A FULLY MASS AND VOLUME CONSERVING CHARACTERISTIC METHOD AND ITS APPLICATIONS

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ABSTRACT

The characteristics-mixed method considers the transport not of a single point or fluid particle, but rather the mass in an entire region of fluid. This mass is transported along the characteristic curves of the hyperbolic part of the transport equation, and the scheme thereby produces very little numerical dispersion, conserves mass locally, and can use long time steps. However, since the shape of a characteristic trace-back region must be approximated in numerical implementation, its volume may be incorrect, resulting in inaccurate concentration densities and, further, inaccurate reaction dynamics. We present a simple modification to the characteristics-mixed method that conserves both mass and volume of the transported fluid regions. Our algorithm also handles boundary conditions through a space-time change of variables in the trace-back routines, which allows the boundary to be treated as if it were interior to the domain. Nearly point sources, such as wells, present special difficulties, since characteristic trace-back curves converge in their vicinity. We also present techniques that allow one to conservatively implement wells. The techniques are illustrated in miscible and immiscible numerical examples and examples of convection by periodic or cellular flows.

INTRODUCTION

We consider the problem of tracer transport in a flow field, as might arise in a porous medium or a shallow water or atmospheric system. We concentrate on the problem as it arises in porous media simulation first, and many of the ideas carry over to the problems of convection by periodic or cellular flow.

Let $\Omega \subset \mathbb{R}^2$ be our bounded domain, and consider an incompressible bulk fluid of velocity $\mathbf{u}(\mathbf{x}, t)$ satisfying the incompressibility condition

$$\nabla \cdot \mathbf{u} = q, \quad \Omega \times J, \tag{1}$$

where $q(\mathbf{x}, t)$ is a given external source or sink function, assumed smooth enough for our purposes, and $J = (0, \infty)$ is the time interval. Our interest lies in the transport of some dilute tracer or other solute species of concentration $c(\mathbf{x}, t)$ within the bulk fluid. We assume that it does not change the overall velocity $\mathbf{u}$. The concentration will generally satisfy an advection-diffusion equation of the form

$$(R\phi c)_t + \nabla \cdot (c\mathbf{u} - D\nabla c) = c_I q_+ + c q_- \equiv q_c(c), \quad \Omega \times J, \tag{2}$$

where $R(\mathbf{x})$ is the retardation factor, $\phi(\mathbf{x})$ is the storage factor of the medium called porosity, subscript t is time partial differentiation, $D(\mathbf{x}, t)$ is the diffusion/dispersion coefficient (that may also depend on $\mathbf{u}$), $q_+(\mathbf{x}, t) \geq 0$ is q when $q > 0$ and 0 otherwise, $q_-(\mathbf{x}, t) = q - q_+ \leq 0$, and $c_I(\mathbf{x}, t)$ is the given concentration of injected fluid.

To apply characteristic methods to (2), one generally uses an operator splitting technique to isolate the hyperbolic and parabolic parts of the equation. That is, over a time step, one approximates the hyperbolic part of the operator,

$$(R\phi c)_t + \nabla \cdot (c\mathbf{u}) = q_c(c), \quad \Omega \times J, \tag{3}$$

and the parabolic part,

$$(R\phi c)_t - \nabla \cdot (D\nabla c) = 0, \quad \Omega \times J, \tag{4}$$

in some order.

Various ELLAM [3] schemes have been developed based on the local mass constraint, including the characteristics-mixed method [1], [2]. The basic idea is to trace back along the characteristics each entire grid element E to $\hat{E}$. In this way, all mass can be accounted for locally; that is, all the mass in $\hat{E}$ is numerically transported forward into E. In the absence of sources, sinks, and external boundaries, the volumes of E and $\hat{E}$ agree. However, to trace $\hat{E}$ back in time requires tracing each boundary point back, which can only be done in one space dimension (unless perhaps the velocity is particularly simple). So, in practice, one must approximate $\hat{E}$ by some simpler shape $\tilde{E}$ by, say, tracing back only the vertices of the element. Almost assuredly the volumes of $\tilde{E}$ and $\hat{E}$ will disagree, violating the volume conservation principle.

Although mass is conserved locally, incorrect local volumes lead to incorrect concentrations, which measure mass per volume. That is, the density is incorrectly approximated and can lead to overshoot or undershoot and seriously degrade the quality of the solution over time, especially when reaction dynamics, based on densities, are also considered.

We present in this paper a simple and relatively computationally efficient method for adjusting the trace-back regions $\hat{E}$ to $\tilde{E}$. The difficulty, of course, is that the set of $\tilde{E}$ must tessellate the region (i.e., they must have no overlaps or gaps).

We also extend the ideas to problems of convection by cellular or periodic flow. It turns out our ideas work well in those problems. Finally, we try to extend this idea to immiscible displacement problems. Some promising preliminary results are obtained.

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