J. KSIAM **Vol.6**, No.1, 1-15, 2002

RELATIONSHIPS AMONG CHARACTERISTIC FINITE ELEMENT METHODS FOR ADVECTION-DIFFUSION PROBLEMS

ZHANGXIN CHEN

Abstract. Advection-dominated transport problems possess difficulties in the design of numerical methods for solving them. Because of the hyperbolic nature of advective transport, many characteristic numerical methods have been developed such as the classical characteristic method, the Eulerian-Lagrangian method, the transport diffusion method, the modified method of characteristics, the operator splitting method, the Eulerian-Lagrangian localized adjoint method, the characteristic mixed method, and the Eulerian-Lagrangian mixed discontinuous method. In this paper relationships among these characteristic methods are examined. In particular, we show that these sometimes diverse methods can be given a unified formulation. This paper focuses on characteristic finite element methods. Similar examination can be presented for characteristic finite difference methods.

1. Introduction

Advection-diffusion transport problems arise in many areas of engineering and applied sciences [16, 25, 30]. These problems have a nondissipative (hyperbolic) advective term and a dissipative (parabolic) part. When the parabolic part dominates, all reasonable numerical methods perform well. When the hyperbolic part dominates, however, strictly parabolic numerical methods do not perform well; they exhibit excessive nonphysical oscillations or excessive numerical diffusions. Although extremely fine mesh refinement is possible to overcome some of the difficulties, it is not a feasible approach due to excessive computational efforts.

Many classes of numerical methods have been developed for solving advection-diffusion transport problems [16, 27, 30]. One of them is the class of characteristic methods.

AMS subject classification: 35K60, 35K65, 65N30, 65N22
Key words: Characteristic methods, Eulerian-Lagrangian, mixed methods, finite elements, advection-diffusion problems, transport diffusion, operator splitting, discontinuous methods
This work is supported in part by National Science Foundation grants DMS-9626179, DMS-9972147, and INT-9901498, and by a gift grant from Mobil Technology Company

Because of the hyperbolic nature of advective transport, it is natural to look to a characteristic treatment in solving these problems. There is a rich family of characteristic methods in the literature, which bear a variety of names, the method of characteristics (MOC) [28, 34, 40], the modified method of characteristics (MMOC) [23], the transport diffusion method (TDM) [5, 29, 35], the Eulerian-Lagrangian method (ELM) [32, 33], the operator splitting method (OSM) [24, 44], the Eulerian-Lagrangian localized adjoint method (ELLAM) [9, 37], the modified method of characteristics with adjusted advection (MMOCAA) [20], the characteristic mixed method (CMM) [1, 22], and the Eulerian-Lagrangian mixed discontinuous method (ELMDM) [12]. The common feature of this class is that the advective part is handled by a characteristic tracking technique (in a Lagrangian framework) and the diffusive part is treated by a spatial (Eulerian) approximation scheme. These characteristic methods can take reasonably large time steps and do not numerically diffuse sharp solution fronts, and some of them can conserve mass. In this paper relationships among these characteristic methods are examined. In particular, we show that these sometimes diverse methods can be given a unified formulation. We start with ELMDM, from which we recover all other methods. This paper focuses on characteristic finite element methods; similar examination can be presented for characteristic finite difference methods. Most of the earlier characteristic methods are based on lowest-order finite elements in their respective setting. In this paper we extend them to general finite elements.

The outline of this paper is as follows. In the next section, we describe a continuous problem. In the third section, we state a unified formulation of characteristic methods. In the fourth section, we deduce all the above mentioned methods from this formulation. In the fifth section, we mention some generalizations. We conclude with two remarks in the last section. We mention that we do not consider stability and convergence properties of these characteristic methods, which can be found in the cited references. Also, it would be interesting to compare the characteristic methods under consideration computationally. This would involve tremendous work and is beyond the scope of this paper. This paper focuses on the theoretical relationships among these methods.

2. A Continuous Problem

We consider the advection-diffusion equation for u on a bounded domain $\Omega \subset \Re^d$, $d \leq 3$, with boundary $\partial\Omega = \Gamma_D \cup \Gamma_N$, $\Gamma_D \cap \Gamma_N = \emptyset$:

$$\begin{aligned} &\partial_t(\phi u) + \nabla \cdot (bu - a\nabla u) = f && \text{in } \Omega \times J, \\ &u = g_D, && \text{on } \Gamma_D \times J, \\ &(bu - a\nabla u) \cdot \nu = g_N, && \text{on } \Gamma_N \times J, \\ &u(x,0) = u^0(x) && \text{in } \Omega, \end{aligned} \tag{2.1}$$

where

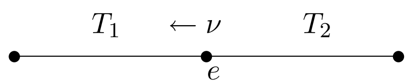

FIGURE 1. An illustration for the jump definition.

$J = (0, T]$ $(T > 0)$, $a(x, t) \in \left(L^\infty(\Omega)\right)^{d\times d}$, $b(x, t) \in \left(L^\infty(\Omega)\right)^{d}$, $\phi(x, t) \in L^\infty(\Omega)$, $g_D(x, t) \in L^\infty(\Gamma_D)$, $g_N(x, t) \in L^\infty(\Gamma_N)$, $f(x, t) \in L^2(\Omega)$ (for each $t \in J$) and $u^0(x) \in L^2(\Omega)$ are given functions (the standard Sobolev spaces $H^k(\Omega) = W^{k,2}(\Omega)$ with the usual norms are used in this paper), and ν is the outer unit normal to $\partial\Omega$.

To introduce a unified formulation, we rewrite this equation as follows:

$$
\begin{aligned}
&\partial_t(\phi u) + \nabla \cdot (bu - \sigma) = f && \text{in } \Omega \times J,\\
&\sigma = a\nabla u && \text{in } \Omega \times J,\\
&u = g_D, && \text{on } \Gamma_D \times J,\\
&(bu - \sigma)\cdot \nu = g_N, && \text{on } \Gamma_N \times J,\\
&u(x, 0) = u^0(x) && \text{in } \Omega.
\end{aligned}
\tag{2.2}
$$

Namely, an auxiliary variable σ is introduced. This variable usually has a physical meaning in applications such as the electric field in semiconductor modeling [13, 14] or the velocity field in petroleum simulation [19, 25]. In the next two sections, we consider the case where $a = (a_{ij})$ is positive definite:

$$
0 < |\xi|^{-2} \sum_{i,j=1}^{d} a_{ij}(x, t)\xi_i\xi_j \le a^* < \infty, \qquad (x, t) \in \Omega \times J,\ \xi \neq 0 \in \Re^d,
\tag{2.3}
$$

with a^* being constant. The situation without this assumption will be addressed in the fifth section.

3. A Unified Formulation

For $h > 0$, let $(T_h)_h$ be a sequence of finite element partitions of Ω; each subdomain $T \in T_h$ has a Lipschitz boundary. Let $\mathcal{E}_h^o$ denote the set of all interior edges (respectively, faces) e of T_h, $\mathcal{E}_h^b$ the set of the edges (respectively, faces) e on $\partial\Omega$, and $\mathcal{E}_h = \mathcal{E}_h^o \cup \mathcal{E}_h^b$. We tacitly assume that $\mathcal{E}_h^o \neq \emptyset$. Finally, each exterior edge or face has imposed on it either Dirichlet or Neumann conditions, but not both.

For $l \geq 0$, define

$$
H^l(T_h) = (v \in L^2(\Omega) : v|_T \in H^l(T), T \in T_h).
$$

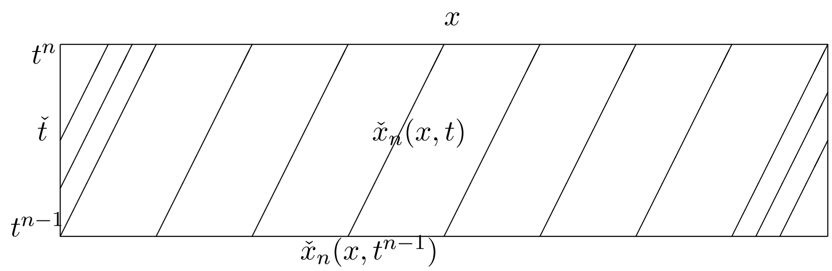

FIGURE 2. An illustration of characteristics.

With each $e \in \mathcal{E}_h$, we associate a unit normal vector ν. For $e \in \mathcal{E}_h^b$, ν is just the outer unit normal to $\partial\Omega$. For $e \in \mathcal{E}_h^o$, with $e = T_1 \cap T_2$ and $T_1, T_2 \in T_h$, ν is the unit normal exterior to T_2 with the corresponding jump definition (see Fig. 1): for $v \in H^l(T_h)$ with $l > 1/2$, we define the average and jump by

$$\{v\} = \frac{1}{2}((v|_{T_1})|_e + (v|_{T_2})|_e), \quad [v] = (v|_{T_2})|_e - (v|_{T_1})|_e.$$

For $e \in \mathcal{E}_h^b$, we utilize the convention (from inside Ω)

$$\{v\} = v|_e \quad \text{and} \quad [v] = \begin{cases} v & \text{if } e \in \Gamma_D, \\ 0 & \text{if } e \in \Gamma_N. \end{cases}$$

For each positive integer $\mathcal{N}$, let $0 = t^0 < t^1 < \cdots < t^{\mathcal{N}} = T$ be a partition of J into subintervals $J^n = (t^{n-1}, t^n]$, with length $\Delta t^n = t^n - t^{n-1}$, $1 \le n \le \mathcal{N}$. Set $v^n = v(\cdot, t^n)$ and

$$\Delta t = \max_{1 \le n \le \mathcal{N}} \Delta t^n.$$

For any $x \in \Omega$ and two times $0 \le t^{n-1} < t^n \le T$, the hyperbolic part of problem (2.1), $\phi\partial_t u + b \cdot \nabla u$, defines the characteristic $\check{x}_n(x,t)$ along the interstitial velocity $\varphi = b/\phi$:

$$\begin{aligned} &\partial_t \check{x}_n = \varphi(\check{x}_n, t), \quad t \in J^n, \\ &\check{x}_n(x, t^n) = x. \end{aligned} \tag{3.1}$$

In general, we cannot follow the characteristic in (3.1) exactly; we can only follow it approximately. There are many ways to solve the first order ordinary differential equation (3.1). Let us consider the Euler method

$$\check{x}_n(x,t) = x - \varphi(x,t^n)(t^n - t), \qquad t \in [\check{t}(x), t^n], \tag{3.2}$$

where $\check{t}(x) = t^{n-1}$ if $\check{x}_n(x,t)$ does not backtrack to the boundary $\partial\Omega$ for $t \in [t^{n-1}, t^n]$; $\check{t}(x) \in (t^{n-1}, t^n]$ is the time instant when $\check{x}_n(x,t)$ intersects $\partial\Omega$, i.e., $\check{x}_n(x, \check{t}(x)) \in \partial\Omega$, otherwise. See Fig. 2, where, for the purpose of demonstration, the characteristics are shown for constant φ in one dimension. If Δt^n is sufficiently small (depending upon the smoothness of φ), the approximate characteristics do not cross each other, which is assumed here. We denote the inverse of $\check{x}_n(\cdot,t)$ by $\hat{x}_n(\cdot,t)$. For a function $v(x,t)$, if $t \in J^n$, we define

$$\hat{v}(x,t) = v(\hat{x}_n(x,t),t^n). \tag{3.3}$$

Note that $\hat{v}(x,t^{n-1,+}) = \hat{v}^{n-1,+}(x)$ follows the characteristics forward from t^{n-1} to t^n to become $v^n(x)$. We shall use this type of functions as test functions below.

Let $V_h \times W_h$ be the finite element spaces for the approximation of σ and u, respectively. They are finite dimensional and defined locally on each element $T \in T_h$, so let $V_h(T) = V_h|_T$ and $W_h(T) = W_h|_T$. Neither continuity constraint nor boundary values are imposed on $V_h \times W_h$. Examples of $V_h \times W_h$ will be given later. Let $(\cdot,\cdot)_S$ denote the $L^2(S)$ inner product (we omit S if $S = \Omega$).

A unified characteristic scheme for (2.1) is: Find $(\sigma_h, u_h) : \{t^1, \dots, t^{\mathcal{N}}\} \to V_h \times W_h$ such that
(3.4)

$$\begin{aligned}
&(\phi^n u_h^n, v) - (\phi^{n-1} u_h^{n-1}, \hat{v}^{n-1,+}) + \sum_{T\in T_h} (\sigma_h^n, \nabla v)_T \,\Delta t^n - \sum_{e\in\mathcal{E}_h} (\{\sigma_h^n\cdot\nu\}, [v])_e \,\Delta t^n \\
&\qquad = \int_{J^n} \left((f,\hat{v}) - \sum_{e\in\Gamma_N} (g_N, \hat{v})_e - \sum_{e\in\Gamma_D} (g_D b\cdot\nu, \hat{v})_e \right) \mathrm{d}t, \qquad v \in W_h, \\
&\sum_{T\in T_h} \left(\left(a^{-1}\right)^n \sigma_h^n - \nabla u_h^n, \tau \right)_T + \sum_{e\in\mathcal{E}_h} ([u_h^n], \{\tau\cdot\nu\})_e = \sum_{e\in\Gamma_D} (g_D^n, \tau\cdot\nu)_e\,, \quad \tau \in V_h,
\end{aligned}$$

where v is extended by zero outside $\bar{\Omega}$. The initial approximation u_h^0 can be defined in any reasonable manner.

System (3.4) has been introduced in [12], and stems from a space-time mixed formulation of (2.2). It can be seen [12] that (3.4) has a unique solution and the stiffness matrix arising from it is positive definite for any pair of V_h and W_h. All characteristic methods under consideration will be derived from (3.4).

4. Relationships

In this section we derive various characteristic methods from (3.4) and discuss their relationships.

4.1. **The Eulerian-Lagrangian mixed discontinuous method (ELMDM).**

Let T_h be a partition into elements, say, simplexes, rectangular parallelepipeds, and/or prisms where edges or faces on $\partial\Omega$ may be curved. In ELMDM, $V_h(T)$ and $W_h(T)$ can be any sets of polynomials. For example, they can be chosen as follows:

$$V_h(T) = (P_{r_1}(T))^d, \quad W_h(T) = P_{r_2}(T), \quad r_1,\, r_2 \geq 0, \tag{4.1}$$

where $P_r(T)$ is the set of polynomials of degree at most r on T. Other choices can be taken:

$$V_h(T) = \left(Q_{r_1}(T)\right)^d, \quad W_h(T) = Q_{r_2}(T), \quad r_1,\, r_2 \geq 0, \tag{4.2}$$

where $Q_r(T)$ is the set of polynomials of degree at most r in each variable on T. With these choices, (3.4) is the Eulerian-Lagrangian mixed discontinuous method (ELMDM) introduced in [12]. For its stability and convergence, refer to [12]. Note that in ELMDM, the set $P_r(T)$ can be used even on rectangular parallelepipeds and prisms. Also, any combination of $P_{r_1}(T)$ and $Q_{r_2}(T)$ can be utilized for $V_h(T)$ and $W_h(T)$. ELMDM expresses local conservation of mass along the characteristics [12]. Moreover, it is totally local, and the partition between adjacent elements does not have to match. Thus ELMDM is of high localizability and parallelizability. While it is in mixed form, it can be implemented in nonmixed form without introducing new variables. ELMDM is based on mixed discontinuous finite element methods [4, 11, 13, 14, 17].

4.2. **The characteristic mixed method (CMM).** Let T_h be as in §4.1 and a regular partition. Associated with the partition T_h, let $V_h \times W_h \subset H(\text{div};\Omega) \times L^2(\Omega)$ be the Raviart-Thomas-Nedelec [31, 36], the Brezzi-Douglas-Fortin-Marini [7], the Brezzi-Douglas-Marini [8] (if $d = 2$), the Brezzi-Douglas-Durán-Fortin [6] (if $d = 3$), or the Chen-Douglas [15] mixed finite element space, where

$$H(\text{div};\Omega) = \left(v \in \left(L^2(\Omega)\right)^d : \nabla \cdot v \in L^2(\Omega)\right).$$

Note that $V_h \subset H(\text{div};\Omega)$ means that the normal components of elements in V_h are continuous across interior boundaries. Because of this feature, (3.4) reduces to: Find $(\sigma_h, u_h) : \{t^1, \dots, t^{\mathcal{N}}\} \to V_h \times W_h$ such that

$$\begin{aligned}
&(\phi^n u_h^n, v) - (\phi^{n-1} u_h^{n-1}, \hat{v}^{n-1,+}) + \sum_{T\in T_h} (\sigma_h^n, \nabla v)_T\, \Delta t^n - \sum_{e\in\mathcal{E}_h} (\sigma_h^n \cdot \nu, [v])_e\, \Delta t^n \\
&\qquad = \int_{J^n} \left((f, \hat{v}) - \sum_{e\in\Gamma_N} (g_N, \hat{v})_e - \sum_{e\in\Gamma_D} (g_D b\cdot\nu, \hat{v})_e \right) \mathrm{d}t, \qquad v \in W_h, \\
&\sum_{T\in T_h} \left(\left(a^{-1}\right)^n \sigma_h^n - \nabla u_h^n, \tau \right)_T + \sum_{e\in\mathcal{E}_h} ([u_h^n], \tau\cdot\nu)_e = \sum_{e\in\Gamma_D} (g_D^n, \tau\cdot\nu)_e\,, \quad \tau \in V_h.
\end{aligned} \tag{4.3}$$

This is a generalization of CMM introduced in [1, 22], where $V_h \times W_h$ was taken to be the lowest-order Raviart-Thomas-Nedelec mixed finite element spaces. In particular, W_h is the space of piecewise constants. With this, (4.3) becomes: Find (σ_h, u_h) :

$\{t^1, \dots, t^{\mathcal{N}}\} \to V_h \times W_h$ such that

$$(\phi^n u_h^n, v) - (\phi^{n-1} u_h^{n-1}, \hat{v}^{n-1,+}) - \sum_{e\in\mathcal{E}_h} (\sigma_h^n \cdot \nu, [v])_e \, \Delta t^n$$

$$= \int_{J^n} \left((f, \hat{v}) - \sum_{e\in\Gamma_N} (g_N, \hat{v})_e - \sum_{e\in\Gamma_D} (g_D b \cdot \nu, \hat{v})_e \right) \mathrm{d}t, \qquad v \in W_h, \tag{4.4}$$

$$\sum_{T\in T_h} \left(\left(a^{-1}\right)^n \sigma_h^n, \tau \right)_T + \sum_{e\in\mathcal{E}_h} ([u_h^n], \tau \cdot \nu)_e = \sum_{e\in\Gamma_D} (g_D^n, \tau \cdot \nu)_e \,, \qquad \tau \in V_h,$$

which is the characteristic mixed method developed in [1, 22]. We remark that a postprocessing procedure similar to that in [38] was used to improve the approximation u_h in [1]. This postprocessing procedure is antidiffusive, so a slope limiting process was exploited to stablize their method. For the stability and convergence analysis of (4.4), see [1]. CMM expresses local conservation of mass along the characteristics as well. Note that with v in place of $\hat{v}^{n-1,+}$, backward Euler integration for the three terms in the right-hand side of the first equation in (4.3), and an explicit treatment of the advection, we can recover the usual mixed finite element method for parabolic problems [39].

4.3. **The Eulerian-Lagrangian localized adjoint method (ELLAM).** To derive ELLAM, we write (3.4) in Galerkin form (nonmixed form). For this, we introduce the coefficient-dependent projections $P_h^n : L^2(\Omega) \to V_h$ by

$$((a^{-1})^n (w - P_h^n w), \tau) = 0 \qquad \forall \tau \in V_h, \tag{4.5}$$

for $w \in L^2(\Omega)$, and $R_h^n : H^1(T_h) \to V_h$ by

$$\sum_{T\in T_h} ((a^{-1})^n R_h^n(v), \tau)_T = - \sum_{e\in\mathcal{E}_h} ([v], \{\tau \cdot \nu\})_e + \sum_{e\in\Gamma_D} (g_D^n, \tau \cdot \nu)_e \qquad \forall \tau \in V_h, \tag{4.6}$$

for $v \in H^1(I_h)$. We remark that the definition of these two projection operators is local.

4.3.1. *The discontinuous case.* Using (4.5) and (4.6), (3.4) can be rewritten as follows [12]: Find $u_h : \{t^1, \dots, t^{\mathcal{N}}\} \to W_h$ such that

(4.7)

$$(\phi^n u_h^n, v) - (\phi^{n-1} u_h^{n-1}, \hat{v}^{n-1,+}) + \sum_{T\in T_h} (P_h^n (a^n \nabla u_h^n), \nabla v)_T \, \Delta t^n$$

$$- \sum_{e\in\mathcal{E}_h} ([u_h^n], \{P_h^n (a^n \nabla v) \cdot \nu\})_e \, \Delta t^n - \sum_{e\in\mathcal{E}_h} (\{(P_h^n (a^n \nabla u_h^n) + R_h^n(u_h^n)) \cdot \nu\}, [v])_e \, \Delta t^n$$

$$= \int_{J^n} \left((f, \hat{v}) - \sum_{e\in\Gamma_N} (g_N, \hat{v})_e - \sum_{e\in\Gamma_D} (g_D b \cdot \nu, \hat{v})_e \right) \mathrm{d}t$$

$$- \sum_{e\in\Gamma_D} (g_D^n, P_h^n (a^n \nabla v) \cdot \nu)_e \, \Delta t^n \qquad \forall v \in W_h,$$

with σ_h given by

$$\sigma_h^n = P_h^n\left(a^n\nabla u_h^n\right) + R_h^n(u_h^n). \tag{4.8}$$

Namely, (3.4) is equivalent to (4.7) and (4.8). When a is piecewise constant and the following relation holds:

$$\nabla W_h(T) \subset V_h(T), \quad T \in T_h, \tag{4.9}$$

(4.7) becomes: Find $u_h : \{t^1, \dots, t^{\mathcal{N}}\} \to W_h$ satisfying

$$\begin{aligned}
&(\phi^n u_h^n, v) - (\phi^{n-1}u_h^{n-1}, \hat{v}^{n-1,+}) + \sum_{T\in T_h}(a^n\nabla u_h^n, \nabla v)_T\,\Delta t^n - \sum_{e\in\mathcal{E}_h}([u_h^n], \{a^n\nabla v\cdot\nu\})_e\,\Delta t^n \\
&\quad - \sum_{e\in\mathcal{E}_h}\left(\{a^n\nabla u_h^n\cdot\nu\}, [v]\right)_e\Delta t^n + \sum_{T\in T_h}\left((a^{-1})^n R_h^n(u_h^n), R_h^n(v)\right)_T\Delta t^n \\
&\quad = \int_{J^n}\left((f,\hat{v}) - \sum_{e\in\Gamma_N}(g_N,\hat{v})_e - \sum_{e\in\Gamma_D}(g_D b\cdot\nu,\hat{v})_e\right)\mathrm{d}t \\
&\quad\quad - \sum_{e\in\Gamma_D}\left(g_D^n, (a^n\nabla v - R_h^n(u_h^n))\cdot\nu\right)_e\Delta t^n \qquad \forall v\in W_h.
\end{aligned} \tag{4.10}$$

While it is derived from (3.4) under the assumption that a is piecewise constant, (4.10) (as it is) is a finite element method regardless of a being variable or constant. When V_h and W_h are chosen as in §4.1, (4.10) can be thought of as ELLAM with discontinuous finite elements. In this case, ELLAM also preserves mass locally. For its analysis, refer to [12].

4.3.2. *The continuous case.* We now consider the case where $W_h \subset H^1(\Omega)$. For simplicity, let

$$\Gamma_D = \left(x\in\partial\Omega : b\cdot\nu \geq 0\right), \quad \Gamma_N = \left(x\in\partial\Omega : b\cdot\nu < 0\right). \tag{4.11}$$

Define

$$M_h = W_h \cap \left(v\in H^1(\Omega) : v|_{\Gamma_D} = 0\right).$$

Note that $[v] = 0$ on $\mathcal{E}_h$ for any $v \in M_h$ by continuity and convention. Consequently, (4.10) reduces to: Find $u_h^n \in M_h + g_D^n$, $n = 1, \dots, \mathcal{N}$, such that

$$\begin{aligned}
&(\phi^n u_h^n, v) - (\phi^{n-1}u_h^{n-1}, \hat{v}^{n-1,+}) + (a^n\nabla u_h^n, \nabla v)\,\Delta t^n \\
&\quad = \int_{J^n}\left((f,\hat{v}) - \sum_{e\in\Gamma_N}(g_N,\hat{v})_e\right)\mathrm{d}t \qquad \forall v\in M_h.
\end{aligned} \tag{4.12}$$

This is an extension of ELLAM devised in [9, 37], where piecewise linear polynomials were used. Also, boundary conditions were treated in an *ad hoc* manner in [9, 37], while they are incorporated into the weak formulation in a natural way in (4.12).

ELLAM with continuous finite elements expresses global conservation of mass. For its convergence with piecewise linear polynomials, refer to [42, 43].

4.4. **The modified method of characteristics (MMOC).** MMOC has an inherent difficulty to handle the general boundary boundary in (2.1) [23]. Traditionally, it was developed for an advection-diffusion transport problem with a periodic boundary condition [18, 23, 26]. To derive it from (3.4), we shall follow this tradition. Define

$$M_h = W_h \cap H^1(\Omega). \tag{4.13}$$

With a periodic boundary condition and backward Euler integration for the first term in the right-hand side of (4.12), this equation becomes: Find $u_h^n \in M_h$, $n = 1, \dots, \mathcal{N}$, such that

$$(\phi^n u_h^n, v) - (\phi^{n-1} u_h^{n-1}, \hat{v}^{n-1,+}) + (a^n \nabla u_h^n, \nabla v)\, \Delta t^n = (f^n, v)\Delta t^n \qquad \forall v \in M_h. \tag{4.14}$$

For each n, let

$$G(x) \equiv G(x, t^n) = x - \varphi(x, t^n)\Delta t^n.$$

We assume that φ has bounded first partial derivatives in space. Then, for Δt^n sufficiently small, $G(\cdot)$ is a differentiable homeomorphism of Ω into itself. Moreover, the Jacobian of this transformation is

$$J(G(x)) = \begin{pmatrix} 1 - \partial_{x_1}\varphi_1^n \Delta t^n & -\partial_{x_2}\varphi_1^n \Delta t^n & -\partial_{x_3}\varphi_1^n \Delta t^n \\ -\partial_{x_1}\varphi_2^n \Delta t^n & 1 - \partial_{x_2}\varphi_2^n \Delta t^n & -\partial_{x_3}\varphi_2^n \Delta t^n \\ -\partial_{x_1}\varphi_3^n \Delta t^n & -\partial_{x_2}\varphi_3^n \Delta t^n & 1 - \partial_{x_3}\varphi_3^n \Delta t^n \end{pmatrix},$$

where $\varphi = (\varphi_1, \varphi_2, \varphi_3)$, and its determinant equals

$$\left|J(G(x))\right| = 1 - \nabla \cdot \varphi^n \Delta t^n + O\left((\Delta t^n)^2\right). \tag{4.15}$$

With a change of variable, Δt^n being sufficiently small, and (4.15), the second term in the left-hand side of (4.14) can be expressed by

$$\begin{aligned} &\left(\phi^{n-1} u_h^{n-1}, \hat{v}^{n-1,+}\right) \\ &\quad = \int_\Omega \phi^{n-1}(x) u_h^{n-1}(x) v\left(\hat{x}_n(x, t^{n-1})\right) \mathrm{d}x \\ &\quad = \int_\Omega \phi^{n-1}\left(\check{x}_n(x, t^{n-1})\right) u_h^{n-1}\left(\check{x}_n(x, t^{n-1})\right) v(x) \left|J(G(x))\right| \mathrm{d}x \\ &\quad = \int_\Omega \phi^{n-1}\left(\check{x}_n(x, t^{n-1})\right) u_h^{n-1}\left(\check{x}_n(x, t^{n-1})\right) v(x) \left(1 - \nabla \cdot \varphi^n \Delta t^n + O\left((\Delta t^n)^2\right)\right) \mathrm{d}x. \end{aligned} \tag{4.16}$$

Consequently, (4.14) can be rewritten as follows: Find $u_h^n \in M_h$, $n = 1, \dots, \mathcal{N}$, such that

$$(4.17)\quad \begin{aligned} (\phi^n u_h^n, v) - \left(\check{\phi}^{n-1}\check{u}_h^{n-1}, v\right) + (a^n \nabla u_h^n, \nabla v)\, \Delta t^n \\ = (f^n, v)\Delta t^n + \left(\check{\phi}^{n-1}\check{u}_h^{n-1}, v\right) O\left(\Delta t^n\right) \qquad \forall v \in M_h, \end{aligned}$$

where $\check{u}_h^{n-1} = u_h^{n-1}\left(\check{x}_n(x, t^{n-1})\right)$. Ignoring the last term in the right-hand side of (4.17), we see that

$$(4.18)\quad (\phi^n u_h^n, v) - \left(\check{\phi}^{n-1}\check{u}_h^{n-1}, v\right) + (a^n \nabla u_h^n, \nabla v)\, \Delta t^n = (f^n, v)\Delta t^n \qquad \forall v \in M_h.$$

Equation (4.18) is an extension of MMOC originally introduced in [23], where ϕ was assumed to be independent of t. As mentioned in §4.3.2, (4.12) conserves mass globally. If the coefficients ϕ and b are constants, it follows from (4.15) that MMOC globally conserves mass as well. However, in general, a systematic conservation error of size $O\left(\Delta t^n\right)$ should be expected from MMOC. In the case where $\nabla \cdot \varphi = 0$, a systematic error of size $O\left((\Delta t^n)^2\right)$ can occur.

MMOC is considered for continuous finite elements; its analysis can be found in [18, 23]. MMOC can be also developed for discontinuous elements [12], as for ELLAM in (4.10). The transport diffusion method (TDM) [5, 29, 35] and the operator splitting method (OSM) [24, 44] are virtually the same as MMOC, although they were presented in slightly different forms.

4.5. **The modified method of characteristics with adjusted advection (MMOCAA).** For MMOC to have a global mass conservation, a scheme different from ELLAM was developed in [20], i.e., the modified method of characteristics with adjusted advection (MMOCAA). MMOCAA is defined from MMOC by perturbing the foot of characteristics slightly [20, 21].

With M_h defined in (4.13) and $u_h^0 \in M_h$ given, for $n \geq 1$ set

$$Q_h^{n-1} = \int_\Omega \phi^{n-1}(x) u_h^{n-1}(x)\mathrm{d}x, \quad \check{Q}_h^{n-1} = \int_\Omega \check{\phi}^{n-1}(x)\check{u}_h^{n-1}(x)\mathrm{d}x.$$

As mentioned above, $Q_h^{n-1} \neq \check{Q}_h^{n-1}$ in general. Set

$$x_n^- = \check{x}_n(x, t^{n-1}) - \gamma\varphi(x, t^n)\left(\Delta t^n\right)^2, \quad x_n^+ = \check{x}_n(x, t^{n-1}) + \gamma\varphi(x, t^n)\left(\Delta t^n\right)^2,$$

where γ is a fixed constant, normally chosen to be less than one [20]. Define

$$\tilde{u}_h^{n-1}(x) = \begin{cases} \max\left(u_h^{n-1}\left(x_n^-\right), u_h^{n-1}\left(x_n^+\right)\right) & \text{if } \check{Q}_h^{n-1} < Q_h^{n-1}, \\ \min\left\{u_h^{n-1}\left(x_n^-\right), u_h^{n-1}\left(x_n^+\right)\right) & \text{if } \check{Q}_h^{n-1} > Q_h^{n-1}, \end{cases}$$

and

$$\tilde{Q}_h^{n-1} = \int_\Omega \check{\phi}^{n-1}(x)\tilde{u}_h^{n-1}(x)\mathrm{d}x.$$

If $\check{Q}_h^{n-1} = \tilde{Q}_h^{n-1}$, we must accept that mass cannot be conserved; otherwise, find $\Lambda^{n-1} \in \Re$ such that

$$Q_h^{n-1} = \Lambda^{n-1}\check{Q}_h^{n-1} + (1 - \Lambda^{n-1})\tilde{Q}_h^{n-1}. \tag{4.19}$$

Define

$$\bar{u}_h^{n-1} = \Lambda^{n-1}\check{u}_h^{n-1} + (1 - \Lambda^{n-1})\tilde{u}_h^{n-1}, \tag{4.20}$$

and

$$\bar{Q}_h^{n-1} = \int_\Omega \check{\phi}^{n-1}(x)\bar{u}_h^{n-1}(x)\mathrm{d}x. \tag{4.21}$$

Clearly, $\bar{Q}_h^{n-1} = Q_h^{n-1}$, so the conservation law is preserved. Now, continue in n with $\bar{u}_h^{n-1}$ in place of $\check{u}_h^{n-1}$ in MMOC (4.18); i.e., find $u_h^n \in M_h$, $n = 1, \dots, \mathcal{N}$, such that

$$(\phi^n u_h^n, v) - \left(\check{\phi}^{n-1}\bar{u}_h^{n-1}, v\right) + (a^n \nabla u_h^n, \nabla v)\,\Delta t^n = (f^n, v)\Delta t^n \qquad \forall v \in M_h. \tag{4.22}$$

For the analysis of MMOCAA, see [21]. Again, MMOCAA can be considered for discontinuous finite elements [12].

4.6. **The method of characteristics (MOC).** The classical method of characteristics is a finite difference method that is based on the forward tracking of particles in cells or elements [28, 34, 40]. Here we extend it to the finite element setting. Again, we consider (2.1) with a periodic boundary condition. With the notation in (3.3) and the above definition of M_h in (4.13), the explicit finite element method of characteristics is defined by: Find $u_h^n \in M_h$, $n = 1, \dots, \mathcal{N}$, such that

$$(\hat{\phi}^n \hat{u}_h^n, v) - \left(\phi^{n-1}u_h^{n-1}, v\right) + \left(a^{n-1}\nabla u_h^{n-1}, \nabla v\right)\Delta t^n = (f^n, v)\Delta t^n \qquad \forall v \in M_h. \tag{4.23}$$

The Eulerian-Lagrangian method (ELM) developed in [32, 33] is similar to (4.23). It is known that the forward tracked characteristic method gives rise to the difficulty of distorted grids. Also, this explicit method requires that a Courant-Friedrich-Lewy (CFL) time step constraint be imposed. An implicit forward tracked characteristic method, i.e., the finite elements incorporating characteristics (FEIC), was introduced in [41]. FEIC uses space-time elements with edges oriented along characteristics. Again, it distorts grids, particularly in multi-dimensional cases. Further, it has restrictions on the space-time elements near the boundary of the space domain. In one dimension, for example, at each time step the treatment of boundary conditions in FEIC exploits one triangular space-time element at the inlet boundary, which effectively limits the Courant number to be of order one.

5. Remarks on a Degenerate Diffusion

So far we have assumed that (2.3) holds. We now consider the case where $a = (a_{ij})$ is symmetric and positive semi-definite:

$$0 \le |\xi|^{-2} \sum_{i,j=1}^{d} a_{ij}(x,t)\xi_i\xi_j \le a^* < \infty, \qquad (x,t) \in \Omega \times J,\ \xi \in \Re^d. \tag{5.1}$$

When (5.1) holds, there is a symmetric, positive semi-definite matrix κ such that

$$a = \kappa\kappa. \tag{5.2}$$

Now, (2.2) is of the form

$$\begin{aligned} &\partial_t(\phi u) + \nabla \cdot (bu - \kappa\sigma) = f && \text{in } \Omega \times J,\\ &\sigma = \kappa \nabla u && \text{in } \Omega \times J,\\ &u = g_D, && \text{on } \Gamma_D \times J,\\ &(bu - \kappa\sigma)\cdot \nu = g_N, && \text{on } \Gamma_N \times J,\\ &u(x,0) = u^0(x) && \text{in } \Omega. \end{aligned} \tag{5.3}$$

Corresponding to (5.3), the counterpart of (3.4) is: Find $(\sigma_h, u_h) : \{t^1, \dots, t^{\mathcal{N}}\} \to V_h \times W_h$ such that

$$\begin{aligned} &(\phi^n u_h^n, v) - (\phi^{n-1}u_h^{n-1}, \hat{v}^{n-1,+}) + \sum_{T\in T_h} (\kappa^n \sigma_h^n, \nabla v)_T\, \Delta t^n - \sum_{e\in\mathcal{E}_h} (\{\kappa^n\sigma_h^n \cdot \nu\}, [v])_e\, \Delta t^n \\ &\quad = \int_{J^n} \left((f,\hat{v}) - \sum_{e\in\Gamma_N} (g_N, \hat{v})_e - \sum_{e\in\Gamma_D} (g_D b\cdot\nu, \hat{v})_e \right) \mathrm{d}t, \qquad v \in W_h,\\ &\sum_{T\in T_h} (\sigma_h^n - \kappa^n \nabla u_h^n, \tau)_T + \sum_{e\in\mathcal{E}_h} ([u_h^n], \{\kappa^n\tau\cdot\nu\})_e = \sum_{e\in\Gamma_D} (g_D^n, \kappa^n \tau\cdot\nu)_e\,, \quad \tau \in V_h. \end{aligned} \tag{5.4}$$

All the characteristic methods considered in the previous section except CMM can be recovered from (5.4) in the same fashion. CMM inherently requires that a be positive definite. To relax this requirement, we can employ the expanded concept in CMM [2, 10]; we do not pursue this.

6. Concluding Remarks

Relationships among various characteristic methods are examined in this paper. We begin with a unified scheme, from which we derive ELMDM, CMM, ELLAM, MMOC (TDM, OSM), MMOCAA, and MOC (ELM, FEIC). While ELMDM is in mixed form, it utilizes any finite element spaces, which do not need to satisfy the *inf-sup* condition. It is also totally local and directly applies to a degenerate diffusion problem. It can be implemented in nonmixed form without introducing new variables. CMM requires a nondegenerate diffusion coefficient. Moreover, it uses the property that the normal components of elements in the vector space are continuous across interior boundaries. The former requirement can be relaxed via the expanded concept, while the latter can be removed by introducing Lagrange multipliers over boundaries [3]. Both ELMDM and CMM conserve mass locally. ELLAM with discontinuous finite elements conserves mass locally, while it with continuous elements conserves mass globally. MMOC has certain difficulties, especially with regard to mass conservation. MMOCAA (with continuous finite elements) evolves from MMOC to conserve mass globally, but it still has the inherent difficulty in the treatment of boundary conditions. The classical MOC gives rise to the usual difficulty of distorted Lagrangian grids in over one dimension, which backtracking methods avoid.

References

[1] T. Arbogast and M. F. Wheeler, A characteristics-mixed finite element for advection-dominated transport problems, *SIAM J. Numer. Anal.* **32** (1995), 404–424.

[2] T. Arbogast, M. F. Wheeler, and I. Yotov, Mixed finite elements for elliptic problems with tensor coefficients as finite differences, *SIAM J. Numer. Anal.* **34** (1997), 828–852.

[3] D. Arnold and F. Brezzi, Mixed and nonconforming finite element methods: implementation, postprocessing and error estimates, *RAIRO Modèl. Math. Anal. Numér.* **19** (1985), 7–32.

[4] F. Bassi and S. Rebay, A high-order accurate discontinuous finite element method for the numerical solution of the compressible Navier-Stokes equations, *J. Comput. Phys.* **131** (1997), 267–279.

[5] J. P. Benque and J. Ronat, Quelques difficultes des modeles numeriques en hydraulique, *Computing Methods in Applied Sciences and Engineering V.*, R. Glowinski and J.-L. Lions (eds.), North-Holland, 1982, 471–494.

[6] F. Brezzi, J. Douglas, Jr., R. Durán, and M. Fortin, Mixed finite elements for second order elliptic problems in three variables, *Numer. Math.* **51** (1987), 237–250.

[7] F. Brezzi, J. Douglas, Jr., M. Fortin, and L. D. Marini, Efficient rectangular mixed finite elements in two and three space variables, *RAIRO Modèl. Math. Anal. Numér* **21** (1987), 581–604.

[8] F. Brezzi, J. Douglas, Jr., and L. D. Marini, Two families of mixed finite elements for second order elliptic problems, *Numer. Math.* **47** (1985), 217–235.

[9] M. A. Celia, T. F. Russell, I. Herrera, and R. E. Ewing, An Eulerian Lagrangian localized adjoint method for the advection-diffusion equation, *Advances in Water Resources* **13** (1990), 187–206.

[10] Z. Chen, Expanded mixed finite element methods for linear second order elliptic problems I, *RAIRO Model. Math. Anal. Numer.* **32** (1998), 479–499.

[11] Z. Chen, On the relationship of various discontinuous finite element methods for second-Order elliptic equations, *East-West Numer. Math.* **9** (2001), 99–122.

[12] Z. Chen, Characteristics-discontinuous finite element methods in mixed form for advection-dominated diffusion problems, *Comp. Meth. Appl. Mech. Engrg.* **191** (2002), 2509–2538.

[13] Z. Chen, B. Cockburn, C. Gardner, and J. W. Jerome, Quantum hydrodynamic simulation of hysteresis in the resonant tunneling diode, *J. Comput. Phys.* **117** (1995), 274–280.

[14] Z. Chen, B. Cockburn, J. W. Jerome, and C.-W. Shu, Mixed-RKDG finite element methods for the 2-D hydrodynamic model for semiconductor device simulation, *VLSI Designs* **3** (1995), 145–158.

[15] Z. Chen and J. Douglas, Jr., Prismatic mixed finite elements for second order elliptic problems, *Calcolo* **26** (1989), 135–148.

[16] Z. Chen, R. E. Ewing, and Z.-C. Shi (eds.), Numerical Treatment of Multiphase Flows in Porous Media, Lecture Notes in Physics, Vol. 552., Springer-Verlag, Heidelberg, 2000.

[17] B. Cockburn and C.-W. Shu, The local discontinuous Galerkin method for time-dependent convection-diffusion systems, *SIAM J. Numer. Anal.* **35** (1998), 2440–2463.

[18] C. N. Dawson, T. F. Russell, and M. F. Wheeler, Some improved error estimates for the modified method of characteristics, *SIAM J. Numer. Anal.* **26** (1989), 1487–1512.

[19] J. Douglas, Jr., R. E. Ewing, and M. Wheeler, The approximation of the pressure by a mixed method in the simulation of miscible displacement, *RAIRO Anal. Numér.* **17** (1983), 17–33.

[20] J. Douglas, Jr., F. Furtado, and F. Pereira, On the numerical simulation of water flooding of heterogeneous petroleum reservoirs, *Computational Geosciences* **1** (1997), 155–190.

[21] J. Douglas, Jr., C.-S. Huang, and F. Pereira, The modified method of characteristics with adjusted advection, Technical Report # 298, Center for Applied Mathematics, Purdue University, Indiana, 1997.

[22] J. Douglas, Jr., F. Pereira, and L. M. Yeh, A locally conservative Eulerian-Lagrangian numerical method and its application to nonlinear transport in porous media, Center for Applied Mathematics Technical Report # 324, Purdue University, Indiana, 1998.

[23] J. Douglas, Jr. and T. F. Russell, Numerical methods for convection dominated diffusion problems based on combining the method of characteristics with finite element or finite difference procedures, *SIAM J. Numer. Anal.* **19** (1982), 871–885.

[24] N. S. Espedal and R. E. Ewing, Characteristic Petrov-Galerkin subdomain methods for two phase immiscible flow, *Comput. Methods Appl. Mech. Engrg.* **64** (1987), 113–135.

[25] R. E. Ewing (ed.), The Mathematics of Reservoir Simulation, SIAM, Philadelphia, 1983.

[26] R. E. Ewing, T. F. Russell, and and M. Wheeler, Convergence analysis of an approximation of miscible displacement in porous media by mixed finite elements and a modified method of characteristics, *Comput. Methods Appl. Mech. Engrg.* **47** (1984), 73–92.

[27] R. E. Ewing and H. Wang, A summary of numerical methods for time-dependent advection-dominated partial differential equations, *Journal of Computational and Applied Mathematics*, to appear.

[28] A. O. Garder, D. W. Peaceman, and A. L. Pozzi, Numerical calculations of multidimensional miscible displacement by the method of characteristics, *Soc. Pet. Eng. J.* **4** (1964), 26–36.

[29] J. M. Hervouet, Application of the method of characteristics in their weak formulation to solving two-dimensional advection equations on mesh grids, *Computational Techniques for Fluid Flow*, Vol. 5, Recent Advances in Numerical Methods in Fluids, T. Taylor *et al.* (eds.), Pineridge Press, 1986, 149–185.

[30] K. W. Morton, Numerical Solution of Convection-Diffusion Problems, Chapman & Hall, 1996.

[31] J. Nedelec, Mixed finite elements in $\Re^3$, *Numer. Math.* **35** (1980), 315–341.

[32] S. P. Neuman, An Eulerian-Lagrangian numerical scheme for the dispersion-convection equation using conjugate-time grids, *J. Comp. Phys.* **41** (1981), 270–294.

[33] S. P. Neuman and S. Sorek, Eulerian-Lagrangian methods for advection-dispersion, *Proc. Fourth Int. Conf. Finite Elements in Water Resources*, P. Holz *et al.* (eds.), Springer-Verlag, 1982, 41–68.

[34] G. F. Pinder and H. H. Cooper, A numerical technique for calculating the transient position of the saltwater front, *Water Resources Research* **6** (1970), 875–882.

[35] O. Pironneau, On the transport-diffusion algorithm and its application to the Navier-Stokes equations, *Numer. Math.* **38** (1982), 309–332.

[36] R. Raviart, and J. Thomas, A mixed finite element method for second order elliptic problems, Lecture Notes in Mathematics, vol. 606, Springer, Berlin, 1977, pp. 292–315.

[37] T. F. Russell, Eulerian-Lagrangian localized adjoint methods for advection-dominated problems, *Proceedings of the* 13th Dundee Conference on Numerical Analysis, D. F. Griffiths and G. A. Watson (eds.), Pitmann Research Notes in Mathematics Series, **228** (1990), Longman Scientific & Technical, Harlow, United Kingdom, 206–228.

[38] S. Stenberg, Some new families of finite elements for the Stokes equations, *Numer. Math.* **56** (1990), 827–838.
[39] V. Thomée, Galerkin Finite Element Methods for Parabolic Problems, Lecture Notes in Mathematics 1054, Springer-Verlag, 1984.
[40] M. R. Todd, P. M. O'Dell, and G. J. Hirasaki, Methods for increased accuracy in numerical reservoir simulators, *Soc. Petrol. Eng. J.* **12** (1972), 515–530.
[41] E. Varoḡlu and W. D. L. Finn, Finite elements incorporating characteristics for one-dimensional diffusion-convection equations, *J. Comp. Phys.* **34** (1980), 371–389.
[42] H. Wang, R. E. Ewing, and T. F. Russell, Eulerian-Lagrangian localized adjoint methods for convection-diffusion equations and their convergence analysis, *IMA J. Numer. Anal.* **15** (1995), 405–459.
[43] H. Wang, An optimal-order error estimate for an ELLAM scheme for two-dimensional linear advection-diffusion equations, *SIAM J. Numer. Anal.* **37** (2000), 1338–1368.
[44] M. F. Wheeler and C. N. Dawson, An operator-splitting method for advection-diffusion-reaction problems, *MAFELAP Proceedings*, Vol. VI, J. A. Whiteman (ed.), Academic Press, 1988, 463–482.

Department of Mathematics
Box 750156, Southern Methodist University
Dallas, TX 75275-0156, U.S.A.
email zchen@mail.smu.edu