DYNAMICALLY ADAPTIVE DISCONTINUOUS GALERKIN METHODS FOR CONTAMINANT TRANSPORT IN POROUS MEDIA

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ABSTRACT

Discontinuous Galerkin (DG) methods are formulated to solve contaminant transport problems. Error indicators-guided dynamic mesh adaptation strategies are presented for efficient DG implementations. Numerical results demonstrate that the dynamic approaches can resolve time-dependent contaminant transport adequately without slope limiting; in particular, the anisotropic mesh adaptation results in well-adapted efficient meshes and small numerical diffusion. Moreover, mass conservation is retained locally during dynamic mesh modification.

KEYWORDS: discontinuous Galerkin methods, contaminant transport, \textit{a posteriori} error estimators, anisotropic adaptation, dynamic adaptations

1. INTRODUCTION

Water is of paramount social and economical value, and its availability and use will considerably influence the development of our world. Sustainable management and protection of water in the environment is one of the key problems of the 21st century, and numerical modeling will contribute significantly to its solution. For instance, natural attenuation is used in tens of thousands of contaminated sites in the United States in place of or in conjunction with engineering remediation systems. Numerical simulation of contaminant transport phenomena play a essential role in furthering the understanding of groundwater remediation and natural attenuation. In addition, transport arises in many other diversified fields, such as petroleum engineering, groundwater hydrology, environmental engineering, soil mechanics, earth sciences, chemical engineering and biomedical engineering. Significant mathematical and computational challenges are imposed by realistic simulations for simultaneous advection, diffusion, dispersion and chemical reaction [2, 9, 11, 15–20, 27–31, 39–41, 44–46].

Discontinuous Galerkin (DG) approximations [3, 4, 8, 21, 23, 25, 26, 42, 43] are finite element methods using piecewise discontinuous polynomial spaces and specialized bilinear forms for the treatment of such discontinuous spaces. Though DG methods first appeared in the late seventies, it was only recently that new schemes using discontinuous approximations have become popular in the scientific and engineering communities. Examples of these schemes include the Bassy and Rebay method [7], the Local Discontinuous Galerkin methods [13], the Oden-Babuska-Bauman (OBB) method [21], the symmetric interior penalty Galerkin (SIPG) methods [32, 38, 42], the non-symmetric interior penalty Galerkin (NIPG) methods [26], and the incomplete interior
penalty Galerkin (IIPG) methods [12, 32, 36, 38]. DG methods are particularly useful for multiscale, adaptive and parallel implementation because they are element-wise conservative, they support local approximations of high order, and they are implementable on unstructured and even non-matching meshes.

In this paper we focus on the four primal DG methods, i.e. OBB, NIPG, SIPG and IIPG, and we investigate three dynamic mesh adaptation strategies, namely, the hierarchic anisotropic (HA), the \(L^2(L^2)\) isotropic (LI), and the hierarchic isotropic (HI). In Section 2 we formulate the primal DG schemes for a general scalar reactive transport equation and present various \textit{a posteriori} error estimators for DG. Section 3 is devoted to the numerical investigation of various dynamic mesh adaptation approaches for DG.

2. DISCONTINUOUS GALERKIN SCHEMES AND ERROR ESTIMATES

2.1. Governing equations

The model problem we consider is single-species reactive transport in a single flowing phase in porous media:

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

where the species concentration \(c\) is the unknown variable to be solved. The final simulation time \(T\), effective porosity \(\phi\), Darcy velocity \(u\) and dispersion/diffusion tensor \(D(u)\) are given parameters. The reaction term \(r(c)\) is a given function to describe the kinetic biogeochemical reaction. The model equation is closed with the boundary conditions

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

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

and the initial condition

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

where \(c_B\) is the inflow boundary concentration and \(c_0\) the initial concentration.

The continuous in time DG approximation \(C^{DG}(\cdot, t) \in \mathcal{D}_r(\mathcal{E}_h)\) of (1)-(4) is the solution of the following ODEs:

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

\[
w \in \mathcal{D}_r(\mathcal{E}_h), \quad t \in (0, T],
\]

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

The bilinear form \(B(c, w; u)\) is given as

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

where \(s_{\text{form}} = -1\) for NIPG or OBB (the non-symmetric formulation), \(s_{\text{form}} = 1\) for SIPG (the symmetric formulation) and \(s_{\text{form}} = 0\) for IIPG (the incomplete interior penalty Galerkin method). The interior penalty term \(J_0^s(c, w)\) is defined by

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

where \(\sigma\) is a discrete positive function that takes a constant value \(\sigma_\gamma\) on the edge or face \(\gamma\). The linear functional \(L(w; \mathbf{u}, c)\) is given as

\[
L(w; \mathbf{u}, c) := \int_\Omega r (\mathcal{M}(c)) w + \int_\Omega c_w q^+ w - \sum_{\gamma \in \Gamma_{h,\text{in}}} \int_\gamma c_B \mathbf{u} \cdot \mathbf{n}_\gamma w.
\]

### 2.2. Residual-based explicit \textit{a posteriori} error estimates

The \textit{a posteriori} error estimates are computed in terms of residual quantities that only depend on the approximate solution and the data. The residuals consist of interior residual \(R_I\), the zeroth order boundary residual \(R_{B0}\) and the first order boundary residual \(R_{B1}\), defined below [34, 37].

\[
R_I := q C^{DG} + r \left( \mathcal{M}(C^{DG}) \right) \quad (9)
\]

\[
R_{B0} := \left\{ \begin{array}{ll}
[C^{DG}] & x \in \gamma, \gamma \in \Gamma_h, \\
0 & x \in \partial \Omega,
\end{array} \right. \quad (10)
\]

\[
R_{B1} := \left\{ \begin{array}{ll}
(c_B \mathbf{u} - C^{DG} \mathbf{u} + \mathbf{D}(\mathbf{u})\nabla C^{DG}) \cdot \mathbf{n} & x \in \gamma, \gamma \in \Gamma_h, \\
\mathbf{D}(\mathbf{u})\nabla C^{DG} \cdot \mathbf{n} & x \in \Gamma_{h,\text{in}}, \\
0 & x \in \Gamma_{h,\text{out}},
\end{array} \right. \quad (11)
\]

where, in element interior, \(C^{DG} = c\) if \(q < 0\) and \(C^{DG} = c_w\) if \(q \geq 0\).

We apply the duality argument to analyze the error in the \(L^2(L^2)\) norm for SIPG [34], where a backward parabolic equation is used and inverse inequality is employed. The results on \textit{a posteriori} error estimates in the \(L^2(L^2)\) norm are stated as follows. Under certain conditions,
there exists a constant $K$, independent of $h$ and $r$, such that

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

(12)

where

$$\eta^2_E = \frac{h_E^4}{r^4} \| R_l \|_{L^2(0,T;L^2(E))}^2 + \frac{1}{2} \sum_{\gamma \in \partial E \setminus \partial \Omega} \left( \frac{h_\gamma}{r} + \delta h_\gamma \right) \| R_{B0} \|_{L^2(0,T;L^2(\gamma))}^2$$

$$+ \frac{1}{2} \sum_{\gamma \in \partial E \setminus \partial \Omega} \frac{h_\gamma^3}{r^3} \| R_{B1} \|_{L^2(0,T;L^2(\gamma))}^2 + \sum_{\gamma \in \partial E \cap \partial \Omega} \frac{h_\gamma^3}{r^3} \| R_{B1} \|_{L^2(0,T;L^2(\gamma))}^2.$$

Here $\delta = 0$ in the case of conforming meshes with triangles or tetrahedra. In general cases, $\delta = 1$. We remark that a posteriori error estimates in the $L^2(L^2)$ norm are shown to be very effective error indicators, in particular for the problems concerning concentration itself rather than transport flux. The advantage of SIPG over the other primal DG methods in adaptive computation is clearly indicated by the fact that the duality argument does not hold for the OBB, NIPG and IIPG methods.

The optimal a posteriori error estimates in the energy norm are obtained for all primal DG methods, i.e. OBB, NIPG, SIPG and IIPG. These error estimates are proved using a new technique that employs a special approximation property of discontinuous finite element spaces by continuous spaces [37]. The results state that, under certain conditions, there exists a constant $K$, independent of $h$, such that

$$\sqrt{\psi} (C_{DG} - c) \|_{L^\infty(0,T;L^2(\Omega))} + \| D^{1/2} (u) \nabla (C_{DG} - c) \|_{L^2(0,T;L^2(\Omega))}$$

$$\leq K \left( \sum_{E \in \mathcal{E}_h} \chi^2_E \right)^{1/2},$$

(13)

where

$$\chi^2_E = \frac{h_E^2}{r^2} \| R_l \|_{L^2(0,T;L^2(E))}^2 + \sum_{\gamma \in \partial E \setminus \partial \Omega} h_\gamma \| R_{B1} \|_{L^2(0,T;L^2(\gamma))}^2$$

$$+ \frac{1}{2} \sum_{\gamma \in \partial E \setminus \partial \Omega} \left( h_\gamma \| R_{B1} \|_{L^2(0,T;L^2(\gamma))}^2 + h^{-1}_\gamma \| R_{B0} \|_{L^2(0,T;L^2(\gamma))}^2 \right)$$

$$+ h_\gamma \| R_{B0} \|_{L^\infty(0,T;L^2(\gamma))}^2 + h_\gamma \| \partial R_{B0} / \partial t \|_{L^2(0,T;L^2(\gamma))}^2.$$

We emphasize that a posteriori error estimates in the energy norm are flexible and apply to all four members of DG. They are explicit and residual-based, thus computationally efficient. General boundary conditions may easily be taken into consideration for these error estimates. In addition, no saturation or regularity assumption for the dual problem is required for these
estimates.

2.3. A posteriori error indicators using hierarchic bases

Residual-based explicit error estimators are efficient to compute and may be used to indicate the subset of elements that need to be refined or coarsened, thus achieving adaptivity. However, these residual-based estimators yield only one piece of information for each element, so they do not provide guidance on anisotropic refinements. In this section we present error estimators using hierarchic bases. Unlike residual-based error estimators, hierarchic error estimators give point-wise information on the error, so they may be used to guide fully anisotropic hp-adaptation. Here, for simplicity, we consider only the anisotropic h-adaptation.

Hierarchic error estimators consist of solving the problem of interest by employing two discretization schemes of different accuracy and using the difference in 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. The reader is referred to [1, 5, 6, 14, 22] for further information.

For a given mesh $\mathcal{E}_h$, we construct the mesh $\mathcal{E}_{h/2}$ by isotropically refining each element of $\mathcal{E}_h$. We denote by $C^{DG}$ the DG solution in the coarse mesh $\mathcal{E}_h$ and by $C^{DG,F}$ the DG solution in the fine mesh $\mathcal{E}_{h/2}$. We make the following saturation assumption:

$$\left\| C^{DG,F} - c \right\|_{L^2(t)} \leq \beta \left\| C^{DG} - c \right\|_{L^2(t)}, \quad 0 \leq \beta < 1. \quad (14)$$

Using the a priori convergence results of DG [24, 32, 38], we observe, for all the four primal DGs, i.e. OBB, SIPG, NIPG and IIPG, that $\beta$ is less than or equal to the following asymptotic value:

$$\beta \leq \frac{1}{2^{r-1}} = \frac{1}{2^{\min(r,s)-1}}.$$

The triangle inequality and the saturation assumption directly imply the following error estimator, which holds for OBB, SIPG, NIPG and IIPG:

$$\frac{1}{1 + \beta} \left( \sum_{E \in \mathcal{E}_h} \eta_E^2 \right)^{1/2} (t) \leq \left\| C^{DG} - c \right\|_{L^2(t)} \leq \frac{1}{1 - \beta} \left( \sum_{E \in \mathcal{E}_h} \eta_E^2 \right)^{1/2} (t), \quad (15)$$

where $\eta_E(t) = \left\| C^{DG,F} - C^{DG} \right\|_{L^2(E)(t)}$.

We now describe the selection of an anisotropic refinement. A uniform degree $r$ of the polynomial space is assumed over the entire domain. The local space for each element $E$ is
denoted by $\mathbb{P}_r(E)$. We further assume that, for an individual element $E$, there are $n$ different refinement options $r_1$, $r_2$, ..., $r_n$. For example, we may refine a rectangular element in the $x$- or $y$-direction. We denote by $r_i(E)$ the set of sub-elements obtained from the refinement $r_i$ applied to the element $E$ and by $\Pi_E$ the $L^2$ projection operator onto $\mathbb{P}_r(E)$. We now compute the error indicator for each refinement option:

$$\eta_{E,r_i}(t) = \sum_{\hat{E} \in r_i(E)} \left\| C_{DG,F} \Phi - \Pi_E C_{DG,F} \Phi \right\|_{L^2(E)}^2(t).$$

Obviously, the smaller the error indicator $\eta_{E,r_i}(t)$, the better the anisotropically refined mesh resolves the higher order accurate solution $C_{DG,F}$ and the better the anisotropically refined mesh is likely to resolve the true solution $c$. Therefore, we choose the refinement $r_i$ at time $t$ such that $\eta_{E,r_i}(t)$ is minimized among all available options.

### 3. DYNAMIC ADAPTIVITIES

#### 3.1. Dynamic mesh adaptation

A non-growing dynamic adaptive strategy [35] is employed here, where the mesh is adaptively adjusted, without changing the number of elements. The initial mesh is chosen to be a uniform fine grid. We denote by $(S)$ the number of elements in a set $S$.

**Algorithm 3.1 (dynamic mesh adaptation)**

*Given an initial mesh $\mathcal{E}_0$, a modification factor $\alpha \in (0, 1)$, time slices $\{(T_0, T_1), (T_1, T_2), \cdots, (T_{N-1}, T_N)\}$, and iteration numbers $\{M_1, M_2, \cdots, M_N\}$:*

1. Let $n = 1$;
2. Let $m = 1$;
3. Compute the initial concentration for time slice $(T_{n-1}, T_n)$ using either the initial condition (if $n = 1$) or the concentration at the end of last time slice (if $n > 1$) by the $L^2$ local projection;
4. Let $\mathcal{E}_{m,n} = \mathcal{E}_0$ if $n = 1$ and $m = 1$; or $\mathcal{E}_{m,n} = \mathcal{E}_{M_{n-1}+1,n-1}$ if $n > 1$ and $m = 1$;
5. Compute the DG approximation of the PDE for time slices $(T_{n-1}, T_n)$ based on mesh $\mathcal{E}_{m,n}$ and compute the error indicator $\eta_E$ for each element $E \in \mathcal{E}_{m,n}$;
6. Select $\mathcal{E}_r \in \mathcal{E}_{m,n}$ such that $(\mathcal{E}_r) = \lceil \alpha #(\mathcal{E}_{m,n}) \rceil$ and $\min\{\eta_E : E \in \mathcal{E}_r\} = \max\{\eta_E : E \in \mathcal{E}_{m,n} \setminus \mathcal{E}_r\}$;
7. Select $\mathcal{E}_c \in \mathcal{E}_{m,n}$ to minimize $\max\{\eta_E : E \in \mathcal{E}_c\}$ subject to $(\mathcal{E}_c) = \lceil \alpha #(\mathcal{E}_{m,n}) \rceil$ and the coarsening-compatible condition with regard to $\mathcal{E}_{m,n}$ and $\mathcal{E}_r$;
8. Refine all $E \in \mathcal{E}_r$ isotropically (or anisotropically guided by the local error indicator), and
Figure 1. DG with LI adaptation (left column: concentration; right column: mesh structure; top row: \( t = 0.01 \); bottom row: \( t = 10 \))

coarsen all \( E \in \mathcal{E}_c \) to form a new mesh \( \mathcal{E}_{m+1,n} \):

9. Let \( m = m + 1 \). If \( m \leq M \), go to step 3;

10. Let \( n = n + 1 \). If \( n \leq N \), go to step 2;

11. Report the solution and stop.

3.2. Numerical examples

Using numerical experiments, we investigate the three dynamic mesh adaptation strategies that are listed below:

- LI approach: the dynamic and isotropic mesh adaptation using the \( L^2 \) norm error
indicator $\eta_E$ in (12);

- HI approach: the dynamic and isotropic mesh adaptation using the error indicator $\eta_E$ of hierarchic bases in (15);
- HA approach: the dynamic and anisotropic mesh adaptation using the error indicator $\eta_E$ of hierarchic bases in (15).

The problem (1) over the domain $\Omega = (0, 1)^2$ is considered. We impose no injection or extraction, i.e. $q = 0$. The initial and inflow boundary concentrations are both zero. The porosity $\phi$ is a constant 0.1, and the diffusion-dispersion tensor $D$ is a diagonal matrix with $D_{ii} = 0.01$. The velocity $u$ is zero at $0.25 < y < 0.5$ and it is $(1, 0)$ uniformly elsewhere. The reaction term is taken to be a constant source: $r(c) = s$, and the contaminant source term $s$ is 1 within the rectangle $(0.25, 0.75) \times (0.25, 0.5)$ and zero elsewhere. The test case represents the coupling of a diffusion process with an advection-dominated process over adjacent domains, where thin concentration layers are formed around the interfaces between these processes.

Figure 2. DG with HI adaptation (left column: concentration; right column: mesh structure; top row: $t=0.01$; bottom row: $t=10$)
Figure 3. DG with HA adaptation (left column: concentration; right column: mesh structure; top row: $t=0.01$; bottom row: $t=10$)

Computations are carried out using SIPG with the three adaptation approaches LI, HI and HA. The number of iterations is chosen to be 5 initially and set to 2 for all other time slices. We set the modification factor $\alpha = 0.05$, and we let a time slice contain 10 time steps. The implicit Euler method is employed for time integration. The initial mesh is a 16x16 uniform rectangular grid. Concentration profiles and mesh structures from the three approaches are shown in Figures 1, 2 and 3, respectively. For each adaptation approach we run a long-term simulation up to $t=10$ using a uniform time step $\Delta t=0.1$ (shown in the two subfigures on the bottom of each figure) and a short-term simulation up to $t=0.01$ using a uniform time step $\Delta t=0.0001$ (shown in the two subfigures on the top of each figure).

Simulation results show that concentration boundary layers, formed almost immediately when the simulation starts, are very thin at early times and spread out spatially with time. The HA approach yields meshes that are dense only around the boundary layers necessary for resolving
the physics in both the long-term and short-term simulations. On the other hand, the LI approach unnecessarily refines the mesh in the center of the middle layer, far away from the boundary layers at early times. Compared with LI, the HI method leads to a better distribution of grids, but HI is still unable to give good concentration profiles at early times. At later times, both LI and HI seem able to provide reasonable concentration predictions. It should be noted that the boundary layers expand during early simulation times, and all three approaches (HA, HI and LI) lead to meshes adapted to this time-evolving phenomena, with HA being the best. In addition, the HA approach does not only provide proper density distribution of the mesh, but it also yields small numerical diffusion and physics-driven element aspect ratios. During early times, most of the elements from HA are narrow, mimicking the shape of the thin boundary layers.

We remark that we have used a very coarse $16 \times 16$ mesh here for convenience in visualizing the differences of the three mesh adaptation approaches. If we use a finer mesh, all three adaptation approaches provide accurate time profiles in both the long-term and short-term simulations (not shown). The successful application of DG to this example occurs because of the effectiveness of DG in treating both advection- and diffusion-dominated problems. In addition, DG offers flexible and effective mesh adaptation in capturing boundary layer phenomena. Finally, we refer the reader to [33–35] for more simulation results of contaminant transport, including dynamically adaptive DG as applied to the ANDRA-Couplex1 case [10].

REFERENCES


