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# Distributed optimal control of time-dependent diffusion–convection–reaction equations using space–time discretization

Z. Kanar Seymen [a], H. Yücel [b,1], B. Karasözen [b,*]

[a] Department of Mathematics, Middle East Technical University, 06800 Ankara, Turkey

[b] Department of Mathematics and Institute of Applied Mathematics, Middle East Technical University, 06800 Ankara, Turkey

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ABSTRACT

We apply two different strategies for solving unsteady distributed optimal control problems governed by diffusion–convection–reaction equations. In the first approach, the optimality system is transformed into a biharmonic equation in the space–time domain. The system is then discretized in space and time simultaneously and solved by an equation-based finite element package, i.e., COMSOL Multiphysics. The second approach is a classical gradient-based optimization method to solve the state and adjoint equations and the optimality condition iteratively. The convection-dominated state and adjoint equations are stabilized using the streamline upwind/Petrov–Galerkin (SUPG) method. Numerical results show favorable accuracy and efficiency of the two strategies for unstabilized and stabilized numerical solutions.



## 1. Introduction

Optimal control problems (OCPs) governed by diffusion–convection–reaction partial differential equations (PDEs) arise in environmental modeling, petroleum reservoir simulation, and in many other applications. A characteristic feature of convection-dominated equations is the presence of sharp boundary and/or interior layers. It is well known that the standard Galerkin finite element method produces nonphysical oscillating solutions when the mesh size is larger than a critical value depending on the ratio between diffusion and convection terms. To enhance the stability while maintaining accuracy, a stabilized term is added to the PDEs. The streamline upwind/Petrov–Galerkin (SUPG) finite element method [1,2] is the most used stabilization technique for convection-dominated PDEs.

Numerical solutions of convection-dominated optimal control problems present an additional challenge since the state and adjoint equations are convection dominated, with opposite signs for the convection terms. As a consequence, errors in the solution can potentially propagate in both directions. Therefore, an effective numerical technique is needed to reduce the errors. Steady-state convection-dominated OCPs have been solved recently with different stabilization methods: with the SUPG method [3,4], local projection stabilization [5], and edge stabilization [6,7]. In [8], stabilization of the Lagrangian was introduced instead of stabilizing the state and adjoint equations separately. It has been recently shown that discontinuous Galerkin discretization [9,10] enjoys a better convergence behavior for convection-dominated OCPs. However, time-dependent convection-dominated OCPs have been studied in few papers. In [11], Dirichlet boundary control problems were

* Corresponding author. Tel.: +90 312 2105653; fax: +90 312 2102985.
*E-mail address:* bulent@metu.edu.tr (B. Karasözen).

1 Present address: Computational Methods in Systems and Control Theory, Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstr. 1, 39106 Magdeburg, Germany.

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studied. For distributed OCPs, the characteristic finite element method was used in [12,13], and the Crank–Nicolson finite element method was applied in [14] with symmetric stabilization.

In PDE constrained optimal control problems, the optimality system consists of the state and adjoint equations, and the optimality condition. Typically, OCPs are solved by using two different approaches: the *optimize-then-discretize* method and the *discretize-then-optimize* method. In the former one, first the necessary optimality conditions are established on the continuous level consisting of the state, the adjoint, and the optimality condition, and then these equations are discretized. In the latter case, only the cost function and the state equation are discretized, and then the optimality system for the finite-dimensional optimization problem is derived. It is well known that both approaches lead to the same discretization scheme provided that a pure Galerkin discretization is used. However, for residual-based stabilization methods like the SUPG method [3,4], the *discretize-then-optimize* approach and the *optimize-then-discretize* approach lead to different discrete problems. For stabilizations based on local projection [5] and on edge stabilization [6,7], discretization and optimization commute, and the optimality system is symmetric. For unsteady OCPs, these two approaches coincide when discretization is based on $H^1$-conforming finite elements in space and $dG(0)$ in time [11].

In this paper, we follow the *optimize-then-discretize* approach. We use two different approaches to solve the optimality system. The first approach is to solve both convection-dominated equations at once as a biharmonic equation in the space–time domain. The transformation of the optimality system into a biharmonic PDE for linear parabolic unconstrained and control constrained OCPs was studied in [15–17] using the equation-based modeling and simulation environment COMSOL Multiphysics. The same approach was used in [18] for distributed optimal control of the unsteady Burgers equation. The second approach is the classic approach called the integrated iteratively forward and backward in time by use of a gradient-based algorithm method. SUPG stabilization terms are added to the state and adjoint equations in both cases.

The rest of the paper is organized as follows. In Section 2, we derive the optimality conditions for the unconstrained and control constrained unsteady distributed convection-dominated OCPs. The full discretization of the optimality system with SUPG stabilization is described in Section 3. The transformation of the optimality system to an elliptic boundary value problem is presented in Section 4. In the final section, we present an implementation of the optimality conditions with stabilization in COMSOL Multiphysics, and we compare the numerical results obtained by the one-shot approach and those produced by the gradient method for the unconstrained and control constrained cases.

## 2. Optimality system

We consider the following unsteady distributed optimal control problem governed by the diffusion–convection–reaction equation with and without control constraints,

$$\underset{u\in U_{\text{ad}}\subseteq L^2(0,T;U)}{\text{minimize}} \; J(y,u) := \frac{1}{2}\,\|y-y_d\|_Q^2 + \frac{\alpha}{2}\,\|u\|_Q^2 \tag{2.1}$$

subject to

$$y_t - \varepsilon\Delta y + \beta\cdot\nabla y + \sigma y = g + u \quad \text{in } Q, \tag{2.2a}$$

$$y = 0 \quad \text{on } \Sigma, \tag{2.2b}$$

$$y(\cdot,0) = y_0 \quad \text{in } \Omega, \tag{2.2c}$$

with the regularization parameter $\alpha > 0$. Here, $y$ and $u$ denote the state and control variables, respectively, and $y_d(x)$ is the desired state. Given the space domain $\Omega \in \mathbb{R}^d (d = 1, 2)$ and the boundary $\partial\Omega$, we define $Q = (0,T)\times\Omega$ and $\Sigma = (0,T)\times\partial\Omega$ with $T > 0$. Let $U = L^2(\Omega)$ and $V = H_0^1(\Omega)$ be Hilbert spaces. We introduce the following Hilbert space:

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

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

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

In the case of pointwise control constraints, the admissible space of control constraints is given by

$$U_{\text{ad}} = \{u \in L^2(0,T;U) : u_a \le u \le u_b,\ \text{a.e. in } \Omega\}$$

with the constant bounds $u_a, u_b \in \mathbb{R}\cup\pm\infty$, with $u_a < u_b$. The source function and initial data are denoted by $g, y_0 \in L^2(\Omega)$, respectively. The diffusion and reaction coefficients are $\varepsilon > 0$ and $\sigma$, respectively. The velocity field $\beta(x,t)$ is taken as being divergence free; i.e., $\nabla\cdot\beta(x,t) = 0$.

By taking the first partial derivatives of the Lagrangian functional [19,20] equal to zero, the following optimality system is obtained, with the state equation

$$y_t - \varepsilon\Delta y + \beta\cdot\nabla y + \sigma y = g + u \quad \text{in } Q, \tag{2.3a}$$

$$y = 0 \quad \text{on } \Sigma, \tag{2.3b}$$

$$y(0) = y_0 \quad \text{in } \Omega, \tag{2.3c}$$