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SOLUTION OF ADVECTION DIFFUSION EQUATIONS IN TWO SPACE DIMENSIONS BY A RATIONAL EULERIAN LAGRANGIAN LOCALIZED ADJOINT METHOD OVER HEXAGONAL GRIDS

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Abstract. We present a characteristic method for the solution of the transient advection diffusion equations in two space-dimensions. This method uses Wachspress-type rational basis functions over hexagonal grids within the framework of the Eulerian Lagrangian localized adjoint methods (ELLAM). It therefore maintains the advantages of previous ELLAM schemes and generates accurate numerical solutions even if large time steps are used in the simulation. Numerical experiments are presented to illustrate the performance of this method and to investigate its convergence numerically.

Key Words. advection-diffusion equations, characteristic methods, Eulerian-Lagrangian methods, rational basis functions

1. Introduction

Advection-diffusion equations are a class of partial differential equations that is mathematically important because they arise in many problems in Science and Engineering. These equations are also important because they present serious computational difficulties, especially when advection dominates the physical process. Standard finite difference and finite element methods, which work well for many other types of equations, generate solutions for this class of equations that exhibit non-physical spurious oscillations and/or artificial numerical diffusion that smears out sharp fronts of the solution where important chemistry and physics take place.

Many specialized methods have been developed which aim at resolving the difficulties mentioned when applied to both linear and nonlinear problems. One large class of methods, usually referred to as *characteristic methods*, makes use of the hyperbolic nature of the governing equations. These methods incorporate Eulerian grids with Lagrangian tracking along the characteristic curves to treat the advective part of the equation [9, 13]. This treatment allows for larger time steps to be used in the simulation. Moreover, it significantly reduces the time truncation errors when compared to methods which rely only on Eulerian grids. However, these methods have difficulty in conserving mass and in treating general boundary conditions.

The Eulerian Lagrangian localized adjoint method was developed by Celia, Russell, Herrera, and Ewing as an improved extension of characteristic methods which maintains their advantages and enhances their performance by conserving mass and treating general boundary conditions naturally in its formulation [6]. This first ELLAM formulation was a finite element formulation for one-dimensional constant

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coefficient advection diffusion equations. The strong potential that this formulation has shown, led to a rapid expansion in all aspects of this class of methods, including the development of various finite element and finite volume formulations for one and higher dimensional problems [1, 3, 10, 14, 26, 27]. Other formulations were also developed including Eulerian-Lagrangian collocation methods [39, 40, 41], and Eulerian Lagrangian discontinuous Galerkin methods [34, 35, 36, 37]. Moreover, convergence properties of the different ELLAM formulations were studied and various optimal order convergence and uniform estimates were established [19, 20, 21, 22, 23, 24, 25, 30, 31, 32, 33].

ELLAM formulations developed for two-dimensional problems have mostly followed the classical polynomial-based finite element approach; which is to discretize the spatial domain into an assembly of triangular or quadrilateral elements and use linear or higher polynomial interpolants as the test functions on each element and the basis for the solution space [12]. However, due to the reliance on polynomial basis, other types of higher-order elements have not been extensively considered even though such elements with large number of sides have been successfully used in a number of applications in Engineering and other fields and have resulted in some cases in better approximations than those obtained by triangular or quadrilateral polynomial based standard finite element codes [7].

In this article we present a rational characteristic method for the solution of variable coefficient advection diffusion equations within the framework of the Eulerian-lagrangian localized adjoint methods. The algorithm is based on a discretization of the spatial domain into a partition of regular hexagonal elements and uses Wachspress-type rational test functions in the space-time domain defined by the characteristics [18]. The derived method generates regularly structured systems which can easily be solved numerically. Numerical experiments are presented to illustrate the performance of the method developed.

2. Development of the Characteristic Schemes

We consider the following two-dimensional unsteady-state advection diffusion equation

$$(\phi(\mathbf{x},t)\,u(\mathbf{x},t))_t + \nabla\cdot\Big(\mathbf{v}(\mathbf{x},t)u(\mathbf{x},t) - \mathbf{D}(\mathbf{x},t)\nabla u(\mathbf{x},t)\Big) = f(\mathbf{x},t) \tag{1}$$

where $\mathbf{x} = (x, y)$, $u_t = \partial u/\partial t$, $\nabla = \langle \partial/\partial x, \partial/\partial y\rangle$, $\phi(\mathbf{x}, t)$ is the retardation coefficient, $\mathbf{v}(\mathbf{x}, t)$ is the velocity field, $\mathbf{D}(\mathbf{x}, t)$ is the diffusion/dispersion tensor, and $f(\mathbf{x}, t)$ is a source/sink term. While the ELLAM method can be developed for any bounded spatial domain which admits a quasi-uniform partition, for simplicity of presentation we consider a spatial domain of the form $\Omega = [a, b] \times [c, d]$. To close the system, we assume that an appropriate initial condition and any proper combination of Dirichlet, Neumann, or flux boundary conditions are specified at the inflow or outflow parts of the boundary.

2.1. Partition and Characteristic Tracking. Eulerian-Lagrangian localized adjoint methods (ELLAM) have previously been developed using triangular and quadrilateral discretizations of the domain [15, 28]. However, in this section we consider a hexagonal discretization, which for simplicity of presentation, we take to be a regular grid. The method uses a time-stepping algorithm, and so, we use the temporal partition

$$t^n = n\,\Delta t, \quad n = 0,\ ...,\ N \quad \text{with } \Delta t = T/N \tag{2}$$

for positive integer N and only focus on the current time interval $(t^n, t^{n+1}]$.