**A Posteriori Error Estimation for Discontinuous Galerkin Approximations of Reactive Transport Problems**

Shuyu Sun and Mary F. Wheeler

Received May 3, 2003; accepted (in revised form) March 2, 2004

Explicit a posteriori residual type error estimators in $L^2(H^1)$ norm are derived for discontinuous Galerkin (DG) methods applied to transport in porous media with general kinetic reactions. They are flexible and apply to all the four primal DG schemes, namely, Oden–Babuška–Baumann DG (OBB-DG), non-symmetric interior penalty Galerkin (NIPG), symmetric interior penalty Galerkin (SIPG) and incomplete interior penalty Galerkin (IIPG). The error estimators use directly all the available information from the numerical solution and can be computed efficiently. Numerical examples are presented to demonstrate the efficiency and the effectivity of these theoretical estimators.

**KEY WORDS:** Discontinuous Galerkin methods; OBB-DG; NIPG; IIPG; SIPG; a posteriori error estimators; $hp$ adaptivity.

**AMS subject classifications:** 65M15; 65M60; 65M50.

**1. INTRODUCTION**

Reactive transport is a fundamental process arising in many diversified fields such as petroleum engineering, groundwater hydrology, environmental engineering, soil mechanics, earth sciences, chemical engineering and biomedical engineering. Realistic simulations for simultaneous transport and chemical reaction present significant computational challenges [13,14,21,27,28,30,33,42,46,53,59,60]. Traditional algorithms employ operator-splitting to treat advection, diffusion–dispersion and chemical reaction independent, while these methods have been shown to be computationally expensive and less accurate.

The authors would like to thank the anonymous referees for their incisive suggestions which contributed toward improving the paper.

The Center for Subsurface Modeling (CSM), The Institute for Computational Engineering and Sciences (ICES), The University of Texas, Austin, Texas 78712, USA.

0885-7474 / 05 / 0600-0501 © 2005 Springer Science+Business Media, Inc.
Godunov and characteristics are popular methods for the advection–diffusion subproblem. While the operator splitting approach allows one to employ different algorithms to each subproblem as well as to implement complicated kinetics in a modular fashion, it can result in slow convergence and a loss of accuracy.

The discontinuous Galerkin method (DG) has recently gained popularity for four main reasons: (1) the flexibility of the method allows for general non-conforming meshes with variable degrees of approximation; (2) the method is locally conservative; (3) the average of the trace of the fluxes along an element edge is continuous; (4) it has a posteriori estimates. Furthermore, DG can handle rough coefficient problems and implement hp-adaptivity more efficiently than conforming approaches. In addition, with appropriate meshing, varying $p$ can yield exponential convergence rates.

DG applied for flow and transport problems in porous media has been studied in [40,48,58]. It has been found that the non-symmetric DG has optimal convergence in $L^2(H^1)$ for both flow and transport problems [40,41]. The $hp$-convergence behaviors of the symmetric DG in $L^2(L^2)$ and in negative norms have been analyzed in [47,50]. In this paper, we consider four commonly used DG schemes, i.e., Oden–Babuška–Baumann DG scheme (OBB-DG), Nonsymmetric Interior Penalty Galerkin (NIPG) [41], Symmetric Interior Penalty Galerkin (SIPG) [55], and Incomplete Interior Penalty Galerkin (IIPG) [24,47].

Unlike a priori error estimates, a posteriori error estimators do not involve knowledge of the exact unknown solution and thus are in general computable. A posteriori error estimators can be used to signify where modifications in discretization parameters need to be made and thus to achieve adaptivity, in particular, the goal-oriented $hp$-adaptivity [2–5,12,15–20,29,32,34,36–39,44]; see also [6,10,54] and references therein. Because the rates of chemical reactions in many complex subsurface systems may vary by several orders of magnitude across the domain and adaptivity is essential, a posteriori error estimators can be particularly useful in reactive transport problems. There are many error estimators for steady-state problems, for example, error estimators based on gradient recovery, the equilibrated residual method, or 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.
Using a duality argument, explicit $L^2(L^2)$ a posteriori error estimates have been developed for SIPG applied to time dependent problems including reactive transport in porous media [51]. These a posteriori error estimates provide valuable error information, which can be used to guide efficient adaptivities. These error estimates are especially valuable in the cases where the primal scalar unknown rather than the flux is of interest. However, they require the regularity assumption of the dual problem, and cannot apply for OBB-DG, NIPG or IIPG.

In this paper we establish a single unified a posteriori error estimation approach for all the four primal DG schemes (i.e., OBB-DG, NIPG, SIPG and IIPG). These explicit a posteriori error estimators do not require a regularity assumption of the dual problem or a saturation assumption. In addition, they can apply to general boundary conditions and general locally Lipschitz continuous kinetic reactions.

The paper is organized as follows. In Sec. 2, we describe the modeling equations. The DG schemes and some of their known properties are introduced in Sec. 3. Section 4 contains explicit a posteriori error estimators in $L^2(H^1)$ norm for the semi-discrete schemes. In Sec. 5, numerical examples based on the explicit a posteriori error estimators are presented. The conclusion is given in Sec. 6.

2. GOVERNING EQUATIONS

In this paper, we consider transport by a single flowing phase in porous media. We again refer to the Darcian flow field a priori and unsaturated case. The stress tensor $q(t)$ is given by the Darcy law:

$$
\nabla \cdot u = q(t),
$$

where $u$ is the Darcy velocity field and $q(t)$ is the imposed external total flow rate. For convenience, a single advection–diffusion-reaction equation is considered. Several single equations of advection, the advective part of which is assumed to be parallel to the boundary conditions, have been presented in [50, 51] with boundary conditions $u \cdot n = 0$, where $n$ denotes the outward normal vector to the boundary.

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

$$
\frac{\partial \phi}{\partial t} + \nabla \cdot (u \phi) - \nabla \cdot (D(u) \nabla \phi) = q(t) + r(c),
$$

where $\phi$ is the concentration, $u$ is the Darcy velocity field, $D(u)$ is the effective diffusion coefficient, $q(t)$ is the imposed external total flow rate, and $r(c)$ is the source term representing kinetic reactions.

The domain is a polyhedral and bounded domain in $\mathbb{R}^d$, ($d = 1, 2$ or 3) with boundary $\partial \Omega = \Gamma_{\text{in}} \cup \Gamma_{\text{out}}$. Here we denote by $\Gamma_{\text{in}}$ the inflow boundary and $\Gamma_{\text{out}}$ the outflow/no-flow boundary, i.e.,

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

$$
\Gamma_{\text{out}} = \{x \in \partial \Omega : u \cdot n \geq 0\}.
$$

Let $n$ denote the unit outward normal vector to $\partial \Omega$. The paper is organized as follows. In Sec. 2, we describe the modeling equations. The DG schemes and some of their known properties are introduced in Sec. 3. Section 4 contains explicit a posteriori error estimators in $L^2(H^1)$ norm for the semi-discrete schemes. In Sec. 5, numerical examples based on the explicit a posteriori error estimators are presented. The conclusion is given in Sec. 6.
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. $q^*c$ is the source term, where the imposed external total flow rate $q$ is a sum of sources (injection) and sinks (extraction), and $c^*$ is the injected concentration if $q \geq 0$ and is the resident concentration $c_w$ if $q < 0$.

We consider the following boundary conditions for this problem.

$$ (u c - D(u) \nabla c) \cdot n = c_B u \cdot n (x,t) \in \Gamma_{in} \times (0,T], \tag{2} $$

$$ (u c - D(u) \nabla c) \cdot n = 0 (x,t) \in \Gamma_{out} \times (0,T], \tag{3} $$

where $c_B$ is the inflow concentration. The initial concentration is specified in the following way.

$$ c(x,0) = c_0(x) x \in \Omega. \tag{4} $$

3. DISCONTINUOUS GALERKIN SCHEME

3.1. Notation

Let $E_h$ 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 $E_j \in E_h$, then each of the subtriangles (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 $h/h_j \leq \tau$ for all $E \in E_h$, where $h$ is the maximum diameter of all elements. The quasi-uniformity is assumed here for convenience of presenting some known DG properties in this section, but it is not required for a posteriori error estimates in the following sections.

We assume no element crosses the boundaries of $\Gamma_{in}$ or $\Gamma_{out}$. The set of all interior edges (for 2 dimensional domain) or faces (for 3-dimensional domain) for $E_h$ are denoted by $\Gamma_h$. On each edge or face $\gamma \in \Gamma_h$, a unit normal vector $n_{\gamma}$ is chosen. The set of all edges or faces on $\Gamma_{out}$ and on $\Gamma_{in}$ for $E_h$ are denoted by $\Gamma_h$, out and $\Gamma_h$, in, respectively, for which the normal vector $n_{\gamma}$ coincides with the outward unit normal vector. For $s \geq 0$ we define $H^s(E_h) = \{ \phi \in L^2(\Omega) : \phi |_{E} \in H^s(E), E \in E_h \}$. \(\tag{5} \)
We now define the average and the jump for $\phi \in H^s(E_h)$, $s > 1/2$. Let $E_i, E_j \in E_h$ and $\gamma = \partial E_i \cap \partial E_j \in \Gamma_h$ with $n_{\gamma}$ exterior to $E_i$. Denote \[
abla_{\gamma} = \frac{1}{2} \left( \nabla_{E_i} \phi \right) \bigg|_{\gamma} + \frac{1}{2} \left( \nabla_{E_j} \phi \right) \bigg|_{\gamma}, \quad (6)\]
and \[
abla_{\gamma} = \nabla_{E_i} \phi \bigg|_{\gamma} - \nabla_{E_j} \phi \bigg|_{\gamma}, \quad (7)\]
Denote the upwind value of concentration $c^\ast$ as follows:
\[
c^\ast \bigg|_{\gamma} = \begin{cases} c \big|_{E_i} & \text{if } u \cdot n_{\gamma} \geq 0, \\ c \big|_{E_j} & \text{if } u \cdot n_{\gamma} < 0. \end{cases} \]
The usual Sobolev norm on $\Omega$ is denoted by $\| \cdot \|_{m,\Omega}$ [1]. The broken norm is defined, for a positive integer $m$, as
\[
||| \phi |||_2^m = \sum_{E \in E_h} \| \phi \|_{2, m,E}^2, \quad (8)\]
The discontinuous finite element space is taken to be $D_r(E_h) \equiv \{ \phi \in L^2(\Omega) : \phi \big|_{E} \in P_r(E), E \in E_h \}$, (9)
where $P_r(E)$ denotes the space of polynomials of (total) degree less than or equal to $r$. Note that we present error estimators in this paper for the local space $P_r$, but the results extend to the local space $Q_r$ because $P_r(E) \subset Q_r(E)$.

The inner product in $(L^2(\Omega))_d$ or $L^2(\Omega)$ is indicated by $(\cdot, \cdot)$ and the inner product in the boundary function space $L^2(\gamma)$ is indicated by $(\cdot, \cdot)_\gamma$.

The “cut-off” operator $M$ is defined as
\[
M(c)(x) = \min(c(x), M), \quad (10)\]
where $M$ is a large positive constant. It is easy to show that the “cut-off” operator $M$ is uniformly Lipschitz continuous in the following sense:

**Lemma 1. (Property of operator $M$)**: The “cut-off” operator $M$, defined as in Eq. (10), is uniformly Lipschitz continuous with a Lipschitz constant one, i.e.,
\[
\| M(c) - M(w) \|_{L^\infty(\Omega)} \leq \| c - w \|_{L^\infty(\Omega)}, \quad (11)\]
We shall use the following inverse inequalities, which can be derived using
the method in [45]. Let \( E \in \mathcal{E}_h \), \( v \in P_r(E) \) and \( h_E \) the diameter of \( E \). Then
there exists a constant \( K \), independent of \( v \), \( r \) and \( h_E \), such that
\[
\| D^q v \|_{0, \partial E} \leq K r h_E^{1/2} \| D^q v \|_{E, q} \geq 0, \quad (12)
\]
\[
\| \partial B^q v \|_{0, E} \leq K r^2 h_E \| D^q v \|_{E, q} \geq 0. \quad (13)
\]

3.2. Continuous in Time Scheme
We introduce the bilinear form \( B(c, w; u) \) defined by
\[
B(c, w; u) = \sum_{E \in \mathcal{E}_h} \int_E (D(u) \nabla c - c u) \cdot \nabla w - \int_\Omega c q - w - \sum_{\gamma \in \Gamma_h} \int_{\gamma} \{ D(u) \nabla c \cdot n \gamma \} \left[ w \right] - s_{\text{form}} \sum_{\gamma \in \Gamma_h} \int_{\gamma} c^* u \cdot n \gamma \left[ w \right] + \sum_{\gamma \in \Gamma_h} \int_{\gamma} c u \cdot n \gamma w + J_{\sigma 0}(c, w), (14)
\]
where \( s_{\text{form}} = -1 \) for NIPG or OBB-DG (the non-symmetric formulation), \( s_{\text{form}} = 1 \) for SIPG (the symmetric formulation) and \( s_{\text{form}} = 0 \) for IIPG method. Here \( q^+ \) is the injection source term and \( q^- \) is the extraction source term, i.e., \( q^+ = \max(q, 0) \), \( q^- = \min(q, 0) \).

By definition, we have \( q = q^+ + q^- \). In addition we define the interior penalty term \( J_{\sigma 0}(c, w) \) as
\[
J_{\sigma 0}(c, w) = \sum_{\gamma \in \Gamma_h} \frac{1}{2} \frac{\sigma_{\gamma}}{h_{\gamma}} \int_{\gamma} \{ c \} [w],
\]
where \( \sigma \) is a discrete positive function that takes the constant value \( \sigma_{\gamma} \) on the edge or face \( \gamma \). For OBB-DG, \( \sigma_{\gamma} \equiv 0 \). We assume \( 0 < \sigma_0 \leq \sigma_{\gamma} \leq \sigma_m \) for SIPG, IIPG or NIPG.

The linear functional \( L(w; u, c) \) is defined as follows:
\[
L(w; u, c) = \int_\Omega r(M(c)) w + \int_\Omega c w q^+ + w - \sum_{\gamma \in \Gamma_h} \int_{\gamma} c B u \cdot n \gamma w. (15)
\]
We give the weak formulation of the reactive transport problem, for which the proof can be found at [47, 50].

**Lemma 2.** (Weak formulation) If \( c \) is the solution of (1)–(3) and \( c \) is essentially bounded, then \( c \) satisfies

\[
\left( \frac{\partial \phi c}{\partial t}, w \right) + B(c, w; u) = L(w; u, c)
\]

\( \forall w \in H^s(\Omega_h), s > \frac{3}{2} \)

\( \forall t \in (0, T] \)

(15)

provided that the constant \( M \) for the "cut-off" operator is sufficiently large.

The continuous in time DG approximation \( C_{DG} \in W^{1, \infty}(0, T; D_r(\Omega_h)) \) of (1)–(4) is defined by

\[
\left( \frac{\partial \phi C_{DG}}{\partial t}, w \right) + B(C_{DG}, w; u) = L(w; u, C_{DG}), \quad w \in D_r(\Omega_h), t \in (0, T]
\]

(16)

\[
(\phi C_{DG}, w) = (\phi c_0, w), \quad w \in D_r(\Omega_h), t = 0
\]

(17)

3.3. Some Known Properties of DG

The element-wise mass conservative property of the DG scheme is described as in the following lemma, which was proved in [47, 50]:

**Lemma 3.** (Local mass balance) The approximation of the concentration satisfies on each element \( E \) the following property of local conservation:

\[
\int_E \frac{\partial \phi C_{DG}}{\partial t} - \int_{\partial E} \left\{ D(u) \nabla C_{DG} \cdot n_E \right\} + \int_{\partial E} C_{DG}^* u \cdot n_E + \sum_{\gamma \subset \partial E} \int_{\gamma} (C_{DG} |_{E} - C_{DG} |_{\Omega}^h) = \int_E C_{DG}^* q + \int_{\Omega_h} (M(C_{DG}))
\]

(18)

We remark that the \( \partial E \) terms in (18) can be extended to a continuous flux defined over the entire domain \( \Omega \). The choices of the parameters \( \sigma_0 \) and \( M \) have been discussed in [47, 50]. The above DG scheme always has a solution (shown in [47, 50]):
Lemma 4. (Existence of solution for DG scheme). Assume that the reaction rate is a locally Lipschitz continuous function of concentration. Then the discontinuous Galerkin scheme (16) and (17) has a unique solution for all $t > 0$.

We recall the following a priori error estimate in $L^2(H^1)$ norm, which was proved for NIPG, SIPG and IIPG in [47, 50]:

Theorem 1. ($L^2(H^1)$ and $L^\infty(L^2)$ error estimate for NIPG, SIPG and IIPG). Let $c$ be the solution to (1)–(4), and assume $c \in L^2(0, T; H^s(Eh))$, $\partial c/\partial t \in L^2(0, T; H^{s-1}(Eh))$ and $c_0 \in H^{s-1}(Eh)$. We further assume that $c$, $u$ and $q$ are essentially bounded, that $\phi$ is time-independent, uniformly bounded above and below by positive numbers, that $D(u)$ is uniformly symmetric positive definite and bounded from above, 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

$$
\| C_{DG} - c \|_{L^\infty(0, T; L^2)} + \| D^{1/2}(u) \nabla (C_{DG} - c) \|_{L^2(0, T; L^2)} + (\int_0^T J_{\sigma_0}(C_{DG} - c, C_{DG} - c))^{1/2} \leq \frac{K}{h} \mu^{-1} r^{-1} \delta^2 \| c \|_{L^2(0, T; H^s)} + \frac{K}{h} \mu^{-1} r^{-1} \left( \| \partial c/\partial t \|_{L^2(0, T; H^{s-1})} + \| c_0 \|_{H^{s-1}} \right),
$$

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, $\delta = 1$.

We recall the following a priori error estimate in $L^2(H^1)$ norm, which is proved for OBB-DG [35] scheme, i.e., the scheme (16) when $s_{form} = -1$ and $\sigma \equiv 0$ in [40]:

Theorem 2. ($L^2(H^1)$ and $L^\infty(L^2)$ error estimate for OBB-DG). Let all assumptions in Theorem 1 hold except $s_{form} = -1$ and $\sigma \equiv 0$. If the constant $M$ for the "cut-off" operator is sufficiently large, then there exists a constant $K$, independent of $h$ and $r$, such that

$$
\| C_{DG} - c \|_{L^\infty(0, T; L^2)} + \| D^{1/2}(u) \nabla (C_{DG} - c) \|_{L^2(0, T; L^2)} \leq \frac{K}{h} \mu^{-1} r^{-5/2} \| c \|_{L^2(0, T; H^s)} + \left( \| \partial c/\partial t \|_{L^2(0, T; H^{s-1})} + \| c_0 \|_{H^{s-1}} \right),
$$

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, $\delta = 1$. 

We define residual quantities that only depend 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 $R_{B1}$, defined below.

$$R_I = qC_{DG}^* + r\left(M(C_{DG})\right) - \phi \frac{\partial C_{DG}}{\partial t} - \nabla \cdot \left(C_{DG} u - D(u) \nabla C_{DG}\right),$$

$$R_{B0} = \begin{cases} [C_{DG}] & x \in \gamma, \gamma \in \Gamma_h, \\ 0 & x \in \partial \Omega, \end{cases}$$

$$R_{B1} = \begin{cases} \left[D(u) \nabla C_{DG} \cdot n\right] & x \in \gamma, \gamma \in \Gamma_h, \\ c_{B}u - C_{DG}u + D(u) \nabla C_{DG} \cdot n & x \in \Gamma_h, \text{in}, \\ D(u) \nabla C_{DG} \cdot n & x \in \Gamma_h, \text{out}. \end{cases}$$

where $C_{DG}^* = c$ if $q < 0$ and $C_{DG}^* = c_w$ if $q \geq 0$.

We remark that all above quantities $R_I$, $R_{B0}$ and $R_{B1}$ can be computed directly and efficiently from the DG solution. The interior residual $R_I$ is the PDE 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 boundary. 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 boundary.

We define the error $\xi$ by

$$\xi = C_{DG} - c.$$
\[
\frac{\partial u}{\partial t} = -\xi u + D(u) \nabla \xi \cdot n, x \in \Gamma_h, \text{in},
\]

\[
\Gamma_h = D(u) \nabla \xi \cdot n, x \in \Gamma_h, \text{out}.
\]

**Proof.** The lemma follows from the fact that all residuals have zero value if \( C_{DG} \) is replaced by the exact solution \( c \).

We define the continuous piece-wise polynomial space as \( D_0^r(E_h) \equiv D_r(E_h) \cap C(\Omega) \) and define \( \Pi \) to be the \( L_2 \) projection from \( D_r(E_h) \) onto \( D_0^r(E_h) \). We will need the approximating property of \( D_r(E_h) \) by \( D_0^r(E_h) \) in order to establish Theorem 3. This approximation result was originally proved in [31] for a non-degenerate and quasi-uniform mesh using a scaling argument. It should be noted that the mesh is seldom quasi-uniform in practice; this is true especially in adaptive computations involving local phenomena. We now rigorously prove that this approximation result extends to a general non-degenerate mesh without a quasi-uniform assumption.

**Lemma 6.** Let \( E_h \) be a general non-degenerate partitions of \( \Omega \) composed of triangles or quadrilaterals if \( d = 2 \), or tetrahedra, prisms or hexahedra if \( d = 3 \), then there exists a constant \( K \), independent of \( h \), such that for every \( w \in D_r(E_h) \), we have

\[
\|w - \Pi w\|_{L_2(\Omega)} \leq K \sum_{\gamma \in \Gamma_h} h_{\gamma} \|\left[ w \right]\|_{L_2(\gamma)}.
\]

**Proof.** Part I. Non-degenerate and quasi-uniform mesh

For the reader's convenience, we give a quick proof of this lemma if, in addition, the mesh is quasi-uniform. We note that, however, part II of this proof alone establishes this lemma. Consider the quotient space \( D_r(E_h) / D_0^r(E_h) \) equipped with the quotient norm

\[
\|w\|_{D_r(E_h) / D_0^r(E_h)} = \inf_{v \in D_0^r(E_h)} \|w - v\|_{L_2(\Omega)}.
\]

To prove this lemma, it is equivalent to show that there exists a constant \( K \), independent of \( h \), such that

\[
\|w - \Pi w\|_{D_r(E_h) / D_0^r(E_h)} \leq K \sum_{\gamma \in \Gamma_h} h_{\gamma} \|\left[ w \right]\|_{L_2(\gamma)}.
\]

By contradiction, we assume that (22) does not hold. Then there is a sequence \( \{w_n\} \) such that

\[
\|w_n\|_{D_r(E_h) / D_0^r(E_h)} = 1 \quad \text{and} \quad \sum_{\gamma \in \Gamma_h} h_{\gamma} \|\left[ w_n \right]\|_{L_2(\gamma)}
\]

(22) for all \( n \).
\[ L_{2}(H^{1}) \text{ norm} \]

\[ \frac{1}{n} \leq 1, \text{ for } n = 1, 2, 3, \ldots \]

Since \( D_{r}(E_{h}) / D_{0}(E_{h}) \) is finite dimensional, \( \{ w_{n} \} \) resides in a compact subset and we may extract a convergent subsequence with limit \( w_{\infty} \). But then it follows that \( w_{\infty} \) is a continuous function and thus \( \| w_{\infty} \|_{D_{r}(E_{h}) / D_{0}(E_{h})} = 0 \), which gives a contradiction. As it is assumed that the mesh is quasi-uniform, we can apply the standard scaling argument to show that \( K \) is independent of \( h \).

**Part II. General non-degenerate mesh**

We now prove the lemma for a general non-degenerate mesh. Since \( E_{h} \) is non-degenerate, we know there exists a constant \( K_{1} \) such that the number of elements sharing any common point, edge or face is bounded by \( K_{1} \). We now let \( \{ \phi_{i} \}, i = 1, 2, \ldots, \dim(D_{0}(E_{h}) / D_{0}(E_{h})) \), be the set of the standard node-based basis functions for the space \( D_{0}(E_{h}) / D_{0}(E_{h}) \), and \( \{ x_{i} \}, i = 1, 2, \ldots, \dim(D_{0}(E_{h}) / D_{0}(E_{h})) \), be the associated node points. That is, \( \text{span}(\{ \phi_{i} \}) = D_{0}(E_{h}) / D_{0}(E_{h}) \), \( \phi_{i}(x_{j}) = \delta_{ij} \), \( \sum_{i = 1}^{\dim(D_{0}(E_{h}) / D_{0}(E_{h}))} \phi_{i} \equiv 1 \), and the support of \( \phi_{i} \) is local and contained in a patch of \( m \) elements (\( m \leq K_{1} \)). We let \( w|_{E} \) be the restriction of \( w \) into the element \( E \in E_{h} \), and \( \phi_{i}|_{E} \) the restriction of \( \phi_{i} \). We have \( w = \sum_{E \in E_{h}} w|_{E} \).

We now decompose \( w|_{E} \) as

\[ w|_{E} = \sum_{i = 1}^{\dim(D_{0}(E_{h}) / D_{0}(E_{h}))} \alpha_{i,E} \phi_{i}|_{E}, \]

where \( \alpha_{i,E} = 0 \) for terms \( \phi_{i}|_{E} \equiv 0 \), and \( \alpha_{i,E} \in \mathbb{R} \) is uniquely determined for terms \( \phi_{i}|_{E} \neq 0 \). Thus we have

\[ w = \sum_{i = 1}^{\dim(D_{0}(E_{h}) / D_{0}(E_{h}))} \sum_{E \in E_{h}} \alpha_{i,E} \phi_{i}|_{E} = \sum_{i \in \Gamma_{h}} \sum_{E \subset \text{supp}(\phi_{i})} \alpha_{i,E} \phi_{i}|_{E}. \]

For each \( i = 1, 2, \ldots, \dim(D_{0}(E_{h}) / D_{0}(E_{h})) \), we consider the following summation of jump terms across the interfaces in the patch \( \text{supp}(\phi_{i}) \):

\[ \sum_{\gamma \subset \text{supp}(\phi_{i})} \sum_{E_{1}(\gamma) \cap E_{2}(\gamma) \subset \Gamma_{h}} (\alpha_{i,E_{1}(\gamma)} - \alpha_{i,E_{2}(\gamma)}) \phi_{i}|_{E_{1}(\gamma)} \|_{L_{2}(\gamma)}, \]

where \( E_{1}(\gamma) \) and \( E_{2}(\gamma) \) denote the two neighboring elements of the edge or face \( \gamma \).
We denote an edge or face with the maximum value of the above term
\( h_{\gamma} \), i.e.,
\[
\hat{\gamma}_i \leq h_{\gamma}(\alpha_{i,E}(\gamma) - \alpha_{i,E}(\hat{\gamma}_i)) \varphi_i \leq 2L_{\gamma}(\gamma)
\]
for all \( \gamma \subseteq \text{supp}(\varphi_i) \cap \Gamma_h \). One can see,
\[
\sum_{E \subseteq \text{supp}(\varphi_i)} \left| h_{\gamma}(\alpha_{i,E} - \alpha_{i,E}(\hat{\gamma}_i)) \varphi_i \right|_{L^2(\Omega)} \leq K \sum_{E \subseteq \Gamma_h} \left| h_{\gamma}(\alpha_{i,E} - \alpha_{i,E}(\hat{\gamma}_i)) \varphi_i \right|_{L^2(\gamma)}.
\]
where \( K \) is a positive constant independent of \( h \).

We now define \( \hat{w} = \dim(D_0^r(E_h)) \sum_{i=1} \alpha_{i,E}(\hat{\gamma}_i) \varphi_i \).
Then \( \hat{w} \in D_0^r(E_h) \) and
\[
\| w - \hat{w} \|_{L^2(\Omega)} \leq \dim(D_0^r(E_h)) \sum_{i=1} \sum_{E \subseteq \text{supp}(\varphi_i)} \left| h_{\gamma}(\alpha_{i,E} - \alpha_{i,E}(\hat{\gamma}_i)) \varphi_i \right|_{L^2(\Omega)} \leq 8 \dim(D_0^r(E_h)) \sum_{i=1} \sum_{E \subseteq \text{supp}(\varphi_i)} \left| h_{\gamma}(\alpha_{i,E} - \alpha_{i,E}(\hat{\gamma}_i)) \varphi_i \right|_{L^2(\Omega)} \leq 16 K \dim(D_0^r(E_h)) \sum_{i=1} \sum_{E \subseteq \text{supp}(\varphi_i)} \left| h_{\gamma}(\alpha_{i,E} - \alpha_{i,E}(\hat{\gamma}_i)) \varphi_i \right|_{L^2(\gamma)} \leq 16 K \dim(D_0^r(E_h)) \sum_{i=1} \sum_{E \subseteq \text{supp}(\varphi_i) \cap \Gamma_h} \left| h_{\gamma}(\alpha_{i,E} - \alpha_{i,E}(\hat{\gamma}_i)) \varphi_i \right|_{L^2(\gamma)} \leq 16 K \sum_{E \subseteq \Gamma_h} \left| h_{\gamma}(\alpha_{i,E} - \alpha_{i,E}(\hat{\gamma}_i)) \varphi_i \right|_{L^2(\gamma)} \leq 16 K \sum_{E \subseteq \Gamma_h} \left| h_{\gamma}(\alpha_{i,E} - \alpha_{i,E}(\hat{\gamma}_i)) \varphi_i \right|_{L^2(\gamma)}.\]
The lemma follows from the minimum distance property of the $L^2$ projection.

\[
\|w - \Pi w\|_{L^2(\Omega)} \leq \|w - \hat{w}\|_{L^2(\Omega)}.
\]

\[\square\]

We now prove a theorem for explicit a posteriori error estimates in $L^2(H^1)$ norm. Because we are not interested in the estimation of the error coming from $L^2$ projection of the initial time data, we assume $c_0 \in D_r(Eh)$. We remark that for many realistic applications $c_0 \in D_r(Eh)$ is indeed satisfied. Throughout the paper, we denote by $K$ a generic positive constant that is independent of $h$. For convenience of presentation we do not track the polynomial degree $r$ and allow $K$ to be dependent on $r$.

**Theorem 3.** (Explicit a posteriori error estimate for OBB-DG, NIPG, SIPG and IIPG). Let all the assumptions in Theorem 2 hold for OBB-DG, or let all the assumptions in Theorem 1 hold for NIPG, SIPG or IIPG. In addition, we assume $c_0 \in D_r(Eh)$. Then there exists a constant $K$, independent of $h$, such that

\[
\sqrt{\phi \xi} \leq K \sum_{E \in Eh} \eta^2_E^{1/2},
\]

where

\[
\eta^2_E = h_E^2 \|R_I\|^2_{L^2(0,T;L^2(E))} + \sum_{\gamma \in \partial E \cap \partial \Omega} h_\gamma \|R_B^1\|^2_{L^2(0,T;L^2(\gamma))} + \sum_{\gamma \in \partial E \setminus \partial \Omega} \|\partial R_B^0/\partial t\|^2_{L^2(0,T;L^2(\gamma))}.
\]
Subtracting the DG scheme equation from the weak formulation, we have for any $w \in D_r(\mathcal{E}_h)$,

$$\left( \partial \phi \xi, w \right) + B(\xi, w; u) = L(w; u, C_{DG}) - L(w; u, c).$$

(23)

Set $w = \hat{\xi},$ we have

$$\left( \partial \phi \xi, \xi \right) + B(\xi, \xi; u) = L(\hat{\xi}; u, C_{DG}) - L(\hat{\xi}; u, c) + \left( \partial \phi \xi, \xi - \hat{\xi} \right) + B(\xi, \xi - \hat{\xi}; u).$$

(24)

Let us first consider the left-hand side of the error equation (24). The first term can be written as

$$\left( \partial \phi \xi, \xi \right) = \frac{1}{2} \frac{d}{dt} \int_{\Omega} \sqrt{\phi \xi} d\Omega.$$

The second term of Eq. (24) is

$$B(\xi, \xi; u) = \sum_{E \in \mathcal{E}_h} \int_E \left( \nabla \xi \cdot \nabla \xi - q \right) \cdot \xi + \sum_{\gamma \in \Gamma_h} \int_{\gamma} \{ \nabla \xi \} \cdot n - \sum_{\gamma \in \Gamma_h} \int_{\gamma} \xi \nabla \nabla \xi \cdot n + \sum_{\gamma \in \Gamma_h} \int_{\gamma} \xi \nabla \nabla \xi \cdot n + \sum_{\gamma \in \Gamma_h} \int_{\gamma} \xi \nabla \nabla \xi \cdot n.$$

We integrate by parts the advection term,

$$- \sum_{E \in \mathcal{E}_h} \int_E \xi \cdot \nabla \xi = - \frac{1}{2} \sum_{E \in \mathcal{E}_h} \int_E \xi \cdot \nabla \xi = - \frac{1}{2} \sum_{E \in \mathcal{E}_h} \int_{\partial E} \xi \cdot n \xi + \sum_{E \in \mathcal{E}_h} \int_E q \xi.$$
Noting that $c_2 = \{ c \}$ and $(c^* - \{ c \}) \text{sign}(u \cdot n) = c_0 / 2$, we have

$$B(\xi, \xi; u) = \left| \int_{\Omega} D_1^2 (u) \nabla \xi \right|^2 + \frac{1}{2} \int_{\Omega} |q_1(\xi)|^2 + \frac{1}{2} \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left| u \cdot n \right|^2 \left( \xi - \hat{\xi} \right)^2 + \frac{1}{2} \sum_{\gamma \in \Gamma_h, \text{in} \cup \Gamma_h, \text{out}} \int_{\gamma} \left| u \cdot n \right|^2 \left( \xi - \hat{\xi} \right)^2 - \frac{1}{2} \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left( D_1 (u) \nabla \xi \cdot n \right) \left( \xi - \hat{\xi} \right) \right).$$

Let us look at the right-hand side of the error equation (24). The first two terms are

$$L_2(\hat{\xi}; u, C_{DG}) - L_2(\hat{\xi}; u, c) = \int_{\Omega} \left( r(M(C_{DG})) - r(M(c)) \right) \hat{\xi} = \int_{\Omega} \left( r(M(C_{DG})) - r(M(c)) \right) \xi + \int_{\Omega} \left( r(M(C_{DG})) - r(M(c)) \right) \left( \hat{\xi} - \xi \right).$$

We expand the last term on the right-hand side of (24) and apply integration by parts

$$B(\xi, \xi - \hat{\xi}; u) = \sum_{E \in E_h} \int_{\partial E} \left| D_1 (u) \nabla \xi - \xi u \right| n \left( \xi - \hat{\xi} \right) \left( \xi - \hat{\xi} \right) - \sum_{E \in E_h} \int_{E} \left| D_1 (u) \nabla \xi - \xi u \right| \left( \xi - \hat{\xi} \right) - \int_{\Omega} \xi q - \left( \xi - \hat{\xi} \right) - \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left( D_1 (u) \nabla \xi \cdot n \right) \left( \xi - \hat{\xi} \right) - \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left( D_1 (u) \nabla \xi \cdot n \right) \left( \xi - \hat{\xi} \right).$$
Using the identities 
\[ \left[ ab \right] \mathbf{= \left( a \right) b + \left( b \right) a \], we have 
B(\xi, \xi - \hat{\xi}; u) = -\sum_{E \in \mathcal{E}} h \int_{E} \nabla \left( D(u) \nabla \xi - \xi u \right)(\xi - \hat{\xi}) - \int_{\Omega} \xi q - (\xi - \hat{\xi})
+ \sum_{\gamma \in \mathcal{G}} h \int_{\gamma} \left\{ \xi - \hat{\xi} \right\} \left[ D(u) \nabla \xi \cdot n_{\gamma} \right]
+ \sum_{\gamma \in \mathcal{G}, \text{in}} h \int_{\gamma} \nabla \left( D(u) \nabla (\xi - \hat{\xi}) \right) \cdot n_{\gamma}(\xi - \hat{\xi})
- \sum_{\gamma \in \mathcal{G}, \text{out}} h \int_{\gamma} \nabla (D(u) \nabla \xi) \cdot n_{\gamma}(\xi - \hat{\xi})
+ J_{\sigma_0}(\xi, \xi - \hat{\xi})
+ \frac{1}{2} \int_{\Omega} |q|^2(\xi) + J_{\sigma_0}(\xi, \xi)
+ \frac{1}{2} \sum_{\gamma \in \mathcal{G}} h \int_{\gamma} |u \cdot n_{\gamma}(\xi)|^2
+ \frac{1}{2} \sum_{\gamma \in \mathcal{G}, \text{in}} h \int_{\gamma} |u \cdot n_{\gamma}(\xi)|^2
+ \frac{1}{2} \sum_{\gamma \in \mathcal{G}, \text{out}} h \int_{\gamma} |u \cdot n_{\gamma}(\xi)|^2.

Substituting all the above terms into the error equation (24), we have 
\[ \frac{1}{2} \frac{d}{dt} \left( \int_{\Omega} \sqrt{\phi \xi} \right)^2 + \frac{1}{2} \int_{\Omega} \left| D^{1/2}(u) \nabla \xi \right|^2 + \int_{\Omega} |q|^2(\xi - \hat{\xi}) + J_{\sigma_0}(\xi, \xi - \hat{\xi})
+ \frac{1}{2} \sum_{\gamma \in \mathcal{G}} h \int_{\gamma} |u \cdot n_{\gamma}(\xi)|^2
+ \frac{1}{2} \sum_{\gamma \in \mathcal{G}, \text{in}} h \int_{\gamma} |u \cdot n_{\gamma}(\xi)|^2
+ \frac{1}{2} \sum_{\gamma \in \mathcal{G}, \text{out}} h \int_{\gamma} |u \cdot n_{\gamma}(\xi)|^2.
\]
\[ \frac{1}{2} \int_{\Omega} \sqrt{\varphi \xi} \, dx + \frac{1}{2} \int_{\Omega} \{ \xi - \hat{\xi} \}^2 \, dx \leq \int_{0}^{\tau} \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left[ D\left( \frac{1}{2} \nabla \xi \right) \cdot n_{\gamma} \right] \{ \xi - \hat{\xi} \} \, d\gamma + \sum_{E \in E_h} \int_{E} R_I \{ \xi - \hat{\xi} \} \, dx \]

Integrating (25) with respect to the time from 0 to \( \tau (0 \leq \tau \leq T) \) and using the fact \( \xi = 0 \) at \( t = 0 \), we have

\[ \frac{1}{2} \int_{\Omega} \sqrt{\varphi \xi} \, dx + \frac{1}{2} \int_{\Omega} \{ \xi - \hat{\xi} \}^2 \, dx \leq \int_{0}^{\tau} \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left[ D\left( \frac{1}{2} \nabla \xi \right) \cdot n_{\gamma} \right] \{ \xi - \hat{\xi} \} \, d\gamma + \sum_{E \in E_h} \int_{E} R_I \{ \xi - \hat{\xi} \} \, dx \]
\[ \int \sum_{\gamma \in \Gamma} h,\text{in} \cup \Gamma h,\text{out} \int_{\gamma} (2\{\tilde{\xi} - \hat{\xi}\} - (\xi - \hat{\xi})^*) u \cdot n_{\gamma} R_B 1 (\xi - \hat{\xi}) = : T_5 \cdot (26) \]

We want to bound each term \( T_i \) on the right-hand side of (26). The second term can be bounded using the property of the cut-off operator.

\[ |T_2| \leq K \int_0^\tau \int_{\Omega} \xi^2 \leq K \int_0^\tau \| \phi \xi \|_0,\Omega \]
The terms $T_6$, $T_7$, and $T_8$ can be bounded in a similar fashion as that in $T_4$.

$$|T_6| \leq K \sum_{\gamma \in \Gamma_h} h_{\gamma} \| R_1 \|_{L^2(0, \tau; L^2(\gamma))}$$

$$+ \epsilon \int_0^\tau \| \sqrt{\phi_\xi} \|_{L^2(0, \Omega)}^2 + \epsilon \| D_{1/2}(u) \nabla \xi \|_{L^2(0, \tau; L^2(\Omega))}^2.$$

$$|T_7| \leq K \sum_{\gamma \in \Gamma_h} h_{\gamma} \| R_0 \|_{L^2(0, \tau; L^2(\gamma))}$$

$$+ \epsilon \int_0^\tau \| \sqrt{\phi_\xi} \|_{L^2(0, \Omega)}^2 + \epsilon \| D_{1/2}(u) \nabla \xi \|_{L^2(0, \tau; L^2(\Omega))}^2.$$

$$|T_8| \leq K \sum_{\gamma \in \Gamma_h} (h_{\gamma} - 1) \| R_0 \|_{L^2(0, \tau; L^2(\gamma))}$$

$$+ \epsilon \int_0^\tau \| \sqrt{\phi_\xi} \|_{L^2(0, \Omega)}^2 + \epsilon \| D_{1/2}(u) \nabla \xi \|_{L^2(0, \tau; L^2(\Omega))}^2.$$
\[
\sum_{\gamma \in \Gamma} \int_{\gamma} \xi u \cdot n_{\gamma} ([C_{DG} - \Pi C_{DG}]) + \sum_{\gamma \in \Gamma_h, \text{out}} \int_{\gamma} \xi u \cdot n_{\gamma} (C_{DG} - \Pi C_{DG}) + J\sigma_0 (\xi, C_{DG} - \Pi C_{DG}).
\]

Noting that 
\[
[C_{DG} - \Pi C_{DG}] = [\xi]
\]
and re-arranging the terms, we have
\[
\sum_{\gamma \in \Gamma} \int_{\gamma} \{D(u) \nabla \xi \cdot n_{\gamma}\} [\xi] = \sum_{\gamma \in \Gamma} \int_{\gamma} \{D(u) \nabla \xi \cdot n_{\gamma}\} [C_{DG} - \Pi C_{DG}].
\]

Integrating by parts the time derivative term, we have
\[
\int_0^\tau (\partial \phi \xi / \partial t, C_{DG} - \Pi C_{DG}) = (\phi \xi, C_{DG} - \Pi C_{DG}) (\tau) - \int_0^\tau (\phi \xi, \partial / \partial t (C_{DG} - \Pi C_{DG})).
\]

Using Lemma 6, we have
\[
\int_0^\tau (\partial \phi \xi / \partial t, C_{DG} - \Pi C_{DG}) \leq \epsilon \| \phi \xi \|_{L^2(\Omega)} + K \sum_{\gamma \in \Gamma} \| R_B \|_{L^2(\gamma)}^2 (\tau).
\]
\[ \| \tau \| R \| (\epsilon + \| \| R + \epsilon \| \tau + \| \| \leq \| \| (\| 1 (\| \tau \| + a \ \text{Posteriori Error Estimation for Discontinuous Galerkin Approximations} \]
522 Sun and Wheeler

\[ \sum_{E \in \mathcal{E}} h^2_E \| R^I \|_{L^2(0,T;L^2(E))} \]

5. NUMERICAL EXAMPLE

In the implementation, we use a simplified version of the error indicator \( \eta^2_E \) defined as follows.

\[ \eta^2_E = \sum_{\gamma \in \partial E \cap \partial \Omega} h_\gamma \| R^B_1 \|_{L^2(0,T;L^2(\gamma))} + \frac{1}{2} \sum_{\gamma \in \partial E \setminus \partial \Omega} (h_\gamma \| R^B_1 \|_{L^2(0,T;L^2(\gamma))} + h^{-1}_\gamma \| R^B_0 \|_{L^\infty(0,T;L^2(\gamma))}) \]

The term \( h_\gamma \| R^B_0 \|_{L^\infty(0,T;L^2(\gamma))} \) is omitted from the original definition of \( \eta^2_E \). This is done because of the simplicity of implementation; namely, the omitted term is in \( L^\infty(0,T;L^2(\gamma)) \) norm, but all other terms are in \( L^2(0,T;L^2(\gamma)) \). All theorems presented in this paper still hold because of the fact \( h_\gamma \| R^B_0 \|_{L^\infty(0,T;L^2(\gamma))} \leq K h_\gamma \| \partial R^B_0 / \partial t \|_{L^2(0,T;L^2(\gamma))} \) + \( K h_\gamma \| R^B_0 \|_{L^2(0,T;L^2(\gamma))} \).

The time derivative \( \frac{\partial C}{\partial t} \) in the interior residual is approximated by

\[ \frac{C_{DG}(t_n+1) - C_{DG}(t_n)}{t_{n+1} - t_n} \]

for \( t \in (t_n, t_n+1) \).

The time derivative of the zeroth order boundary residual is approximated in a similar fashion.
We consider the following example problem:

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

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

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

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

where the domain \( \Omega = (0, 10)^2 \). The porosity \( \phi \) is a constant 0.1, and the tensor \( D \) is a constant and diagonal with \( D_{ii} = 0.01 \). The velocity is \( u = (-0.1, -0.05) \) uniformly, and the initial concentration \( c_0 \) is 1 inside the square centered at (5,5) with the size of 0.3125 \times 0.3125 and is 0 elsewhere (shown in Fig. 1). In this example, we apply the OBB-DG scheme, where we do not need to choose a proper penalty parameter. A 16 \times 16 uniform mesh and polynomial degree \( r = 2 \) are used for spatial discretization. The simulation time interval is \((0, 1)\), and we use the backward Euler's method for time discretization and apply a uniform time step with \( \Delta t = 0.01 \).

The DG solution for the concentration \( c \) at time \( t = 1 \) is plotted in Fig. 2, where the effects of both advection and diffusion can be easily seen. The error of the DG solution is defined as the difference between the DG solution and the exact solution. To approximate the exact solution, we...
Sun and Wheeler employed the OBB-DG scheme with a 64 x 64 uniform mesh and poly-
nomial degree $r = 2$ to compute a higher order accurate solution. The higher order accurate solution and the error of the original DG solution are shown in Figs 3 and 4, respectively. The $L^2$ error indicator $\eta^2_E$ is computed for each element and plotted in Fig. 5. Clearly, the error indicator $\eta^2_E$ is effective in the sense that the error indicator is high in the areas where the error of the DG solution is large. The error indicator provides valuable error information and could allow us to make effective and dynamic grid modifications. The efficient adaptivities guided by the error indicators have been applied to parabolic problems, as presented in [49], where dynamic adaptivity is shown to perform better than static adaptivity for the DG method applied to reactive transport problems. We comment that for dynamic adaptivity, a locally conservative $L^2$ projection will have to be applied to obtain concentration in a new grid for each mesh modification.

6. DISCUSSION AND CONCLUSIONS

Four discontinuous Galerkin schemes have been applied for solving reactive transport in porous media. Because the rates of chemical reactions in many complex subsurface systems might vary by several orders of magnitude across the domain and adaptivity is essential, a posteriori error estimators can be particularly useful in reactive transport problems. Explicit a posteriori error estimators in $L^2(H^1)$ norm have been derived.
Fig. 3. Higher order accurate solution for concentration at \( t = 1 \).

For the combustion scheme depicted in transport with general kinetic reaction. Numerical results demonstrated the efficiency of the \( a \) posteriori error estimator presented. An error estimator or indicator has to be computed efficiently to be practical, and an accurate error estimator, or a good error indicator, needs to use available information as much as possible. We remark that \( a \) posteriori error estimators proposed in this paper use directly all the
available information from the DG solution, and can be computed efficiently. This direct information includes interior residuals and boundary residuals. Interior residuals are coming from the partial differential equation residual in $L^2$ norm for all elements. Boundary residuals can be the zeroth order and the first order, and have contributions from interior element boundary and from domain boundary. Interior element boundary residuals are used to account for the jump of computed concentration (the zeroth order residual) and the jump of computed flux (the first order residual). Domain boundary residuals describe the accuracy of the computed solution in terms of satisfying the imposed boundary conditions.

Like all other explicit a posteriori error estimators, our estimators contain an unknown generic constant, but this approach still allows us to make effective and dynamic grid modifications. The explicit estimators proposed here do not require the regularity assumption of the dual problem or the saturation assumption, and they can apply for general boundary conditions.

We believe implicit a posteriori error estimators for reactive transport can also be interesting for future study. Even though implicit estimators might be more computationally expensive, they can offer tighter bounds on the error. They avoid unknown constants and thus may be used for stopping criteria. In addition, they might offer sharper bounds for the target quantity of interest. For nonlinear problems in particular, implicit a posteriori error estimators are relatively cheaper, compared with the original problems, because the dual problem is linear and computing an approximate solution of the dual problem is much less expensive than solving the original problem.
The combination of explicit and implicit error indicators can be an attractive future work as well. For instance, the computationally cheap explicit error indicators can be used to signal the need for sharp implicit error indicators in different time steps. Error indicators can be applied to multiple time slices, rather than over the entire simulation time, where meshes are modified adaptively in each time slice and thus are dynamic with time. In any case, being able to choose an accurate grid efficiently is of the utmost importance in treating upscaling, uncertainty, inverse problems and optimization, which is a topic we are currently pursuing.

REFERENCES


176 (1–4), 333–361.

40. Rivière, B., and Wheeler, M. F. (2002). Non conforming methods for transport with non-

41. Rivière, B., Wheeler, M. F., and Girault, V. (2001). A priori error estimates for finite ele-
ment methods based on discontinuous approximation spaces for elliptic problems. SIAM

42. Rubin, J. (1983). Transport of reacting solutes in porous media: Relation between math-
ematical nature of problem formulation and chemical nature of reactions. Water Resour.
Res. 19 (5), 1231–1252.

Rice University.


and Fluid Mechanics, Oxford science publications.

natural systems. J. Hydrol. 209 (1-4), 1–388.


48. Sun, S., Rivière, B., and Wheeler, M. F. A combined mixed finite element and discon-
tinuous Galerkin method for miscible displacement problem in porous media. In Recent
progress in computational and applied PDEs, conference proceedings for the international

kin methods applied to reactive transport problems. In Proceedings of the International
Conference on Computing, Communication and Control Technologies (CCCT '04), Austin,
Texas.

50. Sun, S., and Wheeler, M. F. Symmetric and non-symmetric discontinuous Galerkin methods
for reactive transport in porous media. SIAM Journal on Numerical Analysis. submitted.

tinuous Galerkin Approximations of Reactive Transport Problems, TICAM report 03–19,
Institute for Computational Engineering and Sciences, The University of Texas at Austin,
Austin, Texas.


56. Wheeler, M. F., and Darlow, B. L. (1980). Interior penalty Galerkin procedures for mis-
cible displacement problems in porous media. In Computational methods in nonlinear
mechanics (Proc. Second Internat. Conf., Univ. Texas, Austin, Tex., 1979), North-Hol-
land, Amsterdam, pp. 485–506.

diffusion-reaction problems. In Whiteman, J. R. (eds.), The Mathematics of Finite Ele-
