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A discontinuous Galerkin method for optimal control problems governed by a system of convection–diffusion PDEs with nonlinear reaction terms

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ABSTRACT

In this paper, we study the numerical solution of optimal control problems governed by a system of convection–diffusion PDEs with nonlinear reaction terms, arising from chemical processes. The symmetric interior penalty Galerkin (SIPG) method with upwinding for the convection term is used as a discretization method. We use a residual-based error estimator for the state and the adjoint variables. An adaptive mesh refinement indicated by a posteriori error estimates is applied. The arising saddle point system is solved using a suitable preconditioner. Numerical results are presented to illustrate the performance of the proposed error estimator.

1. Introduction

Optimal control problems governed by scalar or coupled partial differential equations (PDEs) have a number of applications in mathematical and physical problems. The equations model a chemical or biological process where the species involved are subject to diffusion, convection and reaction among each other [1–3]. We consider the following model problem

$$A + B \leftrightarrows C,$$

which obeys the law of mass action. To simplify the discussion, we assume that the backward reaction $C \to A + B$ is negligible and that the forward reaction proceeds with a constant (e.g., not temperature dependent) rate. This leads to a coupled convection dominated system for the respective concentrations; see (2) later on.

Let Ω be an open, bounded polygonal domain in $\mathbb{R}^2$ with Lipschitz-continuous boundary $\Gamma = \partial\Omega$, let f_i, β_i, α_i, u^d, v^d, g_i be given functions, and let ε_i, γ_i, ω_u, ω_v, ω_c be given nonnegative diffusion, nonlinear reaction, and regularization parameters, respectively, for $i = u, v$. We here consider a class of distributed optimal control problems governed by a system of convection dominated PDEs

$$\min J(u, v, c) = \frac{\omega_u}{2}\|u - u^d\|^2_{L^2(\Omega)} + \frac{\omega_v}{2}\|v - v^d\|^2_{L^2(\Omega)} + \frac{\omega_c}{2}\|c\|^2_{L^2(\Omega)}, \tag{1}$$

subject to

$$-\varepsilon_u \Delta u + \beta_u \cdot \nabla u + \alpha_u u + \gamma_u uv = f_u + c \quad \text{in } \Omega, \tag{2a}$$

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$$-\varepsilon_v \Delta v + \beta_v \cdot \nabla v + \alpha_v v + \gamma_v uv = f_v \qquad \text{in } \Omega, \tag{2b}$$

$$u = g_u \qquad v = g_v \qquad \text{on } \Gamma, \tag{2c}$$

where u and v refer to the concentration of the reactants. In an optimal control context, we refer to them as state variables, to c as the control variable and to (2) as the state system. The control c enters our state system (2) as a source term for the first reactant u.

In large chemical systems, the nonlinear reaction terms $\gamma_i uv$ are assumed to be expressions given as product of the concentrations of the chemical component u and v with an exponential function of the temperature, called Arrhenius kinetics expression [3]. As an example, the rate of conversion of u and v in the reaction

$$u + v \rightarrow \text{products}$$

can be expressed as

$$k_0 e^{-\frac{E}{\mathcal{R}T}} uv,$$

where u and v are the concentrations of the reactants, pre-exponential factor k_0, the activation energy E, the universal gas constant $\mathcal{R}$, and T is the absolute reaction temperature. We would like to emphasize that the extension of anything derived in this paper to more than two reactants is straightforward. Therefore, we restrict ourselves to two reactants in order to not obscure the presentation by technicalities.

Problems of the form (2) are strongly coupled such that inaccuracies in one unknown directly affect all other unknowns. Therefore, prediction of these unknowns is very important for the safe and economical operation of biochemical and chemical engineering processes. Typically, in (2) the size of the diffusion parameters ε_i is small compared to the size of the velocity fields β_i. Then, such a convection–diffusion system is called convection-dominated.

For convection-dominated problems, especially in the presence of boundary and/or interior layers, the standard finite element methods may result in spurious oscillations causing in turn a severe loss of accuracy and stability. Therefore, we need special techniques to eliminate spurious oscillations. One way to avoid spurious oscillations is the artificial viscosity proposed in [4], which is used in many numerical techniques, i.e., streamline upwind Galerkin method (SUPG) discretization in [5] for linear convection dominated problems and in [6] for nonlinear convection dominated problems, and symmetric interior penalty Galerkin (SIPG) discretization in [7] for scalar and/or coupled convection dominated problems with nonlinear reaction terms. Although adding artificial viscosity reduces spurious oscillations, the accuracy of numerical solutions is not enhanced due to the additional artificial cross-wind diffusion. Another approach is to use adaptive mesh refinement producing generally better accuracy with fewer degrees of freedom.

Adaptive mesh refinement is particularly attractive for the solution of optimal control problems governed by convection dominated PDEs since both state and adjoint PDEs are convection dominated, but the convection term of the adjoint PDE is the negative of the convection term of the state PDE. As a consequence, errors in the solution can potentially propagate in both directions. Adaptivity allows a local mesh refinement in a certain region of the given domain, where the solution is discontinuous or more difficult to approximate, using an a posteriori error estimator or indicator, see e.g., [8]. A posteriori error estimates are computable quantities in terms of the discrete solutions without the knowledge of exact solutions. They are essential in designing algorithms to generate a mesh equidistributing the computational effort and optimizing the computation. Residual-type a posteriori error estimators for convection dominated optimal control problems have been studied in [9–12], but they all use continuous finite element discretizations. The results in [13] show that discontinuous Galerkin (DG) discretizations enjoy a better convergence behavior for convection dominated optimal control problems since optimal convergence orders are obtained if the error is computed away from boundary or interior layers, in contrast to the streamline upwind Petrov Galerkin (SUPG) stabilized finite element discretization [14]. DG methods have several advantages for the solution of the systems of conservation laws [15] over other types of finite element methods. For example, the trial and test spaces are very easy to construct; they can naturally handle inhomogeneous boundary conditions and curved boundaries; and they have flexibility in handling non-matching grids and in designing hp-adaptive mesh refinement. One of the other attractive features of DG methods is the very natural treatment of the convective operators through the stabilizing inter-element jump elements. This avoids the need for cumbersome interior stabilization terms. We would like to refer to [16–19] for discontinuous Galerkin methods in details. DG discretizations have been used in [20–24] for distributed linear optimal control problems governed by convection dominated problems. Our aim here is to extend the adaptive mesh refinement in [21,23], which yields more narrowly refined regions around the layers than the SUPG discretization does, to the optimal control problems governed by a system of convection–diffusion PDEs with nonlinear reaction terms as in (1)–(2).

Here, we consider a class of distributed optimal control problems governed by a system of convection dominated PDEs. Similar optimal control problems without convection terms in the constraints have been discussed in [25–28]. The optimal control problem (1)–(2) can have different local minima since it is a nonconvex programming problem. Therefore, while deriving error estimations, we assume a reference solution $(\tilde{u}, \tilde{v}, \tilde{c})$ satisfying the first- and second-order optimality conditions, which can be derived as in [25,27]. We here apply an inexact Newton method to deal with the nonlinearity of the state system (2). We also propose an effective preconditioner to solve the saddle point system arising from Newton's method.