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A Discontinous 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 for discretization. Residual-based error estimators are used for the state, the adjoint and the control 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 examples are presented for convection dominated problems to illustrate the effectiveness of the adaptivity.

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1 Introduction

Optimal control problems governed by scalar or coupled partial differential equations (PDEs) have a number of applications in mathematical and physical problems. One such field in which these problems can be posed is that of chemical processes. The underlying PDEs are then convection dominated equations with nonlinear reactions terms [12, 13].

Let Ω be a bounded open, convex domain $\mathbb{R}^2$ with boundary $\Gamma = \partial\Omega$, let f_i, β_i, α_i, u_d, v_d, g_i be given functions, and let $\varepsilon_i > 0$, $\omega_z \geq 0$ be given diffusion and regularization parameters, respectively, for $i = 1,2$ and $z \in \{u,v,c\}$. In this paper, we consider a class of distributed optimal control problems governed by a system of convection dominated PDEs

$$\min\ J(u,v,c) = \frac{\omega_u}{2}\|u-u_d\|^2_{L^2(\Omega)} + \frac{\omega_v}{2}\|v-v_d\|^2_{L^2(\Omega)} + \frac{\omega_c}{2}\|c\|^2_{L^2(\Omega)}, \tag{1.1}$$

subject to

$$-\varepsilon_1\Delta u + \beta_1\cdot\nabla u + \alpha_1 u + \gamma_1 r_1(u)r_2(v) = f_1 + c \quad \text{in } \Omega, \tag{1.2a}$$

$$-\varepsilon_2\Delta v + \beta_2\cdot\nabla v + \alpha_2 v + \gamma_2 r_1(u)r_2(v) = f_2 \quad \text{in } \Omega, \tag{1.2b}$$

$$u = g_1 \quad \text{on } \Gamma_1, \tag{1.2c}$$

$$v = g_2 \quad \text{on } \Gamma_2. \tag{1.2d}$$

We refer to u and v as the state variables, to c as the control variable and to (1.2) as the state system. Moreover, we have nonlinear reaction terms $\gamma_i r_1(u)r_2(v)$, in which $r_1(u)$ only depends on the first state variable u, whereas $r_2(v)$ only depends on the second state variable v. The constants γ_i are non-negative for $i = 1,2$.

In large chemical systems, the reaction terms $\gamma_i r_1(u)r_2(v)$ are assumed to be expressions which are products of some function of the concentrations of the chemical component, i.e., u,v, and an exponential function of the temperature, called Arrhenius kinetics expression. As an example, the rate of conversion of u and v in the reaction

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

can be expressed as

$$\gamma r_1(u)r_2(v),$$

where u and v are the concentrations of the reactants, $\gamma = k_0 e^{-\frac{E}{\mathcal{R}T}}$ with pre-exponential factor k_0, the activation energy E, the universal gas constant $\mathcal{R}$, and T is the absolute reaction temperature. For simplicity, we here take γ as non-negative constant. We would like to emphasize that the extension of anything derived in this paper to more than two reactants is straightforward. We restrict ourselves to two reactants in order to not obscure the presentation by technicalities.

Problems of the form (1.2) 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 (1.2) 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 [30], which is used in many numerical techniques, i.e., streamline upwind Galerkin method (SUPG) discretization in [16] for linear convection dominated problems and in [2] for nonlinear convection dominated problems, and symmetric interior penalty Galerkin (SIPG) discretization in [36] 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. Residual-type a posteriori error estimators for convection dominated optimal control problems have been studied in [3, 6, 14, 21, 32], but they all use continuous finite element discretizations. A discontinuous Galerkin (DG) discretization, i.e., SIPG, is used in [33, 35] for distributed linear optimal control problems governed by convection dominated problems. The numerical results obtained in [33, 35] show that the adaptive methods based on the SIPG method refine more narrowly around regions where layers occur than the SUPG discretization does. The reason is that the errors in boundary layers do not propagate into the entire domain [18]. In this paper, 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 [1, 8, 9, 24]. Our goal here is to extend the residual based a posteriori error estimator applied to distributed linear optimal control problems governed by scalar convection dominated equation [33, 35] to optimal control problems governed by a system of convection diffusion PDEs with nonlinear reaction terms as in (1.2).

Our paper is organized as follows. In the next section we specify the problem data and derive the Newton system to solve the optimal control problem. Section 3 introduces the DG discretization, i.e., SIPG discretization for the diffusion term and an upwinding discretization for the convection term. An effective preconditioner is also proposed to solve the saddle point system. The reliability and efficiency estimates of our error estimator are proven in Section 4. The proof uses the reliability and efficiency estimate of a scalar equation, the continuous dependence of the solution of scalar state and adjoint equations on the right hand sides of these equations, boundedness and the locally continuous Lipschitz condition of the nonlinear terms as well as the convexity of the cost functional. Section 5 briefly describes the standard adaptive procedure. In the final section we present numerical results that illustrate the performance of the proposed error estimator.

2 The Nonlinear Optimal Control Problem

In this section, we first discuss some properties of the state equation (1.2), namely existence, uniqueness and regularity of the state solution to prove the existence of the solution of the optimal control problem (1.1)-(1.2). We use the method of ordered upper and lower solutions introduced in [23] and applied in an optimal control context in [1, 8, 9].

The state PDEs (1.2) require a different choice of the state space than linear PDEs due to the nonlinear terms. We need a higher regularity of u and v to make the nonlinearities well defined [8].

Let us start with the weak formulation of the state system (1.2). The state space, the control space and the space of the test functions are

$$Y = H^1(\Omega) \cap L^2(\Omega), \quad C = L^2(\Omega) \quad \text{and} \quad W = H_0^1(\Omega),$$

respectively. Then, it is well known that the weak formulation of the state PDEs (1.2) is such that $\forall w \in W$,

$$\begin{aligned} a_1(u,w) + \int_\Omega \gamma_1 r_1(u) r_2(v) w \, dx + b(c,w) &= l_1(w), \\ a_2(v,w) + \int_\Omega \gamma_2 r_1(u) r_2(v) w \, dx &= l_2(w), \end{aligned}$$

where

$$\begin{aligned} a_i(z,w) &= \int_\Omega \left(\varepsilon_i \nabla z \cdot \nabla w + \beta_i \cdot \nabla z w + \alpha_i z w \right) dx, \quad b(c,w) = -\int_\Omega c w \, dx, \\ l_i(w) &= \int_\Omega f_i w \, dx, \qquad \text{for } i = 1,2. \end{aligned}$$

We make the following assumptions for the functions and parameters on the optimal control problem (1.1)-(1.2) for $i = 1,2$:

A1 $f_i \in L^2(\Omega) \geq 0, u_d, v_d \in L^2(\Omega), g_i \in H^{3/2}(\Gamma_i), \beta_i \in (W^{1,\infty}(\Omega))^2$.

A2 $\alpha_i \in L^\infty(\Omega) \geq 0, \gamma_i \geq 0, \varepsilon_i > 0, \omega_u, \omega_v, \omega_c > 0$.

A3 There exist constants $\kappa_i > 0$ such that

$$\alpha_i(x) - \frac{1}{2} \nabla \cdot \beta_i(x) \geq \kappa_i > 0 \qquad x \in \Omega. \tag{2.1}$$

A4 There also exist constants $\kappa_i^* \geq 0$ such that

$$\| -\nabla \cdot \beta_i + \alpha_i \|_{L^\infty(\Omega)} \leq \kappa_i^* \kappa_i. \tag{2.2}$$

The conditions (**A1**-**A3**) ensure the well-posedness of the linear part of the optimal control problem [11, 18]. The condition (**A4**) is required to prove the efficiency of the error estimator [27, 29]. Although our error estimators can be formulated for $\kappa_i = 0$, we require $\kappa_i > 0$ to prove reliability and efficiency of our estimator. Of course, if $\kappa_i > 0$, we can always find κ_i^* such that (**A4**) holds and the condition (**A4**) is more critical if $\kappa_i = 0$, which is allowed in [27, 29]. In this case, the condition (**A4**) holds only for the case $\alpha_i \equiv \nabla \cdot \beta_i$. Hence, we also require $\nabla \cdot \beta_i \geq 0$ to satisfy the condition (**A3**).

To ensure non-negativity of the concentrations u, v, the source functions f_i and reaction coefficients α_i, γ_i are assumed to be non-negative. Due to the nonlinear terms in (1.2), we also make the following assumptions on the nonlinear terms r_i for $i = 1,2$:

A5 The nonlinear terms r_i satisfy the following assumptions [28, Sec. 4.3.2]:
the boundedness condition of order $k = 0, 1$

$$|D_z^k r_i(z)| \leq C_M, \quad C_M > 0, \ \forall z \in [-M, M], \tag{2.3}$$

and the continuous Lipschitz condition of order $k = 0, 1$, for $s \in [1, \infty]$

$$\|D_z^k r_i(z_1) - D_z^k r_i(z_2)\|_{L^s(\Omega)} \leq L(M)\|z_1 - z_2\|_{L^s(\Omega)}, \quad \forall z_i \in L^\infty(\Omega). \tag{2.4}$$

To show the existence and uniqueness of the system (1.2), we refer to the procedures in [1, 8] for optimal control of a reaction-diffusion system. The main idea follows such that we first find the upper and lower solutions which yield pointwise bounds for the desired solution. Then, we use these bounds as initial iterates to construct two monotonically convergent (nested) sequences. Hence, their common limit is the unique solution of the state system (1.2). In the following theorem, we can state the existence and uniqueness of the state system (1.2) for each control variable c.

Theorem 2.1 *Under the assumptions (**A1**-**A5**), the system (1.2) admits a unique solution $(u, v) \in Y \times Y$ for each $c \in C = L^2(\Omega)$.*

Now, we can give the existence of a solution $(\bar{u}, \bar{v}, \bar{c})$ for the optimal control problem (1.1)-(1.2) in the following theorem.

Theorem 2.2 *There exists at least one global optimizer $(\bar{u}, \bar{v}, \bar{c})$ of the optimal control problem (1.1)-(1.2) provided that the assumptions (**A1**-**A5**) hold.*

Proof. Let us only briefly sketch the proofs done in [Thm. 2.4, Thm. 7.4] [1, 8]. First, the existence of a bounded sequence of state/control pairs whose objective value converges to the overall infimum is established. Then, a subsequence of this sequence is weakly convergent due to the boundedness of this sequence. By compact embedding results, strong convergence of the state components in a weaker norm is obtained. Hence, a feasibility of the limit point can be deduced and finally, a continuity argument is used to obtain convergence of the objective function. □

By taking the Fréchet derivative of the Lagrangian functional of the optimal control problem (1.1)-(1.2) as done in [1, 8, 24], we obtain the following optimality system consisting of the coupled adjoint system

$$\begin{aligned}
-\varepsilon_1 \Delta p - \beta_1 \cdot \nabla p + (\alpha_1 - \nabla \cdot \beta_1) p + \gamma_1 p r_1'(u) r_2(v) & \\
+ \gamma_2 q r_1'(u) r_2(v) = -\omega_u (u - u_d) \ \text{ in } \Omega, & \qquad (2.5a) \\
-\varepsilon_2 \Delta q - \beta_2 \cdot \nabla q + (\alpha_2 - \nabla \cdot \beta_2) q + \gamma_1 p r_1(u) r_2'(v) & \\
+ \gamma_2 q r_1(u) r_2'(v) = -\omega_v (v - v_d) \ \text{ in } \Omega, & \qquad (2.5b) \\
p = 0 \qquad \text{on } \Gamma_1, & \qquad (2.5c) \\
q = 0 \qquad \text{on } \Gamma_2, & \qquad (2.5d)
\end{aligned}$$

the gradient equation

$$\omega_c c - p = 0 \qquad \text{in } \Omega, \tag{2.6}$$

and the coupled state system

$$
\begin{aligned}
-\varepsilon_1 \Delta u + \beta_1 \cdot \nabla u + \alpha_1 u + \gamma_1 r_1(u) r_2(v) &= f_1 + c && \text{in } \Omega, && (2.7a)\\
-\varepsilon_2 \Delta v + \beta_2 \cdot \nabla v + \alpha_2 v + \gamma_2 r_1(u) r_2(v) &= f_2 && \text{in } \Omega, && (2.7b)\\
u &= g_1 && \text{on } \Gamma_1, && (2.7c)\\
v &= g_2 && \text{on } \Gamma_2. && (2.7d)
\end{aligned}
$$

The optimality system (2.5-2.7) can be written in terms of (bi)-linears forms such that

$$
\begin{aligned}
& a_1(w,p) + (\gamma_1 p r_1^{'}(u) r_2(v), w) \\
& \qquad + (\gamma_2 q r_1^{'}(u) r_2(v), w) + \omega_u(u,w) = \omega_u(u_d, w) \quad \forall w \in W, && (2.8a)\\
& a_2(w,q) + (\gamma_1 p r_1(u) r_2^{'}(v), w) \\
& \qquad + (\gamma_2 q r_1(u) r_2^{'}(v), w) + \omega_v(v,w) = \omega_v(v_d, w) \quad \forall w \in W, && (2.8b)\\
& b(w,p) + \omega_c(c,w) = 0 \quad \forall w \in C, && (2.8c)\\
& a_1(u,w) + (\gamma_1 r_1(u) r_2(v), w) + b(c,w) = l_1(w) \quad \forall w \in W, && (2.8d)\\
& a_2(v,w) + (\gamma_2 r_1(u) r_2(v), w) = l_2(w) \quad \forall w \in W. && (2.8e)
\end{aligned}
$$

The optimality system (2.5-2.7) can be described as a set of nonlinear equations with the notation $\Phi(x) = 0$. The Newton's method can be used to solve this problem via the relation $\Phi^{'}(x_k) s_k = -\Phi(x_k)$. Then, an infinite dimensional system is described such that

$$\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix} \mathbf{s} = -\Phi \tag{2.9}$$

with

$$\mathbf{A} = \begin{bmatrix} A_{11} & A_{12} & 0 \\ A_{21} & A_{22} & 0 \\ 0 & 0 & \omega_c \mathbf{I} \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} B_{11} & B_{12} & -\mathbf{I} \\ B_{21} & B_{22} & 0 \end{bmatrix} \quad \text{and} \quad \mathbf{s} = [\Delta p, \Delta q, \Delta c, \Delta u, \Delta v]^T,$$

where $\mathbf{I}$ denotes the identity operator and

$$
\begin{aligned}
A_{11} &= r_1^{''}(u) r_2(v)(\gamma_1 p + \gamma_2 q) + \omega_u,\\
A_{12} = A_{21} &= r_1^{'}(u) r_2^{'}(v)(\gamma_1 p + \gamma_2 q),\\
A_{22} &= r_1(u) r_2^{''}(v)(\gamma_1 p + \gamma_2 q) + \omega_v,\\
B_{12} &= \gamma_1 r_1(u) r_2^{'}(v),\\
B_{21} &= \gamma_2 r_1^{'}(u) r_2(v),\\
B_{11} &= -\varepsilon_1 \Delta + \beta_1 \cdot \nabla + \alpha_1 + \gamma_1 r_1^{'}(u) r_2(v),\\
B_{22} &= -\varepsilon_2 \Delta + \beta_2 \cdot \nabla + \alpha_2 + \gamma_2 r_1(u) r_2^{'}(v).
\end{aligned}
$$

3 Discontinuous Galerkin Discretization

The DG discretization of (2.9) is based on the SIPG discretization for the diffusion and an upwind discretization for the convection. The same discretization is used, e.g., in [15, 27] for a single linear convection diffusion equation and in [18, 33, 34, 35] for linear optimal control problems.

Let $\{\mathcal{T}_h\}_h$ be a family of shape regular meshes such that $\overline{\Omega} = \cup_{K\in\mathcal{T}_h}\overline{K}$, $K_i \cap K_j = \emptyset$ for $K_i, K_j \in \mathcal{T}_h$, $i \neq j$. The diameter of an element K and the length of an edge E are denoted by h_K and h_E, respectively.

We split the set of all edges $\mathcal{E}_h$ into the set $\mathcal{E}_h^0$ of interior edges, and the set $\mathcal{E}_h^\partial$ of boundary edges so that $\mathcal{E}_h = \mathcal{E}_h^\partial \cup \mathcal{E}_h^0$. Let $\mathbf{n}$ denote the unit outward normal to $\partial\Omega$. We define the inflow boundary

$$\Gamma^- = \{x \in \partial\Omega \, : \, \beta \cdot \mathbf{n}(x) < 0\},$$

and the outflow boundary $\Gamma^+ = \partial\Omega \setminus \Gamma^-$. The boundary edges are decomposed into edges $\mathcal{E}_h^- = \left\{E \in \mathcal{E}_h^\partial \, : \, E \subset \Gamma^-\right\}$ that correspond to the inflow boundary and edges $\mathcal{E}_h^+ = \mathcal{E}_h^\partial \setminus \mathcal{E}_h^-$ that correspond to the outflow boundary.

The inflow and outflow boundaries of an element $K \in \mathcal{T}_h$ are defined by

$$\partial K^- = \{x \in \partial K \, : \, \beta \cdot \mathbf{n}_K(x) < 0\}, \quad \partial K^+ = \partial K \setminus \partial K^-,$$

where $\mathbf{n}_K$ is the unit normal vector on the boundary ∂K of an element K.

Let the edge E be a common edge for two elements K and K^e. For a piecewise continuous scalar function u, there are two traces of u along E, denoted by $u|_E$ from inside K and $u^e|_E$ from inside K^e. Then, the jump and average of y across the edge E are defined by:

$$[\![u]\!] = u|_E \mathbf{n}_K + u^e|_E \mathbf{n}_{K^e}, \quad \{\{u\}\} = \frac{1}{2}\big(u|_E + u^e|_E\big). \tag{3.1}$$

Similarly, for a piecewise continuous vector field ∇u, the jump and average across an edge E are given by

$$[\![\nabla u]\!] = \nabla u|_E \cdot \mathbf{n}_K + \nabla u^e|_E \cdot \mathbf{n}_{K^e}, \quad \{\{\nabla u\}\} = \frac{1}{2}\big(\nabla u|_E + \nabla u^e|_E\big). \tag{3.2}$$

For a boundary edge $E \in K \cap \Gamma$, we set $\{\{\nabla u\}\} = \nabla u$ and $[\![u]\!] = u\mathbf{n}$ where $\mathbf{n}$ is the outward normal unit vector on Γ.

3.1 Discretization of State System

We here describe the discretization of the state system (1.2) for a fixed distributed control c.

Let $\mathbb{P}^1(K)$ be the set of all polynomials on $K \in \mathcal{T}_h$ of degree at most 1. Then, we define the discrete state and control spaces to be

$$W_h = Y_h = \left\{y \in L^2(\Omega) \, : \, y\,|_K \in \mathbb{P}^1(K) \quad \forall K \in \mathcal{T}_h\right\}, \tag{3.3a}$$

$$C_h = \left\{c \in L^2(\Omega) \, : \, c\,|_K \in \mathbb{P}^1(K) \quad \forall K \in \mathcal{T}_h\right\}, \tag{3.3b}$$

respectively. The space Y_h of discrete states and the space of test functions W_h are identical due to the weak treatment of boundary conditions for DG methods.

The DG method proposed here is based on the upwind discretization for the convection term and on the SIPG discretization for the diffusion term. This leads to the formulation

$$a_h^1(u,w) + \gamma_1 \sum_{K\in\mathcal{T}_h} \int_K r_1(u_h) r_2(v_h) w_h \, dx + b_h(c,w) = l_h^1(w), \tag{3.4}$$

$$a_h^2(v,w) + \gamma_2 \sum_{K\in\mathcal{T}_h} \int_K r_1(u_h) r_2(v_h) w_h \, dx = l_h^2(w), \tag{3.5}$$

where the (bi)-linear terms are defined as for $i = 1,2$ and $\forall w \in W_h$ as

$$\begin{aligned}
a_h^i(z,w) &= \sum_{K\in\mathcal{T}_h} \int_K \varepsilon_i \nabla z \cdot \nabla w \, dx \\
&\quad - \sum_{E\in\mathcal{E}_h} \int_E \{\{\varepsilon_i \nabla z\}\} \cdot [\![w]\!] \, ds - \sum_{E\in\mathcal{E}_h} \int_E \{\{\varepsilon_i \nabla w\}\} \cdot [\![z]\!] \, ds \\
&\quad + \sum_{E\in\mathcal{E}_h} \frac{\sigma\varepsilon_i}{h_E} \int_E [\![z]\!] \cdot [\![w]\!] \, ds + \sum_{K\in\mathcal{T}_h} \int_K \beta_i \cdot \nabla z w + \alpha_i z w \, dx \\
&\quad + \sum_{K\in\mathcal{T}_h} \int_{\partial K^- \setminus \Gamma} \beta_i \cdot \mathbf{n}(z^e - z) w \, ds - \sum_{K\in\mathcal{T}_h} \int_{\partial K^- \cap \Gamma^-} \beta_i \cdot \mathbf{n} z w \, ds, && (3.6a) \\
b_h(c,w) &= -\sum_{K\in\mathcal{T}_h} \int_K c w \, dx, && (3.6b) \\
l_h^i(w) &= \sum_{K\in\mathcal{T}_h} \int_K f_i w \, dx + \sum_{E\in\mathcal{E}_h^\partial} \frac{\sigma\varepsilon_i}{h_E} \int_E g_i \mathbf{n} \cdot [\![w]\!] \, ds - \sum_{E\in\mathcal{E}_h^\partial} \int_E g_i \{\{\varepsilon_i \nabla w\}\} \, ds \\
&\quad - \sum_{K\in\mathcal{T}_h} \int_{\partial K^- \cap \Gamma^-} \beta_i \cdot \mathbf{n} \, g_i w \, ds && (3.6c)
\end{aligned}$$

with the nonnegative real parameter σ being called the penalty parameter. We choose σ to be sufficiently large, independently of the mesh size h and the diffusion coefficient ε to ensure the stability of the DG discretization as described in [25, Sec. 2.7.1] with a lower bound depending only on the polynomial degree.

Now, we describe the discretized optimal control problem by

$$\min J(u_h, v_h, c_h) = \sum_{K\in\mathcal{T}_h} \left(\frac{\omega_u}{2} \|u_h - u_h^d\|_K^2 + \frac{\omega_v}{2} \|v_h - v_h^d\|_K^2 + \frac{\omega_c}{2} \|c_h\|_K^2 \right) \tag{3.7a}$$

subject to

$$a_h^1(u_h, w_h) + (\gamma_1 r_1(u_h) r_2(v_h), w_h) + b_h(c_h, w_h) = l_h^1(w_h) \quad \forall w \in W_h, \tag{3.7b}$$

$$a_h^2(v_h, w_h) + (\gamma_2 r_1(u_h) r_2(v_h), w_h) = l_h^2(w_h) \quad \forall w \in W_h \tag{3.7c}$$

with $(u_h, v_h, c_h) \in (Y_h, Y_h, C_h)$. Then, the optimality system of the discretized optimal control problem (3.7) is

$$
\begin{aligned}
a_h^1(w_h, p_h) &+ (\gamma_1 p_h r_1^{'}(u_h) r_2(v_h), w_h) \\
&+ (\gamma_2 q_h r_1^{'}(u_h) r_2(v_h), w_h) + \omega_u (u_h, w_h) = \omega_u (u_h^d, w_h) \quad \forall w_h \in W_h, && (3.8a) \\
a_h^2(w_h, q_h) &+ (\gamma_1 p_h r_1(u_h) r_2^{'}(v_h), w_h) \\
&+ (\gamma_2 q_h r_1(u_h) r_2^{'}(v_h), w_h) + \omega_v (v_h, w_h) = \omega_v (v_h^d, w_h) \quad \forall w_h \in W_h, && (3.8b) \\
b_h(w_h, p_h) + \omega_c (c_h, w_h) &= 0 \qquad \forall w_h \in C_h, && (3.8c) \\
a_h^1(u_h, w_h) + (\gamma_1 r_1(u_h) r_2(v_h), w_h) + b_h(c_h, w_h) &= l_h^1(w_h) \qquad \forall w_h \in W_h, && (3.8d) \\
a_h^2(v_h, w_h) + (\gamma_2 r_1(u_h) r_2(v_h), w_h) &= l_h^2(w_h) \qquad \forall w_h \in W_h. && (3.8e)
\end{aligned}
$$

Note that we can neglect the errors introduced by the discretization of coefficients γ_1 and γ_2 since they are taken as constant coefficients. Hence, we take $\gamma_1 = \gamma_h^1$ and $\gamma_2 = \gamma_h^2$ throughout this paper.

3.2 DG Discretization of the Newton System

The DG discretization of the right-hand side $\Phi(x_k)$ of the Newton system in (2.9) is written as

$$
\Phi(x_k) = \begin{bmatrix} A_u^T p_k + \gamma_1 F_{p_k, u_k^{'}, v_k} + \gamma_2 F_{q_k, u_k^{'}, v_k} + \omega_u M u_k - l_p \\ A_v^T q_k + \gamma_1 F_{p_k, u_k, v_k^{'}} + \gamma_2 F_{q_k, u_k, v_k^{'}} + \omega_v M v_k - l_q \\ \omega_c M c_k - M p_k \\ A_u u_k + \gamma_1 F_{u_k, v_k} - M c_k - l_u \\ A_v v_k + \gamma_2 F_{u_k, v_k} - l_v \end{bmatrix}, \tag{3.9}
$$

where

$$
F_{p_k, u_k^{'}, v_k} = \int_\Omega p_k r_1^{'}(u_k) r_2(v_k) \varphi_i \, dx, \quad F_{q_k, u_k^{'}, v_k} = \int_\Omega q_k r_1^{'}(u_k) r_2(v_k) \varphi_i \, dx,
$$

$$
F_{p_k, u_k, v_k^{'}} = \int_\Omega p_k r_1(u_k) r_2^{'}(v_k) \varphi_i \, dx, \quad F_{q_k, u_k, v_k^{'}} = \int_\Omega q_k r_1(u_k) r_2^{'}(v_k) \varphi_i \, dx,
$$

$$
F_{u_k, v_k} = \int_\Omega r_1(u_k) r_2(v_k) \varphi_i \, dx.
$$

A_u and A_v correspond to the bilinear forms $a_h^1(u,w)$ and $a_h^2(v,w)$, whereas l_u and l_v correspond the linear forms $l_h^1(w)$ and $l_h^2(w)$. Further, $l_p = \int_\Omega \omega_u u_d w \, dx$, $l_q = \int_\Omega \omega_v v_d w \, dx$ and mass matrix $M_{ij} = \int\limits_\Omega \varphi_i \varphi_j \, dx$.

The discretized form of the $\Phi^{'}(x_k)$ (2.9) is given by

$$
\Phi^{'}(x_k) = \begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{0} \end{bmatrix} := \mathcal{A} \tag{3.10}
$$

with

$$
\mathbf{A} = \begin{bmatrix} \gamma_1 M_{p,u'',v} + \gamma_2 M_{q,u'',v} + M\omega_u & \gamma_1 M_{p,u',v'} + \gamma_2 M_{q,u',v'} & 0 \\ \gamma_1 M_{p,u',v'} + \gamma_2 M_{q,u',v'} & \gamma_1 M_{p,u,v''} + \gamma_2 M_{q,u,v''} + M\omega_v & 0 \\ 0 & 0 & \omega_c M \end{bmatrix},
$$

$$
\mathbf{B} = \begin{bmatrix} A_u + \gamma_1 M_{u',v} & \gamma_1 M_{u,v'} & -M \\ \gamma_2 M_{u',v} & A_v + \gamma_2 M_{u,v'} & 0 \end{bmatrix},
$$

where

$$
M^{i,j}_{u',v} = \int_\Omega r_1'(u_k) r_2(v_k) \varphi_i \varphi_j \, dx, \quad M^{i,j}_{u,v'} = \int_\Omega r_1(u_k) r_2'(v_k) \varphi_i \varphi_j \, dx,
$$

$$
M^{i,j}_{p,u'',v} = \int_\Omega p_k r_1''(u_k) r_2(v_k) \varphi_i \varphi_j \, dx, \quad M^{i,j}_{q,u'',v} = \int_\Omega q_k r_1''(u_k) r_2(v_k) \varphi_i \varphi_j \, dx,
$$

$$
M^{i,j}_{p,u,v''} = \int_\Omega p_k r_1(u_k) r_2''(v_k) \varphi_i \varphi_j \, dx, \quad M^{i,j}_{q,u,v''} = \int_\Omega q_k r_1(u_k) r_2''(v_k) \varphi_i \varphi_j \, dx,
$$

$$
M^{i,j}_{p,u',v'} = \int_\Omega p_k r_1'(u_k) r_2'(v_k) \varphi_i \varphi_j \, dx, \quad M^{i,j}_{q,u',v'} = \int_\Omega q_k r_1'(u_k) r_2'(v_k) \varphi_i \varphi_j \, dx.
$$

In this paper, we use the SIPG method due to its symmetric property. It guarantees that the discretization of the optimality system is the same as the optimality system of the SIPG discretized optimal control problem, i.e., the "optimize-then-discretize" and the "discretize-then-optimize" commute. This commutative property does not hold for several other popular DG methods (see, e.g., [17, 34]).

3.3 Fast solution of the Newton system and alternatives

We now briefly want to discuss the efficient solution of the linear system (3.10), which is a linear system in saddle point form (see [5, 7] for introductions to this field). As the linear system $\mathcal{A}$ is typically of large dimension, the use of direct solvers is often not feasible. Hence, iterative solvers have to be employed. Here, we focus on methods of Krylov subspace type that build up a low-dimensional subspace, to then find a good approximation to the solution within this subspace. The approximation quality typically depends on the system parameters such as the mesh-size and regularization parameters. In order to achieve robust performance, the linear system $\mathcal{A}x = b$ is multiplied by a preconditioner $\mathcal{P}$ such that the equivalent system $\mathcal{P}^{-1}\mathcal{A}x = \mathcal{P}^{-1}b$ can be solved. Here we assume that the matrix $\mathcal{P}^{-1}\mathcal{A}$ has better numerical properties compared to the original one. For symmetric problems, and in some sense also for nonsymmetric ones, this is achieved by guaranteeing that $\mathcal{P}^{-1}\mathcal{A}$ has a small number of distinct eigenvalues or clusters of eigenvalues. To achieve this, the matrix $\mathcal{P}$ has to resemble $\mathcal{A}$ in some sense while still being easy to invert. For this we follow [20] where it is shown that efficient approximations of the $(1,1)$-block A and the Schur complement $BA^{-1}B^T$ result in good convergence behaviour. For the derivation of the preconditioners we follow [24], where preconditioners for time-dependent reaction-diffusion problems were introduced. We first discuss the approximation of the matrix A. Note that depending on the parameters γ_1, γ_2 and the values of state, control, and adjoint, this block may become indefinite, which means that the reduced Hessian of the overall problem is not symmetric positive definite. One remedy is to apply a Gauss-Newton technique [10, 22], where we ignore second derivatives with respect to the Lagrange multipliers leading to a $(1,1)$-block of the form

$$A_{GN} = \begin{bmatrix} M\omega_u & 0 & 0 \\ 0 & M\omega_v & 0 \\ 0 & 0 & \omega_c M \end{bmatrix}.$$

Note that we denote the original block of the Newton matrix by A_G. It is easy to see that the matrix A_{GN} can trivially be inverted in the case of diagonal mass matrices, which is satisfied for our DG scheme. Otherwise, the Chebyshev semi-iteration is a suitable candidate to approximate the individual sub-blocks [31]. The situation is more complicated when the Newton method is applied as we then need a more involved approximation

$$A_G \approx \hat{A}_G = \begin{bmatrix} A_S & 0 & 0 \\ \gamma_1 M_{p,u',v'} + \gamma_2 M_{q,u',v'} & \gamma_1 M_{p,u,v''} + \gamma_2 M_{q,u,v''} + M\omega_v & 0 \\ 0 & 0 & \omega_c M \end{bmatrix},$$

where we assume that the blocks $\omega_c M$ and $\gamma_1 M_{p,u'',v} + \gamma_2 M_{q,u'',v} + M\omega_u$ can easily be inverted as the matrices are diagonal. The matrix A_S represents the Schur complement of the upper left block, i.e.,

$$\begin{aligned} A_S = \gamma_1 M_{p,u'',v} + \gamma_2 M_{q,u'',v} + M\omega_u - \left(\gamma_1 M_{p,u',v'} + \gamma_2 M_{q,u',v'}\right) \\ \left(\gamma_1 M_{p,u,v''} + \gamma_2 M_{q,u,v''} + M\omega_v\right)^{-1} \left(\gamma_1 M_{p,u',v'} + \gamma_2 M_{q,u',v'}\right), \end{aligned}$$

where we assume that all matrices involved are diagonal and hence trivially invertible. We now have to efficiently approximate the Schur complement, which in general is a more difficult task. Following [24], we derive a preconditioner that approximates all terms of the Schur complement

$$S = BA^{-1}B^T = KL^{-1}K^T + \frac{1}{\omega_c}\mathcal{M},$$

where we use the notation that

$$\begin{aligned} K &= \begin{bmatrix} A_u + \gamma_1 M_{u',v} & \gamma_1 M_{u,v'} \\ \gamma_2 M_{u',v} & A_v + \gamma_2 M_{u,v'} \end{bmatrix}, \quad \mathcal{M} = \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix}, \\ L &= \begin{bmatrix} \gamma_1 M_{p,u'',v} + \gamma_2 M_{q,u'',v} + M\omega_u & \gamma_1 M_{p,u',v'} + \gamma_2 M_{q,u',v'} \\ \gamma_1 M_{p,u',v'} + \gamma_2 M_{q,u',v'} & \gamma_1 M_{p,u,v''} + \gamma_2 M_{q,u,v''} + M\omega_v \end{bmatrix}. \end{aligned}$$

A technique that has proven to provide good convergence uses an approximation of the following form

$$\hat{S} = (K + \hat{\mathcal{M}}_1)\hat{L}^{-1}(K + \hat{\mathcal{M}}_2)^T,$$

where $\hat{L}$ approximates the upper 2×2-block of $A_{G/GN}$. The goal is for

$$\hat{\mathcal{M}}_1 \hat{L}^{-1} \hat{\mathcal{M}}_2^T \approx \frac{1}{\omega_c} \mathcal{M},$$

which is achieved when

$$\hat{\mathcal{M}}_1 = \begin{bmatrix} \frac{1}{\sqrt{\omega_c}} M & 0 \\ 0 & 0 \end{bmatrix} \text{ and } \hat{\mathcal{M}}_2 = \begin{bmatrix} \frac{1}{\sqrt{\omega_c}} A_S & 0 \\ 0 & 0 \end{bmatrix}.$$

Note that this approximation can be used for both the Newton and Gauss-Newton approach. In the Gauss-Newton approach the matrix A_S is simply given by $M\omega_u$. Note that we now need to approximate the inverse of $(K + \hat{\mathcal{M}}_{1,2})$, which we can efficiently do using a fixed number of steps of a preconditioned Uzawa method with a block-diagonal preconditioner where the diagonal blocks of $(K + \hat{\mathcal{M}}_{1,2})$ need to be approximated. We currently use a proof-of-concept implementation that uses a factorisation of these block but appropriately chosen multigrid schemes are of course possible.

The above mentioned preconditioner is embedded into a Krylov subspace solver. These solvers approximate the solution within the Krylov subspace

$$\operatorname{span}\left\{ r_0, \mathcal{P}^{-1}\mathcal{A}r_0, \left(\mathcal{P}^{-1}\mathcal{A}\right)^2 r_0, \dots \right\},$$

where r_0 is the initial residual. In our case we employed GMRES [26], which minimizes the norm of the residual over the current Krylov subspace.

4 A Posteriori Error Estimator

Our a posteriori error estimator builds upon the work by Schötzau and Zhu [27] for the SIPG method and by Verfürth [29] for continuous finite element methods. Similar error estimators are also used in the optimal control context [33, 35]. Here, we extend this concept to optimal control problems governed by a system of convection diffusion PDEs with nonlinear reaction terms.

We measure the error of control c in the L^2 norm, while we measure the error of the state variables (u, v) and the adjoint variables (p, q) in the norm $|||\cdot|||$ and the semi-norm $|\cdot|_A$ [27], which are defined by

$$|||z|||^2 = \sum_{K \in \mathcal{T}_h} (\|\varepsilon \nabla z\|^2_{L^2(K)} + \kappa \|z\|^2_{L^2(K)}) + \sum_{E \in \mathcal{E}_h} \frac{\sigma\varepsilon}{h_E} \|[\![z]\!]\|^2_{L^2(E)}, \tag{4.1}$$

$$|z|^2_A = |\beta z|^2_* + \sum_{E \in \mathcal{E}_h} (\kappa h_E + \frac{h_E}{\varepsilon}) \|[\![z]\!]\|^2_{L^2(E)}, \tag{4.2}$$

where

$$|q|_* = \sup_{w \in H^1_0(\Omega) \setminus \{0\}} \frac{\int_\Omega q \cdot \nabla w dx}{|||w|||} \qquad \text{for } q \in L^2(\Omega)^2. \tag{4.3}$$

The terms $|\beta z|_*^2$ and $h_E\varepsilon^{-1}\|[\![z]\!]\|_{L^2(E)}^2$ of the semi-norm $|\cdot|_A$ will be used to bound the convective derivative, similar to [27, 29]. The other term $\kappa h_E\|[\![z]\!]\|_{L^2(E)}^2$ is related to the linear reaction term.

Let

$$f_h^i, u_h^d, v_h^d, \alpha_h^i, \gamma_h^i \in W_h, \quad \beta_h^i \in W_h^2$$

denote approximations to the right hand sides f_i, the desired states u_d, v_d, the linear reaction terms α_i, the nonlinear reaction coefficients γ_i, and the convection terms β_i, respectively, for $i = 1,2$.

We define weights by $\rho_{K,i} = \min\{h_K\varepsilon_i^{-\frac{1}{2}}, \kappa_i^{-\frac{1}{2}}\}$ and $\rho_{E,i} = \min\{h_E\varepsilon_i^{-\frac{1}{2}}, \kappa_i^{-\frac{1}{2}}\}$, for $i = 1,2$. When $\kappa_i = 0$, $\rho_{K,i} = h_K\varepsilon_i^{-\frac{1}{2}}$ and $\rho_{E,i} = h_E\varepsilon_i^{-\frac{1}{2}}$ are taken.

For each element $K \in \mathcal{T}_h$, the error indicators of the state η_K^u, η_K^v and the adjoint η_K^p, η_K^q are given by

$$(\eta_K^z)^2 = \left[(\eta_{R_K}^z)^2 + (\eta_{E_K}^z)^2 + (\eta_{J_K}^z)^2\right], \qquad z \in \{u,v,p,q\},$$

where for $K \in \mathcal{T}_h$ the interior residual terms are defined by

$$\begin{aligned}
\eta_{R_K}^u &= \rho_{K,1}\|f_h^1 + c_h + \varepsilon_1\Delta u_h - \beta_h^1\cdot\nabla u_h - \alpha_h^1 u_h - \gamma_h^1 r_1(u_h)r_2(v_h)\|_{L^2(K)},\\
\eta_{R_K}^v &= \rho_{K,2}\|f_h^2 + \varepsilon_2\Delta v_h - \beta_h^2\cdot\nabla v_h - \alpha_h^2 v_h - \gamma_h^2 r_1(u_h)r_2(v_h)\|_{L^2(K)},\\
\eta_{R_K}^p &= \rho_{K,1}\| - \omega_u(u_h - u_h^d) + \varepsilon_1\Delta p_h + \beta_h^1\cdot\nabla p_h - (\alpha_h^1 - \nabla\cdot\beta_h^1)p_h\\
&\qquad - \gamma_h^1 p_h r_1'(u_h)r_2(v_h) - \gamma_h^2 q_h r_1'(u_h)r_2(v_h)\|_{L^2(K)},\\
\eta_{R_K}^q &= \rho_{K,2}\| - \omega_v(v_h - v_h^d) + \varepsilon_2\Delta q_h + \beta_h^2\cdot\nabla q_h - (\alpha_h^2 - \nabla\cdot\beta_h^2)q_h\\
&\qquad - \gamma_h^1 p_h r_1(u_h)r_2'(v_h) - \gamma_h^2 q_h r_1(u_h)r_2'(v_h)\|_{L^2(K)},
\end{aligned}$$

the edge residuals for $z = u,p$ and $s = v,q$ are

$$\begin{aligned}
(\eta_{E_K}^z)^2 &= \frac{1}{2}\sum_{E\in\partial K\setminus\Gamma}\varepsilon_1^{-\frac{1}{2}}\rho_{E,1}\|[\![\varepsilon_1\nabla z_h]\!]\|_{L^2(E)}^2,\\
(\eta_{E_K}^s)^2 &= \frac{1}{2}\sum_{E\in\partial K\setminus\Gamma}\varepsilon_2^{-\frac{1}{2}}\rho_{E,2}\|[\![\varepsilon_2\nabla s_h]\!]\|_{L^2(E)}^2,
\end{aligned}$$

and the terms measuring the jumps for $(z,i) \in \{(u,1),(v,2),(p,1),(q,2)\}$ are

$$\begin{aligned}
(\eta_{J_K}^z)^2 =& \frac{1}{2}\sum_{E\in\partial K\setminus\Gamma}\Big(\frac{\sigma\varepsilon_i}{h_E} + \kappa_i h_E + \frac{h_E}{\varepsilon_i}\Big)\|[\![z_h]\!]\|_{L^2(E)}^2\\
&+ \sum_{E\in\partial K\cap\Gamma}\Big(\frac{\sigma\varepsilon_i}{h_E} + \kappa_i h_E + \frac{h_E}{\varepsilon_i}\Big)\|[\![z_h]\!]\|_{L^2(E)}^2.
\end{aligned}$$

Finally, our a posteriori error indicators of the optimal control problem (1.1)-(1.2) are given by

$$\eta^z = \Big(\sum_{K\in\mathcal{T}_h}(\eta_K^z)^2\Big)^{1/2} \quad z \in \{u,v,p,q\}. \tag{4.4}$$

The data approximation errors are

$$\theta^z = \Big(\sum_{K \in \mathcal{T}_h} (\theta_K^z)^2 \Big)^{1/2} \quad z \in \{u, v, p, q\}, \tag{4.5}$$

where

$$\begin{aligned}
(\theta_K^u)^2 &= \rho_{K,1}^2 \Big(\|f_1 - f_h^1\|_{L^2(K)}^2 + \|(\beta_1 - \beta_h^1) \cdot \nabla u_h\|_{L^2(K)}^2 + \|(\alpha_1 - \alpha_h^1) u_h\|_{L^2(K)}^2 \Big), \\
(\theta_K^v)^2 &= \rho_{K,2}^2 \Big(\|f_2 - f_h^2\|_{L^2(K)}^2 + \|(\beta_2 - \beta_h^2) \cdot \nabla v_h\|_{L^2(K)}^2 + \|(\alpha_2 - \alpha_h^2) v_h\|_{L^2(K)}^2 \Big), \\
(\theta_K^p)^2 &= \rho_{K,1}^2 \Big(\|\omega_u (u_h^d - u_d)\|_{L^2(K)}^2 + \|(\beta_1 - \beta_h^1) \cdot \nabla v_h\|_{L^2(K)}^2 \\
&\qquad + \|\big((\alpha_1 - \nabla \cdot \beta_1) - (\alpha_h^1 - \nabla \cdot \beta_h^1)\big) p_h\|_{L^2(K)}^2 \Big), \\
(\theta_K^q)^2 &= \rho_{K,2}^2 \Big(\|\omega_v (v_h^d - v_d)\|_{L^2(K)}^2 + \|(\beta_2 - \beta_h^2) \cdot \nabla q_h\|_{L^2(K)}^2 \\
&\qquad + \|\big((\alpha_2 - \nabla \cdot \beta_2) - (\alpha_h^2 - \nabla \cdot \beta_h^2)\big) q_h\|_{L^2(K)}^2 \Big).
\end{aligned}$$

Assume that (**A1**)-(**A5**) are satisfied. Let (u, v, c, p, q) and $(u_h, v_h, c_h, p_h, q_h)$ be the solutions of (2.8) and (3.8), respectively. Furthermore, let the error estimators η^z (4.4) and the data approximation errors θ^z (4.5) be defined for $z \in \{u, v, p, q\}$. We will prove the reliability estimate

$$\|c - c_h\|_{L^2(\Omega)} + \sum_z |||z - z_h||| + |z - z_h|_A \lesssim \sum_z (\eta^z + \theta^z)$$

(see Theorem 4.6) and the efficiency estimate

$$\sum_z \eta^z \lesssim \|c - c_h\|_{L^2(\Omega)} + \sum_z |||z - z_h||| + |z - z_h|_A + \theta^z.$$

(see Theorem 4.7).

Remark 4.1 *Our a posteriori error indicators are defined for* $\kappa_i \geq 0, \ i = 1, 2$. *Although the a posteriori error indicators (4.4) work in numerical examples, we need* $\kappa_i > 0$ *to prove the constants independent of* ε_i *in the proof of our reliability and efficiency estimates. We note that this assumption is also made for analysis of optimal control problems governed by convection dominated equations [4, 14, 18, 32, 33, 35].*

Throughout this section we use the symbols $\lesssim$ and $\gtrsim$ to denote bounds that are valid up to positive constants independent of the local mesh sizes, the diffusion coefficients ε_i, $i = 1, 2$, and the penalty parameter σ, provided that $\sigma \geq 1$.

The reliability and efficiency estimates of our estimator are proven provided that the state equations (1.2) have homogeneous boundary conditions, i.e., $g_i = 0$, $i = 1, 2$ as proven in [27, 33, 35].

4.1 Reliability of a Posteriori Error Estimator

The following reliability results (4.6-4.9) are obtained by adapting the notation in [27, Thm. 3.2]. Nonlinear terms are eliminated by using the boundedness and continuous Lipschitz conditions given in assumption (**A5**).

Theorem 4.2 *Let (**A1**-**A5**) be satisfied. If $u[c_h]$ is the solution of (2.8d) with $v = v_h$, $c = c_h$ and u_h is the solution of (3.8d), then*

$$|||u[c_h] - u_h||| + |u[c_h] - u_h|_A \lesssim \eta^u + \theta^u. \tag{4.6}$$

If $\tilde{v}$ is the solution of (2.8e) with $u = u_h$ and v_h is the solution of (3.8e), then

$$|||\tilde{v} - v_h||| + |\tilde{v} - v_h|_A \lesssim \eta^v + \theta^v. \tag{4.7}$$

If $\tilde{p}$ is the solution of (2.8a) with $u = u_h, v = v_h, q = q_h$ and p_h is the solution of (3.8a), then

$$|||\tilde{p} - p_h||| + |\tilde{p} - p_h|_A \lesssim \eta^p + \theta^p. \tag{4.8}$$

If $\tilde{q}$ is the solution of (2.8b) with $u = u_h, v = v_h, p = p_h$ and q_h is the solution of (3.8b), then

$$|||\tilde{q} - q_h||| + |\tilde{q} - q_h|_A \lesssim \eta^q + \theta^q. \tag{4.9}$$

We also need the following result on the continuous dependence of the solution to the scalar linear state equation with homogeneous boundary conditions, and of the solution to the adjoint equation.

Lemma 4.3 *Let (**A1**-**A5**) be satisfied and let $g \in L^2(\Omega)$. If $z \in Y$ solves $a_i(z,w) = (g,w)$ for all $w \in W$ and $i = 1,2$, then*

$$|||z||| + |z|_A \lesssim \|g\|_{L^2(\Omega)}, \quad z \in \{u,v\}. \tag{4.10}$$

If $s \in Y$ solves $a_i(w,s) = (g,w)$ for all $w \in V$ and $i = 1,2$, then

$$|||s||| + |s|_A \lesssim \|g\|_{L^2(\Omega)}, \quad s \in \{p,q\}. \tag{4.11}$$

Proof. The papers [29, L. 3.1] and [27, L. 4.4] prove the existence of a constant $C > 0$ such that

$$\inf_{z \in H_0^1(\Omega)\setminus\{0\}} \sup_{w \in H_0^1(\Omega)\setminus\{0\}} \frac{a_i(z,w)}{(|||z||| + |u|_A)|||w|||} \geq C > 0.$$

Since $\kappa > 0$ we have $(g,w) \leq \|g\|_{L^2(\Omega)}\|w\|_{L^2(\Omega)} \lesssim \|g\|_{L^2(\Omega)}|||w|||$. If $z \in Y$ solves $a_i(z,w) = (g,w)$ for all $w \in W$ and $i = 1,2$, then the inf − sup condition implies

$$(|||z||| + |z|_A)|||w||| \lesssim a_i(z,w) = (g,w) \lesssim \|g\|_{L^2(\Omega)}|||w|||,$$

which is the desired inequality (4.10).

The inequality (4.11) can be proven analogously. □

To prove our reliability result, we need the following auxiliary equations. For given $c \in L^2(\Omega)$ we let $u[c] \in H^1(\Omega) \cap L^2(\Omega)$ denote the solution of

$$a_1(u[c],w) + (\gamma_1 r_1(u[c])r_2(v),w) - (c,w) = (f_1,w) \quad \forall w \in W, \tag{4.12a}$$
$$a_2(v,w) + (\gamma_2 r_1(u[c])r_2(v),w) = (f_2,w) \quad \forall w \in W, \tag{4.12b}$$

and let $p[c] \in H^1(\Omega) \cap L^2(\Omega)$ denote the solution of

$$\begin{aligned} a_1(w,p[c]) &+ (\gamma_1 p[c]r_1'(u[c])r_2(v),w) \\ &+ (\gamma_2 q r_1'(u[c])r_2(v),w) + \omega_u(u[c],w) = \omega_u(u_d,w) \quad \forall w \in W, \end{aligned} \tag{4.13a}$$
$$\begin{aligned} a_2(w,q) &+ (\gamma_1 p[c]r_1(u[c_h])r_2'(v),w) \\ &+ (\gamma_2 q r_1(u[c])r_2'(v),w) + \omega_v(v,w) = \omega_v(v_d,w) \qquad \forall w \in W. \end{aligned} \tag{4.13b}$$

The next result is a common ingredient in error analyses for optimal control problems (see, e.g., [19, pp. 1328,1329]) and essentially uses the convexity of the cost functional and boundedness and the locally continuous Lipschitz condition of the nonlinear terms in assumption (**A5**).

Lemma 4.4 *Assume that (**A1-A5**) are satisfied. If (u,v,c,p,q) and (u_h,v_h,c_h,p_h,q_h) are the solutions of (2.8) and (3.8), respectively, then*

$$\|c-c_h\|^2_{L^2(\Omega)} \lesssim \|p_h - p[c_h]\|^2_{L^2(\Omega)} + \|u[c_h]-u\|^2_{L^2(\Omega)} + \|p-p[c_h]\|^2_{L^2(\Omega)}. \tag{4.14}$$

Proof. Let $u[c_h], p[c_h]$ solve (4.12a) and (4.13a) with $c = c_h$. For any $w \in W$ we have

$$(w, \omega_c c - p) - (w, \omega_c c_h - p[c_h]) = (w, p[c_h]-p) + \omega_c(c-c_h,w)$$

Setting $w = c - c_h$ this leads to

$$\begin{aligned} &(c-c_h, \omega_c c - p) - (c-c_h, \omega_c c_h - p[c_h]) \\ &\quad = \quad (c-c_h, p[c_h]-p) + \omega_c\|c-c_h\|^2_{L^2(\Omega)}. \end{aligned} \tag{4.15}$$

From (4.12a) and (4.13a) we can deduce

$$\begin{aligned} (c-c_h, p[c_h]-p) &= (c, p[c_h]-p) - (c_h, p[c_h]-p) \\ &= a_1(u-u[c_h], p[c_h]) - a_1(u-u[c_h], p) \\ &\quad +(\gamma_1 r_2(v)(r_1(u)-r_1(u[c_h])), p[c_h]-p) \\ &= \omega_u\|u-u[c_h]\|^2_{L^2(\Omega)} \\ &\quad +\big(\gamma_1 r_2(v)(p r_1'(u) - p[c_h]r_1'(u[c_h])), u-u[c_h]\big) \\ &\quad +\big(\gamma_2 q r_2(v)(r_1'(u) - r_1'(u[c_h])), u-u[c_h]\big) \\ &\quad +\big(\gamma_1 r_2(v)(r_1(u)-r_1(u[c_h])), p[c_h]-p\big). \end{aligned} \tag{4.16}$$

Using equations (4.15) and (4.16), the gradient equations (2.8c) and (3.8c), we obtain

$$
\begin{aligned}
\omega_c\|c-c_h\|^2_{L^2(\Omega)} \;\le\;& (c-c_h,\omega_c c-p)-(c-c_h,\omega_c c_h-p[c_h]) \\
&+\big(\gamma_1 r_2(v)(p[c_h]r_1'(u[c_h])-pr_1'(u)),u-u[c_h]\big) \\
&+\big(\gamma_2 q r_2(v)(r_1'(u[c_h])-r_1'(u)),u-u[c_h]\big) \\
&+\big(\gamma_1 r_2(v)(r_1(u[c_h])-r_1(u)),p[c_h]-p\big) \\
=\;& (c-c_h,p[c_h]-p_h)-(\omega_c c_h-p_h,c-c_h) \\
&+\big(\gamma_1 r_2(v)(p[c_h]r_1'(u[c_h])-pr_1'(u)),u-u[c_h]\big) \\
&+\big(\gamma_2 q r_2(v)(r_1'(u[c_h])-r_1'(u)),u-u[c_h]\big) \\
&+\big(\gamma_1 r_2(v)(r_1(u[c_h])-r_1(u)),p[c_h]-p\big). \qquad (4.17)
\end{aligned}
$$

With the help of the assumption (**A5**), the boundedness of the solutions and Young's inequality, we obtain

$$
\begin{aligned}
&\big(\gamma_1 r_2(v)(p[c_h]r_1'(u[c_h])-pr_1'(u)),u-u[c_h]\big) \\
&\lesssim \|p[c_h]r_1'(u[c_h])-pr_1'(u)\|^2_{L^2(\Omega)}+\|u[c_h]-u\|^2_{L^2(\Omega)} \\
&= \|r_1'(u[c_h])(p[c_h]-p)+p(r_1'(u[c_h])-r_1'(u))\|^2_{L^2(\Omega)}+\|u[c_h]-u\|^2_{L^2(\Omega)} \\
&\lesssim \|p[c_h]-p\|^2_{L^2(\Omega)}+\|u[c_h]-u\|^2_{L^2(\Omega)}. \qquad (4.18)
\end{aligned}
$$

Similarly, the last two terms of (4.17) are bounded by

$$\big(\gamma_2 q r_2(v)(r_1'(u[c_h])-r_1'(u)),u-u[c_h]\big) \lesssim \|u[c_h]-u\|^2_{L^2(\Omega)}. \qquad (4.19)$$

$$\big(\gamma_1 r_2(v)(r_1(u[c_h])-r_1(u)),p[c_h]-p\big) \lesssim \|u[c_h]-u\|^2_{L^2(\Omega)}. \qquad (4.20)$$

Inserting (4.18-4.20) into (4.17) and applying Young's inequality, the desired result is obtained. □

Lemma 4.5 *Let (**A1-A5**) be satisfied. If $(u[c_h],v,p[c_h],q)$ solves (2.8) and (u_h,v_h,p_h,q_h) solves (3.8), then we have*

$$
\begin{aligned}
|||u[c_h]-u_h|||+|u[c_h]-u_h|_A \;&\lesssim\; \eta^u+\theta^u+\|v-v_h\|_{L^2(\Omega)}, && (4.21a)\\
|||v-v_h|||+|v-v_h|_A \;&\lesssim\; \eta^v+\theta^v+\|u-u_h\|_{L^2(\Omega)}, && (4.21b)\\
|||p[c_h]-p_h|||+|p[c_h]-p_h|_A \;&\lesssim\; \eta^p+\theta^p+\|u[c_h]-u_h\|_{L^2(\Omega)} \\
&\quad +\|v-v_h\|_{L^2(\Omega)}+\|q-q_h\|_{L^2(\Omega)}, && (4.21c)\\
|||q-q_h|||+|q-q_h|_A \;&\lesssim\; \eta^q+\theta^q+\|u-u_h\|_{L^2(\Omega)} \\
&\quad +\|v-v_h\|_{L^2(\Omega)}+\|p-p_h\|_{L^2(\Omega)}. && (4.21d)
\end{aligned}
$$

Proof. Let $\tilde u\in H^1(\Omega)\cap L^2(\Omega)$ solve (2.8d) with $v=v_h, c=c_h$. The difference $u[c_h]-\tilde u\in H^1(\Omega)\cap L^2(\Omega)$ solves

$$a_1(u[c_h]-\tilde u,w)+(\gamma_1 r_1(u[c_h])r_2(v)-\gamma_1 r_1(\tilde u)r_2(v_h),w)=0 \quad \forall w\in W.$$

Note that we can write

$$\gamma_1 r_1(u[c_h])r_2(v) - \gamma_1 r_1(\tilde{u})r_2(v_h) = \gamma_1 r_1(\tilde{u})\big(r_2(v_h) - r_2(v)\big) + \gamma_1 r_2(v)\big(r_1(\tilde{u}) - r_1(u[c_h])\big).$$

Then, Lemma 4.3, assumption (**A5**) and $\|u[c_h] - \tilde{u}\|_{L^2(\Omega)} \lesssim |||u[c_h] - \tilde{u}|||$ yield

$$|||u[c_h] - \tilde{u}||| + |u[c_h] - \tilde{u}|_A \lesssim \|v - v_h\|_{L^2(\Omega)}. \tag{4.22}$$

Moreover, Theorem 4.2 implies

$$|||\tilde{u} - u_h||| + |\tilde{u} - u_h|_A \lesssim \eta^u + \theta^u. \tag{4.23}$$

Hence, the desired inequality (4.21a) follows from (4.22) and (4.23).

Similarly, let $\tilde{p} \in H^1(\Omega) \cap L^2(\Omega)$ solve (2.8a) with $u = u_h, v = v_h, q = q_h, c = c_h$. The difference $p[c_h] - \tilde{p} \in H^1(\Omega) \cap L^2(\Omega)$ solves

$$\begin{aligned} a_1(w, p[c_h] - \tilde{p}) &+ (\gamma_1 p[c_h] r_1'(u[c_h]) r_2(v) - \gamma_1 \tilde{p} r_1'(u_h) r_2(v_h), w) \\ &+ (\gamma_2 q r_1'(u[c_h]) r_2(v) - \gamma_2 q_h r_1'(u_h) r_2(v_h), w) = 0 \quad \forall w \in W. \end{aligned}$$

By adding and subtracting suitable terms and then using Lemma 4.3, assumption (**A5**), the boundedness of solutions, $\|p[c_h] - \tilde{p}\|_{L^2(\Omega)} \lesssim |||p[c_h] - \tilde{p}|||$ and Theorem 4.2, the desired result (4.21b) is obtained. The inequalities (4.21c-4.21d) can be proven analogously.

□

Theorem 4.6 *Assume that assumptions (**A1-A5**) are satisfied. Let (u, v, c, p, q) and $(u_h, v_h, c_h, p_h, q_h)$ be the solutions of (2.8) and (3.8), respectively. If the error estimators η^z and θ^z are defined by (4.4) and (4.5) for $z \in \{u, v, p, q\}$, then we have the a posteriori error bound*

$$\|c - c_h\|_{L^2(\Omega)} + \sum_z |||z - z_h||| + |z - z_h|_A \lesssim \sum_z (\eta^z + \theta^z).$$

Proof. From (4.12)-(4.13) and (2.8), we have $\forall w \in W_h$

$$a_1(u - u[c_h], w) = \big(\gamma_1 r_2(v)(r_1(u[c_h]) - r_1(u)), w\big) + (c - c_h, w), \tag{4.24}$$

$$\begin{aligned} a_1(w, p - p[c_h]) = &\big(\gamma_1 r_2(v)(p[c_h] r_1'(u[c_h]) - p r_1'(u)), w\big) \\ &+ \big(\gamma_2 q r_2(v)(r_1'(u[c_h]) - r_1'(u)), w\big) - \omega_u(u - u[c_h], w). \end{aligned} \tag{4.25}$$

By the continuity results in Lemma 4.3 and assumption (**A5**) we have

$$|||u - u[c_h]||| + |u - u[c_h]|_A \lesssim \|c - c_h\|_{L^2(\Omega)}, \tag{4.26}$$

$$|||p - p[c_h]||| + |p - p[c_h]|_A \lesssim \|u - u[c_h]\|_{L^2(\Omega)}. \tag{4.27}$$

Now, using the estimate $\|w\|_{L^2(\Omega)} \lesssim |||w|||$ for $w \in W_h$ and applying Lemma 4.4, Lemma 4.5, and Theorem 4.2, we obtain the desired bound. □

4.2 Efficiency of a Posteriori Error Estimator

Theorem 4.7 *Assume that assumptions (**A1**-**A5**) are satisfied. Let (u,v,c,p,q) and (u_h,v_h,c_h,p_h,q_h) be the solutions of (2.8) and (3.8), respectively. If the error estimators η^z and θ^z are defined by (4.4) and (4.5) for $z \in \{u,v,p,q\}$, then we have the upper bound*

$$\sum_z \eta^z \lesssim \|c - c_h\|_{L^2(\Omega)} + \sum_z |||z - z_h||| + |z - z_h|_A + \theta^z.$$

Proof. The proof of the efficiency result is similar to Thm. 3.2 in [27]. For each variable, that is, u,v,p,q, the bounds are found by applying the same procedure. The nonlinear terms are bounded by the assumption (**A5**) and the inequality $\|z - z_h\|_{L^2(\Omega)} \lesssim |||y - y_h|||$ is used. □

5 The Adaptive Loop

The adaptive procedure consists of successive execution of the several steps:

SOLVE → **ESTIMATE** → **MARK** → **REFINE**.

The **SOLVE** step is the numerical solution of the optimal control problem with respect to the given triangulation $\mathcal{T}_h$ using the DG discretization. For the **ESTIMATE** step, the residual error estimator $(\eta_K^u)^2 + (\eta_K^v)^2 + (\eta_K^p)^2 + (\eta_K^q)^2$, $K \in \mathcal{T}_h$ defined in Section 4 is used. In the **MARK** step, the edges and elements for the refinement are specified by using the a posteriori error indicator (4.4) and by choosing subsets $\mathcal{M}_K \subset \mathcal{T}_h$ such that the following bulk criterion is satisfied for the given marking parameter θ:

$$\sum_{K \in \mathcal{T}_h} (\eta_K^u)^2 + (\eta_K^v)^2 + (\eta_K^p)^2 + (\eta_K^q)^2 \leq \theta \sum_{K \in \mathcal{M}_K} (\eta_K^u)^2 + (\eta_K^v)^2 + (\eta_K^p)^2 + (\eta_K^q)^2. \tag{5.1}$$

Finally, in the **REFINE** step, the marked elements are refined by longest edge bisection, where the elements of the marked edges are refined by bisection.

6 Numerical Results

We present numerical results for optimal control problems governed by a system of convection-diffusion PDEs with nonlinear reaction terms. When the analytical solutions of the state and the adjoint variables are given, the Dirichlet boundary data g_i, the source functions f_i and the desired states u_d, v_d are computed from (2.5-2.7) using the exact state, adjoint and control. We use piecewise linear polynomials for discretization of the state, adjoint and control variables. The penalty parameter in the SIPG method is chosen as $\sigma = 6$ on interior edges and $\sigma = 12$ on boundary edges. The marking parameter θ in (5.1) varies between 0.3 and 0.6.

6.1 Example with Interior Layers

The following example is constructed by using the examples in [14, 32]. The problem data are

$$\Omega = (0,1)^2, \quad \omega_u = \omega_v = 1, \quad \omega_c = 0.1, \quad \varepsilon_1 = \varepsilon_2 = 10^{-6},$$

$$\beta_1 = (2,3)^T, \quad \beta_2 = (1,0)^T, \quad \alpha_1 = \alpha_2 = 1, \quad r_1(u) = u \quad \text{and} \quad r_2(v) = v.$$

The exact state solutions

$$u(x_1,x_2) = \frac{2}{\pi}\arctan\left(\frac{1}{\sqrt{\varepsilon_1}}\left[-\frac{1}{2}x_1 + x_2 - \frac{1}{4}\right]\right),$$
$$v(x_1,x_2) = 4e^{\frac{-1}{\sqrt{\varepsilon_2}}\left((x-0.5)^2+3(y-0.5)^2\right)}\sin(x\pi)\cos(y\pi)$$

are constructed to have a straight interior layer and an interior layer at the center, respectively, whereas the exact adjoint solutions

$$\begin{aligned} p(x_1,x_2) =& 16x_1(1-x_1)x_2(1-x_2) \\ & \times \left(\frac{1}{2} + \frac{1}{\pi}\arctan\left[\frac{2}{\sqrt{\varepsilon}}\left(\frac{1}{16} - \left(x_1 - \frac{1}{2}\right)^2 - \left(x_2 - \frac{1}{2}\right)^2\right)\right]\right), \\ q(x_1,x_2) =& e^{\frac{-1}{\sqrt{\varepsilon_2}}\left((x-0.5)^2+3(y-0.5)^2\right)}\sin(x\pi)\cos(y\pi) \end{aligned}$$

are constructed to have a circular interior layer and an interior layer at the center, respectively.

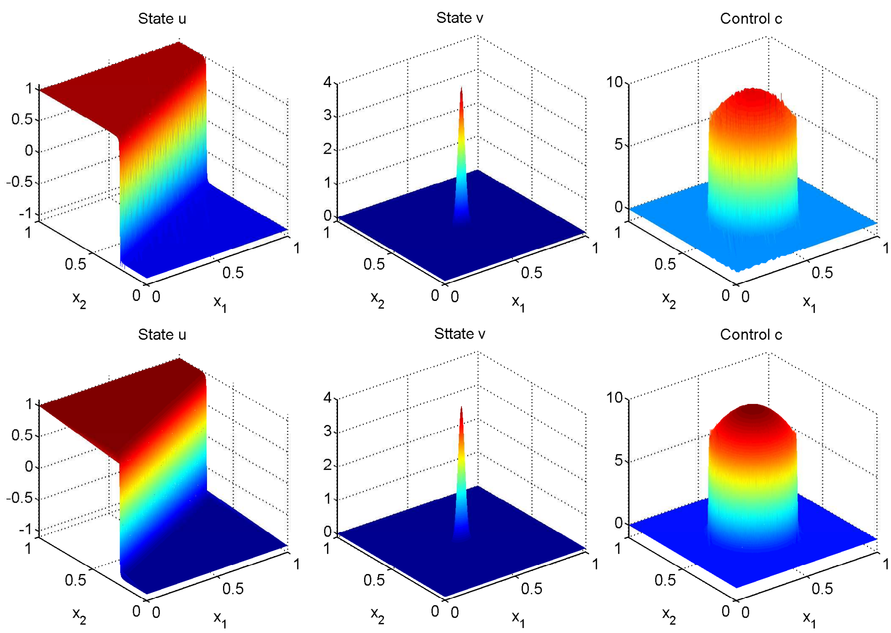


Figure 1: Example 6.1: The plots in the top row show the computed states u, v and control c on a uniformly refined mesh with 16641 vertices for $\gamma_i = 0.1$, $i = 1,2$. The plots in the bottom row show the computed states u, v and control c on an adaptively refined mesh with 15826 vertices for $\gamma_i = 0.1$, $i = 1,2$.

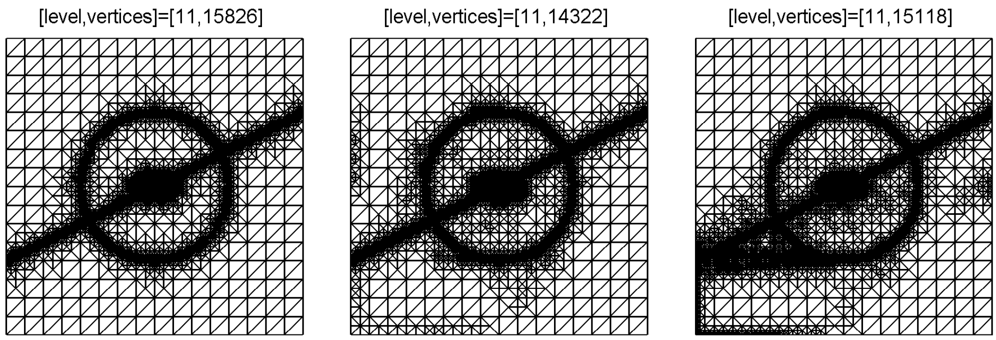


Figure 2: Example 6.1: Adaptively refined meshes for $\gamma_i = 0.1, 1, 5$, $i = 1, 2$ (from left to right).

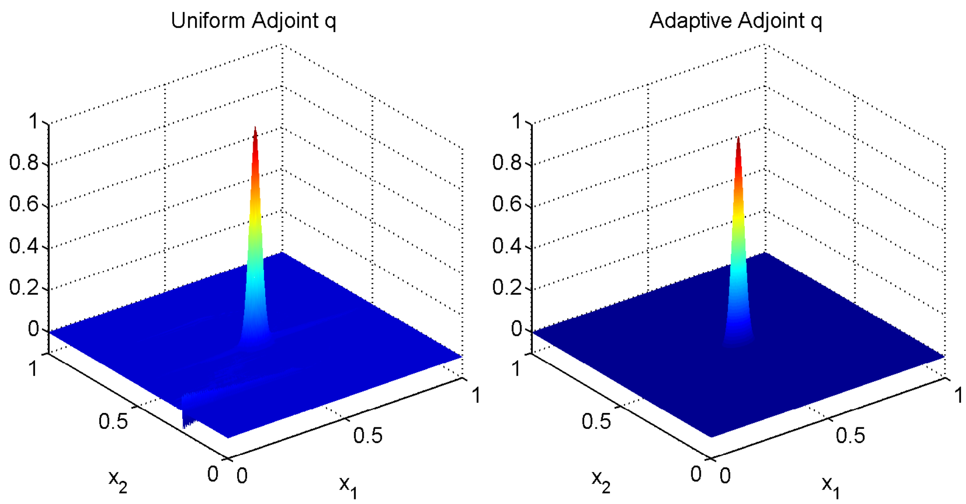


Figure 3: Example 6.1: The plots show the L_2 errors of the adjoint q on a uniformly refined mesh with 16641 vertices and on an adaptively refined mesh with 15118 vertices, respectively, for $\gamma_i = 5$, $i = 1, 2$.

The example having exact solutions of the state u and adjoint p has been used in [14] with an edge stabilization for the control constraint and in [33] with SIPG discretization for the unconstrained case. Also, the example having exact solutions of the state v and adjoint q has been studied in [32] with an edge stabilization and in [35] with SIPG discretization for the control constraint. We here construct a coupled state system with a nonlinear reaction term by combining these two examples.

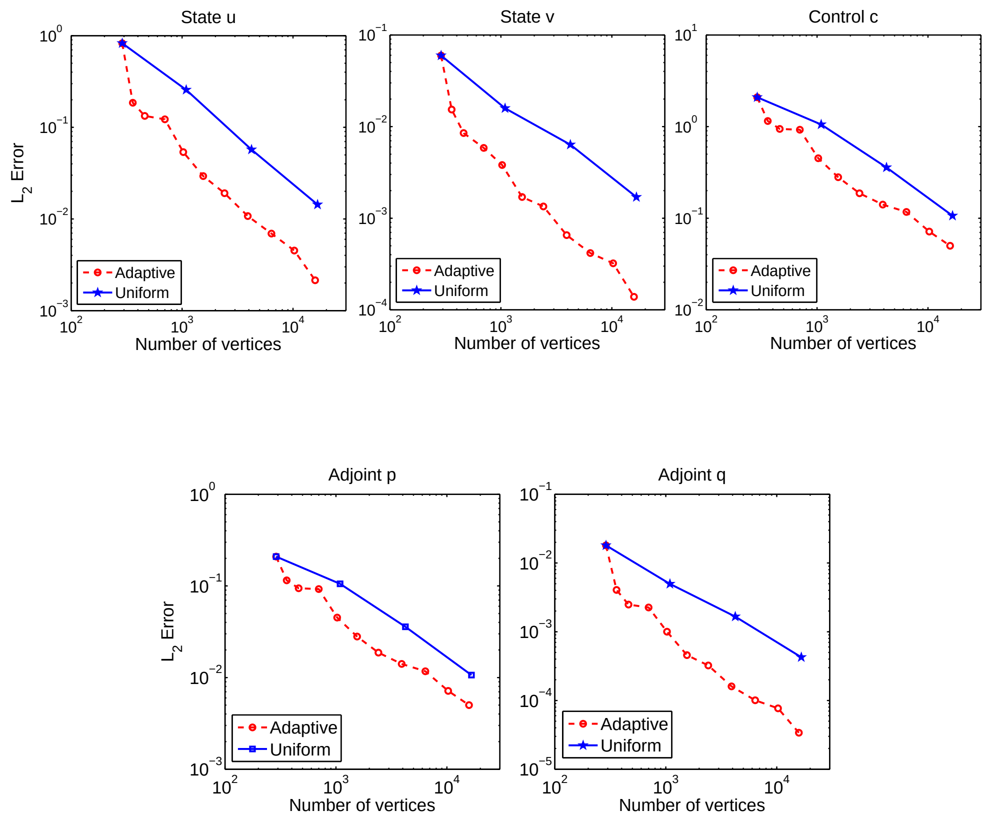
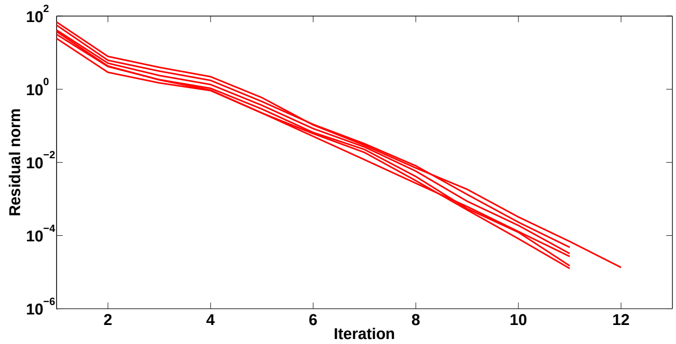
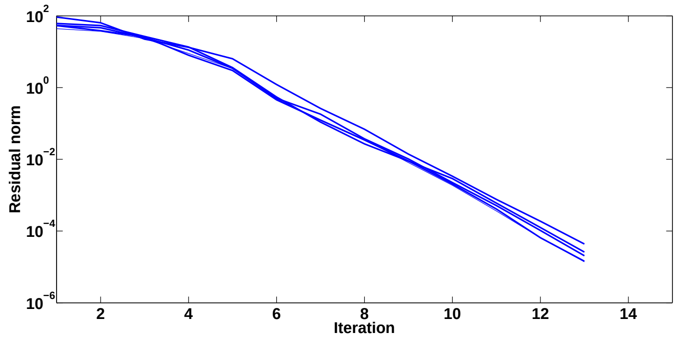


Figure 4: Example 6.1: The plots in the top row show the L_2 errors of the states u, v and control c on a uniformly refined mesh with 16641 vertices for $\gamma_i = 0.1$, $i = 1,2$. The plots in the bottom row show the L_2 errors of the adjoints p, q on an adaptively refined mesh with 15826 vertices for $\gamma_i = 0.1$, $i = 1,2$.

Figure 1 shows that oscillations occur on the interior layers when the initial mesh is refined uniformly with 16641 vertices for $\gamma_i = 0.1$. However, picking out the layers by using the error indicators given in (4.4), the oscillations are reduced. This proves the performance of the adaptive refinement over the uniform refinement. Figure 2 reveals adaptively refined meshes for $\gamma_1 = 0.1, 1, 5$ for $i = 1,2$, respectively. The adaptive mesh obtained for $\gamma_i = 0.1$ is similar to the numerical results obtained in [33] for the linear problems. However, extra regions are refined when we increase values of γ_i. The reason is that the interaction of variables increases with higher values of γ_i. We also observe that the unexpected oscillations occur for the adjoint q when the values of γ_i are increased as shown in Figure 3.



(a) Iteration numbers for $\omega_c = 1e-1$



(b) Iteration numbers for $\omega_c = 1e-3$

Figure 5: Example 6.1: Iteration numbers for the second step of the Gauss-Newton method and a variety of adaptively refined meshes.

The errors measured in the L_2 norm for the state, adjoint and control are decreasing faster for the adaptively refined mesh than for the uniformly refined mesh as shown in Figure 4 for $\gamma_i = 0.1$. We also observe that the errors of adaptive refinement decrease monotonically.

Additionally, we want to briefly illustrate the performance of the proposed preconditioner shown in Figure 5, where we show the GMRES iteration numbers for the second step of the Gauss-Newton method on a variety of adaptively refined meshes and two different values of the regularization parameter ω_c. The convergence of GMRES is measured in the relative norm of the preconditioned residual and the iterations are stopped when the relative residual norm is smaller than $1e-6$. It can be seen that the iteration numbers for both problems are almost constant with respect to the mesh-size and the value of the regularization parameter.

At the moment we only have a proof-of-concept implementation as we have not yet used multigrid techniques to approximate the preconditioning sub-blocks. Also, the presented examples are all set up in two dimensions, where typically sparse factorisations show outstanding performance. This is no longer the case for three-dimensional examples, whereas our preconditioners do utilize the two-dimensional nature of the problem.

6.2 Example with Boundary Layers

The problem data are

$$\Omega = (0,1)^2, \quad \omega_u = \omega_v = 1, \quad \omega_c = 10^{-4}, \quad \varepsilon_1 = \varepsilon_2 = 10^{-6},$$

$$\beta_1 = (1,1)^T, \quad \beta_2 = (-1,-2)^T, \quad \alpha_1 = 0 \quad \text{and} \quad \alpha_2 = 1.$$

The source functions and desired state functions are defined by

$$f_1 = 0, \quad f_2 = 1, \quad u_d = 1 \quad \text{and} \quad v_d = 1.$$

The Dirichlet boundary conditions, i.e., $g_i = 0$ for $i = 1,2$, are homogeneous. The nonlinear reaction term is defined by

$$r_1(u) = u \quad \text{and} \quad r_2(v) = \frac{-v}{1+v}.$$

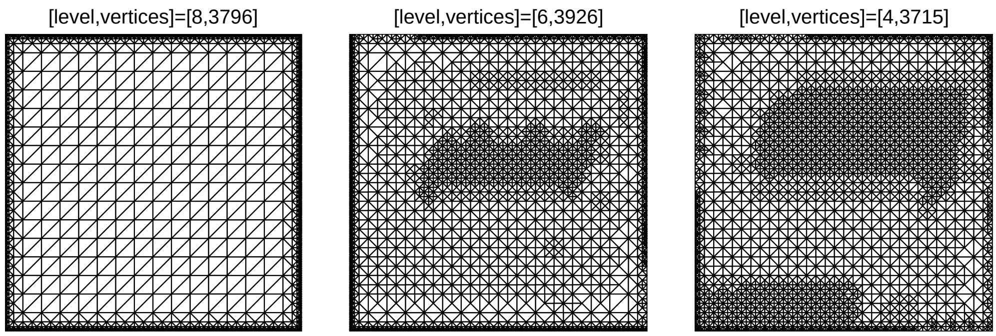


Figure 6: Example 6.2: Adaptively refined meshes for $\gamma_i = 0.1, 1, 5$ for $i = 1,2$ (from left to right).

Figure 7 reveals the computed solutions of the control c on the uniformly refined mesh with 4225 vertices and on an adaptively refined mesh with 3796 vertices for $\gamma_i = 0.1$, $i = 1,2$. The numerical solution on the uniform mesh exhibits oscillations due to the boundary layers as shown in Figure 6. By resolving the boundary layers, the oscillations are reduced as illustrated in Figure 7. From Figure 7, it is evident that substantial computing work can be saved by using efficient adaptive mesh refinement.

As in the previous example, the error estimator (4.4) refines extra regions when the values of the coefficients γ_i of the nonlinear terms are increased, see Figure 6.

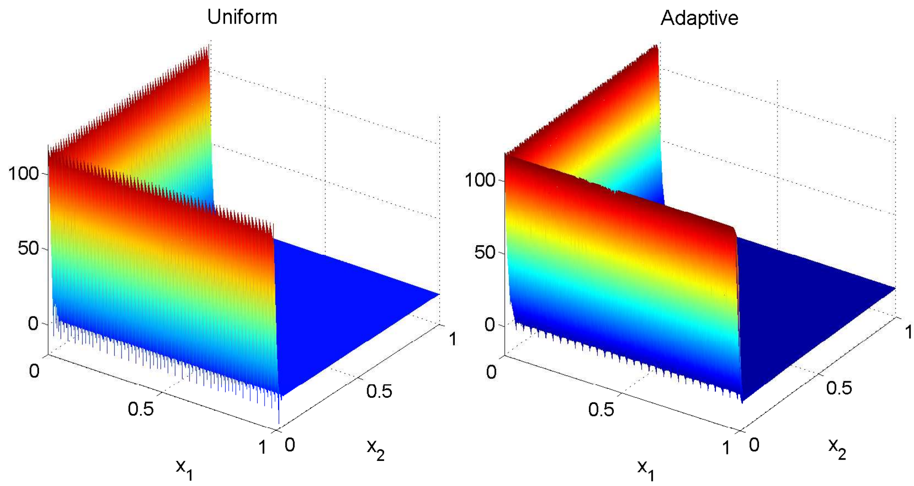


Figure 7: Example 6.2: The computed control c on a uniformly refined mesh (4225 vertices) and on an adaptively refined mesh (3796 vertices) for $\gamma_i = 0.1$, $i = 1,2$.

7 Conclusions

In this paper, we have studied a posteriori error estimates of the symmetric interior penalty Galerkin (SIPG) method for the optimal control problems governed by a system of convection-diffusion PDEs with nonlinear reaction terms, arising from chemical process engineering. The saddle point system resulting from the optimality conditions and discretized with piecewise linear polynomials is solved by using a suitable preconditioner within a Krylov subspace method. We have proven the reliability and efficiency of our estimator. The extension of the results here to unsteady optimal control problems with state and/or control constraints in 2D and 3D is the topic of current investigations and will be addressed in coming work.

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