.29328	27

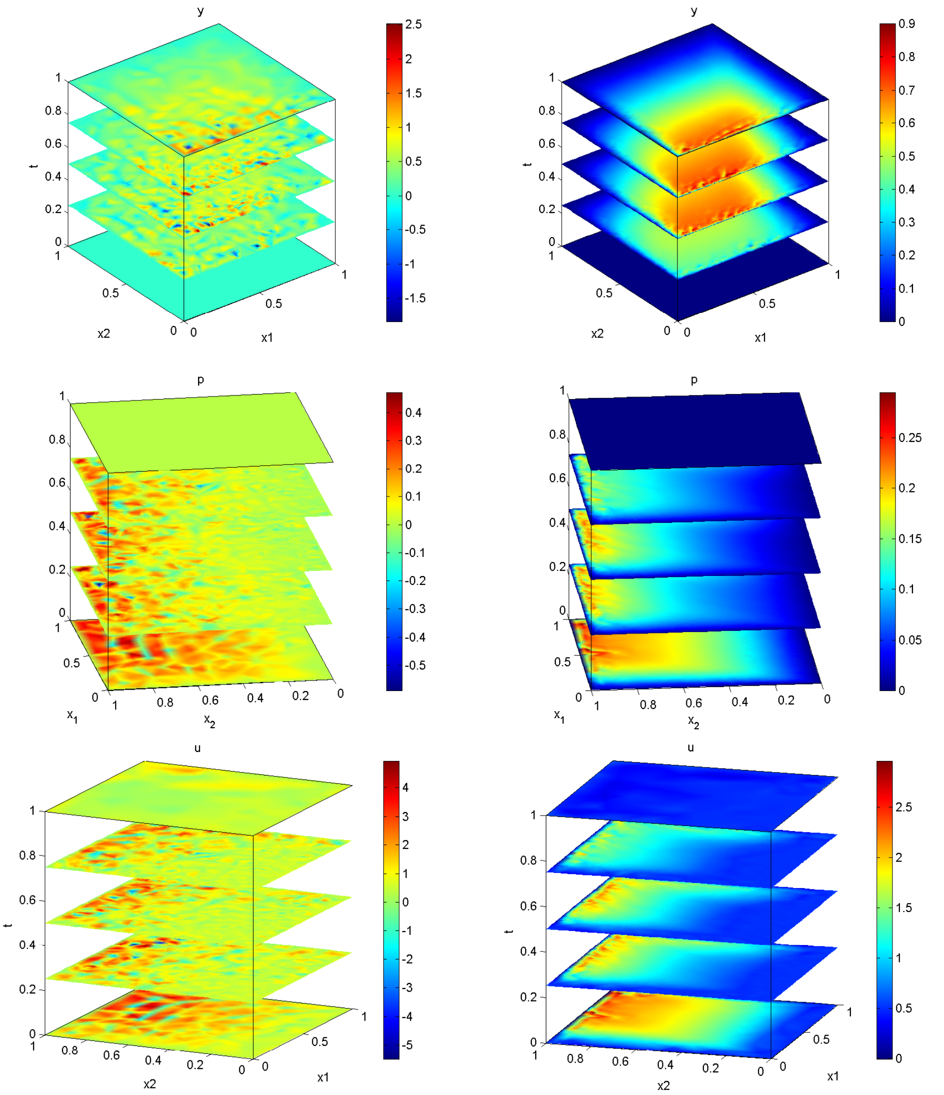


Figure 3.3: One-shot-approach for 2D control constrained problem: unstabilized (left), stabilized (right), optimal state (top), optimal adjoint state (middle), optimal control (bottom)

3.2 Boundary optimal control problem

In this section we consider the boundary (OCP) (2.20) and its optimality system (2.22)-(2.24). As in previous section we apply the same two approaches: *one shot approach and iterative approach.* The classical iterative approach is same as previous section. So we continue with one shot approach.

3.2.1 The one-shot approach

As we mentioned in the previous section, for time-dependent OCPs first the state equation (2.20b) is solved forward in time and the adjoint equation (2.22) backward in time and the control is updated by a gradient based algorithm. This approach requires storage and retrieval of the data containing the state and adjoint variables computed at each discrete time point, which would be infeasible for two-dimensional and three-dimensional problems. In order to apply the first approach, we have to show how the time-dependent diffusion-convection-reaction equation can be interpreted as an elliptic (biharmonic) equation in the time and space variables. In this approach, the time is defined as an additional space dimension. In this sense, we consider the space-time domain Q, where space and time are treated equivalently. Here, we follow the approach [63, 65] for linear parabolic equations. The main difference to the work [63, 65], is that we have additional convection term; moreover, there is a non-symmetric bilinear form with the contribution of this convection term. In Section 3.1, we consider the distributed control problem as in [63, 65] and we follow similar steps with homogenized boundary conditions. However, in this case, there are additional non-homogenous boundary terms as a result of boundary control.
We again start with the homogenization of the state equation (2.20b) by setting $\gamma = (\gamma_0, \gamma_1)^T$, $\mathbf{u} = (u, v)^T$, $\tilde{y} = y - y_d$ with $f = f(y_d, y_0)$ fixed:

$$\begin{aligned} \tilde{y}_t - \epsilon\Delta\tilde{y} + \beta\cdot\nabla\tilde{y} + \sigma\tilde{y} &= f - (y_d)_t + \epsilon\Delta y_d - \beta\cdot\nabla y_d - \sigma y_d, && \text{in } Q, \\ \epsilon\nabla\tilde{y} + \gamma\tilde{y} &= \mathbf{u} - \epsilon\nabla\tilde{y_d} - \gamma\tilde{y_d}, && \text{on } \Sigma, \\ \tilde{y}(\cdot, 0) &= y_0 - y_d(0), && \text{in } \Omega. \end{aligned} \tag{3.8}$$

We assume the existence of a function $\tilde{f}$ fulfilling the initial and boundary conditions of (3.8) and after defining $y := \tilde{y} + \tilde{f}$ we obtain

$$\begin{aligned} y_t - \epsilon\Delta y + \beta\cdot\nabla y + \sigma y &= f - (y_d)_t + \epsilon\Delta y_d - \beta\cdot\nabla y_d - \sigma y_d, && \\ &+ \tilde{f}_t - \epsilon\Delta\tilde{f} + \beta\cdot\nabla\tilde{f} + \sigma\tilde{f}, && \text{in } Q, \\ \epsilon\nabla y + \gamma y &= \mathbf{u}, && \text{on } \Sigma, \\ y(\cdot, 0) &= 0 && \text{in } \Omega. \end{aligned}$$

By rewriting

$$f = f - (y_d)_t + \epsilon\Delta y_d - \beta\cdot\nabla y_d - \sigma y_d + \tilde{f}_t - \epsilon\Delta\tilde{f} + \beta\cdot\nabla\tilde{f} + \sigma\tilde{f},$$

the homogenized state equation is obtained:

$$\begin{aligned} y_t - \epsilon\Delta y + \beta\cdot\nabla y + \sigma y &= f, && \text{in } Q, \\ \epsilon\nabla y + \gamma y &= \mathbf{u}, && \text{on } \Sigma, \\ y(\cdot, 0) &= 0 && \text{in } \Omega. \end{aligned} \tag{3.9}$$

Then the adjoint equation becomes

$$\begin{aligned} -p_t - \epsilon\Delta p - \beta\cdot\nabla p + \sigma p &= y, && \text{in } Q \\ \epsilon\nabla p + (\gamma + \beta)p &= 0, && \text{on } \Sigma \\ p(\cdot, T) &= 0 && \text{in } \Omega. \end{aligned} \tag{3.10}$$

The spaces $H^{2,1}(Q)$ and $\bar{H}^{2,1}(Q)$ are given in the previous section. Let us define

$$\tilde{H}^{2,1}(Q) := \left\{ y \in H^{2,1}(Q) : \epsilon\nabla y + (\beta + \gamma)y = 0 \ \text{ on } \ \Gamma \ \text{ and } \ y(T) = 0 \right\}.$$

We will extend the following results from [63, 65] to the boundary control problem (2.20)

Theorem 3.2.1 *Let us assume that the variables (u, y, p) are sufficiently smooth functions of our OCP problem (3.9)-(3.10) with $y, p \in \tilde{H}^{2,1}(Q)$ and $u \in L^2(0, T)$. Then p satisfies the following biharmonic pde:*

$$-p_{tt} + \epsilon^2\Delta^2 p - (2\sigma\epsilon + \beta^T\beta)\Delta p - 2\beta \cdot (\nabla p)_t + \sigma^2 p = f, \ \textit{in } Q, \tag{3.11a}$$

with the boundary conditions

$$-\epsilon^2\nabla(\Delta p) - \epsilon(\beta + \gamma)\Delta p + (\epsilon\sigma - \gamma\beta)\nabla p + \beta p_t + \gamma\sigma p = \boldsymbol{u}, \ \textit{on } \Sigma, \tag{3.11b}$$

$$\epsilon\nabla p + (\gamma + \beta)p = 0, \ \textit{on } \Sigma, \tag{3.11c}$$

$$-p_t(\cdot, 0) - \epsilon\Delta p(\cdot, 0) - \beta \cdot \nabla p(\cdot, 0) + \sigma p(\cdot, 0) = 0, \ \textit{in } \Omega, \tag{3.11d}$$

$$p(\cdot, T) = 0, \ \textit{in } \Omega. \tag{3.11e}$$

Proof. Taking the partial derivative of $-p_t - \epsilon\Delta p - \beta \cdot \nabla p + \sigma p = y$ with respect to t gives

$$-p_{tt} - \epsilon(\Delta p)_t - \beta \cdot (\nabla p)_t + \sigma p_t = y_t.$$

After replacing y and y_t from the adjoint and state equations we obtain

$$\begin{aligned}
- \quad & p_{tt} - \epsilon\Delta p_t - \beta \cdot (\nabla p)_t + \sigma p_t - \epsilon\Delta y + \beta \cdot \nabla y + \sigma y = f, \\
- \quad & p_{tt} - \epsilon\Delta p_t - \beta \cdot (\nabla p)_t + \sigma p_t - \epsilon\Delta(-p_t - \epsilon\Delta p - \beta \cdot \nabla p + \sigma p), \\
+ \quad & \beta \cdot \nabla(-p_t - \epsilon\Delta p - \beta \cdot \nabla p + \sigma p) + \sigma(-p_t - \epsilon\Delta p - \beta \cdot \nabla p + \sigma p) = f.
\end{aligned}$$

Finally, after rearranging the terms we get

$$-p_{tt} + \epsilon^2\Delta^2 p - (2\sigma\epsilon + \beta^T\beta)\Delta p - 2\beta \cdot (\nabla p)_t + \sigma^2 p = f.$$

After evaluating $y = -p_t - \epsilon\Delta p - \beta \cdot \nabla p + \sigma p$ on the boundary and we obtain the boundary condition for the biharmonic pde

$$\epsilon(-\nabla(p_t) - \epsilon\nabla(\Delta)p - \beta\Delta p + \sigma\nabla p) + \gamma(-p_t - \epsilon p - \beta\nabla p + \sigma p) = \mathbf{u}.$$

Using the original boundary condition for the adjoint equation, (3.11b) and (3.11c) are obtained. By setting $t = 0$ and $t = T$, we obtain (3.11d) and (3.11e). ■

Now, we can continue with the following lemmas which give the bilinear form, its ellipticity and its boundness, respectively.

Lemma 3.2.2 *The solution p of equation (3.11a) satisfies the non-symmetric bilinear form*

$$\boldsymbol{a}\left[p, w\right] = F(w) \ \forall \ w \in \tilde{H}^{2,1}(Q) \ \textit{ and } F \in (\tilde{H}^{2,1}(Q))^*,$$

where

$$F(w) = \iint_Q fw \, dxdt + \iint_\Sigma \vec{n} \cdot \boldsymbol{u}w \, dsdt$$

and

$$
\begin{aligned}
[p,w] &= \iint_Q \left(p_t w_t + \epsilon^2 \Delta p \Delta w + (2\sigma\epsilon + \beta^T\beta)\nabla p \nabla w + 2\beta\cdot(\nabla p) w_t + \sigma^2 p w\right) dxdt \\
&+ \int_\Omega (\epsilon \nabla p(x,0)\nabla w(x,0) + \beta\cdot\nabla p(x,0) w(x,0) + \sigma p(x,0) w(x,0))\, dx \\
&+ \iint_\Sigma (\vec{n}\cdot(\xi p + \beta p_t) w)\, dsdt.
\end{aligned}
$$

Proof. The test function $w \in \tilde{H}^{2,1}(Q)$ is applied to (3.11a) to obtain the weak form

$$
\iint_Q \left(-p_{tt} w + \epsilon^2 \Delta^2 p w - (2\sigma\epsilon + \beta^T\beta)\Delta p w - 2\beta\cdot\nabla p_t w + \sigma^2 p w\right) dxdt = \iint_Q f dxdt.
$$

Using integration by parts, we obtain :

$$
\begin{aligned}
& \iint_Q \left(-p_{tt} w + \epsilon^2 \Delta^2 p w - (2\sigma\epsilon + \beta^T\beta)\Delta p w - 2\beta\cdot(\nabla p)_t w + \sigma^2 p w\right) dxdt \\
=& \iint_Q \left(p_t w_t + \epsilon^2 \Delta p \Delta w + (2\sigma\epsilon + \beta^T\beta)\nabla p \nabla w + 2\beta\cdot(\nabla p) w_t\right) dxdt \\
+& \iint_Q \left(\sigma^2 p w dxdt - \int_\Omega p_t w|_0^T dx - \int_\Omega 2\beta\cdot\nabla p w|_0^T dx + \iint_Q (2\sigma\epsilon + \beta^T\beta)\nabla p \nabla w\right) dxdt \\
-& \iint_\Sigma (2\sigma\epsilon + \beta^T\beta)\vec{n}\cdot\nabla p w) dsdt - \epsilon^2 \iint_\Sigma (\vec{n}\cdot(\nabla(\Delta p)) w dsdt + \vec{n}\cdot((\Delta p)\nabla w))\, dsdt.
\end{aligned}
$$

Let us set $\gamma = \gamma_1$ or $\gamma = \gamma_2$.

We obtain $\nabla w = -\frac{\gamma+\beta}{\epsilon} w$ from the boundary conditions (3.11c). Using (3.11b) and letting $\xi = \frac{\sigma\epsilon(\beta+2\gamma)+\gamma\beta(\gamma+2\beta)}{\epsilon}$ gives

$$
\iint_\Sigma -(2\sigma\epsilon + \beta^T\beta)\vec{n}\cdot\nabla p w - \epsilon^2(\vec{n}\cdot(\nabla(\Delta p)) w + \vec{n}\cdot((\Delta p)\nabla w)) dsdt = \iint_\Sigma (\xi p + \beta p_t - \mathbf{u}) w\, dsdt.
$$

Furthermore from $w(x,T) = 0$ and (3.11d) we have
$-\int_\Omega p_t w|_0^T dx = -\int_\Omega p(x,T)_t w(x,T) + (\epsilon\Delta p(x,0) + \beta\cdot\nabla p(x,0) - \sigma p(x,0)) w(x,0) dx,$
$-\int_\Omega 2\beta\cdot\nabla p w|_0^T dx = -2\beta(\int_\Omega \cdot\nabla p(x,T) w(x,T) - \nabla p(x,0) w(x,0) dx.)$
The right-hand side

$$
\iint_Q f w\, dxdt + \iint_\Sigma \vec{n}\cdot\mathbf{u} w\, dsdt =: F(w)
$$

is a functional from $(\tilde{H}^{2,1}(Q))^*$. ■

Lemma 3.2.3 *The bilinear form is $\tilde{H}^{2,1}$-elliptic, i.e., there is a constant $c > 0$ such that*

$$
\boldsymbol{a}[v,v] \geq c\|v\|^2_{\tilde{H}^{2,1}(Q)} \quad \textit{for all } v \in \tilde{H}^{2,1}(Q).
$$

Proof. We choose $v \in \tilde{H}^{2,1}(Q)$ and estimate $\mathbf{a}[v,v]$:

$$
\begin{aligned}
\mathbf{a}[v,v] &= \iint_Q (\left(v_t^2 + \epsilon^2(\Delta v)^2 + (2\sigma\epsilon + \beta^T\beta)(\nabla v)^2 + 2\beta\cdot(\nabla v) v_t + \sigma^2 v^2\right) dxdt \\
&+ \int_\Omega (\epsilon(\nabla v(x,0))^2 + \beta\cdot\nabla v(x,0) v(x,0) + \sigma(v(x,0))^2\, dx + \iint_\Sigma \vec{n}\cdot(\xi v^2 + \beta v_t v)) dsdt \\
&\geq \min\left\{1, \epsilon^2, (2\sigma\epsilon + \beta^T\beta), \sigma^2\right\} \iint_Q v_t^2 + (\Delta v)^2 + (\nabla v)^2 + v^2\, dxdt \\
&\geq c\|v\|^2_{H^{2,1}(Q)}.
\end{aligned}
$$

Let us assume $\xi \geq 0$, and so $\iint_\Sigma \vec{n} \cdot \xi v^2 \geq 0$. As the convective term is divergence free, we obtain $\iint_\Sigma \vec{n} \cdot \beta v_t v = -\iint_Q \frac{\beta}{2} v^2 \geq 0$. We assume $\int\int_Q 2\beta \cdot (\nabla v) v_t \geq 0$, and since also the constant term β ispositive, $\beta > 0$, we receive

$$\int_\Omega \beta \cdot \nabla v(x,0) v(x,0) = -\int_\Omega div\beta \; v(x,0)^2 = 0.$$

■

Lemma 3.2.4 *The bilinear form $a[v,w]$ is bounded in $\tilde{H}^{2,1}(Q)$,i.e.*

$$a[p,w] \leq c\|p\|^2_{H^{2,1}(Q)} \|w\|^2_{H^{2,1}(Q)} \quad \textit{for all } v, w \in \tilde{H}^{2,1}(Q).$$

Proof. In the following, we let $c > 0$ be a generic constant. We have by $v, w \in H^{2,1}(Q)$

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

By a similar argument, we obtain the following bounds:

$$\beta(\nabla p(x,0), w(x,0))_{L^2(\Omega)} \leq c\,\|p\|_{H^{2,1}(Q)}\,\|w\|_{H^{2,1}(Q)}\,,$$

$$\sigma(p(x,0), w(x,0))_{L^2(\Omega)} \leq c\,\|p\|_{H^{2,1}(Q)}\,\|w\|_{H^{2,1}(Q)}\,.$$

By definition of the inner product defined on the space $H^{2,1}(Q)$, we can bound $\|w_t\|_{L^2(Q)}$ so that

$$2\beta(\nabla p, w_t)_{L^2(Q)} \leq c\,\|p\|_{H^{2,1}(Q)}\,\|w\|_{H^{2,1}(Q)}\,.$$

Furthermore, $\xi(\vec{n} \cdot p, w)_{L^2(\Sigma)}$ *and* $\beta(\vec{n} \cdot p_t, w)_{L^2(\Sigma)}$ are be bounded by $c\,\|p\|_{H^{2,1}(Q)}\,\|w\|_{H^{2,1}(Q)}$.

Using all the bounds above we obtain as in [63, 65]

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

■

By the Lemma 3.2.3, Lemma 3.2.4 and the Lax-Milgram Theorem our Main Theorem can be stated as:

Theorem 3.2.5 *For all $F \in (\tilde{H}^{2,1}(Q))$, the bilinear equation*

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

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

Now we introduce a regularized projection formula to make regularization of control constrained problem. We use again the projection $\mathbb{P}_{[a,b]}\{z\}$ given in the previous section.
Let write $\mathbf{u} := (u,v)^T$ and we may represent as follows:

$$u^* = \mathbb{P}_{[u_a,u_b]}\{\frac{p(0,t)}{\alpha_u}\}, \quad \text{and } v^* = \mathbb{P}_{[v_a,v_b]}\{-\frac{p(1,t)}{\alpha_v}\},$$

Now we obtain the biharmonic equation, where a nondifferentiable, nonlinear terms appear at the left hand side:

$$\begin{array}{rcll} -p_{tt} + \epsilon^2\Delta^2 p - (2\sigma\epsilon + \beta^T\beta)\Delta p - 2\beta\cdot(\nabla p)_t + \sigma^2 p & = & f, & \text{in } Q, \\ -\epsilon^2\nabla(\Delta p) - \epsilon(\beta+\gamma)\Delta p + (\epsilon\sigma - \gamma\beta)\nabla p + \beta p_t + \gamma\sigma p & = & \mathbb{P}_{[u_a,u_b]}\{\frac{p(0,t)}{\alpha_u}\}, & \text{on } \Sigma, \\ -\epsilon^2\nabla(\Delta p) - \epsilon(\beta+\gamma)\Delta p + (\epsilon\sigma - \gamma\beta)\nabla p + \beta p_t + \gamma\sigma p & = & \mathbb{P}_{[v_a,v_b]}\{-\frac{p(1,t)}{\alpha_v}\}, & \text{on } \Sigma, \\ \epsilon\nabla p + (\gamma+\beta)p & = & 0, & \text{on } \Sigma, \\ -p_t(\cdot,0) - \epsilon\Delta p(\cdot,0) - \beta\cdot\nabla p(\cdot,0) + \sigma p(\cdot,0) & = & 0, & \text{in } \Omega, \\ p(\cdot,T) & = & 0 & \text{in } \Omega. \end{array} \tag{3.12}$$

By the same technique as used in Lemma 3.2.2, we can show that the above biharmonic equation can be written in weak formulation as follows:

Corollary 3.2.6 *We define the operators $A = A_1 + A_2$, where*

$$\langle A_1 v, w\rangle = a[v,w],\ \langle A_2 v, w\rangle = \int_\Sigma (\mathbb{P}_{[-v_b,-v_a]}\{\frac{v(1,t)}{\alpha_v}\}w(1,t) + \mathbb{P}_{[u_a,u_b]}\{\frac{v(0,t)}{\alpha_u}\}w(0,t))dt.$$

Then biharmonic form (3.12) is equivalent to

$$Ap = F,$$

where $F \in (\tilde{H}^{2,1}(Q))^*$.

Lemma 3.2.7 *The operator A defined in Corollary 3.2.6 is strongly monotone, coercive, and hemicontinuous.*

Proof. The proof employs the results of Lemma 3.2.2 and Lemma 3.2.3. Let us first show that A is strongly monotone: From Lemma 3.2.3 we have

$$\langle A_1(v_1 - v_2), v_1 - v_2\rangle = a[v_1 - v_2, v_1 - v_2] \geq c\,\|v_1 - v_2\|^2_{H^{1,2}(Q)}.$$

By monotonicity of $\mathbb{P}_{[u_a,u_b]}\{v\}$ in v we have

$$\int_0^T (\mathbb{P}_{[u_a,u_b]}\{-\frac{v_1(0,t)}{\alpha_u}\} - \mathbb{P}_{[u_a,u_b]}\{\frac{v_2(0,t)}{\alpha_u}\})(v_1(0,t) - v_2(0,t))dt \geq 0,$$

similarly, we receive

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

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

$$\mathbb{P}_{[u_a,u_b]}\{\frac{v}{\alpha_u}\}v = \begin{cases} u_a v \ \text{ in } \Sigma_{u_a} := \{t \in (0,T)\ : v < u_a\}, \\ u_b v \ \text{ in } \Sigma_{u_b} := \{t \in (0,T)\ : v > u_b\}, \\ \frac{v^2}{\alpha_u} \text{ in } (0,T)\backslash\{\Sigma_{u_a} \cup \Sigma_{u_b}\}. \end{cases}$$

Similarly, we get

$$\mathbb{P}_{[-v_b,-v_a]}\{\frac{v}{\alpha_v}\}v = \begin{cases} -v_a v \ \text{ in } \Sigma_{v_a} := \{t \in (0,T)\ : v > -v_a\}, \\ -v_b v \ \text{ in } \Sigma_{v_b} := \{t \in (0,T)\ : v < -v_b\}, \\ \frac{v^2}{\alpha_v} \text{ in } (0,T)\backslash\{\Sigma_{v_a} \cup \Sigma_{v_b}\}. \end{cases}$$

Hence, we arrive it

$$\int_0^T \left(\mathbb{P}_{[u_a,u_b]}\{\frac{v(0,t)}{\alpha_u}\} v(0,t) \right) dt$$
$$= \int_{\Sigma_{u_a}} u_a(0,t)v(0,t)dt + \int_{\Sigma_{u_b}} u_b(0,t)v(0,t)dt + \int_{(0,T)\setminus\{\Sigma_{u_a}\cup\Sigma_{u_b}\}} v(0,t)^2 dt$$
$$\geq \int_{\Sigma_{u_a}} u_a(t,0)v(t,0)dt + \int_{\Sigma_{u_b}} u_b(t,0)v(t,0)dt$$

and, similarly,

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

By lemma 3.2.3, we have

$$\langle Av, v\rangle = \langle A_1 v, v\rangle + \langle A_2 v, v\rangle$$
$$= a[v,v] + \int_0^T \left(\mathbb{P}_{[-v_b,-v_a]}\{\frac{v(t,1)}{\alpha_v}\} v(t,1) \right) dt + \int_0^T \left(\mathbb{P}_{[u_a,u_b]}\{\frac{v(t,0)}{\alpha_u}\} v(t,0) \right) dt$$
$$\geq c\,\|v\|_{H^{2,1}(Q)} - \int_{\Sigma_{v_a}} v_a(t,1)v(t,1)dt - \int_{\Sigma_{v_b}} v_b(t,1)v(t,1)dt$$
$$+ \int_{\Sigma_{u_a}} u_a(t,0)v(t,0)dt + \int_{\Sigma_{u_b}} u_b(t,0)v(t,0)dt$$
$$\geq c\,\|v\|_{H^{2,1}(Q)} - \int_{\Sigma_{v_a}} v_a(t,1)v(t,1)dt - \int_{\Sigma_{v_b}} v_b(t,1)v(t,1)dt,$$

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

which results in

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

with $c_{a,b} = \|v_a\|_{L^2(Q_a)} + \|v_b\|_{L^2(Q_b)}$. Therefore, we obtain

$$\frac{\langle Av, v\rangle}{\|v\|_{H^{2,1}(Q)}} \to \infty \text{ if } \|v\|_{H^{2,1}(Q)} \to \infty$$

A is hemi-continuous which is shown in [63]. ■

Here, we have the following theorem.

Theorem 3.2.8 *The biharmonic equation (3.12) has a unique solution $p \in \tilde{H}^{2,1}(Q)$ for all $F \in (\tilde{H}^{2,1}(Q))$.*

Proof. This follows by applying Theorem 4.1, from [83] to

$$Ap = F$$

where A is defined in corollary 3.2.6. ■

In order to avoid the non-differentiability caused by projection, a smoothing technique is considered in [65]. A regularized projection formula is derived by using

$$smsign(z;\epsilon) := \begin{cases} -1, & z < -\epsilon, \\ \mathcal{P}(z), & z \in [-\epsilon, \epsilon], \\ 1, & z > \epsilon, \end{cases}$$

where $\mathcal{P}$ is the polynomial with 7th degree that fulfills

$$\mathcal{P}(\epsilon) = 1, \ \mathcal{P}(-\epsilon) = -1, \mathcal{P}^{(k)}(\pm\epsilon) = 0,$$

for $k = 1, 2$. Furthermore,

$$\int_0^{\epsilon} \mathcal{P}(z)dz = -\int_{-\epsilon}^{0} \mathcal{P}(z)dz = \epsilon.$$

This function fulfills the specifications of the **flsmsing** provided by COMSOL Multiphysics. We refer to [65] for a detailed analysis for smoothing of the projection.

3.2.2 Variational formulation and Stabilization

We consider the boundary (OCP) (2.62) which is convection dominated problem. As in previous section, we use SUPG which stabilizes oscillations and instabilities that arise from the numerical method. If the SUPG method is used to solve optimization problems governed by an advection-dominated pde, however, the convergence properties of the SUPG method can be substantially different from the convergence properties of the SUPG method applied for the solution of an advection-dominated pde.
The SUPG method consists of adding consistent diffusion terms in the state and adjoint equations with the stabilization parameter τ_k, depending on the Peclet number defined in (3.7) and mesh cells [30]:

$$\begin{aligned}
(y_{n+1}^h, v^h) \quad &+ \quad \Delta t[\epsilon(\nabla y_{n+1}, \nabla v^h) + (\beta \cdot \nabla y_{n+1} + \sigma y_{n+1}, v^h)] \\
&+ \quad \Delta t \sum_{K\in\Omega_h} \tau_K(-\epsilon\Delta y_{n+1} + \beta \cdot \nabla y_{n+1} + \sigma y_{n+1}, \beta \cdot \nabla v^h)_K \\
&= \quad (y_n, v^h) + \Delta t \sum_{K\in\Omega_h} \tau_K(-\epsilon\Delta y_n + \beta \cdot \nabla y_n + \sigma y_n, \beta \cdot \nabla v^h)_K \\
&+ \quad \Delta t(f_{n+1}, v^h)) + \Delta t \sum_{K\in\Omega_h} \tau_K((f_{n+1}), \beta \cdot \nabla v^h)_K \\
&\qquad\qquad (n = 0, 1, \cdots, N)
\end{aligned}$$

$$\begin{aligned}
-(p_{n-1}^h, v^h) \quad &+ \quad \Delta t[\epsilon(\nabla p_{n-1}, \nabla v^h) - (\beta \cdot \nabla p_{n-1} + \sigma p_{n-1}, v^h)] \\
&+ \quad \Delta t \sum_{K\in\Omega_h} \tau_K(-\epsilon\Delta p_{n-1} - \beta \cdot \nabla p_{n-1} + \sigma p_{n-1}, \beta \cdot \nabla v^h)_K \\
&= \quad (p_n, v^h) + \Delta t \sum_{K\in\Omega_h} \tau_K(-\epsilon\Delta p_n - \beta \cdot \nabla p_n + \sigma p_n, \beta \cdot \nabla v^h)_K \\
&+ \quad \Delta t((y_n - y_d), v^h)) + \Delta t \sum_{K\in\Omega_h} \tau_K((y_n - y_d), \beta \cdot \nabla v^h)_K, \\
&\qquad\qquad (n = N, N-1, \cdots, 1)
\end{aligned}$$

3.2.3 Implementation and Numerical Examples

In this section, we provide the details of the implementation of numerical realization of the one-shot method in COMSOL Multiphysics for time-dependent convection dominated OCPs. We consider unconstrained and control constrained OCPs for the diffusion-convection-reaction equation in one space dimension by comparing the numerical results for the one-shot approach with and without stabilization.

Table 3.9: One-shot approach with adaption-femlin for the unconstraint boundary control problem

h	adaptive solver $J(y_h, u_h)$ without stabilization	$J(y_h, u_h)$ with stabilization	non-adaptive solver $J(y_h, u_h)$ without stabilization	$J(y_h, u_h)$ with stabilization
2^{-3}	0.0292	0.0155	0.0304	0.0160
2^{-4}	0.0285	0.0156	0.0273	0.0159
2^{-5}	0.0269	0.0157	0.0267	0.0158
2^{-6}	0.0289	0.0158	0.0267	0.0158
2^{-7}	out of memory	out of memory	0.0273	0.0158

Example 3.2.1 (Boundary control problem without control constraints)
For the optimal control problem without control constraints we take $\alpha_Q = 1$,$\alpha_u = \alpha_v = 0.5$ and $\epsilon = 10^{-5}$, $f = 0$, $\beta = -1$, $\sigma = 1$, $\sigma_0 = \sigma_1 = 0.1$, $y_d(x) = x(x-1)$, $y_0(x) = y_d(x)$
We apply the solvers of COMSOL Multiphysics; **adaption**, which solves the elliptic PDE using adaptive mesh refinement, and the **femnlin** that solves nonlinear problems without adaptation.

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

SUPG is implemented in COMSOL Multiphysics for the adaptive and non-adaptive solvers as

```
fem.equ.weak={{'-h*(yx_test)/20*(yx+y+ytime)'
'-h*(px_test)/20*(px+p-ptime-y+zd(x,time))' }  };
```

The exact solution of the optimal control problem above is not known. Therefore, the evolution of the values of the cost function $J(y_h, u_h)$ is shown for a sequence of uniformly refined meshes tending to zero as in [4]. The numerical results for the nonadaptive and adaptive elliptic solvers with and without the stabilization are given in Table 3.9 and in Figure 3.4 for $\Delta x = \Delta t = 2^{-5}$ at $T = 1$. Figure 3.4 shows that the stabilized problem contains slight oscillatory solutions only in a thin region on boundary layer, whereas the unstabilized solutions exhibit strong oscillations in a larger region near the boundary layer. An important characteristic of nonlinear iterative solvers is the mesh independence of the solutions, which shows that the convergence behavior of the iterations for the discrete problem is the same as for the infinite dimensional problem. It allows to predict the convergence to the discretized problem and it can be applied the increase of the performance of the method employing mesh refinement techniques [48]. It asserts that the number of iterations to reach a specified tolerance is independent of the mesh size. Mesh independence OCP's with Burgers equation was observed numerically in [89] using Lagrangian-SQP method and COMSOL Multiphysics in [91]. Different values of tolerances were applied to stop the solver ***femnlin***, which is an affine invariant form of the damped Newton method. The relative tolerances are based on a weighted Euclidean norm for the estimated relative error. The mesh-independence of the stabilized OCP is observed numerically for all mesh size and tolerances in Table 3.10. We consider now control constrained problem modified from [4], where the distributed control problem was considered.
Example 3.2.2 (Boundary control problem with control constraints)

Table 3.10: Mesh independence for the unconstrained boundary control problem

h/tol	2^{-1}	2^{-2}	2^{-3}	2^{-4}	2^{-5}
$1e^{-2}$	2	2	2	2	2
$1e^{-4}$	2	2	2	2	2
$1e^{-6}$	2	2	2	2	2
$1e^{-8}$	2	2	2	2	2
$1e^{-10}$	2	2	2	2	2

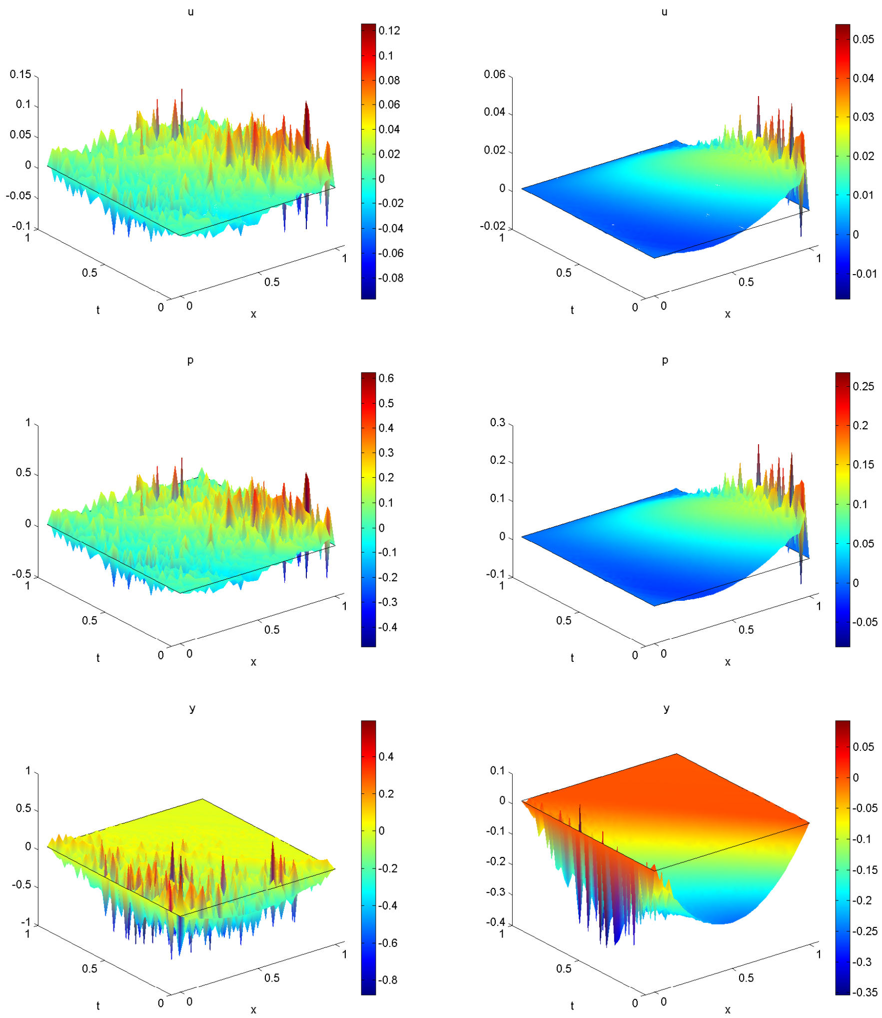


Figure 3.4: One-shot-approach for the unconstrained problem: unstabilized (left), stabilized (right), optimal control (top), optimal adjoint state (middle), optimal state (bottom)

Table 3.11: One-shot approach with adaption-nonadaption for the boundary control constraint problem

h	adaptive solver $J(y_h, u_h)$ without stabilization	$J(y_h, u_h)$ with stabilization	non-adaptive solver $J(y_h, u_h)$ without stabilization	$J(y_h, u_h)$ with stabilization
2^{-3}	0.2345	0.0731	0.1164	0.0780
2^{-4}	0.0873	0.0730	0.2249	0.0758
2^{-5}	out of memory	0.0734	0.1129	0.0748
2^{-6}	out of memory	out of memory	out of memory	0.0743

Table 3.12: Mesh independence for the boundary control constrained problem

h/tol	2^{-1}	2^{-2}	2^{-3}	2^{-4}	2^{-5}
$1e^{-4}$	2	2	2	2	2
$1e^{-6}$	2	2	2	2	2
$1e^{-8}$	2	2	2	2	2
$1e^{-10}$	3	3	3	3	3
$1e^{-12}$	3	3	3	3	3

We set $\alpha_Q = 1$, $\alpha_u = \alpha_v = 0.5$ and $\epsilon = 10^{-5}$, $f = 0$, $\beta = -1$, $\sigma = 1$, $\sigma_0 = \sigma_1 = 0.1$,

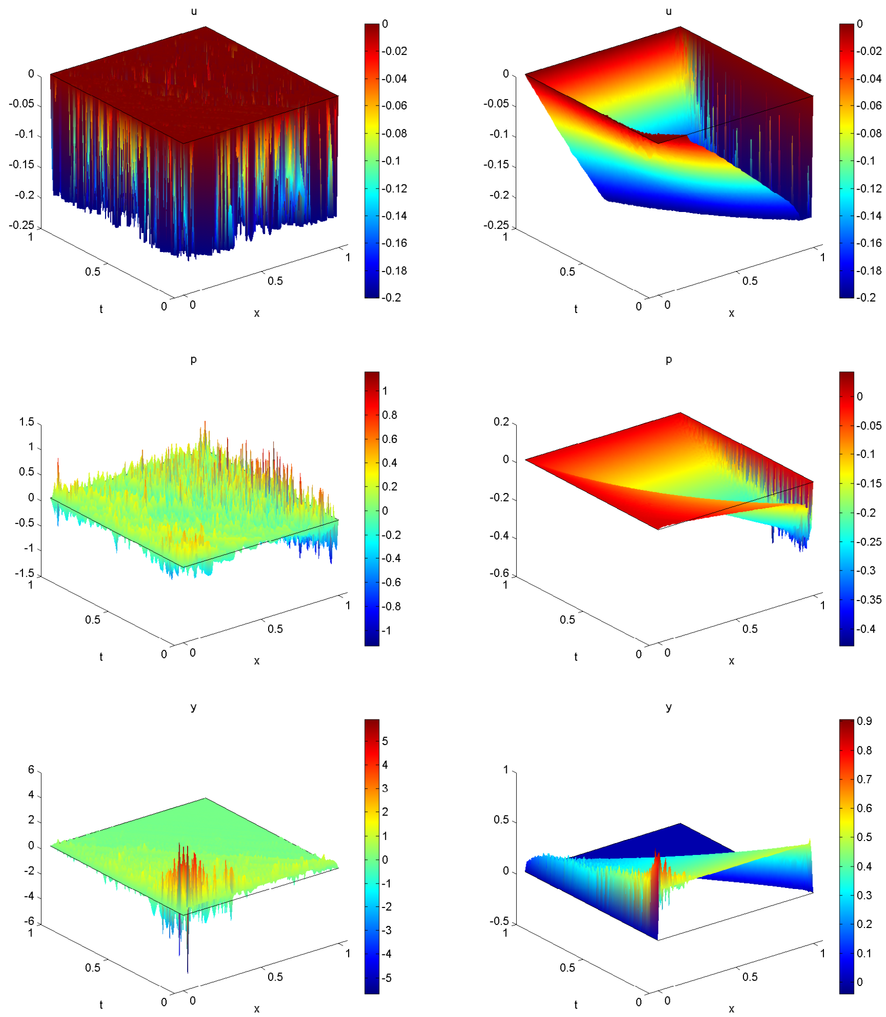
$$y_0(\cdot, 0) = \begin{cases} 1/2, & \text{in } (0,1), \\ 0, & \text{otherwise}, \end{cases}$$

$y_d(x) = y_0(x)$, $u_a = -0,2$ $u_b = 0$, $v_a = -0.25$, $v_b = 0$.
We employ quadratic finite elements for the control constrained problem like in the unconstraint case for state and adjoint state variables, but for the Lagrange multiplier μ, linear finite elements are taken as in [64].
The projection method [61] that is an implementation of the active set strategy as a semi-smooth Newton method [49] for a boundary control problem, is implemented in COMSOL multiphysics as follows:

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

Numerical results for the nonadaptive and adaptive elliptic solvers with and without the stabilization are given in Table 3.9 and in Figure 3.4 for $h = 2^{-5}$. As in the case of unconstrained problem, SUPG stabilization removes the oscillations caused by the boundary layer. Oscillations appear on a thin layer near the boundary.

Table 3.12 shows again the mesh-independence for control constrained problem similar to the unconstrained case.



4

Figure 3.5: One-shot-approach for the control constrained problem: unstabilized (left), stabilized (right), optimal control (top), optimal adjoint state (middle), optimal state (bottom)

CHAPTER 4

DISCRETIZE-THEN-OPTIMIZE

In this chapter, we apply the DO approach mentioned in Chapter 2. In this sense, we use the optimality systems of the finite-dimensional optimization problem obtained by this approach. When we apply SUPG method to the convection dominated state equation, we get the symmetric matrix by this approach of the system. We employ *all-at-once* method for using this approach. In this sense, the optimality system is solved at once for all time steps. This method is applied to elliptic linear optimal control problems in [72, 73, 74] and to parabolic control problems in [78].

Even this approach does not satisfy the adjoint consistency, it leads to a symmetric saddle point form $\mathcal{A}x = b$:

$$\underbrace{\begin{pmatrix} A & B^T \\ B & 0 \end{pmatrix}}_{\mathcal{A}} x = b. \tag{4.1}$$

Here $A \in \mathbb{R}^{n\times n}$ is symmetric and positive definite or positive semi-definite and $B \in \mathbb{R}^{m\times n}, m < n$, is a matrix of full rank. If the block $\mathcal{A}$ is positive definite on the kernel of B, the linear system (4.1) is well defined and has a unique solution [6]. For two and three dimensional evolutionary OCPs, (4.1) can be solved using iterative methods efficiently. We use MINRES as the iterative method with the symmetric and positive block diagonal preconditioner to speed up the convergence of the solution. This method is applied to both distributed and boundary OCPs with and without control constraints. The second part of the chapter deals with the stabilization parameter and a priori error estimates for the fully discrete optimality system. The stabilization parameter is chosen to be proportional to mesh size as in steady-state case for Crank-Nicolson. In the case of backward Euler and semi-implicit scheme, we select the stabilization parameter proportional to the length of the time step size. Finally, the numerical examples are given to illustrate the theoretical results. Hence, the numerical results with the special choice of stabilization parameters confirm the predicted convergence rates.

4.1 Distributed optimal control problems

4.1.1 All-at-Once Method

The optimality systems of distributed OCPs with Θ scheme and semi-implicit scheme obtained in Chapter 2 can be defined in the saddle point form (4.1). As an example we consider the optimality system (2.29) in which SUPG stabilized spatial discretization and the Θ scheme as a time discretization are used: We define

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

and furthermore,

$$x := \begin{pmatrix} Y \\ U \\ P \end{pmatrix}, \; B := \begin{pmatrix} -E_s & \Delta t Z_s \end{pmatrix} \text{ and } b := \begin{pmatrix} \Delta t \mathcal{M}_{1/2} Y_d \\ 0 \\ -F_s \end{pmatrix},$$

where A, B are given in (4.1). Similarly, the other optimality systems can be reformulated in the saddle point form by changing a matrix B and a vector b for each one.

The saddle point system can be solved by direct methods or iterative solvers. Direct methods perform very well for one-dimensional parabolic problem, whereas they are likely to run out of memory for two-dimensional parabolic problem. Although direct methods are faster than iterative solvers, we apply iterative solvers for two-dimensional parabolic problem because of the huge dimension. When we use iterative solvers, the convergence can be slow and so a preconditioner is needed to accelerate the convergence rate.

4.1.1.1 Preconditioning the saddle point system

The preconditioner transforms the saddle point system into a better spectral system such that $\mathcal{P}^{-1}\mathcal{A}X = \mathcal{P}^{-1}F$, where $\mathcal{P}$ is preconditioner which has to be cheap to be inverted and has to cluster the eigenvalues of $\mathcal{P}^{-1}\mathcal{A}$ [6, 41].
There are two effective preconditioners for $\mathcal{A}$ demonstrated in [60] such that

$$\mathcal{P}_1 = \begin{pmatrix} A & 0 \\ 0 & S \end{pmatrix}, \; \mathcal{P}_2 = \begin{pmatrix} A & 0 \\ B & -S \end{pmatrix}, \tag{4.2}$$

where S is the (negative) Schur complement defined by $S = BA^{-1}B^T$. The spectra of $\mathcal{P}_1^{-1}\mathcal{A}$ and $\mathcal{P}_2^{-1}\mathcal{A}$ are given by

$$\lambda(\mathcal{P}_1^{-1}\mathcal{A}) = \frac{1}{2}(1 - \sqrt{5}), 1, \frac{1}{2}(1 + \sqrt{5}), \; \lambda(\mathcal{P}_2^{-1}\mathcal{A}) = 1,$$

and $\mathcal{P}_1^{-1}\mathcal{A}$ and $\mathcal{P}_2^{-1}\mathcal{A}$ are nonsingular [60].

We use the minimal residual method (MINRES) to solve the optimality systems, which are symmetric and indefinite. For MINRES, the form of block-diagonal preconditioner $\mathcal{P}_1$, symmetric and positive definite, is considered generally. Because, we need to compute the preconditioner $\mathcal{P}$ at each iteration, and this process can be done cheaply by choosing the symmetric and positive definite $\mathcal{P}$. MINRES constructs a Krylov subspace given by

$$\text{span}\,\{r_0, \mathcal{A}r_0, \mathcal{A}^2 r_0, ..., \mathcal{A}^k r_0\},$$

and computes the solution to the linear system for every iteration step $k = 1, 2, ...,$ by minimizing the Euclidean norm of the residual r_k over the Krylov subspace. In [76, 87], there is a more detail on the properties of MINRES.

A nonstandard CG method [73] is employed with the block-triangular preconditioner $\mathcal{P}_2$ which is also effective for saddle point systems with symmetric and positive definite A. If A is semi-definite, nonsymmetric methods such as GMRES [92] or BICG [26] can be considered with the block triangular preconditioner. We also note that if we can construct a good approximation to A and S using the Chebyshev semi-iterative method discussed in [85], such as $\hat{A}$ and $\hat{S}$; then we have

$$\hat{\mathcal{P}}_1 = \begin{pmatrix} \hat{A} & 0 \\ 0 & \hat{S} \end{pmatrix}, \quad \hat{\mathcal{P}}_2 = \begin{pmatrix} \hat{A} & 0 \\ B & -\hat{S} \end{pmatrix},$$

and so two preconditioners based on $\hat{\mathcal{P}}_1$ and $\hat{\mathcal{P}}_2$ can be derived for the OCPs. The approximation $\hat{A}$, given by

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

where the approximation of $\widehat{\mathcal{M}}_{1/2}$, a Chebyshev semi-iteration process is taken to approximate the mass matrices.

In our choice, we use the form of $\mathcal{P}_1$ in (4.2), and for the saddle point systems (2.29) we have the following preconditioner proposed in [81]:

$$\mathcal{P} = \begin{pmatrix} \Delta t \mathcal{M}_{1/2} & 0 & 0 \\ 0 & \alpha \Delta t \mathcal{M}_{1/2} & 0 \\ 0 & 0 & S \end{pmatrix} \tag{4.3}$$

with $S := (1/\Delta t) E_s \mathcal{M}_{1/2}^{-1} E_s^T + (\Delta t/\alpha) Z_s \mathcal{M}_{1/2}^{-1} Z_s^T$. For the other optimality systems, we obtain preconditioners in a similar way.

4.1.2 A priori error estimate of fully discrete scheme

The most popular SUPG method was introduced for steady-state diffusion-convection-reaction problem in [40]. The steady-state formulation of SUPG was extended in [47] to fully discrete space-time formulation for time-dependent problem using discontinuous Galerkin method in time. Because the space-time coupled formulation increase the computation of cost significantly, the spatial and temporal discretization is usually separated [33].

In [31, 32], we can find the comparison of the SUPG method and other stabilized finite element methods. The approach given in these studies shows that by discretizing the equation in time and considering the equation as a steady-state diffusion-convection-reaction equation for each time steps and using the spatial discretization with a stabilization method, the methodology leads to a stabilization parameter which is proportional to the time step size and cause large spurious oscillations. When the time and space grid is comparable $k \sim h$, the stabilization parameter can be of the same order in the steady-state problem. However, in many applications, such as the application with fast reactions, very small time step have to be used. Additionally, in this case, the spatial and temporal errors have to be balanced. Moreover, when we derive the fully discrete equation, we can start by discretizing in space with a stabilized method and choose the appropriate stabilization parameter proportional to the mesh size and then discretize in time. In [33], as an insight in the time-continuous case, the stabilization parameter is chosen like $\tau = O(h)$ for all cells for evolutionary diffusion-convection-reaction equations. Then, this choice of the stabilization parameter fullfill the convergence of the discrete solution for the time-continuous case.

A priori error estimation of OCPs has a recent history. In [53, 54], a priori error analysis for OCPs is examined using discontinuous Galerkin methods in space and in time. In [84], a priori error analysis for both semi discrete scheme and the fully discrete schemes of parabolic problems are given and piecewise-linear polynomials are considered for spatial discretization, and the Θ scheme and the semi-implicit scheme are used for temporal discretization. SUPG discretization is applied to elliptic OCPs and evolutionary equations, respectively, in [21, 33], and then a priori error analysis is conducted.

We extend the error analysis [33] which has given for a single PDEs to parabolic OCPs which have extra difficulty because of the adjoint equation, also diffusion-convection-reaction equation with an opposite convection field. We have presented the analysis of the fully discrete case using the Crank-Nicolson, backward Euler and semi-implicit scheme as temporal discretization. We derive a priori error estimates for the SUPG stabilized full discrete scheme of distributed OCPs (2.15), governed by unsteady diffusion-convection-reaction equation. When we use the backward Euler and semi-implicit scheme, the stabilization parameter depends on the length of the time step, and for Crank-Nicolson scheme the parameter is chosen the same as in the steady-state case, i.e., it is proportional to the mesh size. The stability bounds and error estimates are derived based on energy arguments for all these schemes. According to our knowledge, error estimates of this kind for SUPG method applied to OCPs governed by unsteady diffusion-convection-reaction equation have not yet been available before. Moreover, in the most papers, the backward Euler and Crank-Nicolson schemes are used as a temporal discretization generally, and this is the first time we give the error estimates for SUPG with semi-implicit scheme applied to parabolic OCPs.

4.1.2.1 Θ scheme

We first give the stability bounds for the Θ scheme by taking $\Theta = 1/2$ and $\Theta = 1$. We consider a similar argument as in [33] to obtain stability bounds and introduce the preliminaries for the analysis. The elliptic projection $\pi_h : V \to V_h$ is defined by $(\nabla(y - \pi_h y), \nabla v_h) = 0$ for all $v_h \in V_h$. Now, we have the following condition:

$$(\pi_h y)_t = \pi_h(y_t) = \pi_h y_t, \tag{4.4}$$

and the following inverse inequality holds for each $v_h \in V_h$ with the assumption of a quasi uniform mesh (see, e.g., [19]):

$$\|v_h\|_{W^{m,q}(K)} \leq c_{inv} h_K^{l-m-d(\frac{1}{q'}-\frac{1}{q})} \|v_h\|_{W^{l,q'}(K)}. \tag{4.5}$$

Here, $0 \leq l \leq m \leq 1,\ 1 \leq q' \leq q \leq \infty$, h_K is the mesh size diameter of $K \in \mathfrak{T}_h$; we note that we take the same step size $h_K = h$ for all mesh cell K. The interpolation error estimate for $y \in V \cap H^{r+1}$ is well-known [20]:

$$\|y - \pi_h y\|_0 + h\|y - \pi_h y\|_1 \leq C h^{r+1} \|y\|_{r+1}, \tag{4.6}$$

where r is the degree of local polynomials and $\|\cdot\|_r$ denotes the norm in $H^r(\Omega)$.
Before giving the coercivity of a_h^s defined in (2.12a), we note that there is a constant $\mu_0 > 0$ such that

$$\sigma - \frac{1}{2}\nabla \cdot \beta \geq \mu_0 \ \text{ a.e. in } \Omega, \tag{4.7}$$

to ensure the well-posedness of the OCPs (2.1).

Lemma 4.1.1 *(**Coercivity of** $a_h^s(\cdot,\cdot)$) (see, e.g., [77], Lemma 10.3). Let (4.7) be satisfied. If the SUPG parameter τ is chosen such that*

$$\tau \leq \frac{\mu_0}{2\|\sigma\|_{K,\infty}^2}, \tag{4.8}$$

then the bilinear form $a_h^s(\cdot,\cdot)$ associated with SUPG method satisfies

$$a_h^s(y_h, y_h) \geq \frac{1}{2}\|y_h\|_s^2, \tag{4.9}$$

where

$$\|y_h\|_s^2 := \epsilon\|\nabla y_h\|_0^2 + \sum_{K\in\mathfrak{T}_h} \tau\|\beta\cdot\nabla y_h\|_{0,K}^2 + \mu_0\|y_h\|_0^2. \tag{4.10}$$

Now, we will derive the stability estimates for the state and adjoint equations. We take a fixed time step $k = \Delta t$, and the fully discrete state adjoint and control solution at time $t_n = nk$ will be denoted by y_h^n, p_h^n and u_h^n, respectively.
Let us first consider the stability bounds for the state equations and find approximate solution $y_h^n \in V_h$ obtained by using the Θ scheme and SUPG method for $n = 1, 2, ..., N$:

$$\begin{aligned}
&\left(\frac{y_h^n - y_h^{n-1}}{k}, \varphi\right) + \Theta\left(\epsilon(\nabla y_h^n, \nabla\varphi) + (\beta\cdot\nabla y_h^n, \varphi) + (\sigma y_h^n, \varphi)\right) \qquad (4.11)\\
&+ (1-\Theta)\left(\epsilon(\nabla y_h^{n-1}, \nabla\varphi) + (\beta\cdot\nabla y_h^{n-1}, \varphi) + (\sigma y_h^{n-1}, \varphi)\right) = \Theta\left(f^n + u_h^n, \varphi\right) + (1-\Theta)\left(f^{n-1} + u_h^{n-1}, \varphi\right)\\
&+ \sum_{K\in\mathfrak{T}_h} \tau\left(-\frac{y_h^n - y_h^{n-1}}{k}, \beta\cdot\nabla\varphi\right)_K\\
&+ \sum_{K\in\mathfrak{T}_h} \tau\left(\Theta\left(f^n + u_h^n + \epsilon\Delta y_h^n - \beta\cdot\nabla y_h^n - \sigma y_h^n\right), \beta\cdot\nabla\varphi\right)_K\\
&+ \sum_{K\in\mathfrak{T}_h} \tau\left((1-\Theta)\left(f^{n-1} + u_h^{n-1} + \epsilon\Delta y_h^{n-1} - \beta\cdot\nabla y_h^{n-1} - \sigma y_h^{n-1}\right), \beta\cdot\nabla\varphi\right)_K
\end{aligned}$$

for all $\varphi \in V_h$ and $y_h^0 = y_h(0, x)$. Then, (4.11) can be written equivalently in the form

$$\begin{aligned}
&(y_h^n - y_h^{n-1}, \varphi) + k a_h^s\left(\Theta y_h^n + (1-\Theta)y_h^{n-1}, \varphi\right) = k\left(\Theta(f^n + u_h^n) + (1-\Theta)(f^{n-1} + u_h^{n-1}), \varphi\right)\\
&+ k\left[\sum_{K\in\mathfrak{T}_h} \tau\left(\Theta(f^n + u_h^n) + (1-\Theta)(f^{n-1} + u_h^{n-1}), \beta\cdot\nabla\varphi\right)\right]_K - \sum_{K\in\mathfrak{T}_h} \tau(y_h^n - y_h^{n-1}, \beta\cdot\nabla\varphi)_K. \qquad (4.12)
\end{aligned}$$

Let us introduce the following notation given in [84] and useful for the proof of Theorem 4.1.2 which gives the stability bounds of the state equations for both Crank-Nicolson and backward Euler scheme: for any function $\phi \in L^2(\Omega)$, we define

$$\|\phi\|_{-1,h} := \sup_{v_h\in V_{h v_h\neq 0}} \frac{(\phi, v_h)}{\|v_h\|_1}, \tag{4.13}$$

which is a norm on V_h. We note that $\|\phi\|_{-1,h} \leq \|\phi\|_0$ for each $\phi \in L^2(\Omega)$.

In order to derive a priori error estimate for the OCPs, we firstly provide stability estimates for the fully discrete state and adjoint equations.Afterwards, the convergence estimation are derived.

Theorem 4.1.2 *(***Stability of the state equation***). Let (4.7) and (4.8) be fulfilled and μ_0 be a positive constant such that (4.7) holds. Then there exists constants $C > 0$, and $C^* > 0$, independent of h and k and with the following additional conditions for $\Theta = 1$: backward Euler scheme:*

$$\tau \leq \frac{4k}{5}; \tag{4.14}$$

the solution (4.12) satisfies

$$\|y_h^n\|_0^2 + \frac{3k}{40}\sum_{j=1}^{n} \|y_h^j\|_s^2 \leq C\left(\|y_h^0\|_0^2 + \sum_{j=1}^{n} \|f^j\|_0^2 + \|u_h^j\|_0^2\right); \tag{4.15}$$

for $\Theta = 1/2$: Crank-Nicolson scheme the solution (4.12) satisfies

$$\|y_h^n\|_0^2 \leq C^* \left(\|y_h^0\|_0^2 + k \frac{1+\tau}{1-\tau} \sum_{j=1}^{n} \|f^j\|_0^2 + \|u_h^j\|_0^2 \right), \tag{4.16}$$

with the additional conditions $\tau < 1$.

Proof. Let us take $\varphi = (\Theta y_h^n + (1-\Theta) y_h^{n-1})$ in (4.12). By the coercivity assumption (4.9) and using the following equality

$$\left(y_h^n - y_h^{n-1}, \Theta y_h^n + (1-\Theta) y_h^{n-1} \right) = \frac{1}{2} \left(\|y_h^n\|_0^2 - \|y_h^{n-1}\|_0^2 \right) + \left(\Theta - \frac{1}{2} \right) \|y_h^n - y_h^{n-1}\|_0^2,$$

we obtain

$$\begin{aligned}
&\frac{1}{2} \left(\|y_h^n\|_0^2 - \|y_h^{n-1}\|_0^2 \right) + \left(\Theta - \frac{1}{2} \right) \|y_h^n - y_h^{n-1}\|_0^2 + \frac{k}{2} \|\Theta y_h^n + (1-\Theta) y_h^{n-1}\|_s^2 \\
&\leq \underbrace{\left| k \left(\Theta(f^n + u_h^n) + (1-\Theta)(f^{n-1} + u_h^{n-1}), \Theta y_h^n + (1-\Theta) y_h^{n-1} \right) \right|}_{A_1} \\
&\quad + \underbrace{\left| k \left[\sum_{K \in \mathfrak{T}_h} \tau \left(\Theta(f^n + u_h^n) + (1-\Theta)(f^{n-1} + u_h^{n-1}), \beta \cdot \nabla(\Theta y_h^n + (1-\Theta) y_h^{n-1}) \right) \right]_K \right|}_{A_2} \\
&\quad + \underbrace{\left| \sum_{K \in \mathfrak{T}_h} \tau (y_h^n - y_h^{n-1}, \beta \cdot \nabla(\Theta y_h^n + (1-\Theta) y_h^{n-1}))_K \right|}_{A_3}.
\end{aligned} \tag{4.17}$$

If we take $1/2 < \Theta \leq 1$, we can apply the similar approach in [33] and estimate A_1, A_2 by using the Cauchy-Schwarz and Young's Inequality. The term A_3 can be estimated with the conditions (4.14) for the special case $\Theta = 1$. Inserting all these estimates in (4.17) and after summation of the time steps $j = 1, 2, ..., n$, considering the conditions (4.14), we obtain the statements of Theorem, (4.15) for the backward Euler scheme.
However, when we consider the case $0 \leq \Theta \leq 1/2$, especially the Crank-Nicolson scheme ($\Theta = 1/2$), the approach in [33] does not work because of the term A_3. Therefore, we use the similar approach as in [84] and take $\varphi = (y_h^n - y_h^{n-1})$ in (4.12), then we find:

$$\begin{aligned}
&\|y_h^n - y_h^{n-1}\|_0^2 \\
&= -k a_h^s (\Theta y_h^n + (1-\Theta) y_h^{n-1}, y_h^n - y_h^{n-1}) + k \left(\Theta(f^n + u_h^n) + (1-\Theta)(f^{n-1} + u_h^{n-1}), y_h^n - y_h^{n-1} \right) \\
&\quad + k \left[\sum_{K \in \mathfrak{T}_h} \tau \left(\Theta(f^n + u_h^n) + (1-\Theta)(f^{n-1} + u_h^{n-1}), \beta \cdot \nabla(y_h^n - y_h^{n-1}) \right) \right]_K \\
&\quad - \sum_{K \in \mathfrak{T}_h} \tau (y_h^n - y_h^{n-1}, \beta \cdot \nabla(y_h^n - y_h^{n-1}))_K \\
&\leq \gamma k \|\Theta y_h^n + (1-\Theta) y_h^{n-1}\|_1 \|y_h^n - y_h^{n-1}\|_1 + k \|\Theta(f^n + u_h^n) + (1-\Theta)(f^{n-1} + u_h^{n-1}\|_{-1,h} \|y_h^n - y_h^{n-1}\|_1 \\
&\quad + k \sum_{K \in \mathfrak{T}_h} \tau \left(\|\Theta(f^n + u_h^n) + (1-\Theta)(f^{n-1} + u_h^{n-1})\|_{0,K} \|\beta \cdot \nabla(y_h^n - y_h^{n-1})\|_{0,K} \right) \\
&\quad + \sum_{K \in \mathfrak{T}_h} \tau \|y_h^n - y_h^{n-1}\|_{0,K} \|\beta \cdot \nabla(y_h^n - y_h^{n-1})\|_{0,K},
\end{aligned} \tag{4.18}$$

where γ is the continuity constant defined in [84]. By using the property $\|\nabla(y_h^n - y_h^{n-1})\|_0 \leq \|y_h^n - y_h^{n-1}\|_1$ and the inverse inequality with the condition (4.13) and following the steps in [84], we have

$$\|y_h^n\|_0^2 - \|y_h^{n-1}\|_0^2$$
$$\leq \frac{C_*}{1-\tau} k \left(\|\Theta(f^n + u_h^n) + (1-\Theta)(f^{n-1} + u_h^{n-1}\|_{-1,h} + \sum_{K \in \mathfrak{T}_h} \tau \left(\|\Theta(f^n + u_h^n) + (1-\Theta)(f^{n-1} + u_h^{n-1})\|_{0,K} \right) \right)$$

for a suitable $C_* > 0$. By using the inequality $\|\phi\|_{-1,h} \leq \|\phi\|_0$ and summing from $j = 1, ..., n$, we obtain the desired results (4.16). ■

When we consider the stability estimate of the adjoint equation which is also convection dominated parabolic equation with negative convection term, we apply the Θ scheme to the discrete adjoint equation (2.15a). Then we find an approximate solution $p_h^{n-1} \in V_h$:

$$(p_h^{n-1} - p_h^n, \psi) + k a_h^s \left(\psi, \Theta p_h^{n-1} + (1-\Theta) p_h^n\right) = -k \left(\Theta(y_h^n - y_{h,n}^d) + (1-\Theta)(y_h^{n-1} - y_{h,n-1}^d), \psi\right)$$
$$- \sum_{K \in \mathfrak{T}_h} \tau (p_h^{n-1} - p_h^n, \beta \cdot \nabla \psi)_K \tag{4.19a}$$

for all $\psi \in V_h$. Consider $y_{h,n}^d$ being an approximate solution of y_d and $p_{T,h} = p_h(T, x)$. Finally, the gradient equation looks:

$$(\alpha u_h^n - p_h^{n-1}, w - u_h^n) \geq 0 \qquad \forall w \in U_h^{ad}. \tag{4.19b}$$

Theorem 4.1.3 *(**Stability of the adjoint equation**). Let (4.7) and (4.8) be fulfilled and μ_0 be a positive constant such that (4.7) holds. Then there exists positive constants $C > 0$ and $C^* > 0$ independent of h and k and with the additional conditions for $\Theta = 1$: backward Euler scheme:*

$$\tau \leq \frac{4k}{5}, \tag{4.20}$$

the solution (4.19) satisfies

$$\|p_h^n\|_0^2 + \frac{3k}{40} \sum_{j=1}^{n} \|p_h^{j-1}\|_s^2 \leq C \left(\|P_{T,h}\|_0^2 + \sum_{j=1}^{n} \|y_h^j - y_{h,j}^d\|_0^2 \right). \tag{4.21}$$

for $\Theta = 1/2$: Crank-Nicolson scheme: the solution (4.19) satisfies

$$\|p_h^n\|_0^2 \leq C^* \left(\|P_{T,h}\|_0^2 + \frac{k}{1-\tau} \sum_{j=1}^{n} \|y_h^j - y_{h,j}^d\|_0^2 \right) \tag{4.22}$$

with the additional conditions $\tau < 1$.

Proof. If $1/2 < \Theta \leq 1$, we choose $\psi = (\Theta p_h^{n-1} + (1-\Theta)p_h^n)$ in (4.19), and if $0 \leq \Theta \leq 1/2$ we choose $\psi = (p_h^{n-1} - p_h^n)$ and follow the steps as in the proof of Theorem 4.1.2. Herewith, we obtain the desired results. ■

Now, we shall use two auxiliary variables $y_h^n(u), p_h^n(u) \in V_h \times V_h$, $n = 1, 2, ..., N$, associated with the control variable to derive a priori error estimate of the full-discrete scheme as in [27]:

$$(y_h^n(u) - y_h^{n-1}(u), \varphi) + k a_h^s \left(\Theta y_h^n(u) + (1-\Theta) y_h^{n-1}(u), \varphi\right) = k \left(\Theta(f^n + \mathbf{u}^n) + (1-\Theta)(f^{n-1} + \mathbf{u}^{n-1}), \varphi\right)$$
$$+ k \left[\sum_{K \in \mathfrak{T}_h} \tau \left(\Theta(f^n + \mathbf{u}^n) + (1-\Theta)(f^{n-1} + \mathbf{u}^{n-1}), \beta \cdot \nabla \varphi\right) \right]_K - \sum_{K \in \mathfrak{T}_h} \tau (y_h^n(u) - y_h^{n-1}(u), \beta \cdot \nabla \varphi)_K$$
$$\forall \varphi \in V_h, \;\; y_h^0(u) = y_h^0, \;\; n = 1, 2, ..., N, \tag{4.23}$$

$$(p_h^{n-1}(u) - p_h^n(u), \psi) + ka_h^s\left(\psi, \Theta p_h^{n-1}(u) + (1-\Theta)p_h^n(u)\right)$$
$$= -k\left(\Theta(y_h^n(u) - y_{h,n}^d) + (1-\Theta)(y_h^{n-1}(u) - y_{h,n-1}^d), \psi\right) - \sum_{K\in\mathfrak{T}_h} \tau(p_h^{n-1}(u) - p_h^n(u), \beta\cdot\nabla\psi)_K$$
$$\forall\psi \in V_h, \;\; p_{T,h} = 0, \;\; n = N, ..., 2, 1. \quad (4.24)$$

Let us first consider the connection between the approximation solutions (y_h^n, p_h^n) and the auxiliary solution $(y_h^n(u), p_h^n(u))$. We use the following notation:

$$\theta^n = y_h^n - y_h^n(u), \qquad \zeta^n = p_h^n - p_h^n(u).$$

Furthermore, we need some useful lemmas before deriving the main a priori error estimates for the OCPs.

Lemma 4.1.4 *[24] Suppose us that $f \in L^2(\Omega)$ and $\bar{f}(x) = f(x - g(x)k)$, where we assume that g, and∇g are bounded on $\bar{\Omega}$. Then, for sufficiently small k, we have that*
$\|f(x) - \bar{f}(x)\|_{-1} \leq Ck\|f\|$; here, the constant C depends only on $\|g\|_L^\infty(\Omega)$ and $\|\nabla g\|_L^\infty(\Omega)$, and the negative norm $\|\cdot\|_{-1}$ is defined in (4.13).

Lemma 4.1.5 *Let (y_h, p_h) and $(y_h(u), p_h(u))$ be the solutions of ((4.12),(4.19)) and ((4.23)-(4.24)) respectively. Then there exists a constant C independent of h and k such that following estimates holds:*

$$\|y_h - y_h(u)\|_{L^2(I;L^2(\Omega))} + \|p_h - p_h(u)\|_{L^2(I;L^2(\Omega))} \leq C\|u - u_h\|_{L^2(I;L^2(\Omega))}. \quad (4.25)$$

Proof. As in [27], we firstly substract (4.12) from (4.23) to obtain the following inequality:

$$(\theta^n - \bar{\theta}^{n-1}, \varphi) + ka_h^s\left(\Theta\theta^n + (1-\Theta)\theta^{n-1}, \varphi\right) = k\left(\Theta(u_h^n - \mathbf{u}^n) + (1-\Theta)(u_h^{n-1} - \mathbf{u}^{n-1}), \varphi\right)$$
$$+ k\left[\sum_{K\in\mathfrak{T}_h} \tau\left(\Theta(u_h^n - \mathbf{u}^n) + (1-\Theta)(u_h^{n-1} - \mathbf{u}^{n-1}), \beta\cdot\nabla\varphi\right)\right]_K - \sum_{K\in\mathfrak{T}_h} \tau(\theta^n - \theta^{n-1}, \beta\cdot\nabla\varphi)_K. \quad (4.26)$$

As in the proof of the Theorem 4.1.2, if $1/2 < \Theta \leq 1$, we choose $\varphi = (\Theta\theta^n + (1-\Theta)\theta^{n-1})$ as a test function. From Lemma 4.1.4 we have

$$\|\bar{\theta}^{n-1}\|^2 \leq (1 + Ck)\|\theta^{n-1}\|^2. \quad (4.27)$$

Inserting (4.27) in (4.26) and following the steps in Theorem 4.1.2, we get

$$\|\theta^n\|_0^2 + \frac{3k}{40}\sum_{j=1}^n \|\theta^j\|_s^2 \leq Ck\left(\sum_{j=1}^n \|\theta^j\|_0^2 + \|\theta^{j-1}\|_0^2 + \sum_{j=1}^n \|\mathbf{u}^j - u_h^j\|_0^2\right). \quad (4.28)$$

By applying the discrete Gronwall's Lemma, we have

$$\|y_h - y_h(u)\|_{L^2(I;L^2(\Omega))} \leq C\|u - u_h\|_{L^2(I;L^2(\Omega))}. \quad (4.29)$$

In a similar way, we can obtain (4.29) by following the steps applied for Theorem 4.1.2, refinding the part of $0 \leq \Theta \leq 1/2$ by choosing the test function as $\varphi = (\theta^n - \theta^{n-1})$.
Similarly, we derive from the systems of equations (4.19) and (4.24) that

$$\|\zeta\|_{L^2(I;L^2(\Omega))} \leq C\|y_h - y_h(u)\|_{L^2(I;L^2(\Omega))}. \quad (4.30)$$

Therefore, Lemma 4.1.5 is proved through (4.29)-(4.30). ■

Lemma 4.1.6 *Let* (y, p, u) *and* (y_h^n, p_h^n, u_h^n) *be the solutions of (2.9) and ((4.12),(4.19)), respectively. We assume that* $u \in L^2(I; W^{1,\infty}(\Omega)), u|_{\Omega^*} \in L^2(I; H^2(\Omega^*)), p \in L^2(I; W^{1,\infty}(\Omega))$ *where* $\Omega^* := \{U_K : K \subset \Omega, u_a < u|_K < u_b\}$. *Let* u_h^n *be the piecewise linear element space; then for the backward Euler scheme we have*

$$\|u^n - u_h^n\|_{L^2(I;L^2(\Omega))} \leq C\left(h^{3/2} + k + \|p_h^n(u) - p\|_{L^2(I;L^2(\Omega))}\right). \tag{4.31a}$$

for the Crank-Nicolson scheme:

$$\|u^n - u_h^n\|_{L^2(I;L^2(\Omega))} \leq C\left(h^{3/2} + k^2 + \|p_h^n(u) - p\|_{L^2(I;L^2(\Omega))}\right). \tag{4.31b}$$

Proof. The proof can be found in [27]. ■

Lemma 4.1.7 *Let* (y, p) *and* $y_h(u), p_h(u)$ *be the solutions of (2.9) and (4.23,4.24), respectively. Assume that* $y,\ p \in L^2(I; H_0^1(\Omega) \cap H^2(\Omega)) \cap H^1(I; H^2(\Omega)) \cap H^2(I; L^2(\Omega))$, $y_d \in H^1(I; L^2(\Omega))$. *If* $\Theta = 1$ *(backward Euler scheme), the additional condition (4.14) is satisfied then*

$$\|y^n - y_h^n(u)\|_{L^2(I;L^2(\Omega))} \leq C\left(h^2 + k + \tau^{1/2}(h^2 + h + \epsilon) + h^2\tau^{-1/2}\right) \tag{4.32a}$$

with

$$\left(k\sum_{j=1}^{n} \|y(t_j) - y_h^j(u)\|_s\right)^{1/2} \leq C\left(h^2(\epsilon^{1/2} + \tau^{1/2} + h) + k + \tau^{1/2}(h^2 + h + \epsilon) + h^2\tau^{-1/2}\right).$$

When $\Theta = 1/2$ *(Crank-Nicolson scheme), we assume the stabilization parameter* $\tau \leq \frac{h}{2\|\beta\|}$; *then the following estimate holds:*

$$\|y^n - y_h^n(u)\|_{L^2(I;L^2(\Omega))} + \|p^n - p_h^n(u)\|_{L^2(I;L^2(\Omega))} \leq C(h^{\frac{3}{2}} + k^2), \tag{4.32b}$$

where C *depends on some spatial and temporal derivatives of* y, p, *and* y_d.

Proof. Let us start by substracting (2.9c) from (4.23) to obtain an error equation:

$$\begin{aligned}
(\frac{y^n - y^{n-1}}{k}, \varphi) + a(\Theta y^n + (1 - \Theta y^{n-1}), \varphi) - \left(\frac{y_h^n(u) - y_h^{n-1}(u)}{k}, \varphi\right) \\
- a_h^s(\Theta y_h^n(u) + (1 - \Theta) y_h^{n-1}(u), \varphi) \\
+ \left[\sum_{K \in \mathfrak{T}_h} \tau\left(\Theta(f^n + \mathbf{u}^n) + (1 - \Theta)(f^{n-1} + \mathbf{u}^{n-1}), \beta \cdot \nabla\varphi\right)\right]_K \\
- \sum_{K \in \mathfrak{T}_h} \tau\left(\frac{y_h^n(u) - y_h^{n-1}(u)}{k}, \nabla\varphi\right)_K = 0.
\end{aligned} \tag{4.33}$$

As in [33], we decompose the error $y^n - y_h^n(u)$ into an interpolation error and the difference of the interpolation and the solution

$$y_h^n(u) - y^n = (y_h^n(u) - \pi_h^n y) + (\pi_h^n y - y^n) = e_h^n + \eta_h^n.$$

The interpolation error η_h^n can be estimated with (4.6) by taking the degree of local polynomials $r = 1$. Then we need only to derive an estimate for e_h^n:

$$
\begin{aligned}
&(e_h^n - e_h^{n-1}, \varphi) + k a_h^s(\Theta e_h^n + (1-\Theta) e_h^{n-1}, \varphi) \\
&= k \left(\underbrace{y_t^n - \pi_h^n y_t + \left(\pi_h^n y_t - \frac{\pi_h^n y - \pi_h^{n-1} y}{k} \right)}_{T_1}, \varphi \right) \\
&+ k \left(\underbrace{\Theta\sigma\left(y^n - \pi_h^n y\right) + (1-\Theta)\sigma\left(y^{n-1} - \pi_h^{n-1} y\right) + \Theta\beta\cdot\nabla(y^n - \pi_h^n y) + (1-\Theta)\beta\cdot\nabla(y^{n-1} - \pi_h^{n-1} y)}_{T_{2\Theta}}, \varphi \right) \\
&+ k \sum_{K\in\mathfrak{T}_h} \tau(\underbrace{T_1 + T_{2\Theta} + \Theta\epsilon\Delta(\pi_h^n y - y^n) + (1-\Theta)\epsilon\Delta(\pi_h^{n-1} y - y^{n-1})}_{T_{3\Theta}}, \beta\cdot\nabla\varphi)_K \\
&- \sum_{K\in\mathfrak{T}_h} \tau(e_h^n - e_h^{n-1}, \beta\cdot\nabla\varphi)_K. \qquad (4.34)
\end{aligned}
$$

Particularly for the error estimate of backward Euler scheme, we take $\Theta = 1$ in (4.34) and obtain the error equation similar to (4.12), so that we can apply the techniques of the stability estimate (Theorem 4.1.2) to (4.34) by choosing $\varphi = e_h^n$ with $e_h^0 = 0$:

$$
\|e_h^n\|_0^2 + \frac{3k}{40}\sum_{j=1}^n \|e_h^j\|_s^2 \le Ck\left(\sum_{j=1}^n \|T_1^j\|_0^2 + \|T_{2\Theta}^j\|_0^2 + k\sum_{j=1}^n \|T_{3\Theta}^j\|_0^2 \right). \qquad (4.35)
$$

By inserting the bounds for the right-hand side given in [33] to (4.35) and combining with the well-known estimate (4.6), we finish the proof of one part of (4.32) by the following inequality:

$$
\|y^n - y_h^n(u)\|_{L^2(I;L^2(\Omega))} \le C\left(h^2 + k + \tau^{1/2}(h^2 + h + \epsilon) + h^2\tau^{-1/2}\right). \qquad (4.36)
$$

To show the second part of (4.32), we subtract (2.9a) from (4.24) and proceed as in the first part by using the stability estimate of adjoint equation (Theorem 4.1.3), we find the subsequent inequality:

$$
\|p^n - p_h^n(u)\|_{L^2(I;L^2(\Omega))} \le C\|y^n - y_h^n(u)\|_{L^2(I;L^2(\Omega))}. \qquad (4.37)
$$

Thus, the first part of Lemma 4.1.7 is derived for the backward Euler scheme.
When we take $\Theta = 1/2$ in (4.34), by choosing $\varphi = (e_h^n + e_h^{n-1})/2$ with $e_h^0 = 0$ and using Theorem 5.4 given in [33], we have

$$
\begin{aligned}
\|p^n - p_h^n(u)\|_0^2 + k\sum_{j=1}^n \left\| \frac{y^j + y^{j-1}}{2} - \frac{y_h^j + y_h^{j-1}}{2} \right\|_s^2 \qquad (4.38) \\
\le C(h^3 + k^4).
\end{aligned}
$$

Combining (4.38) with (4.37), we obtain the second part of Lemma 4.1.7 for Crank-Nicolson scheme. ■

Theorem 4.1.8 *Let $y,\ p,\ u$ and $y_h^n,\ p_h^n,\ u_h^n$ be the solutions of (2.9) and (4.12, 4.19) respectively. If $\Theta = 1$ (backward Euler scheme) with additional condition (4.14), we have*

$$
\begin{aligned}
&\|y^n - y_h^n\|_{L^2(I;L^2(\Omega))} + \|p^n - p_h^n\|_{L^2(I;L^2(\Omega))} + \|u^n - u_h^n\|_{L^2(I;L^2(\Omega))} \\
&\qquad \le C\left(h^{\frac{3}{2}} + h^2 + k + \tau^{1/2}(h^2 + h + \epsilon) + h^2\tau^{-1/2}\right). \qquad (4.39a)
\end{aligned}
$$

For $\Theta = 1/2$ (Crank-Nicolson scheme) with the condition $\tau \le h/2\|\beta\|$, we have

$$
\|y^n - y_h^n\|_{L^2(I;L^2(\Omega))} + \|p^n - p_h^n\|_{L^2(I;L^2(\Omega))} + \|u^n - u_h^n\|_{L^2(I;L^2(\Omega))} \le C(h^{\frac{3}{2}} + k^2), \qquad (4.39b)
$$

where C depends on some spatial and temporal derivatives of y, p, y_d and u.

Proof. Combining the bounds given by Lemmas 4.1.5-4.1.7, the Main Result of Theorem 4.1.8 can be established by the triangle inequality. ■

4.1.2.2 Semi-implicit scheme

We first derive the stability bounds for the state and adjoint equations of OCP (2.1) by using the similar argument in [84] which covers the error estimates of parabolic problems using semi implicit scheme. In this sense, as in previous section, we first find the approximate solution $y_h^n,\ p_h^n \in V_h$ and $u_h^n \in U_h^{ad}$ obtained by using semi-implicit scheme and SUPG method, respectively:

$$\left(\frac{y_h^n - y_h^{n-1}}{k}, \varphi\right) + \left(\epsilon(\nabla y_h^n, \nabla\varphi) + (\beta\cdot\nabla y_h^{n-1}, \varphi) + (\sigma y_h^{n-1}, \varphi)\right) \tag{4.40a}$$
$$= \left(f^n + u_h^n, \varphi\right) + \sum_{K\in\mathfrak{T}_h} \tau\left(-\frac{y_h^n - y_h^{n-1}}{k}, \beta\cdot\nabla\varphi\right) + \sum_{K\in\mathfrak{T}_h} \tau\left(f^n + u_h^n + \epsilon\Delta y_h^n - \beta\cdot\nabla y_h^{n-1} - \sigma y_h^{n-1}, \beta\cdot\nabla\varphi\right)_K$$

for all $\varphi \in V_h$ and $y_h^0 = y_h(0, x)$, and

$$\left(\frac{p_h^{n-1} - p_h^n}{k}, \psi\right) + \left(\epsilon(\nabla\psi, \nabla p_h^{n-1}) + (\beta\cdot\nabla\psi, p_h^n) + \sigma(\psi, p_h^n)\right) = \left((y_h^{n-1} - y_{h,n-1}^d), \psi\right)$$
$$+ \sum_{K\in\mathfrak{T}_h} \tau\left(\epsilon\Delta\psi - \beta\cdot\nabla\psi - \sigma\psi, \beta\cdot\nabla p_h^n\right) - \sum_{K\in\mathfrak{T}_h} \tau\left(\frac{p_h^{n-1} - p_h^n}{k}, \beta\cdot\nabla\psi\right)_K \tag{4.40b}$$

for all $\psi \in V_h$. Let us consider $y_{h,n}^d$ is the approximate solution of y_d and $p_{T,h} = p_h(T, x)$, and the gradient equation given by

$$(\alpha u_h^n - p_h^{n-1}, w - u_h^n) \geq 0 \qquad \forall w \in U_h^{ad}. \tag{4.40c}$$

We first present the stability bounds of state equation for semi-implicit scheme in the following theorem.

Theorem 4.1.9 *(**Stability of the state equation**) The semi-implicit approximation scheme (4.40a) is unconditionally stable on any finite time interval $(0, T)$ and the solution y_h^n satisfies*

$$\|y_h^n\|_0^2 \leq \left(\|y_h^0\|_0^2 + Ck(1+\tau)\sum_{j=1}^{n} \|f^j\|_0^2 + \|u_h^j\|_0^2\right)\cdot \exp(C^* k(1+\tau)), \tag{4.41}$$

where $\tau < 1$, $C > 0$, $C^* > 0$ are constants independent of h and k.

Proof. As in backward Euler scheme, we start by choosing the test function $\varphi = y_h^n$ in (4.40a) and using Poincare Inequality and Young Inequality, we have

$$\begin{aligned}
&\frac{1}{2}\|y_h^n\|_0^2 - \frac{1}{2}\|y_h^{n-1}\|_0^2 + \frac{1}{2}\|y_h^n - y_h^{n-1}\|_0^2 + \epsilon k\|\nabla y_h^n\|_0^2 \\
&\quad\leq C_1 k(1+\tau)\|y_h^{n-1}\|_0\|\nabla y_h^n\|_0 + C_2 k(1+\tau)\left(\|f^n\|_0 + \|u_h^n\|_0\right)\|\nabla y_h^n\|_0 \\
&\quad+ \frac{\tau}{2}\|y_h^n - y_h^{n-1}\|_0^2 + \frac{\tau}{2}\|\beta\cdot\nabla y_h^n\|_0^2.
\end{aligned}$$

By following the steps in [84] and choosing $\tau < 1$, we easily obtain that

$$|y_h^n\|_0^2 - \|y_h^{n-1}\|_0^2 \leq C^* k(1+\tau)\|y_h^{n-1}\|_0^2 + Ck(1+\tau)\left(\|f^n\|_0^2 + \|u_h^n\|_0^2\right).$$

Summation of the time steps $j = 1, 2, ..., n$, and using Gronwall Inequality, we obtain the desired result (4.41). ■

Theorem 4.1.10 **(Stability of the adjoint equation**) *The semi-implicit approximation scheme (4.40b) is unconditionally stable on any finite time interval* $(0, T)$ *and the solution* p_h^n *satisfies*

$$\|p_h^n\|_0^2 \le \left(\|p_{T,h}\|_0^2 + Ck \sum_{j=1}^{n} \|y_h^j - y_{h,j}^d\|_0^2 \right) \cdot \exp(C^* k(1+\tau)), \tag{4.42}$$

where $\tau < 1,\ C > 0,\ C^* > 0$ *are constants independent of h and k.*

Proof. By proceeding essentially as in the proof of Theorem 4.1.9, choosing $\psi = p_h^{n-1}$ in (4.40b), we can obtain the desired result. ■

To derive the Main Theorem, we need some lemmas as in previous section. In this sense, we shall use two auxiliary variables $y_h^n(u),\ p_h^n(u) \in V_h \times V_h$:

$$\begin{aligned} &\left(\frac{y_h^n(u) - y_h^{n-1}(u)}{k}, \varphi \right) + \left(\epsilon(\nabla y_h^n(u), \nabla\varphi) + (\beta\cdot\nabla y_h^{n-1}(u), \varphi) + (\sigma y_h^{n-1}(u), \varphi) \right) \\ &= (f^n + \mathbf{u}^n, \varphi) + \sum_{K\in\mathfrak{T}_h} \tau \left(-\frac{y_h^n(u) - y_h^{n-1}(u)}{k}, \beta\cdot\nabla\varphi \right) \\ &+ \sum_{K\in\mathfrak{T}_h} \tau \left(f^n + \mathbf{u}^n + \epsilon\Delta y_h^n(u) - \beta\cdot\nabla y_h^{n-1}(u) - \sigma y_h^{n-1}(u), \beta\cdot\nabla\varphi \right)_K \end{aligned} \tag{4.43a}$$

for all $\varphi \in V_h$ and $y_h^0(u) = y_h^0$, $n = 1, 2, ..., N$, and

$$\begin{aligned} &\left(\frac{p_h^{n-1}(u) - p_h^n(u)}{k}, \psi \right) + \left(\epsilon(\nabla\psi, \nabla p_h^{n-1}(u)) + (\beta\cdot\nabla\psi, p_h^n(u)) + \sigma(\psi, p_h^n(u)) \right) = \left((y_h^{n-1}(u) - y_{h,n-1}^d), \psi \right) \\ &+ \sum_{K\in\mathfrak{T}_h} \tau \left(\epsilon\Delta\psi - \beta\cdot\nabla\psi - \sigma\psi, \beta\cdot\nabla p_h^n(u) \right) - \sum_{K\in\mathfrak{T}_h} \tau \left(\frac{p_h^{n-1}(u) - p_h^n(u)}{k}, \beta\cdot\nabla\psi \right)_K \end{aligned} \tag{4.43b}$$

for all $\psi \in V_h$ and $p_{T,h} = 0$, $n = N, ..., 2, 1$. We use the same notation θ^n and ζ^n as defined in previous section to have the connection between the approximation solution $y_h^n,\ p_h^n$ and auxiliary solution $y_h^n(u),\ p_h^n(u)$.

Lemma 4.1.11 *Let* (y_h, p_h) *and* $(y_h(u), p_h(u))$ *be the solutions of (4.40a-b) and (4.43a-b), respectively. Then there exists a constant C independent of h and k, such that the following estimates hold:*

$$\|y_h - y_h(u)\|_{L^2(I;L^2(\Omega))} + \|p_h - p_h(u)\|_{L^2(I;L^2(\Omega))} \le C\|u - u_h\|_{L^2(I;L^2(\Omega))}. \tag{4.44}$$

Proof. We can estimate (4.44) by proceeding the same approach in Lemma 4.1.5 and using the proof of the stability estimate (Theorem 4.1.9). ■

The bound of $\|u - u_h\|_{L^2(I;L^2(\Omega))}$ is given by Lemma 4.1.6 in the previous section.

Lemma 4.1.12 *Let* (y, p) *and* $y_h(u), p_h(u)$ *be the solutions of (2.9) and (4.43a-b), respectively. We assume that* $y,\ p \in L^2(I; H_0^1(\Omega)\cap H^2(\Omega))\cap H^1(I; H^2(\Omega))\cap H^2(I; L^2(\Omega))$, $y_d \in H^1(I; L^2(\Omega))$. *Furthermore, the additional condition (4.14) be satisfied. Then we have*

$$\|y^n - y_h^n(u)\|_{L^2(I;L^2(\Omega))} \le \exp(C^* k(1+\tau)) \times \left(C\left(h^2 + k + \tau^{1/2}(h^2 + h + \epsilon) + h^2\tau^{-1/2} \right) \right), \tag{4.45}$$

where $C^* > 0$ *and C depends on some spatial and temporal derivatives of* $y,\ p$, *and* y_d.

Proof. As in the Θ scheme, we start the proof by substracting (2.9c) from (4.43a) and we decompose the error $y - y_h(u)$ into an interpolation error and the difference of the interpolation and the solution:

$$y_h^n(u) - y^n = (y_h^n(u) - \pi_h^n y) + (\pi_h^n y - y^n) = e_h^n + \eta_h^n.$$

Now the interpolation error η_h^n can be estimated with (4.6), taking the degree of local polynomials $r = 1$. Then, we only need to derive an estimate for e_h^n :

$$\left(\frac{(e_h^n - e_h^{n-1})}{k}, \varphi\right) + \epsilon(\nabla e_h^n, \nabla\varphi) + (\beta \cdot \nabla e_h^{n-1}) + \sigma(e_h^n, \varphi)$$
$$+ \sum_{K\in\mathfrak{T}_h} \tau\left(\epsilon\Delta e_h^n(u) - \beta \cdot \nabla e_h^{n-1}(u) - \sigma e_h^{n-1}(u), \beta \cdot \nabla\varphi\right)_K = (v_h^n, \varphi), \tag{4.46}$$

where $v_h^n \in V_h$ is defined by the relation

$$(v_h^n, \varphi) = \left(\underbrace{y_t^n - \pi_h^n y_t + \left(\pi_h^n y_t - \frac{\pi_h^n y - \pi_h^{n-1} y}{k}\right) + \sigma\left(y^n - \pi_h^n y\right) + \beta \cdot \nabla(y^n - \pi_h^n y)}_{T_1}, \varphi\right)$$
$$+ \sum_{K\in\mathfrak{T}_h} \tau\left(\underbrace{T_1 + \epsilon\Delta(\pi_h^n y - y^n)}_{T_2}, \beta \cdot \nabla\varphi\right)_K - \sum_{K\in\mathfrak{T}_h} \tau\left(e_h^n - e_h^{n-1}, \beta \cdot \nabla\varphi\right)_K. \tag{4.47}$$

Now, e_h^n satisfies a scheme like (4.40a) and so, as in Theorem 4.1.9, by assuming $e_h^0 = 0$, we get

$$\|e_h^n\|_0^2 \le \left(Ck \sum_{j=1}^{n} \|v_h^j\|_0^2\right) \cdot \exp(C^* k(1+\tau)). \tag{4.48}$$

The bound of $\|v_h^j\|_0$ can be found as in the backward Euler scheme. That is, when we take $\Theta = 1$ in (4.34), the right-hand side of (4.34) is the same as in (4.47). Therefore,

$$k \sum_{j=1}^{n} \|v_h^j\|_0 \le C\left(h^2 + k + \tau^{1/2}(h^2 + h + \epsilon) + h^2\tau^{-1/2}\right). \tag{4.49}$$

By inserting (4.49) into (4.48), we obtain the desired result. ■

Now, we are ready to derive the following theorem.

Theorem 4.1.13 *Let y, p, u and y_h^n, p_h^n, u_h^n be the solutions of (2.9) and (4.40), respectively. Assuming the additional condition (4.14), we have*

$$\|y^n - y_h^n\|_{L^2(I;L^2(\Omega))} + \|p^n - p_h^n\|_{L^2(I;L^2(\Omega))} + \|u^n - u_h^n\|_{L^2(I;L^2(\Omega))}$$
$$\le C\left(h^{\frac{3}{2}} + \exp(C^* k(1+\tau)) \cdot \left(h^2 + k + \tau^{1/2}(h^2 + h + \epsilon) + h^2\tau^{-1/2}\right)\right),$$

where C depends on some spatial and temporal derivatives of y, p, y_d and u.

Proof. Combining the bounds given by Lemmas 4.1.11, 4.1.6, and 4.1.12, the main result of Theorem 4.1.13 can be established by the Triangle Inequality. ■

4.1.3 Numerical Examples

In this section, we consider two-dimensional OCPs governed by diffusion-convection-reaction equation to demonstrate our convergence analysis. For all examples, we give the numerical performance of the SUPG method by choosing an appropriate stabilization parameter. When we take Crank-Nicolson method as a time integrators, we choose the stabilization parameter which is proportional to the mesh width, i.e., $\tau \leq h/2$. Actually, in the application of the SUPG stabilization, the choice of the stabilization parameter τ is significantly important. Hence, in Example 4.1.1, we study SUPG method with different stabilization parameters and compare the effect of these parameters. The equilibration of the terms on the right hand side of (4.32b) gives the length of the time step $k \cong h^{3/4}$ and the expected order of convergence is $O(h^{3/2})$ for the Crank-Nicolson method. As in the case of backward Euler and semi-implicit schemes, we derive the optimal scalings of the mesh size h, and time step k by considering the estimates given in Section 4.1.2. Then, we have the only one asymptotic order of convergence by setting the stabilization parameter proportional to time step k, i.e., $\tau \leq 4k/5$. By scaling $k \cong h^{4/3}$, we balance the terms $O(k)$ and $O(h^2\tau^{-1/2}) = O(h^2k^{-1/2})$ to obtain the optimal L^2 error. Hence, when we take the backward Euler and semi-implicit schemes as a time integrators, the expected order is $O(h^{4/3})$. We use the iterative method, MINRES with the idealized block-diagonal preconditioner (4.28) to solve the fully discrete systems. In the following examples, the state variable y, the control variable u, and the adjoint variable p are approximated by piecewise-linear elements with SUPG in the case of spatial discretization. The results are presented for Crank-Nicolson, backward Euler and semi-implicit methods. For the time-dependent distributed control problem, we use the examples from [27, 28] with known exact solutions. For the time-dependent boundary OCPs, we have constructed from the elliptic OCP given in [3] without exact solutions.

Example 4.1.1 (Two-dimensional control constrained problem)
We choose the OCP in [28]. The distributed OCP (2.1) with $\Omega = (0,1)\times(0,1)$, $T > 0$, $Q = (0,T)\times\Omega$, $\Sigma = (0,T)\times\partial\Omega$. Let us choose $\sigma = 0$, $\beta = (1,0)$, and $f(x,t)$, $y_d(x,t)$ and$y_0(x)$ are chosen such that the state, adjoint state and control solutions are

$$\begin{aligned} y(x,t) &= \exp(-t)\sin(2\pi x_1)\sin(2\pi x_2), \\ p(x,t) &= \exp(-t)(1-t)\sin(2\pi x_1)\sin(2\pi x_2), \\ u(x,t) &= \max\{-p,0\}. \end{aligned}$$

The control constraints (2.1c) is defined as $u \geq 0$.

In Figure 4.1, we can observe the order of convergence for different choices of stabilization parameters. We can note that, the convergence order is estimated by taking the logarithm with base two of the quotient of the error at grid size h and the error at grid size $h/2$.

Table 4.1: Example 4.1.1 with $\tau = 2h/7, \epsilon = 10^{-5}$ via Crank-Nicolson method with SUPG.

h	$\|\|y-y_h\|\|$	order	$\|\|p-p_h\|\|$	order	$\|\|u-u_h\|\|$	order
2^{-2}	6.4921e-2	-	3.1103e-2	-	2.073e-2	-
2^{-3}	3.4807e-2	0.89	1.1993e-2	1.37	8.1020e-3	1.36
2^{-4}	1.3658e-2	1.35	3.7622e-3	1.67	2.5511e-3	1.66
2^{-5}	5.1733e-3	1.40	1.3907e-3	1.44	9.1609e-4	1.48

In Table 4.1, we give the results by considering the stabilization parameter, $\tau = 2h/7$. With this pa-

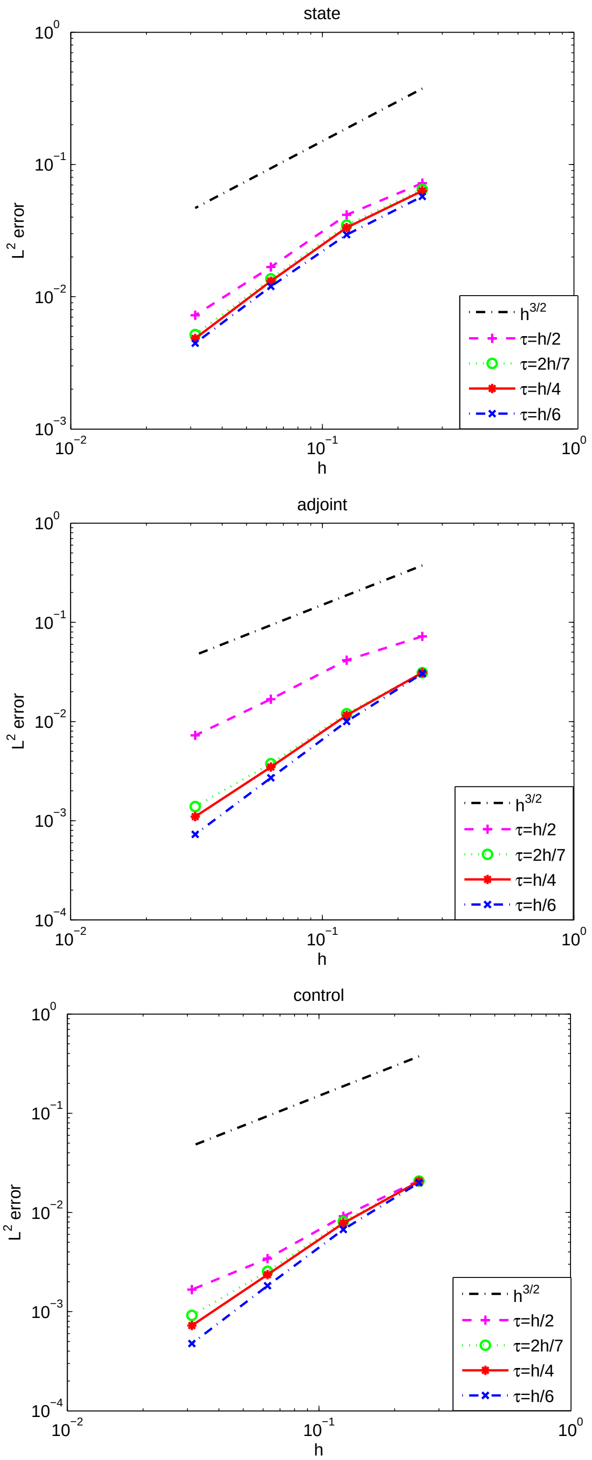


Figure 4.1: L_2 error for SUPG method with $\epsilon = 10^{-5}$.

rameter, we can see the expected order $O(h^{3/2})$ as in observed in Figure 4.1.

In Figure 4.2, 4.3, we use Crank-Nicolson method and take $\epsilon = 10^{-5}$, $\tau = 2h/7$ with $h = 2^{-5}$ and $t = 0.5$. The SUPG stabilized approximate solution are nearly the same as the exact solutions. Moreover, in [28], the same example is discussed and the results which are presented by using the characteristic finite element method in spatial discretization with backward Euler method, are similar to our results. To see the efficieny of SUPG method, we can notice that the oscillations in the contours of the unstabilized approximate state and control equation can be fixed in the contours of the SUPG stabilized state and control equation.

Table 4.2: Example 4.1.1 with $\tau = 2k/3$, $\epsilon = 10^{-5}$ via backward Euler with SUPG.

$h/\sqrt{2}$	$\|y-y_h\|$	order	$\|p-p_h\|$	order	$\|u-u_h\|$	order
2^{-2}	5.9934e-2	-	3.7142e-2	-	3.0848e-2	-
2^{-3}	3.4675e-2	0.78	1.0944e-2	1.76	7.3083e-3	2.07
2^{-4}	1.2344e-2	1.49	2.2452e-3	2.28	1.3397e-3	2.44
2^{-5}	3.9486e-3	1.64	8.7074e-4	1.36	5.358e-4	1.32

Table 4.3: Example 4.1.1 with $\tau = k/3$, $\epsilon = 10^{-2}$ via semi-implicit with SUPG.

$h/\sqrt{2}$	$\|y-y_h\|$	order	$\|p-p_h\|$	order	$\|u-u_h\|$	order
2^{-2}	1.0183e-1	-	5.0774e-2	-	3.3047e-2	-
2^{-3}	3.8663e-2	1.39	1.0921e-2	2.21	7.3658e-3	2.16
2^{-4}	1.2667e-2	1.60	1.5694e-3	2.79	9.8216e-4	2.90
2^{-5}	3.8208e-3	1.72	5.9410e-4	1.40	4.2387e-4	1.21

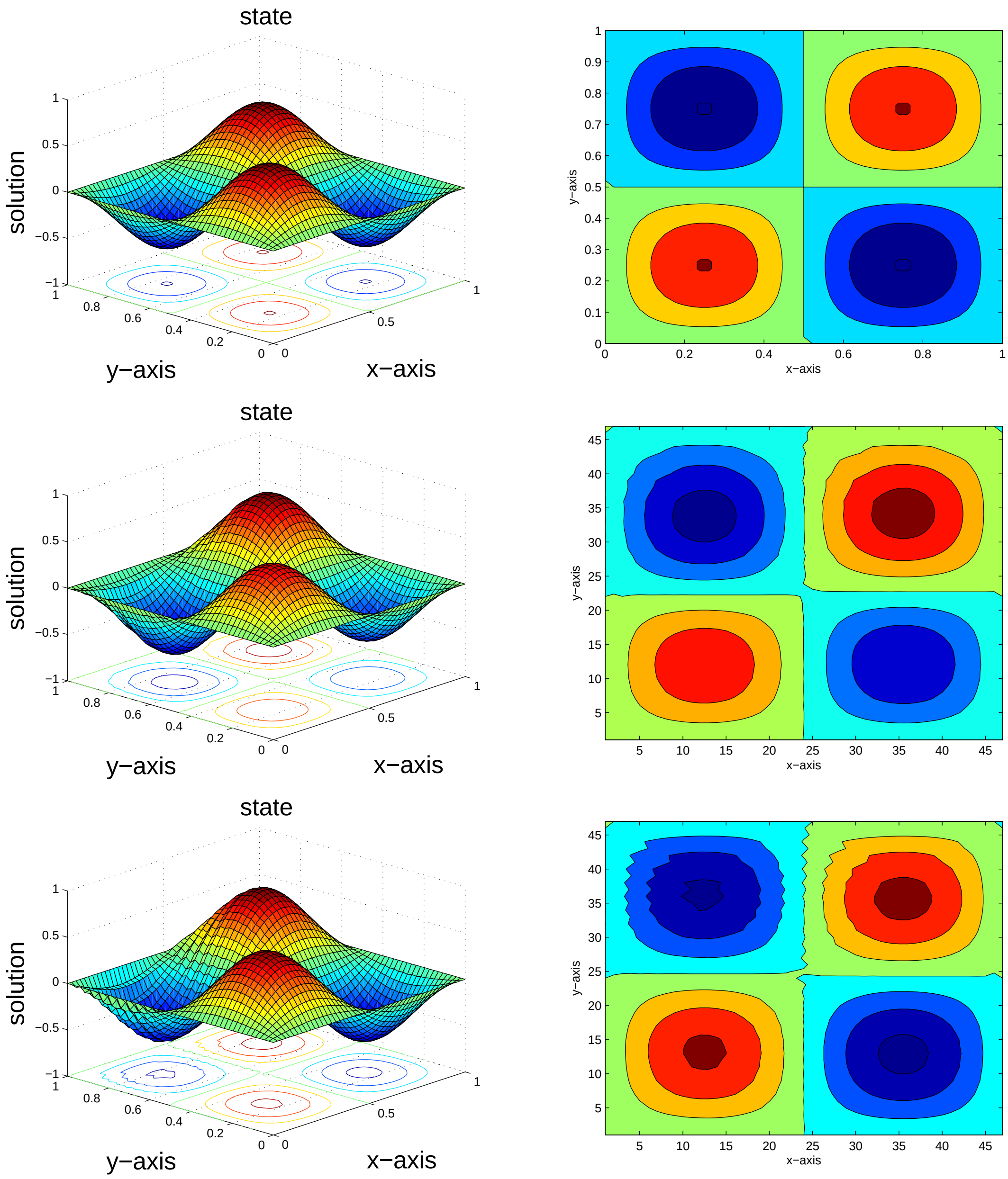


Figure 4.2: Example 4.1.1 via Crank-Nicolson method with $h = 2^{-5}$: The exact state solution (top), the stabilized approximate state solution (middle), the unstabilized approximate state solution (bottom), their contour lines in the left side.

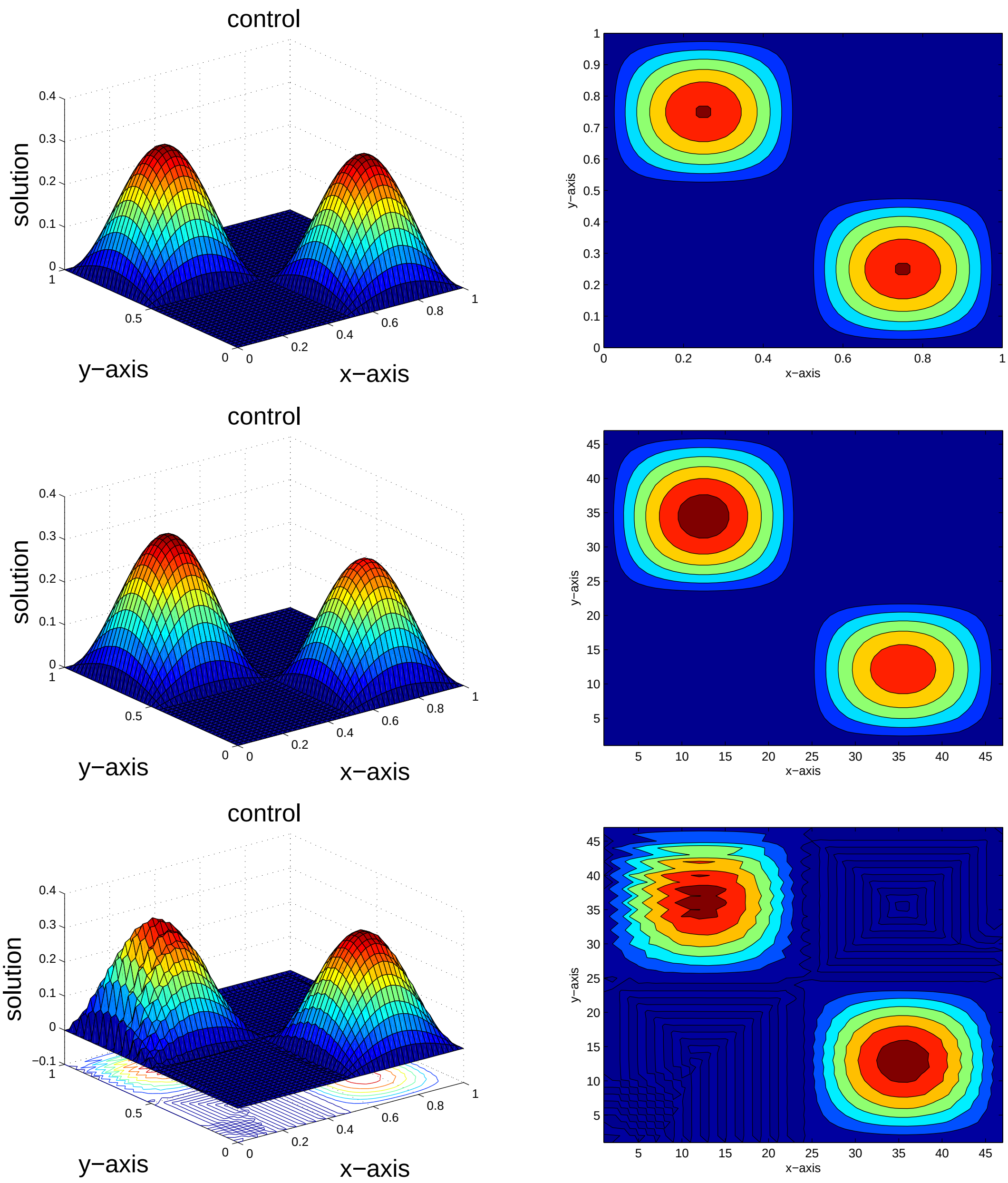


Figure 4.3: Example 4.1.1 via Crank-Nicolson method with $\Delta x = 2^{-5}$: The exact control solution (top), the stabilized approximate control solution (middle), the unstabilized approximate control solution (bottom), their contour lines in the left side.

In Tables 4.2-4.3, we can clearly observe the expected order $O(h^{4/3})$. As it is mentioned in [84], for small ϵ , the convergence of the semi-implicit scheme deteriorates exponentially. Hence, we choose an appropriate value for ϵ with semi-implicit scheme. In this example, by choosing $\epsilon = 10^{-2}$, we get a satisfactory result in terms of convergence.

Example 4.1.2(Two-dimensional control constrained problem)
The basic setting of this example is taken from [28]. The domain, the OCP and control constraint are presented as in the previous example. We choose $\epsilon = 10^{-5}$, $\beta = (0.5, 0.5)$, $\sigma = 0$, and $f(x,t)$ and $y_0(x)$ are chosen such that the state, adjoint state and control solutions are

$$\begin{aligned}
y(x,t) &= p\left(\frac{1}{2\sqrt{\epsilon}}\sin(t_x) - 8\epsilon\pi^2 - \frac{\sqrt{\epsilon}}{2} + \frac{1}{2}\sin(t_x)^2\right) \\
&- \pi\cos(\pi t)\sin(2\pi x_1)\sin(2\pi x_2)\exp\left(\frac{-1+\cos(t_x)}{\sqrt{\epsilon}}\right), \\
p(x,t) &= \sin(\pi t)\sin(2\pi x_1)\sin(2\pi x_2)\exp\left(\frac{-1+\cos(t_x)}{\sqrt{\epsilon}}\right), \\
u(x,t) &= \max\{-p, 0\} \\
y_d(x,t) &= \pi(1 + 2\sqrt{\epsilon}\sin(t_x))\sin(\pi t)\sin(2\pi(x_1+x_2))\exp\left(\frac{-1+\cos(t_x)}{\sqrt{\epsilon}}\right), \\
t_x &= t - 0.5(x_1 + x_2).
\end{aligned}$$

As in the previous example, we first give the numerical studies obtained by using Crank-Nicolson scheme. We take the same proportion between the mesh size h and time step size k, i.e., $k \cong h^{3/4}$. By choosing the stabilization parameter $\tau = h/4$, we obtain the subsequent results supporting our analytical results. In Table 4.4, we obtain the expected order is $O(h^{3/2})$ for Crank-Nicolson method.

Table 4.4: Example 4.1.2 with $\tau = h/4$, $\epsilon = 10^{-5}$ via Crank-Nicolson method with SUPG.

h	$\|y - y_h\|$	order	$\|p - p_h\|$	order	$\|u - u_h\|$	order
2^{-3}	1.0512e-1	-	1.5480e-2	-	1.0661e-2	-
2^{-4}	3.9526e-2	1.41	5.9417e-3	1.38	4.2352e-3	1.33
2^{-5}	1.2448e-2	1.66	2.6355e-3	1.17	1.8845e-3	1.17
2^{-6}	3.2615e-3	1.93	9.219e-4	1.51	6.7908e-4	1.47

In the Figure 4.4, the SUPG stabilized approximate solution has more likeness to the exact solution than the unstabilized solution. Although, the usage of the SUPG method provides us more accurate solution than the unstabilized case, the differences between the exact and stabilized solution can be seen especially in the direction of the convection term.

In Figure 4.5, we can clearly see the efficiency of the SUPG method in the solution of control variable. Howewer as in Figure 4.4, there are some differences in the $x = y$ direction.

In Table 4.5-4.6, we illustrate the numerical studies of backward Euler and semi-implicit scheme, respectively. By choosing the appropriate stabilization parameter $\tau = 4k/5$ for both backward Euler and semi-implicit scheme, we get the orders of convergence, $O(h^{4/3})$.

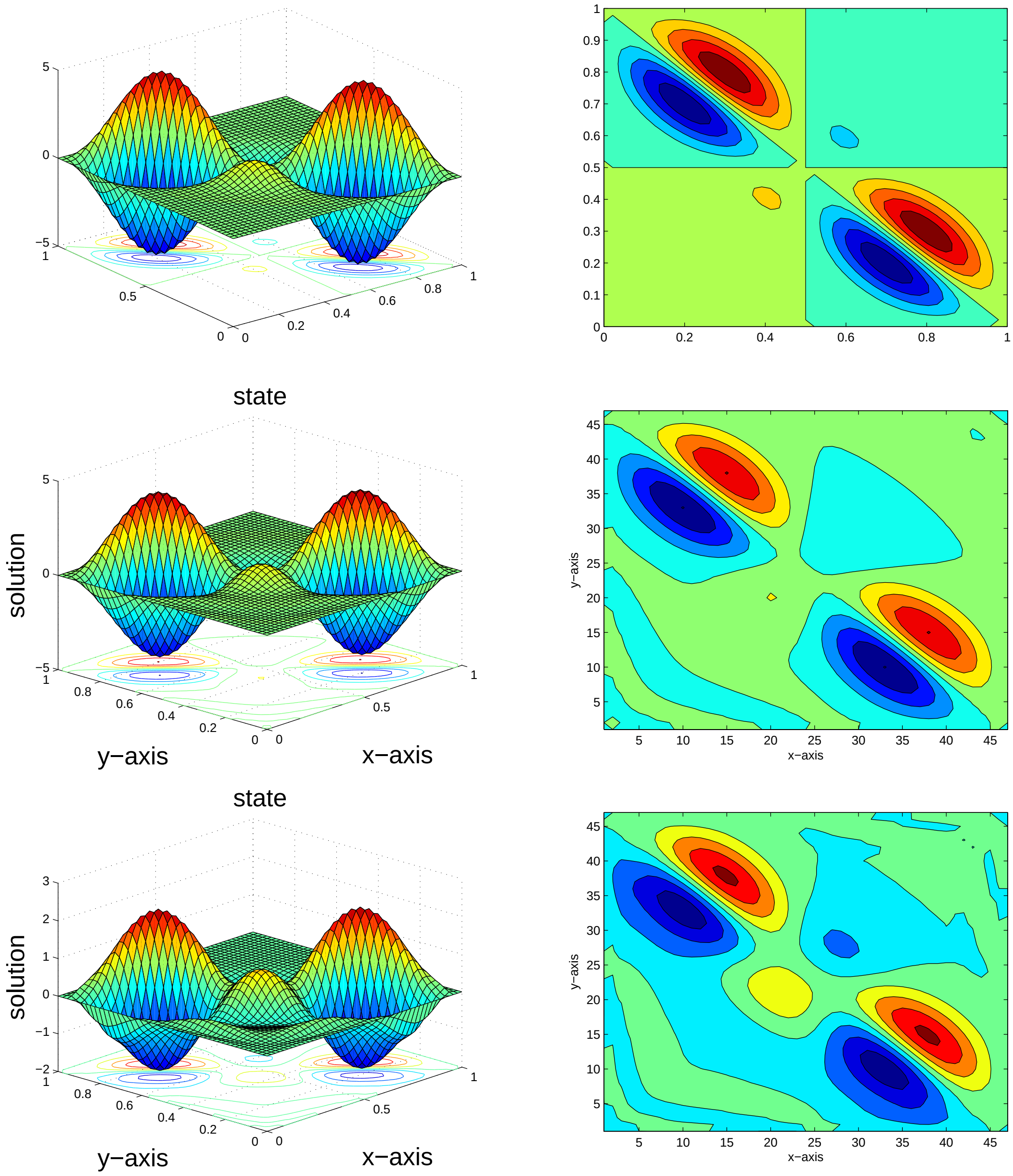


Figure 4.4: Example 4.1.2 via Crank-Nicolson method with $\Delta x = 2^{-5}$: The exact state solution (top), the stabilized approximate state solution (middle), the unstabilized approximate state solution (bottom), their contour lines in the left side.

Table 4.5: Example 4.1.2 with $\tau = 4k/5$, $\epsilon = 10^{-5}$ via backward Euler method with SUPG.

$h/\sqrt{2}$	$\|y - y_h\|$	order	$\|p - p_h\|$	order	$\|u - u_h\|$	order
2^{-2}	2.0462e-1	-	4.2855e-2	-	4.0050e-2	-
2^{-3}	9.2722e-2	1.14	1.0940e-2	1.96	8.4754e-3	2.24
2^{-4}	4.6580e-2	0.99	5.3094e-3	2.04	4.0874e-3	1.05
2^{-5}	2.0143e-2	1.21	2.4378e-3	1.13	1.8015e-3	1.18

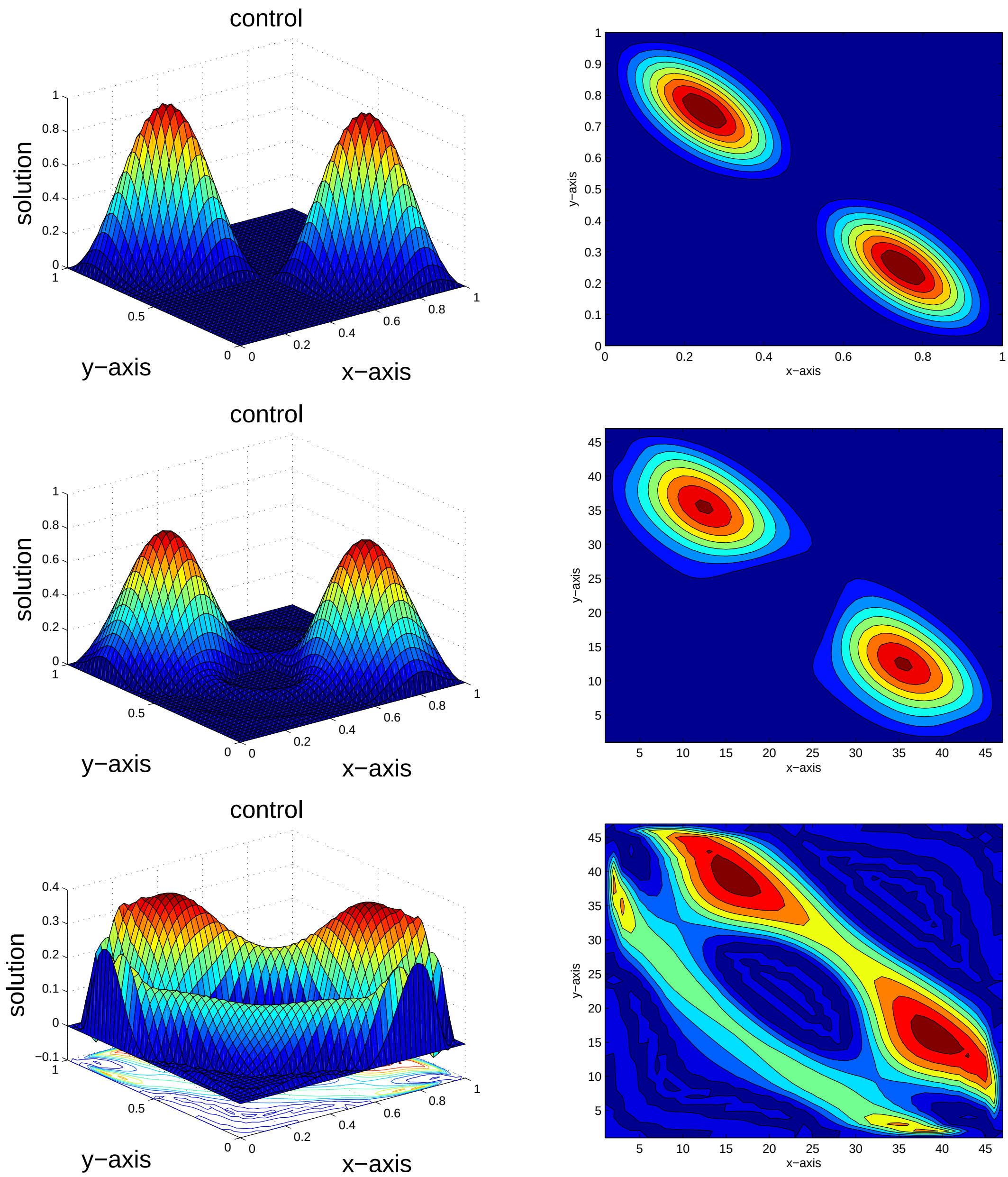


Figure 4.5: Example 4.1.2 via Crank-Nicolson method with $\Delta x = 2^{-5}$: The exact control solution (top), the stabilized approximate control solution (middle), the unstabilized approximate control solution (bottom), their contour lines in the left side.

Table 4.6: Example 4.1.2 with $\tau = 4k/5$, $\epsilon = 0.005$ via semi-implicit method with SUPG.

$h/\sqrt{2}$	$\|y - y_h\|$	order	$\|p - p_h\|$	order	$\|u - u_h\|$	order
2^{-2}	1.5324e-1	-	4.6177e-2	-	3.1771e-2	-
2^{-3}	7.8597e-2	0.96	2.3064e-2	1.00	1.6912e-2	0.90
2^{-4}	2.6199e-2	1.58	1.0275e-2	1.17	7.3080e-3	1.21
2^{-5}	7.2459e-3	1.85	4.1238e-3	1.32	2.9196e-3	1.32

Example 4.1.3(Two-dimensional control constrained problem)
This example is studied in [27]. For this example, we take the control constraints $0 \le u \le 0.5$. We choose $\epsilon = 10^{-5}$, $\beta = (0.5, 0.5)$, $\sigma = 0$, and $f(x,t)$, and $y_0(x)$ are chosen such that the state, adjoint state and control solutions are

$$\begin{aligned}
y(x,t) &= p(\frac{1}{2\sqrt{\epsilon}}\sin(t_x) + 8\epsilon\pi^2 + \frac{\sqrt{\epsilon}}{2} - \frac{1}{2}\sin(t_x)^2) \\
&\quad -\pi\cos(\pi t)\sin(2\pi x_1)\sin(2\pi x_2)\exp(\frac{-1+\cos(t_x)}{\sqrt{\epsilon}}), \\
p(x,t) &= \sin(\pi t)\sin(2\pi x_1)\sin(2\pi x_2)\exp(\frac{-1+\cos(t_x)}{\sqrt{\epsilon}}), \\
u(x,t) &= \max\{0, \min(-p, 0.5)\} \\
y_d(x,t) &= \pi(1 + 2\sqrt{\epsilon}\sin(t_x))\sin(\pi t)\sin(2\pi(x_1+x_2))\exp(\frac{-1+\cos(t_x)}{\sqrt{\epsilon}}), \\
t_x &= t - 0.5(x_1 + x_2).
\end{aligned}$$

This is so similar to Example 4.1.2, except the control constraints. The control constraint defined in Example 4.1.2 has only a lower bound, whereas the control constraint in this example has both lower and upper bound. In the following Table 4.7, we can see the $O(h^{3/2})$ order accuracy for the Crank-Nicolson method by taking the parameter $\tau = h/8$.

Table 4.7: Example 4.1.3 with $\tau = h/8$, $\epsilon = 10^{-5}$ via Crank-Nicolson method with SUPG.

h	$\|y - y_h\|$	order	$\|p - p_h\|$	order	$\|u - u_h\|$	order
2^{-2}	2.6425e-1	-	1.5792e-1	-	6.8394e-3	-
2^{-3}	1.1201e-1	1.24	2.3062e-2	2.77	1.4405e-2	1.07
2^{-4}	3.9680e-2	1.49	6.5409e-3	1.82	4.0418e-3	1.83
2^{-5}	1.2406e-2	1.67	2.8686e-3	1.19	1.7745e-3	1.19
2^{-6}	3.1830e-3	1.36	9.2918e-4	1.62	5.9923e-4	1.56

For the backward Euler and semi-implicit scheme, we again take the stabilization parameter proportional to the length of the time step size, i.e.,$\tau \le 4k/5$. Tables 4.8-4.9 show that the convergence orders of L^2 error in all variables are achieved as expected.

Table 4.8: Example 4.1.3 with $\tau = 4k/5$, $\epsilon = 10^{-5}$ via backward Euler method with SUPG.

$h/\sqrt{2}$	$\|y - y_h\|$	order	$\|p - p_h\|$	order	$\|u - u_h\|$	order
2^{-2}	2.0429e-1	-	4.2832e-2	-	3.8896e-2	-
2^{-3}	9.2702e-2	1.14	1.0957e-2	1.96	7.6304e-3	2.34
2^{-4}	4.6555e-2	0.99	5.3384e-3	1.04	3.3266e-3	1.20
2^{-5}	2.0132e-2	1.21	2.4539e-3	1.12	1.5122e-3	1.14

Table 4.9: Example 4.1.3 with $\tau = 4k/5,\ \epsilon = 0.005$ via semi-implicit method with SUPG.

$h/\sqrt{2}$	$\|\|y - y_h\|\|$	order	$\|\|p - p_h\|\|$	order	$\|\|u - u_h\|\|$	order
2^{-2}	1.4030e-1	-	4.9870e-2	-	2.4990e-2	-
2^{-3}	6.6726e-2	1.07	2.3230e-2	1.10	1.3974e-2	0.83
2^{-4}	2.2837e-2	1.54	1.0395e-2	1.16	6.2149e-3	1.17
2^{-5}	8.4950e-3	1.42	4.1925e-3	1.31	2.5356e-3	1.29

In Figure 4.6-4.7, we clearly present the accuracy of the SUPG method numerically. As a difference of previous example, in this example we have upper bound for control variable which can be observed in Figure 4.7. By correcting the unstabilized solutions, we obtain the good approximation to exact solution with SUPG method except for the direction of convection term.

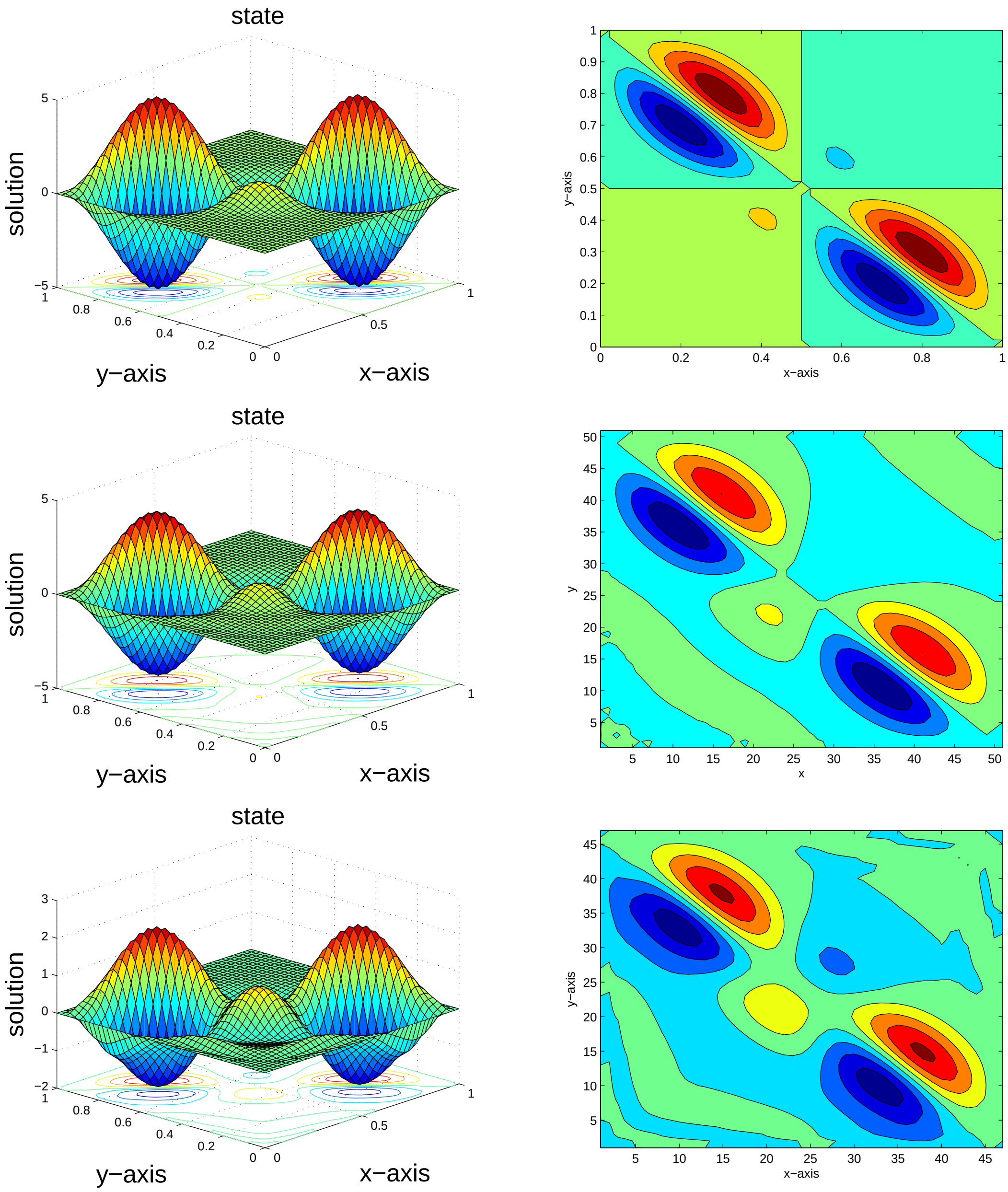


Figure 4.6: Example 4.1.3 via Crank-Nicolson method with $\Delta x = 2^{-5}$: The exact state solution (top), the stabilized approximate state solution (middle), the unstabilized approximate state solution (bottom), their contour lines in the right side.

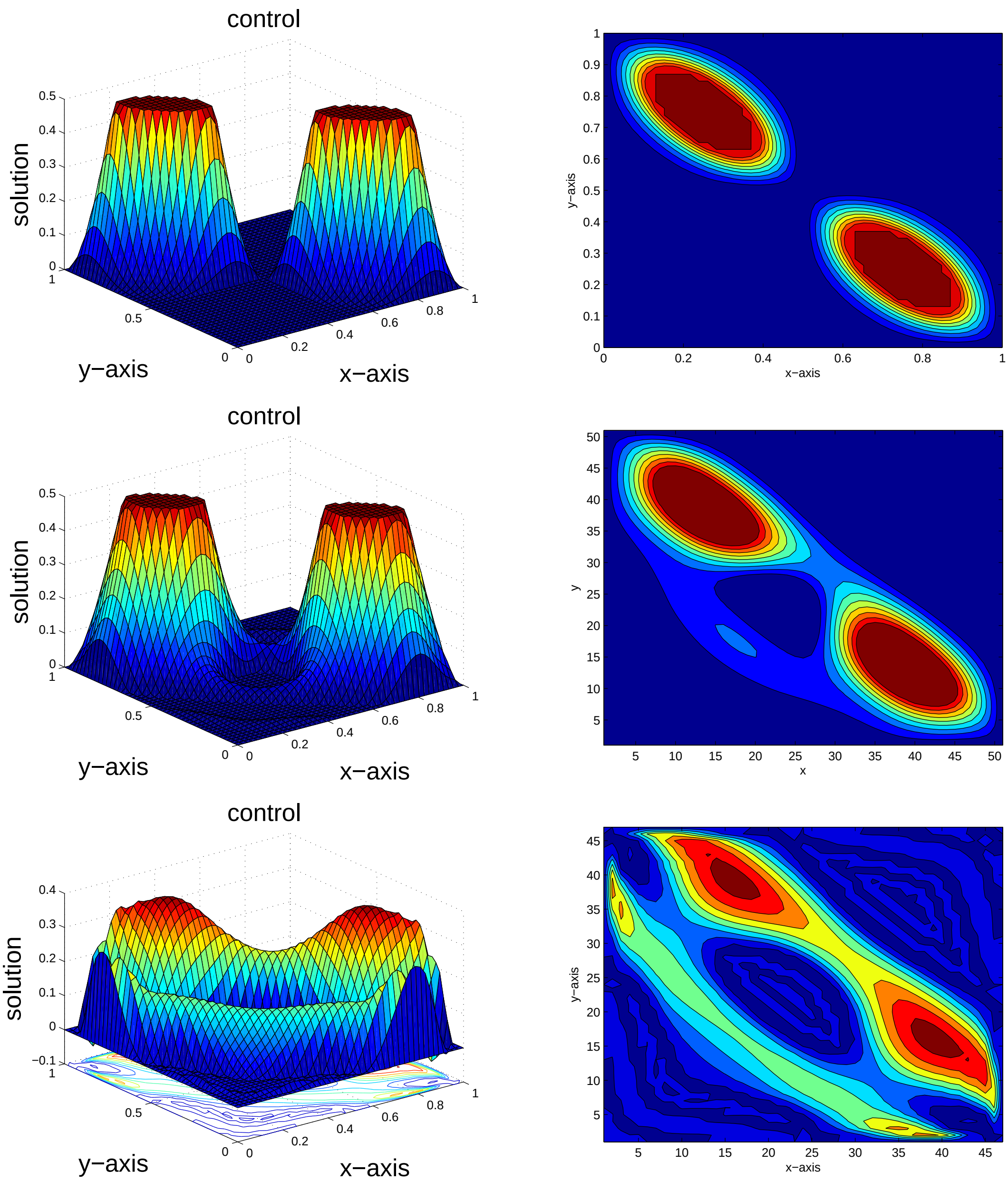


Figure 4.7: Example 4.1.3 via Crank-Nicolson method with $\Delta x = 2^{-5}$: The exact control solution (top), the stabilized approximate control solution (middle), the unstabilized approximate control solution (bottom), their contour lines in the left side.

4.2 Optimal boundary control problem

4.2.1 All-at-Once method and preconditioning

We proceed the boundary OCPs and as we mentioned in the previous section, we apply the all-at-once method to solve the optimality systems which are obtained using the DO approach in Chapter 2. In a similar way, we redefine the optimality systems (2.84) in the saddle point form (4.1).

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

and

$$x := \begin{pmatrix} Y \\ U \\ P \end{pmatrix}, \quad B := \begin{pmatrix} -E_{s,b} & \Delta t Z_{s,b} \end{pmatrix} \text{ and } b := \begin{pmatrix} \Delta t \mathcal{M}_{1/2} Y_d \\ 0 \\ -F_{s,b} \end{pmatrix}$$

We can use both the direct method or the iterative method according to the dimension of the problem. If the dimension is not too big, we can choose the direct method easily. However, if the dimension is huge, we can not use the direct method because of the memory problem, and we choose iterative method with the following preconditioner:

$$\mathcal{P} = \begin{pmatrix} \Delta t \mathcal{M}_{1/2} & 0 & 0 \\ 0 & \alpha \Delta t \mathcal{M}_{1/2,b} & 0 \\ 0 & 0 & S \end{pmatrix} \tag{4.50}$$

In the case of the time-dependent boundary OCPs, we choose the Schur complement $S := (1/\Delta t) E_{s,b} \mathcal{M}_{1/2}^{-1} E_{s,b}^T + (\Delta t/\alpha) Z_{s,b} \mathcal{M}_{1/2,b}^{-1} Z_{s,b}^T$.

We note that as an assumption, all mass matrices are lumbed and $\mathcal{M}_{1/2,b}$, $\mathcal{M}_{1/2}$ are a block-diagonal matrix of lumbed boundary-mass matrices M_b, and a mass matrix over the domain Ω M, respectively. Herewith, we can evaluate our problem efficiently. Moreover, in [81], effective preconditioners are derived by evaluating the effective approximation of the Schur complement of the matrix system.

4.2.1.1 Numerical example

In this section, we consider a two-dimensional boundary OCP governed by convection-dominated diffusion-convection-reaction equation. As in the distributed case, we give the numerical performance of the SUPG method by choosing the appropriate stabilization parameter. The piecewise-linear elements with SUPG are used to approximate the state, the adjoint, and the control variables in the case of spatial discretization. The studies are presented for Crank-Nicolson method.

We generate our time-dependent boundary OCPs from the elliptic boundary OCP given in [3]. The boundary OCP (2.62) and the state equation (2.62b) with the domain $\Omega = (0, 1) \times (0, 0.2)$, $T > 0$, $Q = (0, T) \times \Omega$, and $\Sigma = (0, T) \times \partial\Omega$. Let us choose $\epsilon = 0.001$, $\sigma = 1$, $f = 0$, $\gamma = 10^3$, $\alpha = 10^{-4}$, $\beta' = [1\ 0]$).

The exact solution of the boundary OCP is not known, so we can observe the L^2 error of the cost functional J_{hk} with SUPG for a sequence of uniformly refined meshes and time steps tending to zero.

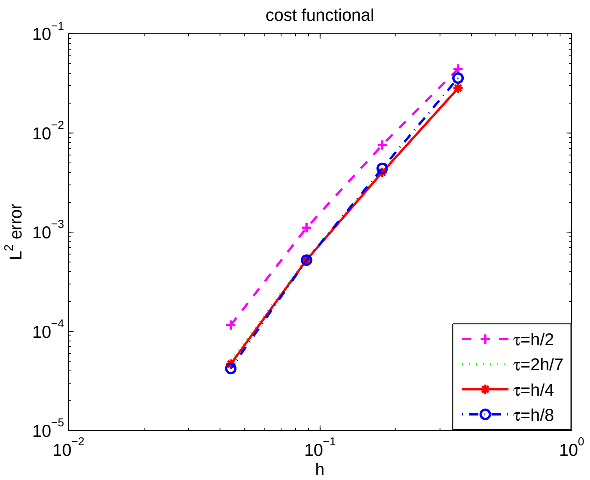


Figure 4.8: L_2 error for SUPG method with $\epsilon = 10^{-3}$.

In Figure 4.8, we indicate the L^2 error of the cost functional for different choice of stabilization parameters. The relation between the mesh size h and the time step size k is taken as $k \cong h^{3/4}$.

In Table 4.10, we demonstrate the L^2 error with different stabilization parameter to see the effect of the parameter on the SUPG method. For this example, the small stabilization parameter tends to a small L^2 error of the cost functional.

Table 4.10: Example 4.2.1 with $\epsilon = 10^{-3}$ via Crank-Nicolson with SUPG.

$h/\sqrt{2}$	$\|\|J_{hk}\|\|$ $(\tau = h/2)$	$\|\|J_{hk}\|\|$ $(\tau = 2h/7)$	$\|\|J_{hk}\|\|$ $(\tau = h/4)$	$\|\|J_{hk}\|\|$ $(\tau = h/8)$
2^{-3}	4.4272e-2	2.7815e-2	2.8312e-2	3.5825e-2
2^{-4}	7.5644e-3	4.0823e-3	4.0136e-3	4.3923e-3
2^{-5}	1.1099e-3	5.4600e-4	5.2514e-4	5.2232e-4
2^{-6}	1.1573e-4	4.9955e-5	4.6880e-5	4.2127e-5

In Figures 4.9-4.11, the approximate solution of the state, the adjoint, and the control variables are shown with and without SUPG. The efficiency of the SUPG method can be seen by its contours lines. Especially in Figure 4.9-4.10, we can observe the decreasing of the oscillation in the contours by applying the SUPG method. In Figure 4.11, its line is given for $y = 0.2$ to illustrate the efficiency on the boundary. Since we do not have exact solution, we can compare the unstabilized and stabilized solution to show the accuracy of the SUPG method. We take $\tau = h/8$, and $t = 0.5$ in the following figures.

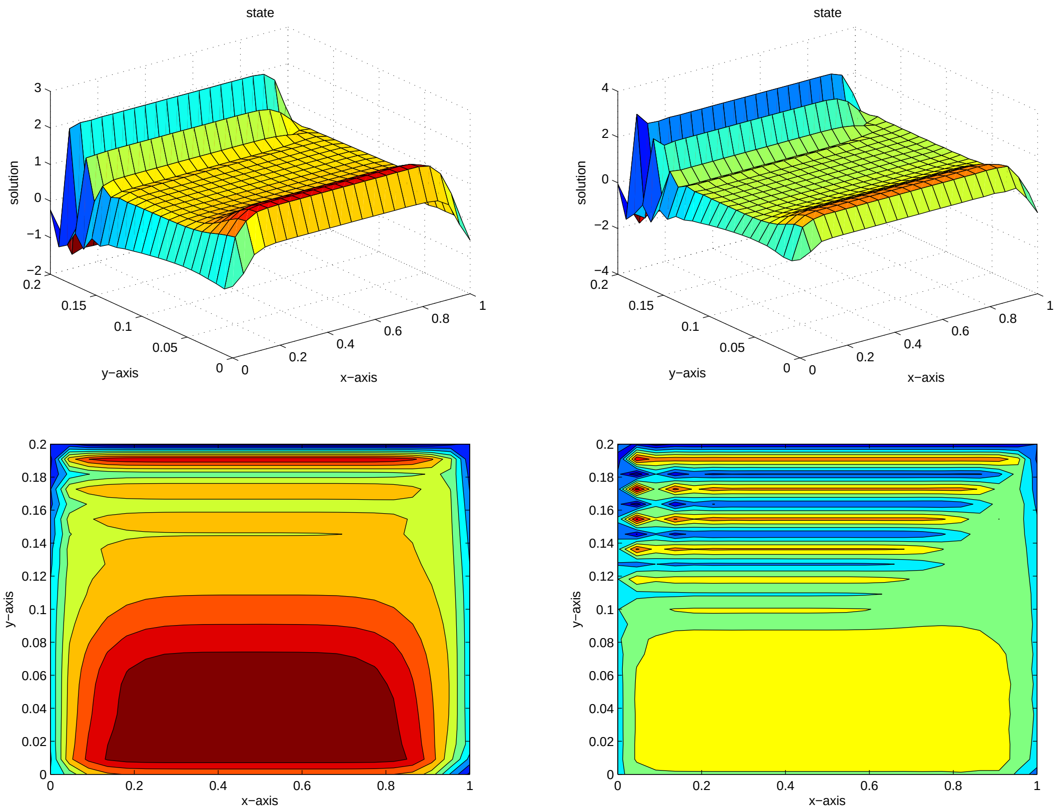


Figure 4.9: Example 4.2.1 via Crank-Nicolson method with $\Delta x = 2^{-5}\sqrt{2}$: The approximate state solution (top), its contour line (bottom), stabilized (left), unstabilized (right).

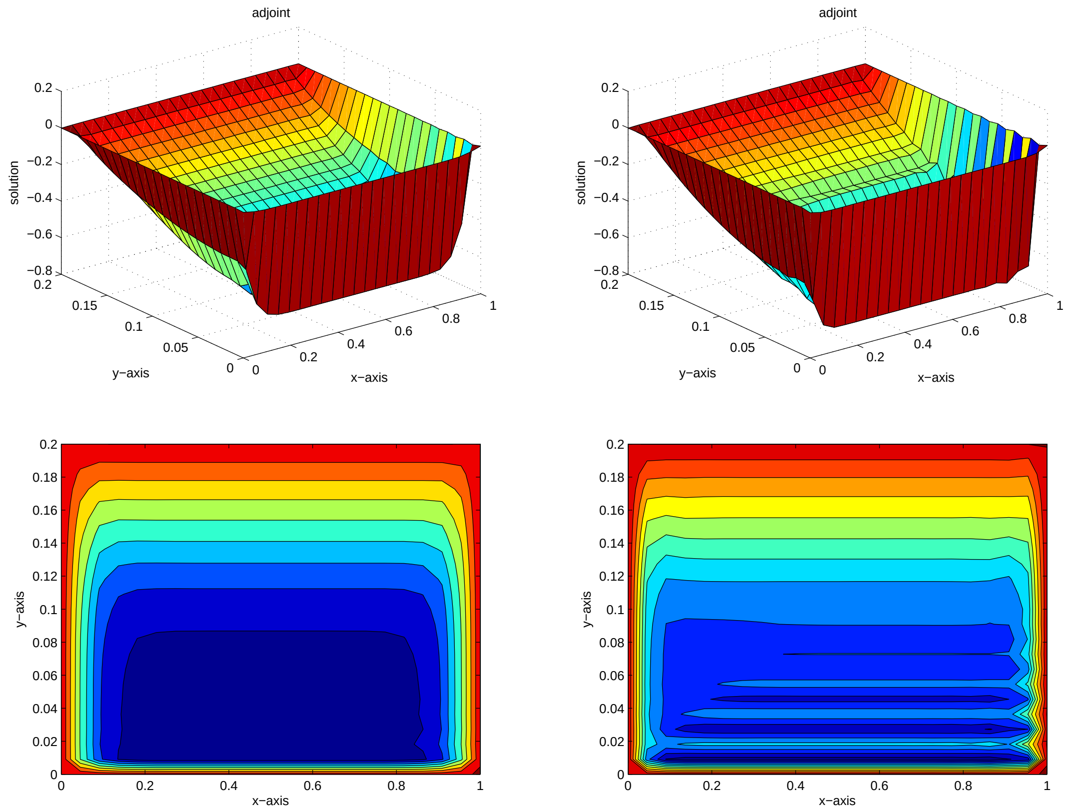


Figure 4.10: Example 4.2.1 via Crank-Nicolson method with $h = 2^{-5}\sqrt{2}$: The approximate adjoint solution (top), its contour line (bottom),stabilized (left), unstabilized (right).

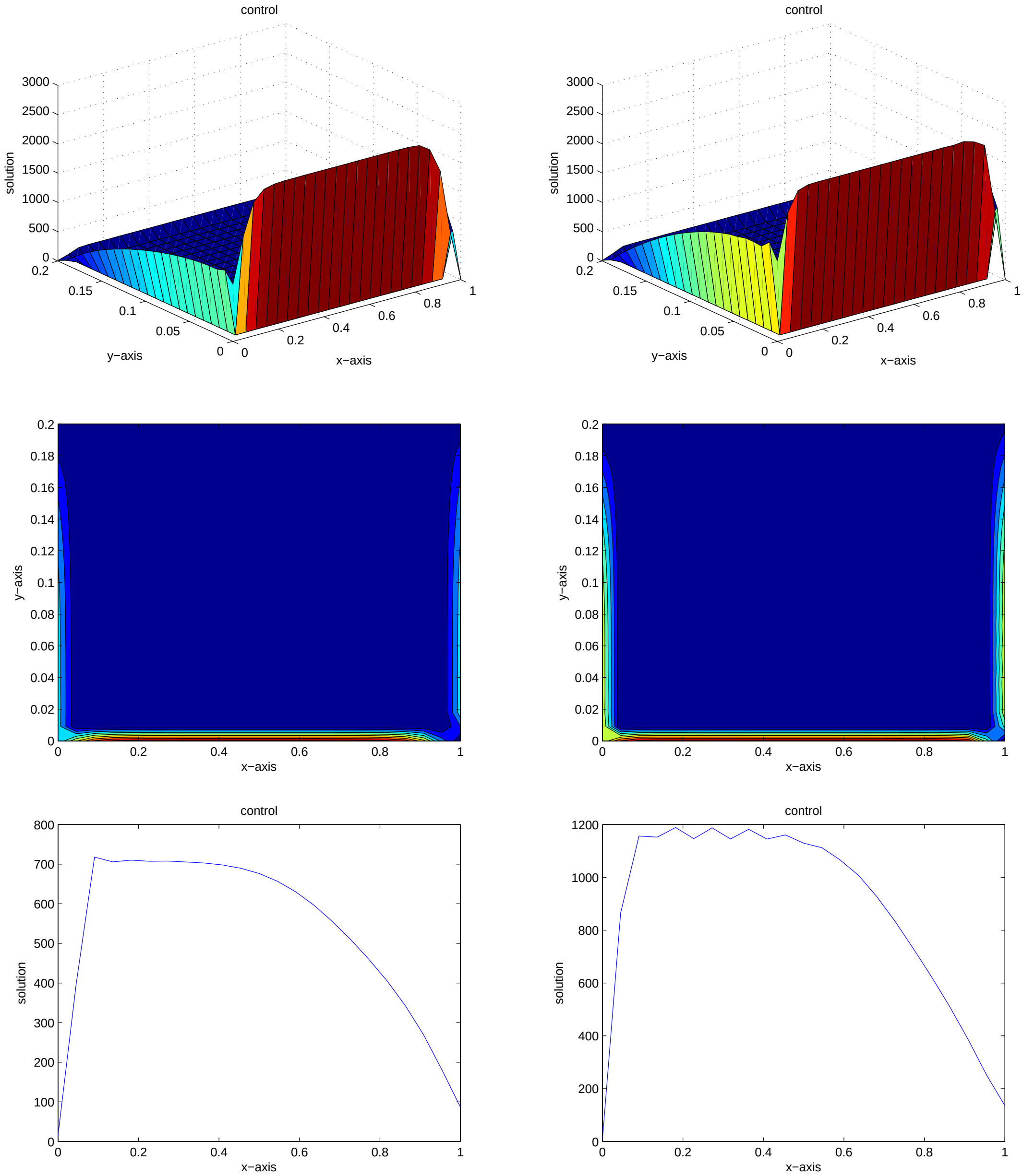


Figure 4.11: Example 4.2.1 via Crank-Nicolson method with $t = 0.5$, $h = 2^{-5}\sqrt{2}$: The approximate control solution(top), its contour line (middle), its line with $y = 0.2$ (bottom), stabilized (left), unstabilized (right)

CHAPTER 5

CONCLUSION AND FUTURE WORK

The optimal control problems (OCPs) consisting of the state, adjoint and control equations are discretized in space by linear finite elements with SUPG stabilization. For time discretization, backward Euler, Crank-Nicolson and semi-implicit methods are considered. We have analyzed the effect of the SUPG method applied to OCPs of evolutionary diffusion-convection-reaction equation using both OD and DO approaches. The OD approach with the adaptive algorithms of COMSOL gives satisfactory results for the optimization problem with and without control constraints. In the DO approach, numerical results obtained by *all-at-once* method with a special choice of SUPG parameter confirm the predicted convergence rates very well. Because the SUPG is a residual based stabilization, OD and DO approaches do not commute.

As a future work, the symmetric stabilization techniques based on continuous interior penalty method and edge stabilization can be applied to convection dominated OCPs governed by evolutionary diffusion-convection-reaction equations.

REFERENCES

[1] N. Arada, and J.P. Raymond, Dirichlet boundary control of semilinear parabolic equations - Part 2: Problems with pointwise state constraints, Applied Mathematics and Optimization, 45:145-167, 2002.

[2] M. Augustin, and A. Caiazzo, and A. Fiebach, and J. Fuhrmann, and V. John, and A. Linke, and R. Umla, An assessment of discretizations for convection dominated convection diffusion equations, 200:3395-3409, 2011.

[3] R. Bartlett, M. Heinkenschloss, D. Ridzal, and B. van Bloemen Waanders, Domain Decomposition Methods for Advection Dominated Linear-Quadratic Elliptic Optimal Control Problems, Computer Methods in Applied Mechanics and Engineering, 195:6428-6447, 2006.

[4] R. Becker, and B. Vexler. Optimal control of the convection-diffusion equation using stabilized finite element methods, Numer. Math., 106:349-367, 2007.

[5] R. Becker, and M. Braack, A finite element pressure gradient stabilization for the Stokes equations based on local projections, Calcolo, 38:173-199,2001.

[6] M. Benzi, G.H. Golub, and J. Liesen, Numerical solution of saddle point problems Acta Numerica., 14:1-137, 2005.

[7] M. Bergounioux, K. Ito, and K. Kunisch, Primal-dual strategy for constrained optimal control problems, SIAM J. Control Optim., 37:1176-1194, 1999.

[8] F. Bonnans, Second-order analysis for control constrained optimal control problems of semilinear elliptic systems. Appl. Math. and Optimization, 38:303-325, 1998.

[9] M. Braack, Optimal control in fluid mechanics by finite elements with symmetric stabilization, SIAM J. Control Optim., 48:672-687, 2009.

[10] A.N. Brooks, and T.J. R. Hughes, Streamline upwind/Petrov Galerkin formulations for convection dominated flows with particular emphasis on the incompressible Navier Stokes equations, Comput. Methods Appl. Mech. Engrg., 32:199-259, 1982.

[11] E. Burman, and P. Hansbo, Edge stabilization for Galerkin approximations of convection-diffusion-reaction problems, Comput. Methods Appl. Mech. Engrg., 193:1437-1453, 2004.

[12] E. Burman, and M. Fernandez, Finite element methods with symmetric stabilization for the transient convection diffusion reaction equation, Computer Methods in Mechanics and Engineering 198:2508-2519, 2009.

[13] E. Burman, Cranck-Nicolson finite element methods using symmetric stabilitization with an application to optimal control problems subject to transient advection-diffusion equation, Commun. Math. Sci., 9:319-329, 2011.

[14] G. Büttner, Ein Mehrgitterverfahren zur optimalen Steuerung parabolischer Probleme. PhD thesis,Technische Universität Berlin, 2004.

[15] E. Casas, and M. Mateos, Second order sufficient optimality conditions for semilinear elliptic control problems with finitely many state constraints. SIAM J. Control and Optimization, 40:1431-1454, 2002.

[16] E. Casas, J.C. de los Reyes, and F. Tröltzsch, Sufficient second-order optimality conditions for semilinear control problems with pointwise state constraints, SIAM J. on Optimization, 19(2):616-643, 2008.

[17] E. Casas, F. Tröltzsch, and A. Unger, Second order sufficient optimality conditions for a nonlinear elliptic control problem. Z. für Analysis und ihre Anwendungen (ZAA), 15:687-707, 1996.

[18] E. Casas, F. Tröltzsch, and A. Unger, Second order sufficient optimality conditions for some state-constrained control problems of semilinear elliptic equations, SIAM J. Control and Optimization, 38:1369-1391, 2000.

[19] P.G. Ciarlet, Basic error estimates for elliptic problems, in Handbook of Numerical Analysis, Vol.2: Finite Element Methods (Part 1), P. Ciarlet and J. Lions,eds., Elsevier/North-Holland, Amsterdam, Newyork, Oxford, Tokyo, 1991.

[20] P.G. Ciarlet, Basic error estimates for elliptic problems, in Handbook of Numerical Analysis 2 P. Ciarlet and J. Lions, eds., Elsevier/North-Holland, Amsterdam, Newyork, Oxford, Tokyo, 17-351, 1991.

[21] S. S. Collis, and M. Heinkenschloss, Analysis of the Streamline Upwind/Petrov Galerkin Method Applied to the Solution of Optimal Control Problems, Rice University, Houston, CAAM TR02-01, March, 2002.

[22] B. Dacorogna, Direct Methods in the Calculus of Variations, Appl. Math.,78, 1989.

[23] L. Dede, and A. Quarteroni, Optimal control and numerical adaptivity for advection-diffusion equations, ESAIM: Mathematical Modelling and Numerical Analysis, 39:1019-1040, 2005.

[24] J. Douglas, and T.F. Russell, Numerical methods for convection-dominated diffusion problems based on combining the method of characteristics with finite element or finite differences procedures, SIAM J. Numer. Anal., 19:871-885, 1982.

[25] M. Engel, and M. Griebel, A multigrid method for constrained optimal control problems, SF-BPreprint, 406, Sonderforschungsbereich 611, Rheinische Friedrich-Wilhelms-Universitat Bonn, Journal of Computational and Applied Mathematics, 235(15):4368-4388, 2011.

[26] R. Fletcher, Conjugate gradient methods for indefinite systems, in Numerical analysis, Springer, Berlin, Lecture Notes in Math., Vol. 506:73-89,1976.

[27] H. Fu, A characteristic finite element method for optimal control problems governed by convection diffusion equations, Journal of Computational and Applied Mathematics, 235:825-836, 2010.

[28] H. Fu, and H. Rui, A Priori Error Estimates for Optimal Control Problems Governed by Transient Advection-Diffusion Equations, J. Sci. Comput., 38:290-315, 2009.

[29] A. V. Fursikov, Optimal control of Distributed systems: Theory and Applications, AMS, 1999.

[30] V. John, and E. Schmeyer, Finite element methods for time dependent convection diffusion reaction equations with small diffusion, Comput. Methods Appl. Mech. Engrg., 198:475-494, 2008.

[31] V. John, and E. Schmeyer, Stabilized finite element methods for time-dependent diffusion-convection-reaction equations, Comput. Methods Appl. Mech. Engrg., 198:475-494, 2008. (2008),

[32] V. John, and E. Schmeyer, On finite element methods for 3d time-dependent diffusion-convection-reaction equations with small diffusion, in BAIL 2008-Boundary and Interior Layers, Lect. Notes Comput. Sci. Eng. 69, Springer, Berlin, 173-182, 2009.

[33] V. John, and J. Novo, Error analysis of the SUPG finite element discretization of evolutionary Convection Diffusion Reaction equations, SIAM J. Numer. Analy., 49:1149-1176, 2011.

[34] C. Johnson, and U. Nävert, An analysis of some finite element methods for advection-diffusion problems, in Analytical and Numerical Approaches to Asymptotic Problems in Analysis, S. Axelsson, L.S. Frank, A. van der Sluis (eds.), North-Holland Publishing Company, Amsterdam, 99-116, 1981.

[35] C. Johnson, and J. Pitkränta, An analysis of the discontinuous Galerkin method for scalar hyperbolic equation, Math. Comp., 46:1-26, 1986.

[36] C. Johnson, Numerical Solution of Partial Differential Equations by the Finite Element Method, Cambridge Univ. Press, Cambridge, (1987).

[37] H. Goldberg, and F. Tröltzsch, Second order optimality conditions for a class of control problems governed by nonlinear integral equations with application to parabolic boundary control, Optimization, 20:687-689, 1989.

[38] R. Grisse, A reduced SQP algorithm for the optimal control of semilinear parabolic equations, System Modeling and Optimization, 130:239-253, 2003.

[39] P. Grisvard, Elliptic problems in nonsmooth domains, Longman Scientific Technical, Harlow, Essex, 1985.

[40] M. Heinkenschloss, and D. Leykekhman, Local Error Estimates for SUPG Solutions of Advection-Dominated Elliptic Linear-Quadratic Optimal Control Problems, Rice University, Houston, CAAM Technical Report, TR08-30, 2008.

[41] R. Herzog, Algorithms and Preconditioning in PDE-Constrained Optimization, Summer school Lectures Notes, Lambrecht, July 2010.

[42] M. Hinze, M. Köster, and S. Turek. A hierarchical space-time solver for distributed control of the stokes equation. Technical report 1253:21-10, 2008.

[43] M. Hintermüller, K. Ito, and K. Kunisch, The primal-dual active set strategy as a semi smooth newton method. SIAM J. Optim., 865-888, 2002.

[44] M. Hintermüller, F. Tröltzsch, and I. Yousept, Mesh-independence of semismooth Newton methods for Lavrentiev-regularized state constrained nonlinear optimal control problems, *Numerische Mathematik*, 108:571-603, 2008.

[45] M. Hinze, N. Yan, and Z. Zhou, Variational discretization for optimal control governed by convection dominated diffusion equations, J. Comput. Math., 27:237-253, 2009.

[46] T.J. R. Hughes, and A. Rooks, Streamline upwind/Petrov Galerkin formulations for the convection dominated flows with particular emphasis on the incompressible Navier-Stokes equations, Comput. Methods Appl. Mech. Engrg., 54:199-259, 1982.

[47] T.J. R. Hughes, L.P. Franca, and M. Mallet, A new finite element formulation for computational fluid dynamics: VI. Convergence analysis of the generalized SUPG formulation for linear time-dependent multidimensional advective-diffusive systems, Comput. Methods Appl. Mech. Engrg., 63:97-112, 1987.

[48] K. Kunisch, and S. Volkwein, Augmented Lagrangian-SQP techniques and their approximations, Optimization methods in partial differential equations Contemp. Math., 209:147-159, 1996.

[49] M. Hintermüller, K. Ito, and K. Kunisch, The Primal-Dual Active Set Strategy as a Semismooth Newton Method, SIAM J. Optim., 13:865-888, 2002.

[50] K. Kunisch, and B. Vexler. Constrained Dirichlet boundary control in L^2 for a class of evolution equations, SIAM J. Control Optim., 46:1726-1753, 2007.

[51] J.L. Lions, Optimal control of systems governed by partial differential equations, Springer, Berlin, 1997.

[52] G. Lube, and B. Tews, Distributed and boundary control of singularly perturbed advection-diffusion-reaction problems, Lecture Notes in Computational Science and Engineering, 69:205-215, 2009.

[53] D. Meidner, and B. Vexler, A priori error estimates for space-time finite element discretization of parabolic optimal control problems part I: Problems without control constraints, SIAM J. on Control and Optimization, 47(3):1150-1177, 2008.

[54] D. Meidner, and B. Vexler, A priori error estimates for space-time finite element discretization of parabolic optimal control problems part II: Problems with control constraints, SIAM J. on Control and Optimization, 47(3):1301-1329, 2008.

[55] T.P. Mathew, M. Sarkis, and C.E. Schaerer, Analysis of block matrix preconditioners for elliptic optimal control problems, Numerical Linear Algebra with Applications, 14(4):257-259, 2007.

[56] T.P. Mathew, M. Sarkis, and C.E. Schaerer, Analysis of Block Parareal Preconditioners for Parabolic Optimal Control Problems, SIAM J. on Scientific Computing archive, 32(3):1180-1200, 2010.

[57] T.P. Mathew, M. Sarkis, and C.E. Schaerer, Block iterative algorithms for the solution of parabolic optimal control problems. In M. Dayd'e et al., editor, 7th International Meeting High Performance Computing for Computational Science, Springer, Lect. Notes Comput. Sci., 4395:452-465, 2007.

[58] D.Meidner, Adaptive Space-Time Finite Element Methods for Optimization Problems Governed by Nonlinear Parabolic Systems, Phd Thesis, University of Heidelberg, 2008.

[59] K.W. Morton, Numerical Solution of Convection-Diffusion Problems, Chapman & Hall, London, Glasgow, New York, (1996).

[60] M.F. Murphy, G. H. Golub, and A. J. Wathen, A Note on Preconditioning for Indefinite Linear Systems, SIAM Journal on Scientific Computing., 21(6):1969-1972, 2000.

[61] I. Neitzel, U. Prüfert, and T. Slawig, Strategies for time-dependent pde control using an integrated modeling and simulation environment, part one: problems without inequality constraints, Technical report, Matheon, Berlin, 2007.

[62] I. Neitzel, U. Prüfert, and T. Slawig, Solving time-dependent optimal control problems in COMSOL multiphysics, Proceedings of the COMSOL Conference Hannover, 2008.

[63] I. Neitzel, U. Prüfert, and T. Slawig, On Solving Parabolic Optimal Control Problems by Using Space-Time Discretization, Technical Report, Matheon, Berlin, 2007.

[64] I. Neitzel, U. Prüfert, and T. Slawig, Strategies for time-dependent pde control with inequality constraints using an integrated modeling and simulation environment, Numer. Algorithms, 50:241-249, 2009.

[65] I. Neitzel, U. Prüfert, and T. Slawig, A Smooth regularization of the projection formula for constrained parabolic optimal control problems, Technical Report, Matheon, Berlin, 2010(21).

[66] I. Neitzel, and F. Tröltzsch, On regularization methods for the numerical solution of parabolic control problems with pointwise state constraints, Esaim-control Optimisation and Calculus of Variations 15:426-453, 2009.

[67] C.C. Paige, and M.A. Saunders, Solution of sparse indefinite systems of linear equations. SIAM J. Numer. Anal., 12(4):617 629, 1975.

[68] J.W Pearson, A.J. Wathen, Fast iterative solvers for convection-diffusion control problems, Technical report, ETNA (2011).

[69] J.P. Raymond and F. Tröltzsch, Second order sufficient optimality conditions for nonlinear parabolic control problems with state constraints, Discrete and Continuous Dynamical Systems, 6:431-450, 2000.

[70] R. Codina, Comparison of some finite element methods for solving the diffusion convection reaction equation, Comput. Methods Appl. Mech. Engrg., 156:185-210, 1998.

[71] R. Codina, On stabilized finite element methods for linear systems of convection diffusion reaction equations, Comput. Methods Appl. Mech. Engrg., 188:61-82, 2000.

[72] T. Rees, S. Dollar, and A. Wathen, Optimal solvers for PDE-constrained optimization, SIAM J. Scientific Computing., 32:271-298, 2010.

[73] M. Stoll and T. Rees, Block-triangular preconditioners for PDE-constrained optimization, Numer. Linear Algebra Appl., 17:977-996, 2010.

[74] T. Rees, M. Stoll, and S. Dollar, All-at-once preconditioning in pde constrained optimization, Kybernetika, 46:341-360, 2010.

[75] H.-G. Roos, M. Stynes and L. Tobiska, Numerical methods for singularly perturbed differential eqyations, vol. 24 of Springer Series in Computational Mathematics Springer-Verlag, Berlin (1996).

[76] Y. Saad. Iterative methods for sparse linear systems. PWS Publishing, Boston, 1996.

[77] M. Stynes, Steady state convection-diffusion problems, in Acta Numerica, AIserles, ed.,Cambridge University Press, Cambridge, UK, 445-508, 2005.

[78] M. Stoll and A. Wathen, All-at-Once Solution if Time-Dependent PDE-Constrained Optimisation Problems, Technical report, OCCAM (Oxford Center for Collaborative Applied Mathematics), 2010.

[79] M. Stoll, One -shot solution of a time dependent time periodic PDE constrained optimization problem, Max Planck Instıtute Magdeburg Preprints MPIMD/10-04, 2011.

[80] M. Stoll and A. Wathen, All-at-Once Solution if Time-Dependent PDE-Constrained Optimization Problems, Kybernetika, 46(2):341-360, 2010.

[81] J.W. Pearson, M. Stoll, A. Wathen, Regularization-robust preconditioners for time-dependent PDE constrained optimization problems, Max Planck Instıtute Magdeburg Preprints MPIMD/11-05, 2011.

[82] F. Tröltzsch , Optimale Steuerung partieller Differentialgleichungen, Vieweg and Sohn,Wiesbaden, 2005.

[83] F. Tröltzsch, Optimal Control of Partial Differential Equations: Theory, Methods and Applications, *Graduate Studies in Mathematics, American Mathematical Society*, 112, 2010.

[84] A. Quarteroni, and A. Valli, Numerical approximation of partial differential equations, vol. 23 of Springer Series in Computational Mathematics, Springer-Verlag, Berlin, (1994).

[85] J. Wathen, and T. Rees, Chebyshev Semi-iteration in Preconditioning for Problems Including the Mass Matrix, Electronic Transactions on Numerical Analysis, 34:125-135, 2009.

[86] J. Wloka, Partial Differential Equations, Cambridge, Cambridge University Press, 2005.

[87] H.A. van der Vorst. Iterative Krylov Methods for Large Linear Systems. Cambridge University Press, 2003.

[88] S. Volkwein, Mesh-independence for an augmented Lagrangian-SQP method in Hilbert spaces, *SIAM J. Control Optim.*, 35:767-785, 2000.

[89] S. Volkwein, Lagrange-SQP techniques for the control constrained optimal boundary control problems for the Burgers equation, *Computational Optimization and Applications*, 26:253-284, 2003.

[90] N. Yan, and Z. Zhou, A priori and a posteriori error analysis of edge stabilization Galerkin method for the optimal control problem governed by convection dominated diffusion equation, Numer. Math. Theor. Meth. Appl., 1:297-320, 2008.

[91] F. Yılmaz, and B. Karasözen, Solving Distributed Optimal Control Problems for the Unsteady Burgers Equation in COMSOL Multiphysics, Journal of Computational and Applied Mathematics, 235(16):4839-4850, 2011.

[92] Y. Saad, and M.H. Schultz, GMRES:a generalized minimal residual algorithm for solving nonsymmetric linear systems, SIAM J.Sci. Statist. Comput., 7:856-869, 1986.

[93] G. Zhou, and R. Rannacher, Pointwise superconvergence of the streamline diffusion finite- element method, Numer. Methods Partial Differential Equations, 12:123-145, 1996.

VITA

PERSONAL INFORMATION

Surname, Name	:	Seymen, Zahire
Nationality	:	Turkish (TC)
Date and Place of Birth	:	13 May 1981 , Ankara
Marital Status	:	Married
Phone	:	+90 532 401 4016
email	:	e118897@metu.edu.tr

ACADEMIC DEGREES

Ph.D. Middle East Technical University, Ankara, TURKEY, 2013 February
Supervisor : Prof. Dr. Bülent Karasözen
Thesis Title : Solving Optimal Control of Convection-Reaction-Diffusion
Equation By Space-Time Discretization

B.S. Department of Mathematics,
Middle East Technical University, Ankara, TURKEY, 2004 June

RESEARCH VISITS

November 2007-February 2008 Department of Mathematics, University of Houston, USA
supervised by Prof.Dr. R.H.W. Hoppe

SCHOLARSHIPS

April 2005 - October 2008 Doctorate Scholarship
Turkish Scientific and Technical Research Council (TÜBİTAK)

EMPLOYMENT

March 2010 - Mathematicians,
Turkish Petroleum Corporation, Ankara (TPAO), TURKEY

FOREIGN LANGUAGES

Advanced English

PUBLICATIONS

1. Z. Seymen, H. Yücel, and B. Karasözen, Distributed Optimal Control of Timedependent Diffusion-Convection-Reaction Equations Using Space-Time Discretization, Journal of Computational and Applied Mathematics, submitted

CONFERENCES

1. Z. Seymen, and B. Karasözen, Optimal Boundary Control of Convection dominated time-dependent partial differential equations, International Conference on Applied Analysis and Algebra, Yildiz Technical University, 29-30 June, 1-2 July 2011,Istanbul-Turkey

2. H. Yücel, F. Yılmaz, Z. Seymen, and B. Karasözen, Distributed Optimal Control of unsteady Burgers and Convection-Diffusion-Reaction Equations using COMSOL Multiphysics, Computational techniques for optimization problems subject to time-dependent PDEs, Brighton, England, 14-16 December 2009.