Comput Geosci (2007) 11:87–101
DOI 10.1007/s10596-007-9041-2

ORIGINAL PAPER

Local problem-based *a posteriori* error estimators for discontinuous Galerkin approximations of reactive transport

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Received: 9 August 2005 / Revised: 3 October 2006 / Accepted: 7 October 2006 / Published online: 16 February 2007

Abstract We consider adaptive discontinuous Galerkin (DG) methods for solving reactive transport problems in porous media. To guide anisotropic and dynamic mesh adaptation, *a posteriori* error estimators based on solving local problems are established. These error estimators are efficient to compute and effective to capture local phenomena, and they apply to all the four primal DG schemes, namely, symmetric interior penalty Galerkin, nonsymmetric interior penalty Galerkin, incomplete interior penalty Galerkin, and the Oden–Babuška-Baumann version of DG. Numerical results are provided to illustrate the effectiveness of the proposed error estimators.

Keywords *a posteriori* error estimators · discontinuous Galerkin methods · IIPG · NIPG · OBB-DG · reactive transport · SIPG

1 Introduction

Estimating numerical errors is of paramount importance to simulations of physical phenomena, as the errors may be large and sometimes even invalidate computational predictions. In addition, quantifying the magnitude and distribution of discretization errors provides a basis for adaptive control of the numerical process, including the meshing and the degrees of approximations, substantially improving computational efficiency. Being generally computable, *a posteriori* error estimators may be used to signify where modifications in discretization parameters need to be made, thus achieving adaptivity, in particular, goal-oriented *hp*-adaptivity [2–9, 12, 18–23, 29, 30, 34, 37, 38, 41, 42, 47, 60].

Among their many appealing properties, discontinuous Galerkin (DG) methods [10, 11, 13, 14, 17, 24, 25, 28, 31–33, 35, 36, 39, 43, 45, 46, 48–50, 61, 62] are well known for their advantages in the ease of implementation for *hp*-adaptivity. Indeed, DG methods employ discontinuous piecewise polynomial spaces to approximate solutions of differential equations, allowing general nonconforming meshes, including nonmatching grids and hanging nodes, to be treated naturally. Moreover, variable degrees of approximations (i.e., *p*-adaptivity) are also substantially easier to implement for DG than for conventional finite element methods. In addition to the ease of adaptive implementation, the flexibility of allowing nonconforming spaces also increases the efficiency of adaptivity because the unnecessary areas do not need to be refined merely to maintain mesh conformity. For time-dependent problems, the employment of discontinuous spaces allows the L^2 projection of the simulated quantity to conserve mass element-wise and involve only local computation, thus realizing solution accuracy and computational efficiency simultaneously during mesh modification.

Adaptivity and *a posteriori* error estimators are particularly useful in solving reactive transport problems because reactive transport systems exhibit rich time-

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dependent local behaviors, such as concentration plumes, sharp fronts, shocks, and layers. Reactive transport phenomena arise from many natural and engineered systems, and they play important roles in numerous engineering and scientific fields, particularly in petroleum, environmental and chemical engineering, as well as in earth and life sciences. DG has recently been applied for flow and transport problems in porous media [44, 52, 54, 58, 63], and an optimal convergence in $L^2(H^1)$ was demonstrated for flow and transport problems [44, 46, 51, 56]. The *hp*-convergence behaviors in the $L^2(L^2)$ and negative norms have also been analyzed [51, 56]. In addition, explicit *a posteriori* error estimates of DG for reactive transport have been studied [53, 55, 59]. In this paper, we study local problem-based *a posteriori* error estimators of DG applied to reactive transport problems.

The paper is organized as follows: In the following section, we formulate the DG schemes for reactive transport problems and review a few properties of DG related to our discussion. In Section 3, we derive the local problem-based *a posteriori* error estimators. Section 4 is devoted to numerical studies, where we illustrate how the proposed error estimators may be used to guide an isotropic or anisotropic refinement of an element and to achieve dynamic mesh adaptation. Finally, in Section 5, our results are summarized, and future work is described.

2 Governing equations and discontinuous Galerkin schemes

2.1 Governing equations

We consider reactive transport with a single flowing phase in porous media. We assume that a time-independent Darcy velocity field $\mathbf{u}$ is given, and that it satisfies $\nabla \cdot \mathbf{u} = q$, where q is the imposed external total flow rate. For simplicity, only a single advection–diffusion–reaction equation is considered. However, results may be extended to systems with kinetic reactions. In addition, for convenience, we assume that Ω is a bounded polygonal domain in $\mathbb{R}^d$ ($d = 2$ or 3) with boundary $\partial\Omega = \overline{\Gamma}_{\text{in}} \cup \overline{\Gamma}_{\text{out}}$. Here, we denote by Γ_{in} the inflow boundary and by Γ_{out} the outflow/no-flow boundary, i.e.,

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

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

where $\mathbf{n}$ represents the unit outward normal vector to $\partial\Omega$. The classical advection–diffusion–reaction equation for a single flowing phase in porous media is given by

$$\frac{\partial \phi c}{\partial t} + \nabla \cdot (\mathbf{u}c - \mathbf{D}\nabla c) = qc^{\#} - \lambda c,$$
$$(x, t) \in \Omega \times (0, T], \tag{1}$$

where the unknown variable c is the concentration of a species (amount per volume). Here, T is the final simulation time. ϕ denotes porosity and is assumed to be time-independent and uniformly bounded, above and below, by positive numbers. The dispersion–diffusion tensor $\mathbf{D}$ is assumed to be uniformly symmetric positive definite and bounded from above. The reaction parameter λ could be a function of time and space, but it is assumed to be nonnegative. $c^{\#}$ is an injected concentration c_{w} if $q \geq 0$, or resident concentration c if $q < 0$. The following boundary conditions are imposed for this problem:

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

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

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

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

2.2 Notation

Let $\mathcal{E}_h$ be a family of nondegenerate and possibly nonconforming partitions of Ω composed of triangles or quadrilaterals if $d = 2$, or tetrahedra, prisms, or hexahedra if $d = 3$. Here h is the maximum element diameter for the mesh. The nondegeneracy 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 subtriangles (for $d = 2$) or subtetrahedra (for $d = 3$) of element E_j contains a ball of radius ρh_j in its interior. We assume that no element crosses the boundaries Γ_{in} and Γ_{out}. The set of all interior edges (for two-dimensional domain) or faces (for three-dimensional domain) for $\mathcal{E}_h$ is denoted by Γ_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 Γ_{out} and Γ_{in} for $\mathcal{E}_h$ are denoted by $\Gamma_{h,\text{out}}$ and $\Gamma_{h,\text{in}}$, respectively, for which the normal vector $\mathbf{n}_\gamma$ coincides with the outward unit normal vector.

We denote by $\|\cdot\|_{m,R}$ the usual Sobolev norm over a domain R [1]. The Sobolev norm $\|\cdot\|_{m,\Omega}$ over the entire domain Ω is also denoted simply by $\|\cdot\|_m$. For $s \geq 0$, we define the broken Sobolev space

$$H^s(\mathcal{E}_h) := \left\{\phi \in L^2(\Omega) : \ \phi|_E \in H^s(E), \ E \in \mathcal{E}_h\right\}.$$

One can show that $H^s(\mathcal{E}_h)$ is a normed linear space with its norm defined by

$$\|\phi\|_{H^s(\mathcal{E}_h)} := \left(\sum_{E\in\mathcal{E}_h} \|\phi\|_{s,E}^2 \right)^{1/2}.$$

Following convention, we also use the notation $|||\cdot|||_{s,\mathcal{E}_h}$ or simply $|||\cdot|||_s$ to denote the broken norm $\|\cdot\|_{H^s(\mathcal{E}_h)}$. For a given normed space X and a number $p \ge 1$, we define

$$L^p(0,T;X) := \left\{\phi : \ \phi(t) \in X, \|\phi\|_X \in L^p(0,T)\right\}.$$

The space $L^p(0,T;X)$ is also a normed linear space with its norm given by

$$\|\phi\|_{L^p(0,T;X)} := \left\|(\|\phi\|_X)\right\|_{L^p(0,T)}.$$

The broken norm $\|\cdot\|_{L^p(0,T;H^s(\mathcal{E}_h))}$ is often also written as $|||\cdot|||_{L^p(0,T;H^s)}$ in the triple bar notation. We denote by $(\cdot,\cdot)_R$ the inner product in $\left(L^2(R)\right)^d$ or $L^2(R)$ over a domain R. The inner product $(\cdot,\cdot)_\Omega$ over the entire domain Ω is also denoted simply by $(\cdot,\cdot)$.

The discontinuous finite element space is taken to be

$$\mathcal{D}_r(\mathcal{E}_h) := \left\{\phi \in L^2(\Omega) : \ \phi|_E \in \mathbb{P}_r(E), \ E \in \mathcal{E}_h\right\}, \tag{5}$$

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 results in this paper for the local space $\mathbb{P}_r$, although the results also apply to $\mathbb{Q}_r$, the local space of tensor-product polynomials.

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. We denote

$$\{\phi\} := \frac{1}{2}\left((\phi|_{E_i})|_\gamma + (\phi|_{E_j})|_\gamma\right),$$

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

The upwind value of a concentration $c^*|_\gamma$ is defined as:

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

We shall use the following inverse inequalities, which can be derived using the method in [50]. Let $E \in \mathcal{E}_h$ and $v \in \mathbb{P}_r(E)$. There exists a constant K independent of v, r, and h_E, such that

$$\begin{cases} \|D^q v\|_{0,\partial E} \le K\frac{r}{h_E^{1/2}}\|D^q v\|_{0,E}, & q \ge 0, \\ \left\|D^{q+1} v\right\|_{0,E} \le K\frac{r^2}{h_E}\|D^q v\|_{0,E}, & q \ge 0. \end{cases} \tag{6}$$

2.3 Continuous-in-time schemes

We introduce a bilinear form $B(c,w)$ defined as

$$\begin{aligned} B(c,w) := &\sum_{E\in\mathcal{E}_h}\int_E (\mathbf{D}\nabla c - c\mathbf{u})\cdot\nabla w + \int_\Omega \left(\lambda - q^-\right) cw \\ &- \sum_{\gamma\in\Gamma_h}\int_\gamma \left\{\mathbf{D}\nabla c\cdot\mathbf{n}_\gamma\right\}[w] \\ &- s_{\text{form}}\sum_{\gamma\in\Gamma_h}\int_\gamma \left\{\mathbf{D}\nabla w\cdot\mathbf{n}_\gamma\right\}[c] \\ &+ \sum_{\gamma\in\Gamma_h}\int_\gamma c^*\mathbf{u}\cdot\mathbf{n}_\gamma [w] \\ &+ \sum_{\gamma\in\Gamma_{h,\text{out}}}\int_\gamma c\mathbf{u}\cdot\mathbf{n}_\gamma w + J_0^\sigma(c,w), \end{aligned} \tag{7}$$

where $s_{\text{form}} = -1$ for the nonsymmetric interior penalty Galerkin (NIPG) method [46] or the Oden–Babuška-Baumann formulation of DG (OBB-DG) [35], $s_{\text{form}} = 1$ for the symmetric interior penalty Galerkin (SIPG) method [51, 56, 61], and $s_{\text{form}} = 0$ for the incomplete interior penalty Galerkin (IIPG) method [26, 51, 56]. Here q^+ is the injection source term, and q^- is the extraction source term, 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 $J_0^\sigma(c,w)$ as

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

where σ is a discrete positive function that takes the constant value σ_γ on the edge or face γ. We let $\sigma_\gamma \equiv 0$ for OBB-DG and assume $0 < \sigma_0 \le \sigma_\gamma \le \sigma_m$ for SIPG, NIPG, and IIPG.

The linear functional $L(w)$ is defined as

$$L(w) := \int_\Omega c_w q^+ w - \sum_{\gamma\in\Gamma_{h,\text{in}}}\int_\gamma c_B\mathbf{u}\cdot\mathbf{n}_\gamma w. \tag{8}$$

We now state the weak formulation of the reactive transport problem for which the proof may be found in [51, 56].

Lemma 2.1 (Weak formulation) *If c is a solution of Eqs. (1)–(3), then c satisfies*

$$\left(\frac{\partial\phi c}{\partial t}, w\right) + B(c,w) = L(w), \forall w \in H^s(\mathcal{E}_h),$$

$$s > \frac{3}{2}, \ \forall t \in (0,T]. \tag{9}$$

The continuous-in-time DG approximation $C^{\mathrm{DG}}(\cdot, t) \in \mathcal{D}_r(\mathcal{E}_h)$ of Eqs. (1)–(4) is defined by

$$\left(\frac{\partial \phi C^{\mathrm{DG}}}{\partial t}, w\right) + B(C^{\mathrm{DG}}, w) = L(w),$$
$$\forall w \in \mathcal{D}_r(\mathcal{E}_h), \ t \in (0, T], \tag{10}$$

$$\left(\phi C^{\mathrm{DG}}, w\right) = (\phi c_0, w), \quad \forall w \in \mathcal{D}_r(\mathcal{E}_h), \quad t = 0. \tag{11}$$

Lemma 2.2 (Existence of a solution) [51, 56] *The discontinuous Galerkin schemes* (10) *and* (11) *have a unique solution for all* $t > 0$.

The element-wise mass conservation of DG schemes is stated in the following lemma [51, 56]. We note that the concentration jump term, i.e., the fourth term in Eq. (12), is considered as part of the computed diffusive flux for SIPG, NIPG, and IIPG.

Lemma 2.3 (Local mass balance) *The DG approximation of the concentration satisfies, on each element E, the following local mass balance property*:

$$\int_E \frac{\partial \phi C^{\mathrm{DG}}}{\partial t} - \int_{\partial E\setminus\partial\Omega} \{\mathbf{D}\nabla C^{\mathrm{DG}} \cdot \mathbf{n}_{\partial E}\} + \int_{\partial E} C^{\mathrm{DG}*}\mathbf{u} \cdot \mathbf{n}_{\partial E}$$
$$+ \sum_{\gamma\subset\partial E\setminus\partial\Omega} \frac{r^2\sigma_\gamma}{h_\gamma} \int_\gamma \left(C^{\mathrm{DG}}|_E - C^{\mathrm{DG}}|_{\Omega\setminus\overline{E}}\right)$$
$$= \int_E (C^{\mathrm{DG}} q^- + c_w q^+) - \int_E \lambda C^{\mathrm{DG}}. \tag{12}$$

2.4 Convergence results of DG

In [51, 56], the following *a priori* error estimates were established for NIPG, SIPG, and IIPG:

Theorem 2.4 ($L^2(H^1)$ *and* $L^\infty(L^2)$ error estimates for NIPG, SIPG, and IIPG) *Let c be the solution to Eqs.* (1)–(4), *and assume* $c \in L^2(0, T; H^s(\mathcal{E}_h))$, $\partial c/\partial t \in L^2(0, T; H^{s-1}(\mathcal{E}_h))$, *and* $c_0 \in H^{s-1}(\mathcal{E}_h)$. *We further assume that c,* $\mathbf{u}$, *and q are essentially bounded. If the penalty parameter* σ_0 *is sufficiently large, then there exists a constant K, independent of h and r, such that*

$$\|\sqrt{\phi}\,(C^{\mathrm{DG}}-c)\|_{L^\infty(0,T;L^2)} + \|\!|\mathbf{D}^{\frac{1}{2}}\nabla\,(C^{\mathrm{DG}}-c)\|\!|_{L^2(0,T;L^2)}$$
$$+ \left(\int_0^T J_0^\sigma\,(C^{\mathrm{DG}}-c, C^{\mathrm{DG}}-c)\right)^{\frac{1}{2}}$$
$$\le K\frac{h^{\mu-1}}{r^{s-1-\frac{\delta}{2}}}\|\!|c\|\!|_{L^2(0,T;H^s)}$$
$$+ K\frac{h^{\mu-1}}{r^{s-1}}\left(\|\!|\partial c/\partial t\|\!|_{L^2(0,T;H^{s-1})} + \|\!|c_0\|\!|_{s-1}\right),$$

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

The following *a priori* error estimates for OBB-DG were derived in [44, 51].

Theorem 2.5 ($L^2(H^1)$ and $L^\infty(L^2)$ error estimates for OBB-DG) *Let all assumptions in Theorem 2.4 hold except* $s_{\mathrm{form}} = -1$ *and* $\sigma \equiv 0$. *There exists a constant K, independent of h and r, such that*

$$\left\|\sqrt{\phi}\,(C^{\mathrm{DG}}-c)\right\|_{L^\infty(0,T;L^2)} + \|\!|\mathbf{D}^{\frac{1}{2}}\nabla\,(C^{\mathrm{DG}}-c)\|\!|_{L^2(0,T;L^2)}$$
$$\le K\frac{h^{\mu-1}}{r^{s-\frac{5}{2}}}\left(\|\!|c\|\!|_{L^2(0,T;H^s)} + \|\!|\partial c/\partial t\|\!|_{L^2(0,T;H^{s-1})}\right.$$
$$\left. + \|\!|c_0\|\!|_s\right),$$

where $\mu = \min(r+1, s)$, $r \ge 2$, *and* $s \ge 3$.

3 *A posteriori* error estimates

3.1 Computationally intensive hierarchic error estimators

We first consider error estimators based on hierarchic bases. Hierarchic error estimators consist of solving the problem of interest by employing two discretizations of different accuracy and using the difference between the approximations as an estimate for the error. The advantages of this approach include its applicability to many classes of problems and the simplicity and ease of its implementation. Unlike residual-based error estimators, hierarchic error estimators give point-wise information on the error and thus may be used to guide fully anisotropic *hp*-adaptation. The reader is referred to [9, 15, 16, 27, 40] for further information.

For a given mesh $\mathcal{E}_h$, we construct the mesh $\mathcal{E}_{h/2}$ by isotropically refining each element in $\mathcal{E}_h$. We denote by C^{DG} the DG solution in the original space $\mathcal{D}_r(\mathcal{E}_h)$. We denote by r' ($r \le r' \le r+K$) the improved approximation degree and by h' ($h/K \le h' \le h$) the refined mesh size. Often we use $r' = r+1$ and/or $h' = h/2$. We now define $C^{\mathrm{DG,F}}$ as the DG solution in the fine space $\mathcal{D}_{r'}(\mathcal{E}_{h'})$. In other words, the fine space solution $C^{\mathrm{DG,F}}(\cdot, t) \in \mathcal{D}_{r'}(\mathcal{E}_{h'})$ is defined by, for $w^{\mathrm{F}} \in \mathcal{D}_{r'}(\mathcal{E}_{h'})$,

$$\left(\frac{\partial \phi C^{\mathrm{DG,F}}}{\partial t}, w^{\mathrm{F}}\right) + B(C^{\mathrm{DG,F}}, w^{\mathrm{F}}) = L(w^{\mathrm{F}}), \tag{13}$$

$$\left(\phi C^{\mathrm{DG,F}}, w^{\mathrm{F}}\right)(0) = \left(\phi c_0, w^{\mathrm{F}}\right). \tag{14}$$

We make the following saturation assumption:

$$\left\|C^{\mathrm{DG,F}} - c\right\|_X \le \beta_X \left\|C^{\mathrm{DG}} - c\right\|_X, \quad 0 \le \beta_X < 1, \qquad (15)$$

where X could be the $L^\infty(L^2)$, $L^2(L^2)$, or $L^2(H^1)$ norm. For example, it is reasonable to expect from Theorem 2.4 that $\beta_{L^2(H^1)}$ is less than or equal to the following value asymptotically for the error of SIPG, NIPG, or IIPG in $L^2(H^1)$:

$$\beta_{L^2(H^1)} \le \left(\frac{h'}{h}\right)^{\mu-1} \left(\frac{r}{r'}\right)^{s-1-\delta/2}.$$

The hierarchic error estimator is defined as

$$\zeta := C^{\mathrm{DG}} - C^{\mathrm{DG,F}}. \qquad (16)$$

Substituting $C^{\mathrm{DG,F}} = C^{\mathrm{DG}} - \zeta$ into Eqs. (13) and (14), we see that, for $w^{\mathrm{F}} \in \mathcal{D}_{r'}(\mathcal{E}_{h'})$,

$$\left(\frac{\partial \phi\zeta}{\partial t}, w^{\mathrm{F}}\right) + B(\zeta, w^{\mathrm{F}}) = \left(\frac{\partial \phi C^{\mathrm{DG}}}{\partial t}, w^{\mathrm{F}}\right) + B(C^{\mathrm{DG}}, w^{\mathrm{F}}) - L(w^{\mathrm{F}}), \qquad (17)$$

$$\left(\phi\zeta, w^{\mathrm{F}}\right)(0) = \left(\phi C^{\mathrm{DG}}, w^{\mathrm{F}}\right)(0) - \left(\phi c_0, w^{\mathrm{F}}\right). \qquad (18)$$

The hierarchic error estimator ζ is close to the true error in the following sense:

Theorem 3.1 (Hierarchic error estimators for OBB-DG, SIPG, NIPG, or IIPG) *Let the saturation assumption (15) be satisfied. Then we have*

$$\frac{1}{1+\beta_X}\|\zeta\|_X \le \left\|C^{\mathrm{DG}} - c\right\|_X \le \frac{1}{1-\beta_X}\|\zeta\|_X.$$

Proof The theorem follows by the saturation assumption (15) together with the triangle inequality. □

Numerical experiments indicate that the hierarchic error estimator ζ is very effective, in particular, for guiding dynamic and anisotropic mesh adaptation [57]. However, the computation of ζ is expensive. This disadvantage motivates us to consider an estimate that is close to ζ but only involves solutions of local problems.

3.2 *A posteriori* error estimators based on solving local problems

We now define a computationally efficient error estimator η to approximate the hierarchic estimator ζ. For each $E \in \mathcal{E}_h$, we use the local space $\mathcal{D}_{r'}(\mathcal{E}_{h'} \cap E)$ obtained by restricting $\mathcal{D}_{r'}(\mathcal{E}_{h'})$ to E. We may also consider $\mathcal{D}_{r'}(\mathcal{E}_{h'} \cap E)$ as the space of functions with an extension of zero to $\Omega \setminus E$. Then $\mathcal{D}_{r'}(\mathcal{E}_{h'} \cap E)$ becomes a subspace of $\mathcal{D}_{r'}(\mathcal{E}_{h'})$. In fact, $\mathcal{D}_{r'}(\mathcal{E}_{h'})$ is the direct sum of $\mathcal{D}_{r'}(\mathcal{E}_{h'} \cap E)$ over all $E \in \mathcal{E}_h$. We now define $\eta_E \in \mathcal{D}_{r'}(\mathcal{E}_{h'} \cap E)$ as the solution of the following local problem for $w_E^{\mathrm{F}} \in \mathcal{D}_{r'}(\mathcal{E}_{h'} \cap E)$,

$$\left(\frac{\partial \phi\eta_E}{\partial t}, w_E^{\mathrm{F}}\right) + B(\eta_E, w_E^{\mathrm{F}}) = \left(\frac{\partial \phi C^{\mathrm{DG}}}{\partial t}, w_E^{\mathrm{F}}\right) + B(C^{\mathrm{DG}}, w_E^{\mathrm{F}}) - L(w_E^{\mathrm{F}}), \qquad (19)$$

$$\left(\phi\eta_E, w_E^{\mathrm{F}}\right)(0) = \left(\phi C^{\mathrm{DG}}, w_E^{\mathrm{F}}\right)(0) - \left(\phi c_0, w_E^{\mathrm{F}}\right). \qquad (20)$$

The function η_E involves only local computation in the element E. The estimators η_E for all elements $E \in \mathcal{E}_h$ may be computed independently of each other and in parallel. Moreover, the function

$$\eta := \sum_{E\in\mathcal{E}_h} \eta_E$$

approximates ζ in the sense of Theorems 3.2 and 3.3. Throughout this section, we denote by K a generic positive constant, independent of h and r, and by ϵ a fixed positive constant that may be chosen as arbitrarily small.

Theorem 3.2 (A *posteriori* lower bound for OBB-DG, SIPG, NIPG, or IIPG) *We assume that the penalty parameter σ_0 may be chosen to be sufficiently large for SIPG and IIPG. We impose no additional assumption for NIPG or OBB-DG. There exists a constant K, independent of h and r, such that*

$$\begin{aligned}
&\left\|\sqrt{\phi}\eta\right\|_{L^\infty(0,T;L^2(E))} + \|\mathbf{D}^{\frac{1}{2}}\nabla\eta\|_{L^2(0,T;L^2(\mathcal{E}_{h'}\cap E))} \\
&\quad\le \left\|\sqrt{\phi}\zeta\right\|_{L^\infty(0,T;L^2(E))} + \|\mathbf{D}^{\frac{1}{2}}\nabla\zeta\|_{L^2(0,T;L^2(\mathcal{E}_{h'}\cap E))} \\
&\qquad + K\frac{r}{h^{1/2}}\left\|\zeta|_{\Omega\setminus E}\right\|_{L^2(0,T;L^2(\partial E\setminus\partial\Omega))} \\
&\qquad + K\left(\frac{h^{1/2}}{r} + \delta_{\mathrm{OBB}}\frac{r}{h^{1/2}}\right) \\
&\qquad \times \left\|\nabla\zeta|_{\Omega\setminus E}\cdot\mathbf{n}_{\partial E}\right\|_{L^2(0,T;L^2(\partial E\setminus\partial\Omega))}, \\
&\forall E \in \mathcal{E}_h,
\end{aligned} \qquad (21)$$

and

$$\begin{aligned}
&\left\|\sqrt{\phi}\eta\right\|_{L^\infty(0,T;L^2(\Omega))} + \|\mathbf{D}^{\frac{1}{2}}\nabla\eta\|_{L^2(0,T;L^2(\mathcal{E}_{h'}))} \\
&\quad\le \left\|\sqrt{\phi}\zeta\right\|_{L^\infty(0,T;L^2(\Omega))} + \|\mathbf{D}^{\frac{1}{2}}\nabla\zeta\|_{L^2(0,T;L^2(\mathcal{E}_{h'}))} \\
&\qquad + K\frac{r}{h^{1/2}}\sum_{E\in\mathcal{E}_h}\|\zeta\|_{L^2(0,T;L^2(\partial E\setminus\partial\Omega))} \\
&\qquad + K\left(\frac{h^{1/2}}{r} + \delta_{\mathrm{OBB}}\frac{r}{h^{1/2}}\right) \\
&\qquad \times \sum_{E\in\mathcal{E}_h}\|\nabla\zeta\cdot\mathbf{n}_{\partial E}\|_{L^2(0,T;L^2(\partial E\setminus\partial\Omega))},
\end{aligned} \qquad (22)$$

where $\delta_{\rm OBB} = 1$ *for OBB-DG or NIPG with arbitrary penalty parameters, and* $\delta_{\rm OBB} = 0$ *for SIPG, IIPG, or NIPG with sufficiently large penalty parameters.*

Proof Comparing Eqs. (17) and (18) with Eqs. (19) and (20), and noting that $\mathcal{D}_{r'}(\mathcal{E}_{h'} \cap E)$ is a subspace of $\mathcal{D}_{r'}(\mathcal{E}_{h'})$, we have, for $w_E^{\rm F} \in \mathcal{D}_{r'}(\mathcal{E}_{h'} \cap E)$,

$$\left(\frac{\partial \phi \eta_E}{\partial t}, w_E^{\rm F}\right) + B\left(\eta_E, w_E^{\rm F}\right) = \left(\frac{\partial \phi \zeta}{\partial t}, w_E^{\rm F}\right) + B\left(\zeta, w_E^{\rm F}\right), \tag{23}$$

$$\left(\phi \eta_E, w_E^{\rm F}\right)(0) = \left(\phi \zeta, w_E^{\rm F}\right)(0). \tag{24}$$

We now break the hierarchic estimator into its element-wise components: $\zeta = \sum_{E \in \mathcal{E}_h} \zeta_E$, $\zeta_E \in \mathcal{D}_{r'}(\mathcal{E}_{h'} \cap E)$. By substituting $w_E^{\rm F} = \eta_E - \zeta_E$ into Eqs. (23) and (24), we obtain

$$\left(\frac{\partial \phi(\eta_E - \zeta)}{\partial t}, \eta_E - \zeta_E\right) + B(\eta_E - \zeta_E, \eta_E - \zeta_E)$$
$$= B(\zeta - \zeta_E, \eta_E - \zeta_E), \tag{25}$$

$$(\phi(\eta_E - \zeta), \eta_E - \zeta_E)(0) = 0. \tag{26}$$

Equation (26) and the strict positiveness of ϕ suggest that $\eta_E - \zeta_E = 0$ at $t = 0$. The first term of Eq. (25) may be written as the time derivative of $\left\|\sqrt{\phi}(\eta_E - \zeta_E)\right\|_0^2/2$. We may rewrite the second term of Eq. (25) as

$$\begin{aligned}
&B(\eta_E - \zeta_E, \eta_E - \zeta_E)\\
&= \sum_{E' \in \mathcal{E}_{h'}} \int_{E'} \mathbf{D}\nabla(\eta_E - \zeta_E) \cdot \nabla(\eta_E - \zeta_E)\\
&\quad - \sum_{E' \in \mathcal{E}_{h'}} \int_{E'} (\eta_E - \zeta_E)\mathbf{u} \cdot \nabla(\eta_E - \zeta_E)\\
&\quad -(1 + s_{\rm form}) \sum_{\gamma \in \Gamma_{h'}} \int_\gamma \left\{\mathbf{D}\nabla(\eta_E - \zeta_E) \cdot \mathbf{n}_\gamma\right\}[\eta_E - \zeta_E]\\
&\quad + \sum_{\gamma \in \Gamma_{h'}} \int_\gamma (\eta_E - \zeta_E)^* \mathbf{u} \cdot \mathbf{n}_\gamma [\eta_E - \zeta_E]\\
&\quad + \sum_{\gamma \in \Gamma_{h',\rm out}} \int_\gamma \mathbf{u} \cdot \mathbf{n}_\gamma (\eta_E - \zeta_E)^2\\
&\quad + \int_\Omega (\lambda - q^-)(\eta_E - \zeta_E)^2 + J_{0,F}^\sigma(\eta_E - \zeta_E, \eta_E - \zeta_E),
\end{aligned}$$

where, to distinguish the penalty term in the fine mesh from the one in the coarse mesh, we denote the former by $J_{0,F}^\sigma(\cdot,\cdot)$, i.e.,

$$J_{0,F}^\sigma(c, w) := \sum_{\gamma \in \Gamma_{h'}} \frac{r'^2 \sigma_\gamma}{h'_\gamma} \int_\gamma [c][w].$$

We integrate the advection term by parts and obtain

$$\begin{aligned}
&- \sum_{E' \in \mathcal{E}_{h'}} \int_{E'} (\eta_E - \zeta_E)\mathbf{u} \cdot \nabla(\eta_E - \zeta_E)\\
&= -\frac{1}{2} \sum_{E' \in \mathcal{E}_{h'}} \int_{E'} \mathbf{u} \cdot \nabla(\eta_E - \zeta_E)^2\\
&= \frac{1}{2} \sum_{E' \in \mathcal{E}_{h'}} \int_{E'} q(\eta_E - \zeta_E)^2\\
&\quad - \frac{1}{2} \sum_{\gamma \in \Gamma_{h'}} \int_\gamma \mathbf{u} \cdot \mathbf{n}_\gamma \left[(\eta_E - \zeta_E)^2\right]\\
&\quad - \frac{1}{2} \sum_{\gamma \in \Gamma_{h',\rm in} \cup \Gamma_{h',\rm out}} \int_\gamma \mathbf{u} \cdot \mathbf{n}_\gamma (\eta_E - \zeta_E)^2.
\end{aligned}$$

In addition, noting that $\left[c^2\right] = 2\{c\}[c]$ and $(c^* - \{c\})$ sign $(\mathbf{u} \cdot \mathbf{n}) = [c]/2$, we have

$$\begin{aligned}
&B(\eta_E - \zeta_E, \eta_E - \zeta_E)\\
&= |\!|\!|\mathbf{D}^{\frac{1}{2}}\nabla(\eta_E - \zeta_E)|\!|\!|_{0,E\cap\mathcal{E}_{h'}}^2 + \frac{1}{2}\int_E |q|\,(\eta_E - \zeta_E)^2\\
&\quad + \frac{1}{2} \sum_{\gamma \in \Gamma_{h'}} \int_\gamma \left|\mathbf{u} \cdot \mathbf{n}_\gamma\right| [\eta_E - \zeta_E]^2\\
&\quad + \frac{1}{2} \sum_{\gamma \in \Gamma_{h',\rm in} \cup \Gamma_{h',\rm out}} \int_\gamma \left|\mathbf{u} \cdot \mathbf{n}_\gamma\right| (\eta_E - \zeta_E)^2\\
&\quad + \int_E \lambda(\eta_E - \zeta_E)^2 + J_{0,F}^\sigma(\eta_E - \zeta_E, \eta_E - \zeta_E)\\
&\quad - (1 + s_{\rm form}) \sum_{\gamma \in \Gamma_{h'}} \int_\gamma \left\{\mathbf{D}\nabla(\eta_E - \zeta_E) \cdot \mathbf{n}_\gamma\right\}[\eta_E - \zeta_E].
\end{aligned}$$

The last term in the above expression vanishes for OBB-DG and NIPG. In the case of SIPG or IIPG, we have assumed that the penalty parameter σ_0 may be chosen to be sufficiently large. We may then bound this term by applying the Cauchy–Schwarz and inverse inequalities:

$$\begin{aligned}
&\left|\sum_{\gamma \in \Gamma_{h'}} \int_\gamma \left\{\mathbf{D}\nabla(\eta_E - \zeta_E) \cdot \mathbf{n}_\gamma\right\}[\eta_E - \zeta_E]\right|\\
&\le \frac{h'}{Kr'^2} \sum_{E' \in \mathcal{E}_{h'}} \left\|\mathbf{D}^{\frac{1}{2}}\nabla(\eta_E - \zeta_E) \cdot \mathbf{n}_{\partial E'}\right\|_{0,\partial E'}^2\\
&\quad + \frac{Kr'^2}{h'} \sum_{\gamma \in \Gamma_{h'}} \|[\eta_E - \zeta_E]\|_{0,\gamma}^2\\
&\le \frac{1}{2}|\!|\!|\mathbf{D}^{\frac{1}{2}}\nabla(\eta_E - \zeta_E)|\!|\!|_{0,E\cap\mathcal{E}_{h'}}^2 + \frac{1}{2}J_{0,F}^\sigma(\eta_E - \zeta_E, \eta_E - \zeta_E).
\end{aligned}$$

The right-hand side of Eq. (25) consists of eight pieces:

$$
\begin{aligned}
B(\zeta - \zeta_E, \eta_E - \zeta_E)
&= \sum_{E' \in \mathcal{E}_{h'}} \int_{E'} \mathbf{D}\nabla(\zeta - \zeta_E) \cdot \nabla(\eta_E - \zeta_E) \\
&\quad - \sum_{E' \in \mathcal{E}_{h'}} \int_{E'} (\zeta - \zeta_E)\mathbf{u} \cdot \nabla(\eta_E - \zeta_E) \\
&\quad + \int_{\Omega} (\zeta - \zeta_E)(\lambda - q^-)(\eta_E - \zeta_E) \\
&\quad - \sum_{\gamma \in \Gamma_{h'}} \int_{\gamma} \left\{\mathbf{D}\nabla(\zeta - \zeta_E) \cdot \mathbf{n}_\gamma\right\} [\eta_E - \zeta_E] \\
&\quad - s_{\text{form}} \sum_{\gamma \in \Gamma_{h'}} \int_{\gamma} \left\{\mathbf{D}\nabla(\eta_E - \zeta_E) \cdot \mathbf{n}_\gamma\right\} [\zeta - \zeta_E] \\
&\quad + J_{0,F}^{\sigma}(\zeta - \zeta_E, \eta_E - \zeta_E) \\
&\quad + \sum_{\gamma \in \Gamma_{h'}} \int_{\gamma} (\zeta - \zeta_E)^* \mathbf{u} \cdot \mathbf{n}_\gamma [\eta_E - \zeta_E] \\
&\quad + \sum_{\gamma \in \Gamma_{h',\text{out}}} \int_{\gamma} (\zeta - \zeta_E)\mathbf{u} \cdot \mathbf{n}_\gamma (\eta_E - \zeta_E) \\
&=: \sum_{i=1}^{8} T_i.
\end{aligned}
$$

It is easy to see that $T_1 = T_2 = T_3 = T_8 = 0$. Let us first consider the cases of SIPG, NIPG, and IIPG with sufficiently large penalty parameters. We may bound the terms T_4 and T_5 by hiding a large constant in the penalty term and by using the inverse inequality, respectively:

$$
\begin{aligned}
|T_4| &\le \epsilon \frac{\sigma_0 r'^2}{h'} \sum_{\gamma \in \Gamma_h} \|[\eta_E - \zeta_E]\|_{0,\gamma}^2 + \frac{Kh'}{r'^2} \|\{\mathbf{D}\nabla(\zeta - \zeta_E) \cdot \mathbf{n}_{\partial E}\}\|_{0,\partial E \setminus \partial\Omega}^2 \\
&\le \epsilon J_{0,F}^{\sigma}(\eta_E - \zeta_E, \eta_E - \zeta_E) + \frac{Kh}{r^2} \left\| \nabla\zeta|_{\Omega\setminus E} \cdot \mathbf{n}_{\partial E} \right\|_{0,\partial E \setminus \partial\Omega}^2, \\
|T_5| &\le \frac{\epsilon h}{Kr^2} \|\{\mathbf{D}\nabla(\eta_E - \zeta_E) \cdot \mathbf{n}_{\partial E}\}\|_{0,\partial E}^2 + \frac{Kr^2}{h} \|[\zeta - \zeta_E]\|_{0,\partial E \setminus \partial\Omega}^2 \\
&\le \epsilon |\!|\!| \mathbf{D}^{\frac{1}{2}} \nabla(\eta_E - \zeta_E) |\!|\!|_{0,E}^2 + \frac{Kr^2}{h} \left\| \zeta|_{\Omega\setminus E} \right\|_{0,\partial E \setminus \partial\Omega}^2.
\end{aligned}
$$

Similar applications of the Cauchy–Schwarz inequality and approximation results give

$$
\begin{aligned}
|T_6| &\le \epsilon J_{0,F}^{\sigma}(\eta_E - \zeta_E, \eta_E - \zeta_E) + K J_{0,F}^{\sigma}(\zeta - \zeta_E, \zeta - \zeta_E) \\
&\le \epsilon J_{0,F}^{\sigma}(\eta_E - \zeta_E, \eta_E - \zeta_E) + \frac{Kr^2}{h} \left\| \zeta|_{\Omega\setminus E} \right\|_{0,\partial E \setminus \partial\Omega}^2, \\
|T_7| &\le \epsilon \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left|\mathbf{u} \cdot \mathbf{n}_\gamma\right| [\eta_E - \zeta_E]^2 + K \left\| (\zeta - \zeta_E)^* \right\|_{0,\partial E \setminus \partial\Omega}^2 \\
&\le \epsilon \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left|\mathbf{u} \cdot \mathbf{n}_\gamma\right| [\eta_E - \zeta_E]^2 + K \left\| \zeta|_{\Omega\setminus E} \right\|_{0,\partial E \setminus \partial\Omega}^2.
\end{aligned}
$$

For OBB-DG or NIPG with arbitrary penalty parameters, the estimates of the terms T_5, T_6, and T_7 remain the same (in fact, T_6 vanishes for OBB-DG). However, we need to bound T_4 differently since a penalty term is not available to hide the error jump:

$$
\begin{aligned}
|T_4| &\le \epsilon \frac{h}{Kr^2} \sum_{\gamma \in \Gamma_h} \|[\eta_E - \zeta_E]\|_{0,\gamma}^2 + \frac{Kr^2}{h} \|\{\mathbf{D}\nabla(\zeta - \zeta_E) \cdot \mathbf{n}_{\partial E}\}\|_{0,\partial E \setminus \partial\Omega}^2 \\
&\le \epsilon \|\eta_E - \zeta_E\|_{0,E}^2 + \frac{Kr^2}{h} \left\| \nabla\zeta|_{\Omega\setminus E} \cdot \mathbf{n}_{\partial E} \right\|_{0,\partial E \setminus \partial\Omega}^2.
\end{aligned}
$$

Substituting all the estimates into Eq. (25), we see that

$$
\begin{aligned}
&\frac{1}{2}\frac{d}{dt} \left\| \sqrt{\phi}(\eta_E - \zeta_E) \right\|_{0,E}^2 + \frac{1}{2} |\!|\!| \mathbf{D}^{\frac{1}{2}} \nabla(\eta_E - \zeta_E) |\!|\!|_{0,E\cap\mathcal{E}_{h'}}^2 \\
&\quad + \frac{1}{2} \int_E |q| (\eta_E - \zeta_E)^2 \\
&\quad + \frac{1}{2} \sum_{\gamma \in \Gamma_{h'}} \int_{\gamma} \left|\mathbf{u} \cdot \mathbf{n}_\gamma\right| [\eta_E - \zeta_E]^2 \\
&\quad + \frac{1}{2} \sum_{\gamma \in \Gamma_{h',\text{in}} \cup \Gamma_{h',\text{out}}} \int_{\gamma} \left|\mathbf{u} \cdot \mathbf{n}_\gamma\right| (\eta_E - \zeta_E)^2 \\
&\quad + \int_E \lambda(\eta_E - \zeta_E)^2 \\
&\quad + \frac{1}{2} J_{0,F}^{\sigma}(\eta_E - \zeta_E, \eta_E - \zeta_E) \\
&\quad \le \epsilon J_{0,F}^{\sigma}(\eta_E - \zeta_E, \eta_E - \zeta_E) \\
&\qquad + \epsilon \sum_{\gamma \in \Gamma_h} \int_{\gamma} \left|\mathbf{u} \cdot \mathbf{n}_\gamma\right| [\eta_E - \zeta_E]^2 \\
&\qquad + \epsilon |\!|\!| \mathbf{D}^{\frac{1}{2}} \nabla(\eta_E - \zeta_E) |\!|\!|_{0,E}^2 \\
&\qquad + \epsilon \|\eta_E - \zeta_E\|_{0,E}^2 + K\frac{r^2}{h} \left\| \zeta|_{\Omega\setminus E} \right\|_{0,\partial E \setminus \partial\Omega}^2 \\
&\qquad + K \left(\frac{h}{r^2} + \delta_{\text{OBB}} \frac{r^2}{h} \right) \left\| \nabla\zeta|_{\Omega\setminus E} \cdot \mathbf{n}_{\partial E} \right\|_{0,\partial E \setminus \partial\Omega}^2. \qquad (27)
\end{aligned}
$$

Integrating Eq. (27) with respect to time t, recalling that $\eta_E - \zeta_E = 0$ at $t = 0$ and that $\Gamma_h \subset \Gamma_{h'}$, and applying Gronwall's inequality, we conclude that

$$
\begin{aligned}
&\left\| \sqrt{\phi}(\eta_E - \zeta_E) \right\|_{L^\infty(0,T;L^2)} + |\!|\!| \mathbf{D}^{\frac{1}{2}} \nabla(\eta_E - \zeta_E) |\!|\!|_{L^2(0,T;L^2(\mathcal{E}_{h'}))} \\
&\quad \le K \frac{r}{h^{1/2}} \left\| \zeta|_{\Omega\setminus E} \right\|_{L^2(0,T;L^2(\partial E \setminus \partial\Omega))} \\
&\qquad + K \left(\frac{h^{1/2}}{r} + \delta_{\text{OBB}} \frac{r}{h^{1/2}} \right) \\
&\qquad \times \left\| \nabla\zeta|_{\Omega\setminus E} \cdot \mathbf{n}_{\partial E} \right\|_{L^2(0,T;L^2(\partial E \setminus \partial\Omega))}.
\end{aligned}
$$

The desired local error estimate (21) follows by applying the triangle inequality. The global error estimate (22) follows by summing Eq. (27) over all $E \in \mathcal{E}_h$, integrating the resultant equation, utilizing Gronwall's inequality, and applying the triangle inequality. □

Theorem 3.3 (*A posteriori* upper bound for OBB-DG, SIPG, NIPG, or IIPG) *We assume that the penalty parameter σ_0 may be chosen to be sufficiently large for SIPG and IIPG. We impose no additional assumption for NIPG or OBB-DG. There exists a constant K, independent of h and r, such that*

$$\begin{aligned}
&\left\|\sqrt{\phi}\zeta\right\|_{L^\infty(0,T;L^2(\Omega))} + |||\mathbf{D}^{\frac{1}{2}}\nabla\zeta|||_{L^2(0,T;L^2(\mathcal{E}_{h'}))} \\
&\quad\le \left\|\sqrt{\phi}\eta\right\|_{L^\infty(0,T;L^2(\Omega))} + |||\mathbf{D}^{\frac{1}{2}}\nabla\eta|||_{L^2(0,T;L^2(\mathcal{E}_{h'}))} \\
&\qquad + K\frac{r}{h^{1/2}}\sum_{E\in\mathcal{E}_h}\|\nabla\eta\cdot\mathbf{n}_{\partial E}\|_{L^2(0,T;L^2(\partial E\setminus\partial\Omega))} \\
&\qquad + K\left(\frac{r}{h^{1/2}}+(1-\delta_{OBB})\frac{r^3}{h^{3/2}}\right) \\
&\qquad \times\sum_{E\in\mathcal{E}_h}\|\eta\|_{L^2(0,T;L^2(\partial E\setminus\partial\Omega))}\,,
\end{aligned} \tag{28}$$

where $\delta_{\mathrm{OBB}} = 1$ for OBB-DG, and $\delta_{\mathrm{OBB}} = 0$ for SIPG, IIPG, or NIPG.

Proof Substituting $w_E^{\mathrm{F}} = \eta_E - \zeta_E$ into Eqs. (23) and (24), then summing over all $E \in \mathcal{E}_h$, we obtain

$$\left(\frac{\partial\phi(\eta-\zeta)}{\partial t}, \eta-\zeta\right) + B(\eta-\zeta,\eta-\zeta) = \sum_{E\in\mathcal{E}_h} B(\eta-\eta_E,\eta_E-\zeta_E), \tag{29}$$

$$\eta-\zeta = 0, \qquad \text{at } t=0. \tag{30}$$

Similar to the proof of Theorem 3.2, we write the first term of Eq. (29) as

$$\left(\frac{\partial\phi(\eta-\zeta)}{\partial t}, \eta-\zeta\right) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left\|\sqrt{\phi}(\eta-\zeta)\right\|_0^2.$$

The second term of Eq. (29) may be expanded as

$$\begin{aligned}
&B(\eta-\zeta,\eta-\zeta) \\
&\quad= \sum_{E\in\mathcal{E}_{h'}}\int_E \mathbf{D}\nabla(\eta-\zeta)\cdot\nabla(\eta-\zeta) \\
&\qquad - \sum_{E\in\mathcal{E}_{h'}}\int_E(\eta-\zeta)\mathbf{u}\cdot\nabla(\eta-\zeta) \\
&\qquad - (1+s_{\mathrm{form}})\sum_{\gamma\in\Gamma_{h'}}\int_\gamma\{\mathbf{D}\nabla(\eta-\zeta)\cdot\mathbf{n}_\gamma\}[\eta-\zeta] \\
&\qquad + \sum_{\gamma\in\Gamma_{h'}}\int_\gamma(\eta-\zeta)^*\mathbf{u}\cdot\mathbf{n}_\gamma[\eta-\zeta] + \sum_{\gamma\in\Gamma_{h',\mathrm{out}}}\int_\gamma\mathbf{u}\cdot\mathbf{n}_\gamma(\eta-\zeta)^2 \\
&\qquad + \int_\Omega(\lambda-q^-)(\eta-\zeta)^2 + J_{0,F}^\sigma(\eta-\zeta,\eta-\zeta)\,.
\end{aligned}$$

Integrating the advection term by parts and noting that $[c^2] = 2\{c\}[c]$ and $(c^* - \{c\})\,\mathrm{sign}\,(\mathbf{u}\cdot\mathbf{n}) = [c]/2$, we conclude that

$$\begin{aligned}
&B(\eta-\zeta,\eta-\zeta) \\
&\quad= |||\mathbf{D}^{\frac{1}{2}}\nabla(\eta-\zeta)|||_0^2 + \frac{1}{2}\int_\Omega|q|(\eta-\zeta)^2 \\
&\qquad + \frac{1}{2}\sum_{\gamma\in\Gamma_{h'}}\int_\gamma|\mathbf{u}\cdot\mathbf{n}_\gamma|[\eta-\zeta]^2 \\
&\qquad + \frac{1}{2}\sum_{\gamma\in\Gamma_{h',\mathrm{in}}\cup\Gamma_{h',\mathrm{out}}}\int_\gamma|\mathbf{u}\cdot\mathbf{n}_\gamma|(\eta-\zeta)^2 \\
&\qquad + \int_\Omega\lambda(\eta-\zeta)^2 + J_{0,F}^\sigma(\eta-\zeta,\eta-\zeta) \\
&\qquad - (1+s_{\mathrm{form}})\sum_{\gamma\in\Gamma_{h'}}\int_\gamma\{\mathbf{D}\nabla(\eta-\zeta)\cdot\mathbf{n}_\gamma\}[\eta-\zeta]\,.
\end{aligned}$$

The last term in the above expression vanishes for OBB-DG and NIPG, and it may be bounded for SIPG and IIPG using the same technique as before:

$$\begin{aligned}
&\left|\sum_{\gamma\in\Gamma_{h'}}\int_\gamma\{\mathbf{D}\nabla(\eta-\zeta)\cdot\mathbf{n}_\gamma\}[\eta-\zeta]\right| \\
&\quad\le \frac{1}{2}|||\mathbf{D}^{\frac{1}{2}}\nabla(\eta-\zeta)|||_0^2 + \frac{1}{2}J_{0,F}^\sigma(\eta-\zeta,\eta-\zeta)\,.
\end{aligned}$$

The right-hand side of Eq. (29) contains four non-zero terms:

$$\begin{aligned}
&\sum_{E\in\mathcal{E}_h}B(\eta-\eta_E,\eta_E-\zeta_E) \\
&\quad= -\sum_{E\in\mathcal{E}_h}\sum_{\gamma\subset\partial E\setminus\partial\Omega}\int_\gamma\{\mathbf{D}\nabla(\eta-\eta_E)\cdot\mathbf{n}_\gamma\}[\eta_E-\zeta_E] \\
&\qquad - s_{\mathrm{form}}\sum_{E\in\mathcal{E}_h}\sum_{\gamma\subset\partial E\setminus\partial\Omega}\int_\gamma\{\mathbf{D}\nabla(\eta_E-\zeta_E)\cdot\mathbf{n}_\gamma\} \\
&\qquad \times[\eta-\eta_E] \\
&\qquad + \sum_{E\in\mathcal{E}_h}\sum_{\gamma\subset\partial E\setminus\partial\Omega}\frac{\sigma r'^2}{h'}\int_\gamma[\eta-\eta_E][\eta_E-\zeta_E] \\
&\qquad + \sum_{E\in\mathcal{E}_h}\sum_{\gamma\subset\partial E\setminus\partial\Omega}\int_\gamma(\eta-\eta_E)^*\mathbf{u}\cdot\mathbf{n}_\gamma[\eta_E-\zeta_E] \\
&\quad=: \sum_{i=1}^4 S_i.
\end{aligned}$$

The term S_2 may be bounded in a similar way as before. However, we must resort to the inverse inequality to estimate S_1, S_3, and S_4, as they cannot be hidden using the penalty term due to $(\eta_E - \zeta_E)|_{\Omega\setminus\overline{E}} = 0$ or $[\eta_E - \zeta_E]|_{\partial E} \neq [\eta - \zeta]|_{\partial E}$. In addition, we note that $S_3 = 0$ for OBB-DG.

$$
\begin{aligned}
|S_1| &\leq \frac{\epsilon h}{Kr^2} \sum_{E\in\mathcal{E}_h} \|[\eta_E - \zeta_E]\|^2_{0,\partial E\setminus\partial\Omega} \\
&\quad + \frac{Kr^2}{h} \sum_{E\in\mathcal{E}_h} \|\{\mathbf{D}\nabla(\eta - \eta_E)\cdot \mathbf{n}_{\partial E}\}\|^2_{0,\partial E\setminus\partial\Omega} \\
&\leq \epsilon \|\eta - \zeta\|^2_{0,\Omega} + \frac{Kr^2}{h} \sum_{E\in\mathcal{E}_h} \left\| \nabla\eta|_{\Omega\setminus E}\cdot \mathbf{n}_{\partial E}\right\|^2_{0,\partial E\setminus\partial\Omega} \\
&\leq \epsilon \|\eta - \zeta\|^2_{0,\Omega} + \frac{Kr^2}{h} \sum_{E\in\mathcal{E}_h} \|\nabla\eta\cdot \mathbf{n}_{\partial E}\|^2_{0,\partial E\setminus\partial\Omega},
\end{aligned}
$$

$$
\begin{aligned}
|S_2| &\leq \frac{\epsilon h}{Kr^2} \sum_{E\in\mathcal{E}_h} \left\|\mathbf{D}^{\frac{1}{2}}\nabla(\eta_E - \zeta_E)\cdot \mathbf{n}_{\partial E}\right\|^2_{0,\partial E} \\
&\quad + \frac{Kr^2}{h} \sum_{E\in\mathcal{E}_h} \|[\eta - \eta_E]\|^2_{0,\partial E\setminus\partial\Omega} \\
&\leq \epsilon |\!|\!|\mathbf{D}^{\frac{1}{2}}\nabla(\eta - \zeta)|\!|\!|^2_0 \\
&\quad + \frac{Kr^2}{h} \sum_{E\in\mathcal{E}_h} \|\eta\|^2_{0,\partial E\setminus\partial\Omega},
\end{aligned}
$$

$$
\begin{aligned}
|S_3| &\leq \frac{\epsilon h}{Kr^2} \sum_{E\in\mathcal{E}_h} \|[\eta_E - \zeta_E]\|^2_{0,\partial E\setminus\partial\Omega} \\
&\quad + \frac{Kr^6}{h^3} \sum_{E\in\mathcal{E}_h} \|[\eta - \eta_E]\|^2_{0,\partial E\setminus\partial\Omega} \\
&\leq \epsilon \|\eta - \zeta\|^2_{0,\Omega} + \frac{Kr^6}{h^3} \sum_{E\in\mathcal{E}_h} \|\eta\|^2_{0,\partial E\setminus\partial\Omega},
\end{aligned}
$$

$$
\begin{aligned}
|S_4| &\leq \frac{\epsilon h}{Kr^2} \sum_{E\in\mathcal{E}_h} \|[\eta_E - \zeta_E]\|^2_{0,\partial E\setminus\partial\Omega} \\
&\quad + \frac{Kr^2}{h} \sum_{E\in\mathcal{E}_h} \left\|(\eta - \eta_E)^*\right\|^2_{0,\partial E\setminus\partial\Omega} \\
&\leq \epsilon \|\eta - \zeta\|^2_{0,\Omega} + \frac{Kr^2}{h} \\
&\quad \times \sum_{E\in\mathcal{E}_h} \|\eta\|^2_{0,\partial E\setminus\partial\Omega}.
\end{aligned}
$$

Substituting all the estimates into Eq. (29), we see that

$$
\begin{aligned}
&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left\|\sqrt{\phi}(\eta - \zeta)\right\|^2_0 + \frac{1}{2}|\!|\!|\mathbf{D}^{\frac{1}{2}}\nabla(\eta - \zeta)|\!|\!|^2_0 + \frac{1}{2}\int_\Omega |q|\,(\eta - \zeta)^2 \\
&\quad + \frac{1}{2}\sum_{\gamma\in\Gamma_{h'}} \int_\gamma \left|\mathbf{u}\cdot\mathbf{n}_\gamma\right| [\eta - \zeta]^2 \\
&\quad + \frac{1}{2}\sum_{\gamma\in\Gamma_{h',\mathrm{in}}\cup\Gamma_{h',\mathrm{out}}} \int_\gamma \left|\mathbf{u}\cdot\mathbf{n}_\gamma\right| (\eta - \zeta)^2 \\
&\quad + \int_\Omega \lambda(\eta - \zeta)^2 + \frac{1}{2} J^\sigma_{0,F}(\eta - \zeta, \eta - \zeta) \\
&\leq \epsilon \|\eta - \zeta\|^2_{0,\Omega} + \epsilon |\!|\!|\mathbf{D}^{\frac{1}{2}}\nabla(\eta - \zeta)|\!|\!|^2_0 \\
&\quad + K\frac{r^2}{h}\sum_{E\in\mathcal{E}_h} \|\nabla\eta\cdot\mathbf{n}_{\partial E}\|^2_{0,\partial E\setminus\partial\Omega} \\
&\quad + K\left(\frac{r^2}{h} + (1 - \delta_{\mathrm{OBB}})\frac{r^6}{h^3}\right)\sum_{E\in\mathcal{E}_h} \|\eta\|^2_{0,\partial E\setminus\partial\Omega}. \qquad (31)
\end{aligned}
$$

Integrating Eq. (31) with respect to time t, and applying Gronwall's inequality, we conclude that

$$
\begin{aligned}
&\left\|\sqrt{\phi}(\eta - \zeta)\right\|_{L^\infty(0,T;L^2(\Omega))} + |\!|\!|\mathbf{D}^{\frac{1}{2}}\nabla(\eta - \zeta)|\!|\!|_{L^2(0,T;L^2(\mathcal{E}_{h'}))} \\
&\leq K\frac{r}{h^{1/2}}\sum_{E\in\mathcal{E}_h} \|\nabla\eta\cdot\mathbf{n}_{\partial E}\|_{L^2(0,T;L^2(\partial E\setminus\partial\Omega))} \\
&\quad + K\left(\frac{r}{h^{1/2}} + (1 - \delta_{\mathrm{OBB}})\frac{r^3}{h^{3/2}}\right) \\
&\quad \times \sum_{E\in\mathcal{E}_h} \|\eta\|_{L^2(0,T;L^2(\partial E\setminus\partial\Omega))}.
\end{aligned}
$$

The desired error estimate (28) follows by applying the triangle inequality.

4 Numerical results

We consider problems (1)–(4) over the domain $\Omega = (0, 10)^2$. The domain is divided into two parts, i.e., the lower half $\Omega_l = (0, 10) \times (0, 5)$ and the upper half $\Omega_u = (0, 10) \times (5, 10)$. Adsorption occurs only in the lower part of the domain, which results in an effective porosity ϕ of 0.2 in Ω_l. The effective porosity ϕ in Ω_u is 0.1. The diffusion–dispersion tensor $\mathbf{D}$ is a diagonal matrix with $\mathbf{D}_{ii} = 0.01$, and the velocity is $\mathbf{u} = (-0.2, 0)$. We impose no injection or extraction, and we ignore kinetic reactions; that is, we assume that $q = \lambda = 0$. Due to contamination, the initial total concentration ϕc_0 is 0.1 inside the square centered at (5,5) with a side of length 0.3125 and 0.0 elsewhere. The inflow concentration c_{B} is zero.

SIPG with the implicit Euler time integration is employed to solve this problem. The penalty parameter is chosen to be 0.1, based on an error bound established in [56]. The simulation time interval is (0, 2) with a uniform time step size $\Delta t = 0.01$. The complete quadratic basis function is used for each element. We apply the following dynamic mesh adaptation, starting with a

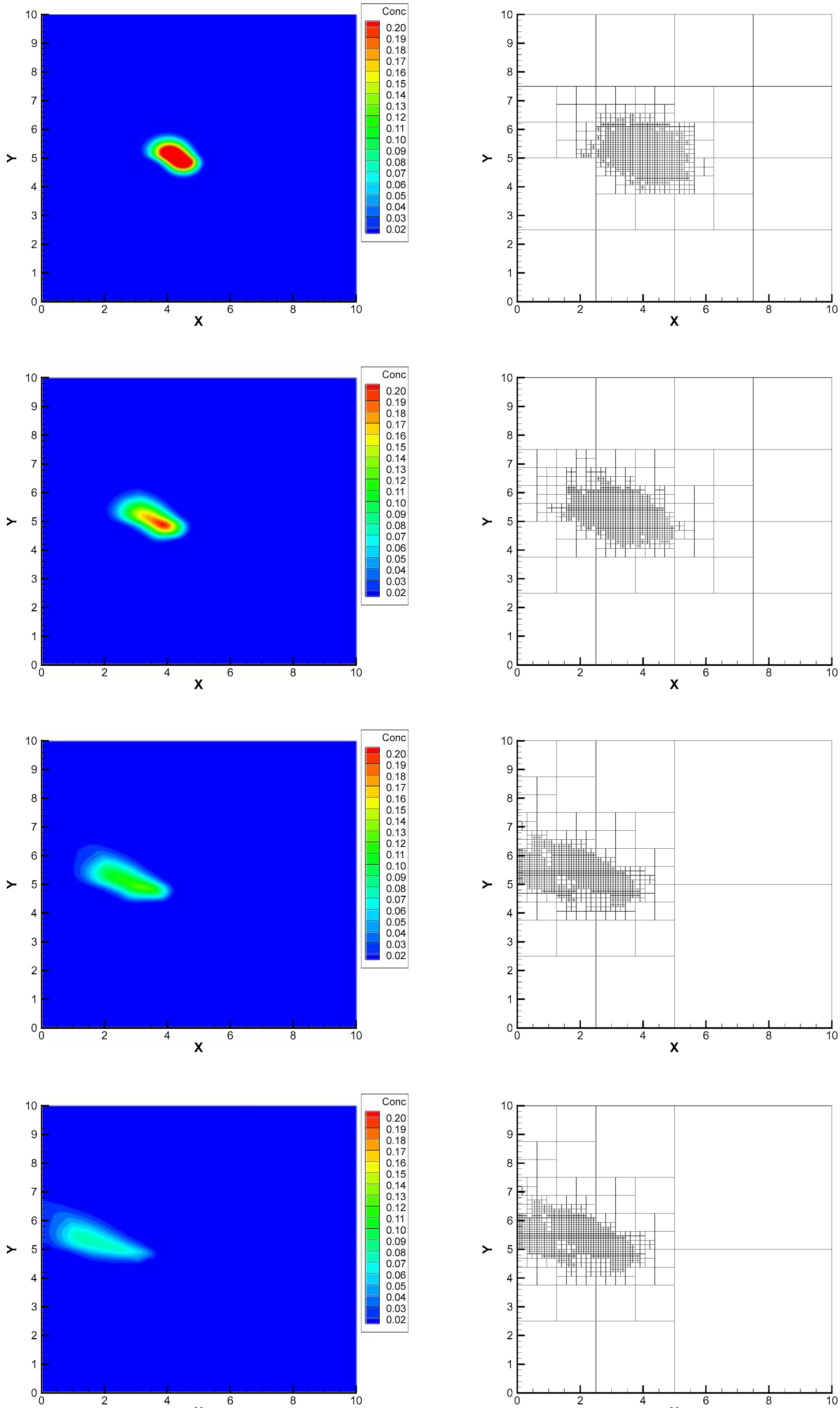

Fig. 1 DG results with the LP-I mesh adaptation (left column: the concentration in fluid; right column: the mesh structure; from top row to bottom: $t = 0.5$, 1, 1.5, and 2, respectively)

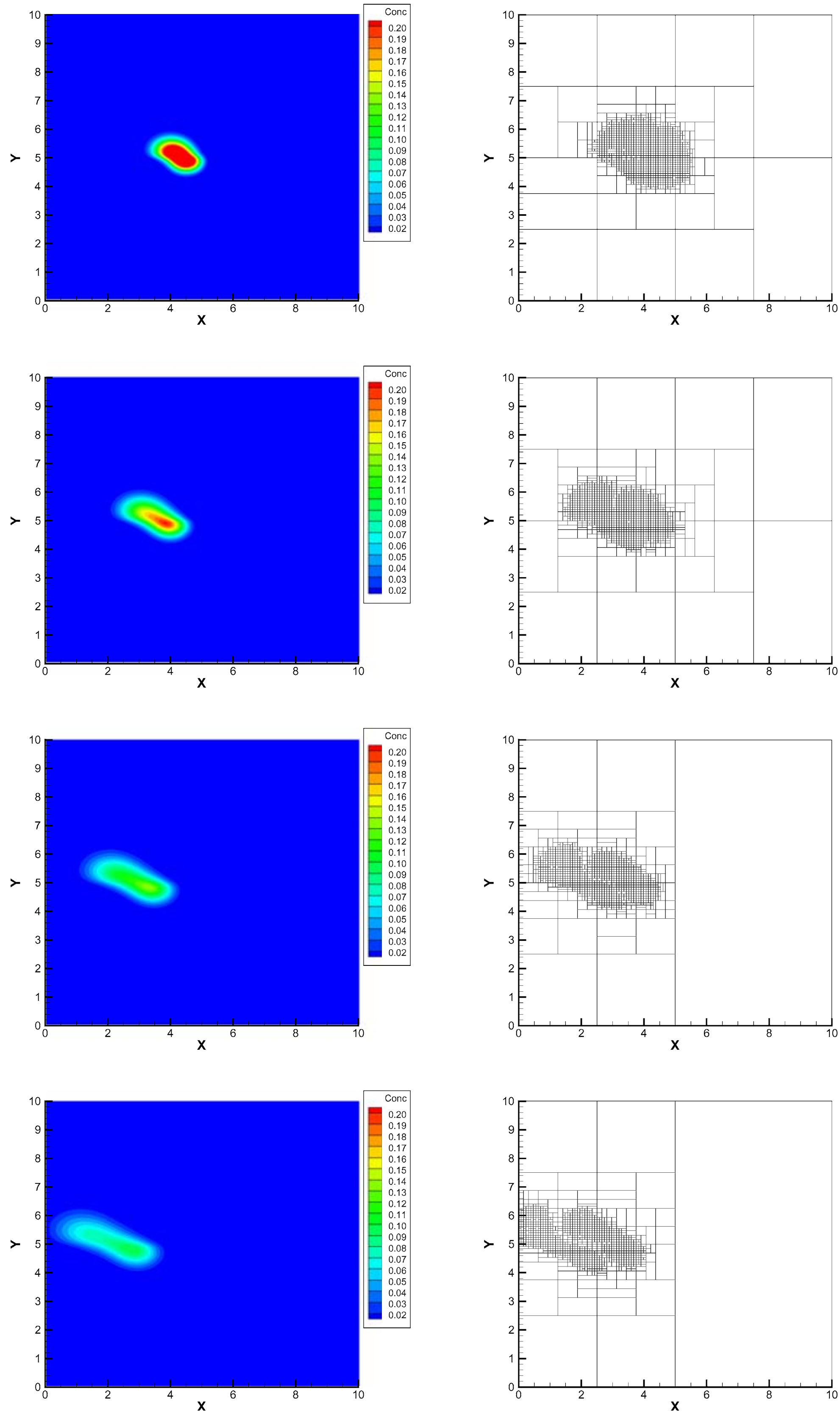

Fig. 2 DG results with the LP-A mesh adaptation (left column: the concentration in fluid; right column: the mesh structure; from top row to bottom: $t = 0.5$, 1, 1.5, and 2, respectively)

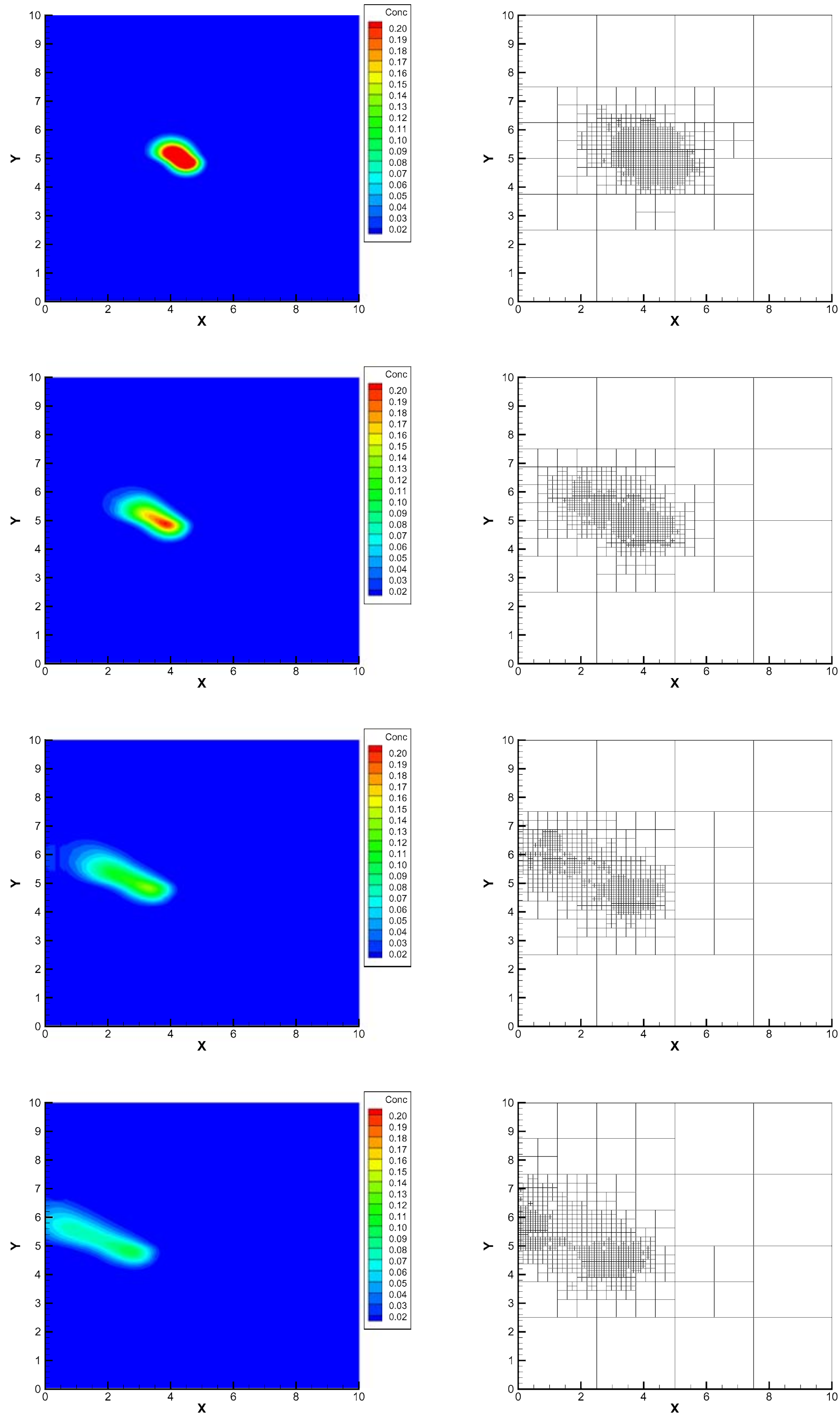

Fig. 3 DG results with the ER-I mesh adaptation (left column: the concentration in fluid; right column: the mesh structure; from top row to bottom: $t = 0.5$, 1, 1.5, and 2, respectively)

32×32 uniform rectangular mesh. The local problem-based error indicator η in the $L^2\left(t_{n-1}, t_n; L^2(E)\right)$ norm is computed for each element E at time step t_n using $h' = h/2$ and $r' = r$. Then, 5% of elements with the largest error indicator values are refined either isotropically (each element is refined into four congruent sub-elements) or anisotropically (each element is refined into two sub-elements in either x or y direction as guided by the error indicator η; see [57] for details on anisotropic refinements), and another 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 during each mesh modification.

Results on the concentration profiles and the mesh structures as functions of time are shown in Figs. 1 and 2, respectively, for the isotropic (LP-I adaptive scheme, in short) and the anisotropic (LP-A, in short) mesh adaptations, both guided by the local problem-based error indicator η. In addition, for comparison, we present in Fig. 3 the result from adaptive SIPG as guided by the explicit residual-type error indicator in the $L^2(L^2)$ norm [59] (ER-I, in short) with all other parameters unchanged. Simulation results show that a contaminant plume moves to the left due to advection, expanding its area with time due to diffusion and dispersion. Clearly, the mesh from each of the three simulations follows the movement of the plume. Due to the retardation effect arising from adsorption, the advection of the contaminant is slower in the lower part of the domain. Nevertheless, a continuous concentration profile is formed because of non-zero diffusion–dispersion over the entire domain.

A close investigation of the shape, size, and center of the plume reveals that the LP-A approach has the least numerical diffusion among the three, and that it is most effective in characterizing the plume structure. Between the two isotropic mesh adaptations, it is clear that the ER-I approach performs better than LP-I. However, it was found in our previous numerical results [57] that both the isotropic and anisotropic mesh adaptations with hierarchic error estimators perform better than the ER-I approach. Thus, one sees that the approximation of hierarchic error estimators by the local problem-based alternative indeed introduces a pronounced reduction of effectiveness. Nevertheless, being more efficient than hierarchic error estimators in computational cost, the local problem-based estimators are still very useful for guiding adaptivity. In particular, local problem-based estimators are important in guiding anisotropic mesh adaptation and p-adaptivity, as residual-type indicators may provide information only for isotropic mesh adaptation. Our results here indicate that, due to the advantage of anisotropic over isotropic mesh adaptation, local problem-based estimators are preferred over the explicit residual-type $L^2(L^2)$ indicators, at least for the test example.

5 Discussion and conclusions

We have established local problem-based *a posteriori* error estimators for DG to approximate the effective, but computationally expensive, hierarchic estimators. Both upper and lower bounds of the errors in the proposed estimators are derived. The local problem-based estimators involve only local computation and are far more efficient than hierarchic estimators in computational cost. Moreover, the local problem-based estimators over an element may be computed independently of other elements; thus, they are completely parallelizable. Numerical experiments have been conducted to study the effectiveness of the proposed estimators in terms of guiding dynamic mesh adaptation of DG as applied to reactive transport problems. Our numerical investigation suggested that the local problem-based estimators are effective in guiding anisotropic mesh adaptation, resulting in small numerical diffusion and sharp resolution of concentration fronts. However, for isotropic mesh adaptation, the local problem-based estimators might be inferior to explicit residual-type indicators. As a future extension, we propose to study local problem-based *a posteriori* error estimators for DG methods as applied to transport coupled with kinetic and local-equilibrium reactions and to multiphase flow in porous media.

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