A posteriori error estimation and dynamic adaptivity for symmetric discontinuous Galerkin approximations of reactive transport problems

Shuyu Sun*, Mary F. Wheeler

The Center for Subsurface Modeling (CSM), The Institute for Computational Engineering and Sciences (ICES), The University of Texas at Austin, 201 E. 24th Street, Austin TX 78712, USA

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Abstract

A symmetric discontinuous Galerkin scheme is applied for solving reactive transport problems. An explicit a posteriori error estimator in $L^2(L^2)$ is derived for the semi-discrete scheme applied to transport with general kinetic reactions. Explicit a posteriori error estimators in terms of linear functionals and negative norms are also obtained for transport problems with simple reactions. An adaptive approach based on the a posteriori error estimators is proposed to modify the mesh dynamically. Numerical examples demonstrate the efficiency and effectivity of the estimators. Moreover, it is shown in this study that the proposed adaptivity eliminates the need of slope limiters.

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1. Introduction

Numerical modeling of reactive transport in porous media has important applications in numerous diverse fields, such as petroleum recovery, groundwater hydrology, environmental protection, rock mechanics, soil chemistry, and biomedical engineering. In particular, the numerical simulation of reactive transport contributes considerably to solutions for sustainable water management and protection [47]. Its importance cannot be overemphasized, as water is of paramount social and economic value, and the availability and use of water will considerably influence the global development of our society. For
instance, natural attenuation is used in tens of thousands of contaminated sites in the United States in place of or in conjunction with engineering remediation systems. Another important application of reactive transport is in geological carbon sequestration \[16,46\], which represents one of the most promising approaches for mitigating the harmful greenhouse effect of carbon dioxide. In addition, the decision on how and where to store radioactive nuclear waste relies on the prediction of transport behaviors of radioactive species after thousands or even millions of years \[36,37\]. Similarly, the distillation operation in a packed column commonly used in chemical industry concerns the heat and mass transfer in porous media \[51,50,56\] and is thus appropriate for the application of numerical modeling methods for reactive transport. Furthermore, reactive transport and flow have found many uses in the medical sciences since most parts of the human body are themselves porous media. In particular, modeling of blood flow, nutrient transport and angiogenesis in the porous tissues of the human body assists medical doctors gain a better understanding of blood-vessel formation during cancer development, and may help pharmaceutical engineers design effective drug delivery systems \[54,55\]. However, realistic simulations for simultaneous transport and chemical reaction present significant mathematical and computational challenges \[10,25,61,47,43,30,24\].

Discontinuous Galerkin (DG) methods \[17,33,59,42,11,12,58,28\] have recently gained popularity for a wide variety of problems, and they are of particular interest for multiscale, adaptive and parallel implementation because they have several appealing properties: (1) they are element-wise conservative; (2) they support local approximations of high orders; (3) they are robust and non-oscillatory in the presence of high gradients; (4) they are implementable on unstructured and even non-matching meshes; and (5) with the appropriate meshing, they are capable of delivering exponential rates of convergence. In addition, the mass matrices are block diagonal for DG applied to time-dependent problems, which provides a substantial computational advantage, especially if explicit time integrations are used.

DG applications for flow and transport problems in porous media have been studied in \[49,41,60\]. It has been found that DG methods have optimal convergence in \(L^2(H^1)\) for both flow and transport problems \[41,42,48\]. The optimal \(hp\)-convergence behaviors in \(L^2(L^2)\) and in negative norms have also been established for the symmetric DG formulations with a jump term (commonly referred to as the SIPG) \[52,48\]. In this paper, we propose and study a posteriori error estimators and dynamic and adaptive strategies guided by the estimators for SIPG.

Unlike a priori error estimates, a posteriori error estimators do not involve knowledge of the exact unknown solution and are thus in general computable. A posteriori error estimators can be used to signify where modifications in discretization parameters need to be made, thus achieving adaptivity, in particular, goal-oriented \(hp\)-adaptivity \[31,39,20,8,5–7,19,21–23,26,32,35,38,40,44,27,18,4,2,3\], see also \[57,9,13\] and references therein. Because the rates of chemical reactions in many complex sub-surface systems may vary by several orders of magnitude across the domain, adaptivity is essential and a posteriori error estimators can be particularly useful in reactive transport problems. There are many error estimators for steady state problems (e.g., error estimators based on gradient recovery, equilibrated residual methods, implicit and explicit estimators), however, the investigation of a posteriori error estimators for transient problems, especially for reactive transport problems, is limited. While implicit estimators attempt to compute tight bounds on the error through the use of a dual problem with the residuals as data and to avoid a generic constant, explicit estimators can be computed efficiently directly from the computed solution and given data. It should be noted that explicit estimators serve as error indicators for adaptation but cannot be used to perform an actual assessment of the error due to the presence of an unknown constant, whereas implicit estimators, although computationally more expensive, would provide such error assessments. Explicit a posteriori error estimators in the \(L^2(H^1)\) norm have been derived for DG methods applied to reactive transport \[53\]. This paper is primarily devoted to explicit a posteriori estimators in \(L^2(L^2)\). We remark that error indicators in the \(L^2(L^2)\) norm are preferred over indicators in \(L^2(H^1)\) for problems concerning the concentration itself rather than the transport flux.
The paper is organized as follows. In the following section, we describe the modeling equations. The DG scheme and some of its known properties are introduced in Section 3. Section 4 contains an explicit a posteriori error estimator in the $L^2(L^2)$ norm for the semi-discrete scheme. In Section 5, explicit a posteriori error estimators in terms of linear functionals for the semi-discrete scheme are derived. Based on that, explicit a posteriori error estimators in negative norms are also obtained. In Section 6, numerical examples based on the explicit a posteriori error estimator in the $L^2(L^2)$ norm are presented. The conclusions are summarized in Section 7.

2. Governing equations

For convenience, we consider reactive transport with a single flowing phase in porous media, though our results extend to reactive transport in surface water. We assume that the Darcy velocity field $u$ is given, is time-independent, and satisfies $\nabla \cdot u = q$, where $q$ is the imposed external total flow rate.

We consider only a single advection–diffusion–reaction equation. Results for a system of equations with kinetic reactions can be derived by similar arguments. In addition, for convenience, we assume that $X$ is a polygonal and bounded domain in $\mathbb{R}^d$, $(d = 1, 2$ or $3)$ with boundary $\partial X = \Gamma_\text{in} \cup \Gamma_\text{out}$. Here, we denote by $\Gamma_\text{in}$ the inflow boundary and by $\Gamma_\text{out}$ the outflow/no-flow boundary, i.e.,

$\Gamma_\text{in} = \{x \in \partial X : u \cdot n > 0\},$

$\Gamma_\text{out} = \{x \in \partial X : u \cdot n < 0\},$

where $n$ denotes the unit outward normal vector to $\partial X$.

Let $T$ be the final simulation time. The classical advection–diffusion–reaction equation for a single flowing phase in porous media is given by

$$\frac{\partial \phi c}{\partial t} + \nabla \cdot (uc - D(u)\nabla c) = qc^* + r(c), \quad (x, t) \in \Omega \times (0, T],$$

where the unknown variable $c$ is the concentration of a species (amount per volume). Here, $\phi$ is the effective porosity and is assumed to be time-independent, uniformly bounded above and below by positive numbers; $D(u)$ is the dispersion/diffusion tensor and is assumed to be uniformly symmetric positive definite and bounded from above; $r(c)$ is the reaction term; $qc^*$ is the source/sink term, where the imposed external total flow rate $q$ is a sum of sources (injection) and sinks (extraction); and $c^*$ is the injected concentration $c_w$ if $q > 0$ or is the resident concentration $c$ if $q < 0$.

We consider the following boundary conditions for this problem:

$$(uc - D(u)\nabla c) \cdot n = c_\text{in}u \cdot n, \quad (x, t) \in \Gamma_\text{in} \times (0, T],$$

$$(-D(u)\nabla c) \cdot n = 0, \quad (x, t) \in \Gamma_\text{out} \times (0, T],$$

where $c_\text{in}$ is the inflow concentration. The initial concentration is specified in the following way:

$c(x, 0) = c_0(x), \quad x \in \Omega.$

3. Discontinuous Galerkin schemes

3.1. Notation

Let $\mathcal{E}_h$ be a family of non-degenerate, quasi-uniform and possibly non-conforming partitions of $\Omega$ composed of triangles or quadrilaterals if $d = 2$, or tetrahedra, prisms or hexahedra if $d = 3$. The
non-degeneracy requirement (also called regularity) is that the element is convex and that there exists $\rho > 0$ such that, if $h_j$ is the diameter of $E_j \in \mathcal{E}_h$, then each of the sub-triangles (for $d = 2$) or sub-tetrahedra (for $d = 3$) of element $E_j$ contains a ball of radius $\rho h_j$ in its interior. The quasi-uniformity requirement is that there is $\tau > 0$ such that $\frac{1}{\tau} \leq \frac{1}{h}$ for all $E_j \in \mathcal{E}_h$, where $h$ is the maximum diameter of all elements. It should be noted that the quasi-uniformity is assumed here only for the convenience of quoting some known DG properties in this section, but it is not required for the a posteriori error estimates in the following sections. We assume that no element crosses the boundaries in $\Gamma_{in}$ and $\Gamma_{out}$. The set of all interior edges (for a 2-dimensional domain) or faces (for a 3-dimensional domain) for $\mathcal{E}_h$ is denoted by $\Gamma_h$. On each edge or face $\gamma \in \Gamma_h$, a unit normal vector $\mathbf{n}_\gamma$ is chosen. The sets of all edges or faces on $\Gamma_{out}$ and on $\Gamma_{in}$ for $\mathcal{E}_h$ are denoted by $\Gamma_{h,out}$ and $\Gamma_{h,in}$, respectively. The normal vector $\mathbf{n}_\gamma$ for $\gamma \in \Gamma_{h,out} \cup \Gamma_{h,in}$ coincides with the outward unit normal vector.

For $s \geq 0$, we define

$$H^s(\mathcal{E}_h) = \{ \phi \in L^2(\Omega) : \phi|_{E} \in H^s(E), E \in \mathcal{E}_h \}. \tag{3.1}$$

The usual Sobolev norm on $\Omega$ is denoted by $\| \cdot \|_{m,\Omega}$ [1]. The broken norms are defined, for $m \geq 0$, as

$$\|\|\phi\||_m^2 = \sum_{E \in \mathcal{E}_h} \|\phi\|_{m,E}^2. \tag{3.2}$$

We now define the average and jump for $\phi \in H^s(\mathcal{E}_h)$, $s > 1/2$. Let $E_i, E_j \in \mathcal{E}_h$ and $\gamma = \partial E_i \cap \partial E_j \in \Gamma_h$ with $\mathbf{n}_\gamma$ exterior to $E_i$. Denote

$$\{ \phi \} = \frac{1}{2}((\phi|_{E_i})|_\gamma + (\phi|_{E_j})|_\gamma), \tag{3.3}$$

$$[\phi] = (\phi|_{E_i})|_\gamma - (\phi|_{E_j})|_\gamma. \tag{3.4}$$

Denote the upwind value of the concentration $c^*|_\gamma$ as follows:

$$c^*|_\gamma = \begin{cases} c|_{E_i} & \text{if } \mathbf{u} \cdot \mathbf{n}_\gamma > 0 \\ c|_{E_j} & \text{if } \mathbf{u} \cdot \mathbf{n}_\gamma < 0. \end{cases}$$

The discontinuous finite element space is taken to be

$$\mathcal{D}_r(\mathcal{E}_h) \equiv \{ \phi \in L^2(\Omega) : \phi|_{E} \in \mathbb{P}_r(E), E \in \mathcal{E}_h \}, \tag{3.5}$$

where $\mathbb{P}_r(E)$ denotes the space of polynomials of (total) degree less than or equal to $r$ on $E$. Note that we present $hp$-results in this paper for the local space $\mathbb{P}_r$, but the results also apply to the local space $\mathbb{Q}_r$ because $\mathbb{P}_r(\subset \mathbb{Q}_r(E))$.

We denote by $(\cdot, \cdot)_R$ the inner product in $(L^2(R))^d$ or $L^2(R)$ over a domain $R$. The inner product $(\cdot, \cdot)_\Omega$ over the entire domain $\Omega$ is also denoted simply by $(\cdot, \cdot)$. The “cut-off” operator $\mathcal{M}$ is defined as

$$\mathcal{M}(c)(x) = \min(c(x), M), \tag{3.6}$$

where $M$ is a large positive constant. It is easy to show that the “cut-off” operator $\mathcal{M}$ is uniformly Lipschitz continuous in the following sense:

**Lemma 3.1** (Property of operator $\mathcal{M}$). The “cut-off” operator $\mathcal{M}$ defined in Eq. (3.6) is uniformly Lipschitz continuous with a Lipschitz constant of one; that is

$$\|\mathcal{M}(c) - \mathcal{M}(w)\|_{L^\infty(\Omega)} \leq \|c - w\|_{L^\infty(\Omega)}. \tag{3.7}$$

We use the following $hp$-approximation results, which can be proved using the techniques in [14,15]. Let $E \in \mathcal{E}_h$ and $\phi \in H^s(E)$, and let $h_E$ denote the diameter of $E$. Then there exists a constant $K$, independent of $\phi$, $r$, and $h_E$, and a sequence of $V_r^h \in \mathbb{P}_r(E), r = 1, 2, \ldots$, such that
\[
\begin{aligned}
\left\{ \begin{array}{l}
\| \phi - z_h^q \|_{q,E} \leq K \frac{h_E^{r-q}}{r^{q+1}} \| \phi \|_{s,E} & 0 \leq q < \mu, \\
\| \phi - z_h^q \|_{q,\partial E} \leq K \frac{h_E^{r-q-1}}{r^{q+\frac{3}{2}}} \| \phi \|_{s,E} & 0 \leq q < \mu - \frac{1}{2},
\end{array} \right.
\end{aligned}
\]  

(3.8)

where \( \mu = \min(r + 1, s) \).

We shall also use the following inverse inequalities, which can be derived using the method in [45]. We let \( E \in \mathcal{E}_h \) and \( v \in \mathcal{P}_r(E) \). There exists a constant \( K \), independent of \( v, r \) and \( h_E \), such that

\[
\begin{aligned}
\| D^q v \|_{0,\partial E} & \leq K \frac{r}{h_E^{\frac{3}{2}}} \| D^q v \|_{0,E}, \quad q \geq 0 \\
\| D^{q+1} v \|_{0,E} & \leq K \frac{r^2}{h_E} \| D^q v \|_{0,E} \quad q \geq 0.
\end{aligned}
\]

(3.9)

3.2. Continuous-in-time schemes

We introduce the bilinear form \( B(c, w; u) \) defined as

\[
B(c, w; u) = \sum_{E \in \mathcal{E}_h} \int_E (D(u) \nabla c - cu) \cdot \nabla w \, dx - \int_D cq^- w \, dx \\
- \sum_{\gamma \in \Gamma_h} \int_{\gamma} \{D(u) \nabla c \cdot n \}_{\gamma} [w] \, ds - s_{\text{form}} \sum_{\gamma \in \Gamma_h} \int_{\gamma} \{D(u) \nabla w \cdot n\}_{\gamma} [c] \, ds \\
+ \sum_{\gamma \in \Gamma_h} \int_{\gamma} c^+ u \cdot n_{\gamma} [w] \, ds + \sum_{\gamma \in \Gamma_h} \int_{\gamma} cu \cdot n \, w \, ds + J_0^s(c, w),
\]

(3.10)

where \( s_{\text{form}} = -1 \) for the non-symmetric formulation and \( s_{\text{form}} = 1 \) for the symmetric scheme. For convenience of presentation, we denote \( B(c, w; u) \) as \( B_3(c, w; u) \) when \( s_{\text{form}} = 1 \). Here \( q^+ \) and \( q^- \) are the injection and extraction source terms, respectively, i.e.,

\[
q^+ = \max(q, 0), \quad q^- = \min(q, 0).
\]

By definition, we have \( q = q^+ + q^- \). In addition, we define the interior penalty term \( J_0^s(c, w) \) as

\[
J_0^s(c, w) = \sum_{\gamma \in \Gamma_h} \frac{r^2 \sigma_{\gamma}}{h_{\gamma}} \int_{\gamma} [c][w] \, ds,
\]

where \( \sigma \) is a discrete positive function that takes the constant value \( \sigma_{\gamma} \) on the edge or face \( \gamma \). We assume that \( \sigma \) is bounded from above and below: \( 0 < \sigma_0 \leq \sigma_{\gamma} \leq \sigma_m \), \( \forall \gamma \in \Gamma_h \).

The linear functional \( L(w; u, c) \) is defined by

\[
L(w; u, c) = \int_D r(M(c))w \, dx + \int_D c_w q^+ w \, dx - \sum_{\gamma \in \Gamma_{h,m}} \int_{\gamma} c_{\gamma} u \cdot n_{\gamma} w \, ds.
\]

(3.11)

We give the weak formulation of the reactive transport problem, for which a proof has been derived [52,48].

**Lemma 3.2** (Weak formulation). If \( c \) is a solution of (2.1)–(2.3) and \( c \) is essentially bounded, then \( c \) satisfies

\[
\left( \frac{\partial c}{\partial t}, w \right) + B(c, w; u) = L(w; u, c) \quad \forall w \in H^s(\mathcal{E}_h), s > \frac{3}{2} \quad \forall t \in (0, T)
\]

(3.12)

provided that the constant \( M \) for the “cut-off” operator is sufficiently large.
The continuous-in-time DG approximation \(C^{DG} \in W^{1,\infty}(0, T; \mathcal{D}_r(\mathcal{E}_h))\) of (2.1)–(2.4) is defined by

\[
\left( \partial_t \phi C^{DG}, w \right) + B(C^{DG}, w; u) = L(w; u, C^{DG}), \quad w \in \mathcal{D}_r(\mathcal{E}_h), \quad t \in (0, T],
\]

\[
(\phi C^{DG}, w) = (\phi c_0, w), \quad w \in \mathcal{D}_r(\mathcal{E}_h), \quad t = 0.
\]

3.3. Some known properties of DG

The above DG scheme always has a solution \([52,48]\).

**Lemma 3.3** (Existence of solution for DG scheme). Assume that the reaction rate is a locally Lipschitz continuous function of the concentration. Then the discontinuous Galerkin scheme (3.13) and (3.14) has a unique solution for all \(t > 0\).

We also recall an a priori error estimate in the energy norm \([52,48]\) for DG with a penalty term.

**Theorem 3.4** \((L^2(H^1)\) and \(L^\infty(L^2)\) error estimates). Let \(c\) be the solution to (2.1)–(2.4), and assume \(c \in L^2(0, T; H^s(\mathcal{E}_h)), \partial c / \partial t \in L^2(0, T; H^{r-1}(\mathcal{E}_h))\) and \(c_0 \in H^{s-1}(\mathcal{E}_h)\). We further assume that \(c, u\) and \(q\) are essentially bounded and that the reaction rate is a locally Lipschitz continuous function of \(c\). If the constant \(M\) for the “cut-off” operator and the penalty parameter \(\sigma_0\) are sufficiently large, then there exists a constant \(K\), independent of \(h\) and \(r\), such that

\[
\begin{align*}
\|C^{DG} - c\|_{L^\infty(0, T; L^2)} + \|D^1(u)\nabla(C^{DG} - c)\|_{L^2(0, T; L^2)} + \left( \int_0^T J^2_0(C^{DG} - c, C^{DG} - c) \, \mathrm{d}t \right)^{1/2} \\
\leq K \frac{h^{r-1}}{r^{r-1-\delta}} \|c\|_{L^2(0, T; H^r)} + K \frac{h^{r-1}}{r^{r-1-\delta}} \left( \|\partial c / \partial t\|_{L^2(0, T; H^{r-1})} + \|c_0\|_{H^{s-1}} \right),
\end{align*}
\]

where \(\mu = \min(r + 1, s), r \geq 1, s \geq 2,\) and \(\delta = 0\) in the case of conforming meshes with triangles or tetrahedra. In general cases, \(\delta = 1\).

4. An a posteriori error estimate in \(L^2(L^2)\)

From now on, we only consider the symmetric DG formulation (i.e. \(s_{form} = 1\)). We make additional assumptions on \(\phi\) and \(D : \phi \in W^{2,\infty}(\Omega)\) and \(D_{ij} \in W^{1,0}_{\infty}((0, T) \times \Omega)\), where

\[
W^{r,s}_{\infty}((0, T) \times \Omega) \equiv \{ f \in L^2((0, T) \times \Omega) \| f \|_{W^{r,s}_{\infty}} < \infty \},
\]

\[
\|f\|_{W^{r,s}_{\infty}} \equiv \sum_{|\alpha| \leq r, |\beta| \leq s} \text{ess sup}_{(0, T) \times D} (|D^\alpha_x f| + |D^\beta_x f|).
\]

We first recall a theorem proven in \([34,29]\):

**Theorem 4.1.** Consider the parabolic equation

\[
\frac{\partial \phi \Phi}{\partial t} + \nabla \cdot (u \Phi - D \nabla \Phi) + a \Phi = f, \quad x \in \Omega, \quad t \in (0, T],
\]

\[
D \nabla \Phi \cdot n = 0, \quad x \in \partial \Omega, \quad t \in (0, T],
\]

\[
\phi = 0, \quad x \in \Omega, \quad t = 0.
\]
Assume that $0 < \phi_0 \leq \phi(x) \leq \phi_m$, $D$ is uniformly symmetric positive definite and bounded from above, $\phi \in W^{2,\infty}(\Omega)$, $D_{ij} \in W^{1,0}((0, T) \times \Omega)$, $u \in L^\infty(\Omega)$ ($u$ being independent of time), $a \in L^2(0, T; L^\infty(\Omega))$ and $f \in L^2(0, T; L^2(\Omega))$. Then there exists a unique solution $\Phi$ satisfying the above equation and the regularity bounds given by

$$
\| \Phi \|_{L^\infty(0,T,H^1)} + \| \Phi \|_{L^2(0,T,H^2)} \leq K \| f \|_{L^2(0,T,L^2)},
$$
where $K$ is a constant independent of the input data $f$.

We define residual quantities that depend only on the approximate solution and the data. The residuals consist of the interior residual $R_i$, the zeroth order boundary residual $R_{B0}$ and the first order boundary residual $R_{B1}$, as defined below:

$$
R_i = q C^{DG} + r\cdot(\mathcal{M}(C^{DG})) - \phi \frac{\partial C^{DG}}{\partial t} - \nabla \cdot (C^{DG} u - D(u) \nabla C^{DG}), \quad (4.1)
$$

$$
R_{B0} = \begin{cases}
[C^{DG}], & x \in \gamma, \gamma \in \Gamma_h, \\
0, & x \in \partial \Omega.
\end{cases} \quad (4.2)
$$

$$
R_{B1} = \begin{cases}
[D(u) \nabla C^{DG}] \cdot \mathbf{n}, & x \in \gamma, \gamma \in \Gamma_h, \\
D(u) \nabla C^{DG} \cdot \mathbf{n}, & x \in \partial \Omega.
\end{cases} \quad (4.3)
$$

We remark that all the above quantities $R_i$, $R_{B0}$ and $R_{B1}$ are computed directly and efficiently from the DG solution. The interior residual $R_i$ is the PDE (partial differential equation) residual of the DG solution, and it is defined at every interior point of all mesh elements. The zeroth order boundary residual $R_{B0}$ is the numerical (non-physical) discontinuity or Dirichlet boundary condition residual of the DG solution, and it is defined at almost every point on the mesh element boundaries. The first order boundary residual $R_{B1}$ is the numerical (non-physical) discontinuity of the DG normal flux or Neumann boundary condition residual of the DG solution, and it is also defined at almost every point on the mesh element boundaries.

We now prove a theorem for an explicit a posteriori error estimate in the $L^2(L^2)$ norm. For simplicity of presentation, we consider the problem with only the no-flow boundary condition, but the result may be generalized. Because we are not interested in the estimation of the error coming from the $L^2$ projection of initial time data, we assume $c_0 \in \mathcal{D}_r(\mathcal{E}_h)$. We remark that for many realistic applications, the condition $c_0 \in \mathcal{D}_r(\mathcal{E}_h)$ is indeed satisfied. Throughout the paper, we denote by $K$ a generic positive constant that is independent of $h$ and $r$.

**Theorem 4.2** (Explicit a posteriori error estimate in $L^2(L^2)$). Let the assumptions in Theorem 3.4 hold. In addition, we assume $\phi \in W^{2,\infty}(\Omega)$, $D_{ij} \in W^{1,0}((0, T) \times \Omega)$, $u \in L^\infty(\Omega)$ ($u$ being independent of time), $u \cdot \mathbf{n}|_{\partial \Omega} = 0$ and $c_0 \in \mathcal{D}_r(\mathcal{E}_h)$. Then there exists a constant $K$, independent of $h$ and $r$, such that

$$
\| C^{DG} - c \|_{L^2(0,T,L^2)} \leq K \left( \sum_{E \in \mathcal{E}_h} \eta_E^2 \right)^{1/2},
$$

where

$$
\eta_E^2 = \frac{h_E^4}{r^4} \| R_i \|_{L^2(0,T,L^2(\mathcal{E}_h))}^2 + \frac{1}{2} \sum_{\gamma \in \mathcal{E}_h \setminus \partial \Omega} \frac{h_{\gamma}^4}{r^4} \| R_{B0} \|_{L^2(0,T,L^2(\gamma))}^2
$$

$$
+ \frac{1}{2} \sum_{\gamma \in \mathcal{E}_h \setminus \partial \Omega} \frac{h_{\gamma}^4}{r^4} \| R_{B1} \|_{L^2(0,T,L^2(\gamma))}^2.
$$
Here, \( h_1 = \max (h_{E_1}, h_{E_2}) \) for \( \gamma = \partial E_1 \cap \partial E_2 \), and \( h_2 = h_E \) for \( \gamma = \partial E \cap \partial \Omega \), \( r \geq 1 \) and \( \delta = 0 \) in the case of conforming meshes with triangles or tetrahedra. In general cases, \( \delta = 1 \).

**Proof.** We denote the error in the DG method by \( \xi \):

\[
\xi = \xi_{DG} - c.
\]

Subtracting the DG scheme equation by the weak formulation, we have for any \( w \in \mathcal{D}_r(\delta_h) \) the following orthogonality equation:

\[
\left( \frac{\partial \xi}{\partial t}, w \right) + B_S(\xi, w; u) = L(w; u, \xi_{DG}) - L(w; u, c). \tag{4.4}
\]

Now we consider the “backward” or adjoint parabolic equation

\[
- \frac{\partial \phi \xi}{\partial t} + \nabla \cdot (-u \Phi - D(u)\nabla \Phi) + (a + q^+) \Phi = \xi, \quad x \in \Omega, \quad t \in [0, T),
\]

\[
D \nabla \Phi \cdot n = 0, \quad x \in \partial \Omega, \quad t \in [0, T),
\]

\[
\Phi = 0, \quad x \in \Omega, \quad t = T,
\]

where \( a \) is defined by

\[
a(x, t) = - \frac{r(M(C_{DG}(x, t))) - r(M(c(x, t)))}{C_{DG}(x, t) - c(x, t)} \quad \text{if} \quad C_{DG}(x, t) - c(x, t) \neq 0
\]

and \( a(x, t) = 0 \) if \( C_{DG}(x, t) - c(x, t) = 0 \).

We note that

\[
L(w; u, \xi_{DG}) - L(w; u, c) = - \int_D (\xi_{DG} - c) a \, dx = - \int_D a \xi \, dx
\]

and

\[
\|a\|_{L^2(0,T;L^\infty)} \leq \sqrt{T} \|a\|_{L^\infty(0,T;L^\infty)} \leq K_L < \infty,
\]

where \( K_L \) is a fixed constant.

From Theorem 4.1, we know that there exists a unique solution \( \Phi \) for the adjoint equation satisfying

\[
\|\Phi\|_{L^\infty(0,T;H^1)} + \|\Phi\|_{L^2(0,T;H^2)} \leq K \|\xi\|_{L^2(0,T;L^2)}.
\]  \tag{4.5}

The \( L^2 \) norm of the error at \( t \in (0, T) \) is

\[
\|\xi\|_{0, \Omega}^2 = \sum_{E \in \delta_h} \left( \zeta, \frac{\partial \phi \xi}{\partial t} \right)_E + \sum_{E \in \delta_h} \nabla \cdot (-u \Phi - D(u)\nabla \Phi)_E + \sum_{E \in \delta_h} (\zeta, (a + q^+) \Phi)_E.
\]

Integrating by parts and observing that \( D(u) \nabla \Phi \cdot n = 0 \) on \( \partial \Omega \), \( \nabla \cdot u = q \), and \( [D(u) \nabla \Phi \cdot n] = [\Phi] = 0 \), we see

\[
\|\xi\|_{0, \Omega}^2 = \frac{d}{dt} \sum_{E \in \delta_h} (\zeta, \Phi)_E + \sum_{E \in \delta_h} \left( \frac{\partial \xi}{\partial t}, \Phi \right)_E + \sum_{E \in \delta_h} ((a - q^-) \zeta, \Phi)_E + \sum_{E \in \delta_h} (\nabla \zeta, D(u) \nabla \Phi)_E
\]

\[
- \sum_{E \in \delta_h} \int_E \{D(u) \nabla \Phi \cdot n\} [\zeta] \, ds - \sum_{E \in \delta_h} (\zeta, u \cdot \nabla \Phi)_E
\]

\[
= \frac{d}{dt} \sum_{E \in \delta_h} (\zeta, \Phi)_E + \left( \frac{\partial \xi}{\partial t}, \Phi \right)_E + (a \zeta, \Phi) + B_S(\zeta, \Phi; u).
\]
Applying the orthogonality Eq. (4.4), we obtain
\[
\|\xi\|^2_{0,\Omega} = - \frac{d}{dr} \sum_{E \in \mathcal{E}_h} \left( \xi, \phi \Phi \right)_E + \left( \phi \frac{\partial \xi}{\partial t}, \Phi - \hat{\Phi} \right) + (a \xi, \Phi - \hat{\Phi}) + B_S(\xi, \Phi - \hat{\Phi}; \mathbf{u}),
\]
(4.6)
where \( \hat{\Phi} \in \mathcal{P}_r(\mathcal{E}_h) \) is an interpolant satisfying (3.8) element-wise.

The bilinear term may be expanded as follows:
\[
B_S(\xi, \Phi - \hat{\Phi}; \mathbf{u}) = \sum_{E \in \mathcal{E}_h} \int_E \left( \mathbf{D}(\mathbf{u}) \nabla \xi - \xi \nabla \phi \right) \cdot \nabla (\Phi - \hat{\Phi}) \, dx - \int_{\partial \Omega} \hat{\xi}^q (\Phi - \hat{\Phi}) \, ds
\]
\[
- \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left\{ \mathbf{D}(\mathbf{u}) \nabla \xi \cdot \mathbf{n}_\gamma \right\} [\Phi - \hat{\Phi}] \, ds - \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left\{ \mathbf{D}(\mathbf{u}) \nabla (\Phi - \hat{\Phi}) \cdot \mathbf{n}_\gamma \right\} [\xi] \, ds
\]
\[
+ \sum_{\gamma \in \Gamma_h} \int_{\gamma} \hat{\xi}^s \mathbf{u} \cdot \mathbf{n}_\gamma [\Phi - \hat{\Phi}] \, ds + J_0^s(\xi, \Phi - \hat{\Phi}).
\]

Applying a further integration by parts to the bilinear term, we have
\[
B_S(\xi, \Phi - \hat{\Phi}; \mathbf{u}) = \sum_{E \in \mathcal{E}_h} \int_E \nabla \cdot \left( -\mathbf{D}(\mathbf{u}) \nabla \xi + \xi \nabla \phi \right)(\Phi - \hat{\Phi}) \, dx
\]
\[
+ \sum_{E \in \mathcal{E}_h} \int_E \left( \mathbf{D}(\mathbf{u}) \nabla \xi - \xi \nabla \phi \right) \cdot \mathbf{n}_E (\Phi - \hat{\Phi}) \, ds - \int_{\partial \Omega} \hat{\xi}^q (\Phi - \hat{\Phi}) \, ds
\]
\[
- \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left\{ \mathbf{D}(\mathbf{u}) \nabla \xi \cdot \mathbf{n}_\gamma \right\} [\Phi - \hat{\Phi}] \, ds - \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left\{ \mathbf{D}(\mathbf{u}) \nabla (\Phi - \hat{\Phi}) \cdot \mathbf{n}_\gamma \right\} [\xi] \, ds
\]
\[
+ \sum_{\gamma \in \Gamma_h} \int_{\gamma} \hat{\xi}^s \mathbf{u} \cdot \mathbf{n}_\gamma [\Phi - \hat{\Phi}] \, ds + J_0^s(\xi, \Phi - \hat{\Phi}).
\]

Using the identities \([ab] = [a][b] + [a]b \) and \( a \mathbf{b} - [ab] = -(2\mathbf{b} - b^*)[a] \), we obtain
\[
B_S(\xi, \Phi - \hat{\Phi}; \mathbf{u}) = \sum_{E \in \mathcal{E}_h} \int_E \nabla \cdot \left( -\mathbf{D}(\mathbf{u}) \nabla \xi + \xi \nabla \phi \right)(\Phi - \hat{\Phi}) \, dx - \int_{\partial \Omega} \hat{\xi}^q (\Phi - \hat{\Phi}) \, ds
\]
\[
- \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left( \phi - 2\Phi + \hat{\Phi} \right) \cdot \mathbf{n}_\gamma [\xi] \, ds + \sum_{\gamma \in \Gamma_h} \int_{\gamma} \mathbf{D}(\mathbf{u}) \nabla \xi \cdot \mathbf{n}_\gamma (\Phi - \hat{\Phi}) \, ds
\]
\[
- \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left\{ \mathbf{D}(\mathbf{u}) \nabla (\Phi - \hat{\Phi}) \cdot \mathbf{n}_\gamma \right\} [\xi] \, ds + \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left\{ \mathbf{D}(\mathbf{u}) \nabla \xi \cdot \mathbf{n}_\gamma \right\} (\Phi - \hat{\Phi}) \, ds + J_0^s(\xi, \Phi - \hat{\Phi}).
\]

Substituting this result back into (4.6) and employing the residual notations, we observe
\[
\|\xi\|^2_{0,\Omega} = - \frac{d}{dr} \sum_{E \in \mathcal{E}_h} \left( \xi, \phi \Phi \right)_E - \sum_{E \in \mathcal{E}_h} \int_E R_1(\Phi - \hat{\Phi}) \, dx
\]
\[
- \sum_{\gamma \in \Gamma_h} \int_{\gamma} R_{B0} \mathbf{u} \cdot \mathbf{n}_\gamma (2\Phi - 2\hat{\Phi} + \Phi^*) \, ds
\]
\[
+ \sum_{\gamma \in \Gamma_h} \int_{\gamma} R_{B1} (\Phi - \hat{\Phi}) \, ds - \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left\{ \mathbf{D}(\mathbf{u}) \nabla (\Phi - \hat{\Phi}) \cdot \mathbf{n}_\gamma \right\} R_{B0} \, ds
\]
\[
+ \sum_{\gamma \in \Gamma_h} \int_{\gamma} R_{B1} (\Phi - \hat{\Phi}) \, ds + \sum_{\gamma \in \Gamma_h} \frac{r^2 \sigma_{\gamma}}{h_{\gamma}} \int_{\gamma} R_{B0} (\Phi - \hat{\Phi}) \, ds,
\]
(4.7)
where we have used the fact
\[ R_1 = qC^{DG} + r \mathcal{H}(C^{DG}) - \phi \frac{\partial C^{DG}}{\partial t} - \nabla : (C^{DG} u - D(u) \nabla C^{DG}) \]
\[ = \tilde{\xi} q - a \tilde{\xi} - \phi \frac{\partial \tilde{\xi}}{\partial t} - \nabla : (\tilde{\xi} u - D(u) \nabla \tilde{\xi}), \]
which may be obtained by using the fact that the exact solution possesses a zero residual.

Integrating (4.7) over the time interval \([0, T]\), applying the Cauchy–Schwarz inequality, and recalling (3.8), we get
\[ \| \tilde{\xi} \|_{L^2(0,T,L^2)}^2 \leq K \| \phi \|_{L^2(0,T,L^2)}^2 \left( \sum_{E \in \mathcal{E}_h} \frac{h_E^4}{r_E^3} \| R_1 \|^2_{L^2(0,T,L^2)} + \sum_{\gamma \in \mathcal{F}_h} \frac{h_{\gamma}^3}{r_{\gamma}^3} \| R_{\mathcal{B}_1} \|^2_{L^2(0,T,L^2(\gamma))} \right) \]
\[ + \sum_{\gamma \in \mathcal{F}_h} \frac{h_{\gamma}^3}{r_{\gamma}^3} \| R_{\mathcal{B}_1} \|^2_{L^2(0,T,L^2(\gamma))} + \sum_{\gamma \in \mathcal{F}_h} \frac{h_{\gamma}^3}{r_{\gamma}^3} \| R_{\mathcal{B}_0} \|^2_{L^2(0,T,L^2(\gamma))} \left( \sum_{\gamma \in \mathcal{F}_h} \frac{h_{\gamma}^3}{r_{\gamma}^3} \| R_{\mathcal{B}_1} \|^2_{L^2(0,T,L^2(\gamma))} \right)^{1/2}, \]
We note that for triangles or tetrahedra, we may choose a continuous interpolant \( \tilde{\phi} \) such that the \( \int_{0}^{T} J_0^\alpha (\xi, \phi - \tilde{\phi}) \, dt \) term disappears. Thus we have
\[ \| \tilde{\xi} \|_{L^2(0,T,L^2)}^2 \leq K \| \phi \|_{L^2(0,T,L^2)}^2 \left( \sum_{E \in \mathcal{E}_h} \frac{h_E^4}{r_E^3} \| R_1 \|^2_{L^2(0,T,L^2)} + \sum_{\gamma \in \mathcal{F}_h} \frac{h_{\gamma}^3}{r_{\gamma}^3} \left( \frac{h_{\gamma}^3}{r_{\gamma}^3} + \delta h_{\gamma} \right) \right) \| R_{\mathcal{B}_0} \|^2_{L^2(0,T,L^2(\gamma))} \]
\[ + \sum_{\gamma \in \mathcal{F}_h} \frac{h_{\gamma}^3}{r_{\gamma}^3} \| R_{\mathcal{B}_1} \|^2_{L^2(0,T,L^2(\gamma))} + \sum_{\gamma \in \mathcal{F}_h} \frac{h_{\gamma}^3}{r_{\gamma}^3} \| R_{\mathcal{B}_1} \|^2_{L^2(0,T,L^2(\gamma))} \left( \sum_{\gamma \in \mathcal{F}_h} \frac{h_{\gamma}^3}{r_{\gamma}^3} \| R_{\mathcal{B}_1} \|^2_{L^2(0,T,L^2(\gamma))} \right)^{1/2}, \]
where \( \delta = 0 \) in the case of conforming meshes with triangles or tetrahedra; \( \delta = 1 \) in general cases.

The theorem is then obtained by using the regularity (4.5) of the adjoint problem. □

5. Estimates in terms of linear functionals and negative norms

5.1. A posteriori error estimates in terms of linear functionals

For many applications, one is interested in a linear functional of the solution \( F(c) \) in the form of
\[ F(c) = \int_{0}^{T} \int_{\Omega} c(x,t) f(x,t) \, dx \, dt. \]

We now prove the following theorem of explicit a posteriori error estimates in terms of linear functionals. We comment that explicit a posteriori error estimates presented here do not use the detailed information about linear functionals and are less effective than implicit a posteriori error estimates that require to solve an adjoint problem.

Theorem 5.1 (Linear functional a posteriori error estimates). Let the assumptions in Theorem 4.2 hold. In addition, we assume \( \phi \in W^{n_1+2,\infty}(\Omega), D_{ij} \in W^{n_1+1,0}_\infty((0,T) \times \Omega), u_i \in W^{n_1}_\infty(\Omega), \) and that the chemical reaction
term has a linear form $r(c) = k_0 + k_1 c$, where $k_0 = k_0(x, t)$ and $k_1 = k_1(x, t) \in W^{1,0}_\infty((0, T) \times \Omega)$ are parameters for reaction. Then there exists a constant $K$, independent of $h$ and $r$, such that

$$|F(C^{DG}) - F(c)| \leq K \|f\|_{L^2(0, T; H^1)} \left( \sum_{E \in \mathcal{E}_h} \eta_E^2 \right)^{1/2},$$

where

$$\eta_E^2 = \frac{h_{E,2r+4}^2}{r_{E,2r+4}^2} \|R_{1,E} R_{2,E} \|^2_{L^2(0, T; L^2(\Omega))} + \frac{1}{2} \sum_{E \in \mathcal{E}_h : \partial E = \partial E_1} \left( \frac{h_{E,2r+1}^2}{r_{E,2r+1}^2} + \frac{h_{E,2r+2}^2}{r_{E,2r+2}^2} + \frac{1}{2} \sum_{E \in \mathcal{E}_h : \partial E \cap \partial E = \partial E_2} \|R_{2,E} \|^2_{L^2(0, T; L^2(\gamma_1))} \right) + \frac{1}{2} \sum_{E \in \mathcal{E}_h : \partial E = \partial \Omega} \|R_{1,E} \|^2_{L^2(0, T; L^2(\gamma_1))}.$$

Here, $h = \max(h_{E_1}, h_{E_2})$ for $\gamma = \partial E_1 \cap \partial E_2$, and $h = h_{E_2}$ for $\gamma = \partial E \cap \partial \Omega$, $\mu_1 = \min(r - 1, s_1)$, $r \geq 1$, $s_1 \geq 0$, and $\delta = 0$ in the case of conforming meshes with triangles or tetrahedra. In general cases, $\delta = 1$.

**Proof.** Again, we denote the error in the DG method by $\xi$ and have for any $w \in \mathcal{D}_r(\mathcal{E}_h)$ the following orthogonality equation:

$$\left( \frac{\partial \phi_\xi}{\partial t}, w \right) + B_S(\xi, w; u) = L(w; u, C^{DG}) - L(w; u, c). \tag{5.1}$$

We consider the “backward” or adjoint parabolic equation

$$-\frac{\partial \phi}{\partial t} + \nabla \cdot (-u \Phi - D(u) \nabla \Phi) + (a + q^+) \Phi = f, \quad x \in \Omega, \ t \in [0, T),$$

$$D \nabla \Phi \cdot n = 0, \quad x \in \partial \Omega, \ t \in [0, T),$$

$$\Phi = 0, \quad x \in \Omega, \ t = T,$$

where $a$ is defined as

$$a(x, t) = -k_1(x, t) \in W^{1,0}_\infty((0, T) \times \Omega).$$

By using Theorem 4.1 repeatedly, we obtain a unique solution $\Phi$ for the adjoint equation satisfying

$$\|\Phi\|_{L^\infty(0, T; H^1)} + \|\Phi\|_{L^2(0, T; H^1) + \Omega)} \leq K \|f\|_{L^2(0, T; H^1)}. \tag{5.2}$$

We note that we can always choose the constant $M$ for the “cut-off” operator sufficiently large such that

$$L(w; u, C^{DG}) - L(w; u, c) = -(C^{DG} - c)a = -a \xi.$$

Now, let us consider the $L^2$ inner product $(\xi, f)$ at $t \in (0, T]$,

$$(\xi, f) = \sum_{E \in \mathcal{E}_h} (\xi, f)_E = \sum_{E \in \mathcal{E}_h} \left( \xi, \frac{\partial \phi}{\partial t} \right)_E + \sum_{E \in \mathcal{E}_h} \left( \xi, \nabla \cdot (-u \Phi - D(u) \nabla \Phi) \right)_E + \sum_{E \in \mathcal{E}_h} \left( \xi, (a + q^+) \Phi \right)_E.$$

Integrating by parts and observing that $D \nabla \Phi \cdot n = 0$ on $\partial \Omega$, $\nabla \cdot u = q$, and $[D(u) \nabla \Phi \cdot n.] = [\Phi] = 0$, we know
where the orthogonality Eq. (5.1) has been used, and \( \hat{\Phi} \in \mathcal{D}_r(E_h) \) is an interpolant satisfying (3.8) element-wise.

Applying further integration by parts to the bilinear term in the same way as in the previous section, we have

\[
B_S(\zeta, \Phi - \hat{\Phi}; u) = \sum_{E \in E_h} \int_E \nabla \cdot (-\mathbf{D}(u) \nabla \zeta + \zeta u)(\Phi - \hat{\Phi}) \, dx - \int_\Omega \zeta q^- (\Phi - \hat{\Phi}) \, dx
\]

\[
- \sum_{\gamma \in F_h} \int_{\gamma} (\Phi - 2\{\hat{\Phi}\} + \hat{\Phi}^*) u \cdot n_\gamma [\zeta] \, ds
\]

\[
+ \sum_{\gamma \in \partial \Omega} \int_{\gamma} \mathbf{D}(u) \nabla \zeta \cdot n_\gamma (\Phi - \hat{\Phi}) \, ds - \sum_{\gamma \in F_h} \int_\gamma \{\mathbf{D}(u) \nabla (\Phi - \hat{\Phi}) \cdot n_\gamma \} [\zeta] \, ds
\]

\[
+ \sum_{\gamma \in F_h} \int_{\gamma} \{\mathbf{D}(u) \nabla \zeta \cdot n_\gamma \} \{\Phi - \hat{\Phi}\} \, ds + J_0^\gamma(\zeta, \Phi - \hat{\Phi}).
\]

By back-substituting this result into (5.3) and integrating over the time interval \([0, T]\), we get

\[
\int_0^T (\zeta, f) \, dt = - \sum_{E \in E_h} \int_0^T \int_E R_1(\Phi - \hat{\Phi}) \, dx \, dt - \sum_{\gamma \in F_h} \int_0^T \int_{\gamma} R_{B0} u \cdot n_\gamma (\Phi - 2\{\hat{\Phi}\} + \hat{\Phi}^*) \, ds \, dt
\]

\[
+ \sum_{\gamma \in \partial \Omega} \int_0^T \int_{\gamma} R_{B1}(\Phi - \hat{\Phi}) \, ds \, dt - \sum_{\gamma \in F_h} \int_0^T \int_{\gamma} \{\mathbf{D}(u) \nabla (\Phi - \hat{\Phi}) \cdot n_\gamma \} R_{B0} \, ds \, dt
\]

\[
+ \sum_{\gamma \in F_h} \int_0^T \int_{\gamma} R_{B1} \{\Phi - \hat{\Phi}\} \, ds \, dt + \sum_{\gamma \in \partial \Omega} \frac{r_0^2}{h_\gamma} \int_0^T \int_{\gamma} R_{B0}(\Phi - \hat{\Phi}) \, ds \, dt.
\]

Applying the Cauchy–Schwarz and interpolation inequalities of (3.8), we obtain

\[
|F(C^{DG}) - F(c)| = \int_0^T (\zeta, f) \, dt
\]

\[
\leq K \|\Phi\|_{L^2(0,T; H^1(\Omega))} \left( \sum_{E \in E_h} \frac{h_E^{2\mu_1+4}}{r^{2\mu_1+4}} \|R_1\|_{L^2(0,T; L^2(E))} + \sum_{\gamma \in F_h} \left( \frac{h_{B0}^{2\mu_1+1}}{r^{2\mu_1+1}} + \delta \frac{h_{B0}^{2\mu_1+1}}{r^{2\mu_1+1}} \right) \|R_{B0}\|_{L^2(0,T; L^2(\gamma))} \right)^{1/2}
\]

\[
+ \sum_{\gamma \in \partial \Omega} \frac{h_\gamma^{2\mu_1+3}}{r^{2\mu_1+3}} \|R_{B1}\|_{L^2(0,T; L^2(\gamma))} + \sum_{\gamma \in F_h} \frac{h_\gamma^{2\mu_1+3}}{r^{2\mu_1+3}} \|R_{B1}\|_{L^2(0,T; L^2(\gamma))} \right)^{1/2},
\]

where \( \delta = 0 \) in the case of conforming meshes with triangles or tetrahedra; \( \delta = 1 \) in general cases. The theorem follows directly from this and (5.2).
5.2. A posteriori error estimates in negative norms

Assume $m$ is a positive integer, we define the negative Sobolev norm $\| \cdot \|_{H^{-m}(\Omega)}$ in the usual way:

$$\|c\|_{H^{-m}(\Omega)} = \sup_{v \in C_0^m(\Omega) \setminus \{0\}} \frac{|(c, v)|}{\|v\|_{H^m(\Omega)}},$$

$$\|c\|_{L^2(0,T;H^{-m})} = \sup_{v \in C_0^m((0,T) \times \Omega) \setminus \{0\}} \frac{|(c, v)|}{\|v\|_{L^2(0,T,H^m)}}.$$

Then there exists a constant $K$, independent of $h$ and $r$, such that

Theorem 5.2 (A posteriori error estimates in negative norms). Let the assumptions in Theorem 5.1 hold. Then there exists a constant $K$, independent of $h$ and $r$, such that

$$\|C^{DG} - c\|_{L^2(0,T;H^{-m})} \leq K \left( \sum_{E \in \mathcal{T}_h} \eta_E^m \right)^{1/2},$$

where

$$\eta_E^m = \frac{h_{2\text{min}(r-1,m)+4}}{p^{2m+4}} \|R_1\|_{L^2(0,T,L^2(\gamma))}^2 + \frac{1}{2} \sum_{\gamma \in \partial E \cap \partial \Omega} \left( \frac{h_{2\text{min}(r-1,m)+1}^2}{p^{2m+1}} + \delta \frac{h_{2\text{min}(r-1,m)+1}^2}{p^{2m-1}} \right) \|R_{B1}\|_{L^2(0,T,L^2(\gamma))}^2 \right),$$

Here, $h_{\gamma} = \max(h_{E_1}, h_{E_2})$ for $\gamma = \partial E_1 \cap \partial E_2$, and $h_{\gamma} = h_{E}$ for $\gamma = \partial E \cap \partial \Omega$, $r \geq 1$, $m \geq 0$, and $\delta = 0$ in the case of conforming meshes with triangles or tetrahedra. In general cases, $\delta = 1$.

Proof. The theorem follows by the definition of negative norms and Theorem 5.1. □

6. Adaptive numerical examples

6.1. Adaptive strategies

We consider the $h$-adaptivity for DG applied to reactive transport problems in this section. For transient reactive transport problems, especially for these problems involving a long period of simulation time, the location of strong physics (or biogeochemistry) usually moves with time. Naturally, we want error indicators to account for the physics at the current time. Thus it is favorable to compute error indicators only for the location of strong physics (or biogeochemistry) usually moves with time. Because it is very expensive to modify the mesh each time step, we divide the total simulation time into a collection of time slices, each of which may contain a varying number of time steps. For convenience, we start with a uniform rectangular mesh in the following examples. The error indicator $\eta_E$ in $L^2(L^2)$ is computed for each element in each time slice. The time derivative term in the interior residual $R_I$ is approximated by

$$\frac{\partial C^{DG}}{\partial t} \approx \frac{(C^{DG})_{t_{n+1}} - (C^{DG})_{t_n}}{t_{n+1} - t_n}, \quad t \in (t_n, t_{n+1}).$$
At the end of each time slice, 5% of elements with the largest error indicator values are refined isotropically (i.e., each element is refined into 4 congruent sub-elements), and 5% of elements with the smallest error indicator values are coarsened. The total number of elements remains constant. The concentration is projected in a locally conservative manner using the $L^2$ projection each time the mesh is modified.

6.2. A simple advection–diffusion example

We consider the following problem (6.1)–(6.4):

$$\frac{\partial \phi c}{\partial t} + \nabla \cdot (uc - D\nabla c) = 0, \quad (x, t) \in \Omega \times (0, T],$$

$$\left(uc - D\nabla c \right) \cdot n = c_B u \cdot n, \quad (x, t) \in \Gamma_{in} \times (0, T],$$

$$(-D\nabla c) \cdot n = 0, \quad (x, t) \in \Gamma_{out} \times (0, T],$$

$$c(x, 0) = c_0(x), \quad x \in \Omega,$$

where the domain $\Omega = (0, 10)^2$. The porosity $\phi$ is a constant 0.1, and the tensor $D$ is a constant diagonal tensor with $D_{ii} = 0.01$. The velocity is $u = (-0.2, -0.1)$ uniformly. The initial total concentration $\phi c_0$ is 0.1 inside the square centered at (5, 5) with a size of $0.3125 \times 0.3125$, and it is 0.0 elsewhere. The inflow concentration is $c_B = 0$. The penalty parameter is chosen according to the method presented in [48, 52]. The simulation time interval is (0, 2), and we use the backward Euler method to integrate with respect to time with a uniform time step $\Delta t = 0.01$. We divide the time interval into 20 time slices, where each time slice contains 10 time steps. Polynomials of degree $r = 2$ are used in each element. An $h$-adaptive DG simulation is performed using the uniform rectangular $16 \times 16$ grid as an initial mesh. For comparison, DG without adaptivity is also applied to the problem using a fixed uniform rectangular $16 \times 16$ grid.

The numerical solutions of the concentration using DG with and without adaptivity are shown in Fig. 1. A contaminant plume moves in the direction of the velocity due to advection, and the plume expands with time due to diffusion. Evidently, the adaptive DG method, using the same number of degrees of freedom, resolves the concentration profiles much more sharply than the non-adaptive DG. It should be noted that significant overshoots and undershoots are observed in the concentration profiles from the non-adaptive DG; this is especially true during early time steps. Though this can be partially avoided using slope limiting techniques, overshoots and undershoots are eliminated inherently in the adaptive DG. Comparing the grid distribution and the concentration contour, we find that the mesh is locally adaptive to the areas with high concentrations (advection) and large concentration gradients (diffusion). Clearly, the results indicate that the error indicator in $L^2$ is effective in guiding efficient adaptivity for DG as applied to reactive transport problems.

6.3. A transport example with heterogeneous adsorption

In this example, we consider the problem (6.1)–(6.4) with all the parameters the same as those in the advection–diffusion example, except that we let the velocity $u = (-0.2, 0)$ uniformly, and we let the effective porosity $\phi$ be 0.2 for $y \leq 5$ and let $\phi$ be 0.1 elsewhere. The variation on the effective porosity is a result of heterogeneous adsorption in different layers of the domain. The numerical solutions of the concentration using DG with and without adaptivity are shown in Fig. 2; both use the same number of degrees of freedom.

We observe that the retardation effect, arising from adsorption, results in slow contaminant transport in the lower part of the domain. The concentrations in the lower and upper parts communicate by the diffusion process, leading to continuous concentration profiles. Again, the adaptive DG method resolves the solution much better than the non-adaptive DG. Significant overshoths and undershoots are formed in
Fig. 1. The advection–diffusion example (Left: concentration profiles from the DG with dynamic adaptivity guided by the $L^2(L^2)$ error indicator; Central column: the meshes from the adaptive DG; Right: the DG with a uniform mesh. From top to bottom: $t = 0.5, 1.0, 1.5, 2.0$, respectively.)
Fig. 2. The transport example with heterogeneous absorption (Left: concentration profiles from the DG with dynamic adaptivity guided by the $L^2(L^2)$ error indicator; Central column: the meshes from the adaptive DG; Right: the DG with a uniform mesh. From top to bottom: $t = 0.5, 1.0, 1.5, 2.0$, respectively.)
the concentration profiles from the non-adaptive DG, in particular during early time steps. In contrast, overshoots and undershoots are not noticeable in the adaptive DG. Obviously, adaptivity eliminates the need of a slope limiter in this example. The time evolution of the grid distribution matches up with that of the concentration contour, demonstrating again that the error indicator in the $L^2(L^2)$ norm is effective in guiding efficient adaptivity for DG.

6.4. A transport example with strong adsorption

In this example, we consider the problem (6.1)–(6.4) in which all the parameters are the same as in the transport example with heterogeneous adsorption, except that we let the effective porosity $\phi$ be 10 for $4.6875 \leq y \leq 5.3125$ and let $\phi$ be 0.1 elsewhere. The variation on the effective porosity is a result of strong adsorption in the thin central layer. In Fig. 3, the DG solutions for the concentration fields are shown, with and without using adaptivity.

Due to the strong retardation effect from the adsorption in the central thin layer, it is observed that the contaminant plume is basically detained in the center of the domain with little advection noticeable there. The contaminant is leaked to the other two layers from the central layer through diffusion. Once the contaminant reaches the top or bottom layers, it advects quickly to the left. Unlike the previous examples, overshoots and undershoots are quite small, even for the non-adaptive DG. Still, we see that the adaptive DG method does a better job than the non-adaptive DG in predicting the concentration profiles. The effectiveness of the error indicator in $L^2(L^2)$ is reflected in the grid distribution that is intensively refined around the area with high concentrations and concentration gradients.

7. Discussion and conclusions

A symmetric discontinuous Galerkin scheme has been applied for solving reactive transport problems in porous media. Because the rates of chemical reactions in many complex sub-surface systems may vary by several orders of magnitude across the domain and adaptivity is essential, a posteriori error estimators may be particularly useful in reactive transport systems. An explicit a posteriori error estimator in $L^2(L^2)$ has been derived for the semi-discrete scheme applied to transport with general kinetic reactions. Explicit a posteriori error estimators in terms of linear functionals and negative norms have also been obtained for transport problems with a linear chemical reaction term. Numerical examples demonstrated the effectiveness of the a posteriori error estimators presented.

The error estimators in $L^2(L^2)$, in terms of linear functionals and in negative norms have similar structure, i.e., all draw contributions from the PDE residuals, the interior boundary discontinuity residuals of the DG concentration and flux, and the residuals from imposed boundary conditions. However, they have different weight coefficients for these contributions. Clearly, this may result in different adaptive meshes for distinct error estimators. The choice of error estimators depends upon our goal in solving the problem. For example, the error estimator in the $L^2(L^2)$ norm is preferred if the goal is to minimize the numerical error in $L^2(L^2)$. It should be noted that SIPG is the only primal DG scheme to possess an optimal $L^2(L^2)$ error estimator.

It is found that the dynamic and adaptive DG resolves the solution much better than the non-adaptive counterpart. This is the case especially for reactive transport problems involving a long period of simulation time. Overshoots and undershoots often occur for non-adaptive DG with coarse grids. These overshoots and undershoots can be eliminated using adaptivity without increasing the number of degrees of freedom. It should be observed that DG errors including overshoots and undershoots are localized; in other words, there is less pollution of errors, even in the non-adaptive case. In addition, for transient problems involving diffusion, the DG errors tend to decay with time.
Fig. 3. The transport example with strong adsorption (Left: concentration profiles from the DG with dynamic adaptivity guided by the $L^2$ error indicator; Central column: the meshes from the adaptive DG; Right: the DG with a uniform mesh. From top to bottom: $t = 0.5, 1.0, 1.5, 2.0$, respectively.)
For future work, implicit a posteriori error estimators for reactive transport are of interest as they offer tighter bounds and may be used for stopping criteria. We are also looking at applications of a posteriori error estimators and adaptivity to multiple component, multiple flowing phase systems with mixed kinetic and equilibrium type reactions.

References


