Available online at www.sciencedirect.com
SCIENCE DIRECT®
Advances in Water Resources 28 (2005) 1292–1309
Advances in Water Resources
www.elsevier.com/locate/advwatres

On a monotonicity preserving Eulerian–Lagrangian localized adjoint method for advection–diffusion equations

Thimo Neubauer *,[1], Peter Bastian

Interdisziplinäres Zentrum für Wissenschaftliches Rechnen, Universität Heidelberg, Im Neuenheimer Feld 368, 69120 Heidelberg, Germany

Received 22 October 2004; received in revised form 11 March 2005; accepted 14 March 2005
Available online 24 June 2005

Abstract

Eulerian–Lagrangian localized adjoint methods (ELLAMs) provide a general approach to the solution of advection-dominated advection–diffusion equations allowing large time steps while maintaining good accuracy. Moreover, the methods can treat systematically any type of boundary condition and are mass conservative. However, all ELLAMs developed so far suffer from non-physical oscillations and are usually implemented on structured grids. In this paper, we propose a finite volume ELLAM which incorporates a novel correction step rendering the method monotone while maintaining conservation of mass. The method has been implemented on fully unstructured meshes in two space dimensions. Numerical results demonstrate the applicability of the method for problems with highly non-uniform flow fields arising from heterogeneous porous media.

Keywords: Advection–diffusion equation; ELLAM; Characteristic methods; Porous media; Contaminant transport

1. Introduction

Despite many years of research, the efficient and accurate solution of the advection–dominated advection–diffusion equation is still a formidable task. Among the more recent developments in the field is the Eulerian–Lagrangian localized adjoint method (ELLAM) introduced in [1]. ELLAMs can be cast in the form of (discontinuous in time) space–time Petrov–Galerkin finite element methods where the test functions locally solve the homogeneous adjoint equation of the advective part. For problems without reaction or adsorption term that are treated in this paper, the test functions are constant along the characteristics. ELLAM treats the advection part in a Lagrangian and the diffusion part in an Eulerian way thus combining the best of both worlds with the aim of allowing large time-steps to be taken without sacrificing accuracy. In contrast to one of its precursors, the modified method of characteristics (MMOC) introduced in [2], it allows a consistent treatment of all types of boundary conditions through a weak formulation. The current state-of-the-art of the method is collected in [3].

ELLAM schemes were implemented in different space dimensions with varying test and trial functions [3] but still share a significant drawback: they are not guaranteed to produce monotone solutions. For many practical purposes, especially when a reaction term is coupled with the transport, this property is mandatory. In the following we will shortly discuss the main reasons why these non-physical oscillations occur, the in-depth discussion is contained in Section 4. We will focus on zero- and first-order test and trial functions, however the reasoning can be applied to higher-order approaches

* Corresponding author.
E-mail addresses: thimo.neubauer@iwr.uni-heidelberg.de (T. Neubauer), peter.bastian@iwr.uni-heidelberg.de (P. Bastian).
[1] Supported by the BMBF-project "Entwicklung eines Simulationsmodells zur Prognose des Selbstreinigungsvermögens eines belasteten Grundwasserleiters" 03-BAM1HD.

0309-1708/$ - see front matter © 2005 Elsevier Ltd. All rights reserved.
doi:10.1016/j.advwatres.2005.04.010

as well. As is common in literature, we will use the term finite volume ELLAM (FVELLAM) for schemes with piecewise constant test functions.

One major reason for the oscillations is that for non-orthogonal trial functions with overlapping support, e.g. the piecewise (bi-)linears, the mass matrix is non-diagonal. As is well known from standard finite elements this results in oscillations for non-smooth right-hand sides. The standard approach for this problem is to use lumping which fixes the oscillations but increases numerical diffusion. Binning and Celia compared normal ELLAM and FVELLAM with and without lumping for some 3D examples in [4]. Russell and Binning [5] proposed a selective lumping scheme which adds the minimum amount of numerical diffusion to the mass matrix so that for a given right-hand side no oscillations will occur. This approach was shown to work for a 1D ELLAM, however generalization for higher dimensions or unstructured grids will require some effort due to current assumptions on the matrix shape and properties.

The second reason for oscillations is the error made when tracking the mass along the characteristics to integrate on the old time level. Backward tracking, which uses a quadrature defined on the new time level, does not suffer from this integration error but cannot guarantee global mass conservation. With forward tracking the quadrature points are defined on the old time level but the quadrature weights will not necessarily sum up to the correct volume for each grid element on the new time level. For piecewise linear test functions and any other test functions with overlapping support this effect is reduced because the tracked mass is spread over several neighboring nodes. This however leads, especially for a lumped mass matrix, to numerical diffusion. FVELLAMs on the other hand are less diffusive but very susceptible to this integration error due to the test function discontinuities. A simple fix for this problem is to increase the number of quadrature points but this has a severe impact on the computational efficiency. A different approach is to smooth out the discontinuous test functions for the right-hand side integral: the approximate test functions proposed by Healy and Russell [6] change shape between linear test functions for coarse quadratures and constant test functions with a small linear overlap to the neighboring function for finer quadratures. Together with strategic space integration points (SSIP) which are backtracked from the new time level to be included in the quadrature on the old time level the method is reported to minimize oscillations but does not provably remove them.

A different approach to reduce the integration error after characteristic tracking is to change the grid on the old time level. For each grid element on the new time level an approximation of the backtracked image with the same volume but not necessarily the correct shape can be constructed. This ensures a local mass conservation in the transport step. A work by Chilakapati [7] shows a way to compute this modified grid during the flow computation.

In this paper, we will propose a FVELLAM scheme using consistent lumping on the left- and right-hand side of the equation so that non-smooth solutions can be modeled appropriately. As this method is clearly sensitive to the aforementioned integration error we will further present a novel postprocessing scheme which, for a given quadrature and arbitrary concentration distribution, constructs a monotone solution. A further advantage of the postprocessing scheme is that it is purely algebraic and therefore independent of the underlying mesh.

ELLAMs are very attractive for the solution of contaminant transport problems in highly heterogeneous porous media with their resulting highly non-uniform velocity fields. Traditional Eulerian methods, even high resolution schemes [8], produce a large amount of numerical diffusion in this case. In one of our examples we show that the proposed ELLAM is clearly superior even to state-of-the-art higher-order discontinuous Galerkin methods [9,10] for this type of problem.

This paper is organized as follows. First, we describe the continuous problem in Section 2. Section 3 presents a general framework for ELLAMs and applies this framework to yield two formulations of ELLAM, one based on the vertex-centered finite volume scheme, the other based on the higher-order discontinuous Galerkin method. Then Section 4 concentrates on the numerical evaluation of critical integrals in the scheme and Section 5 introduces the new postprocessing scheme to ensure monotonicity of the solution. Finally the numerical results with the proposed techniques are shown in Section 6.

2. Continuous model problem

Let $\Xi = \Omega \times T$ be a space–time domain with $\Omega \subset \mathbb{R}^2$ the spatial domain and $T = (0, T_{\text{end}})$ a time interval. We consider the advection–diffusion equation

$$\begin{aligned} &\frac{\partial (R(\mathbf{x},t)C)}{\partial t} + \nabla \cdot \mathbf{j}(\mathbf{x},t) = r, \\ &\mathbf{j}(\mathbf{x},t) = \mathbf{v}(\mathbf{x},t)C - \mathscr{D}(\mathbf{x},t)\nabla C \quad \text{in } \Xi \end{aligned} \tag{1}$$

for the unknown concentration $C : \Xi \to \mathbb{R}$ where $\mathscr{D}(\mathbf{x},t)$ is the hydrodynamic dispersion tensor, $\mathbf{v}(\mathbf{x},t)$ is a given divergence free velocity field, $R(\mathbf{x},t)$ is the retardation factor and $r(\mathbf{x},t)$ is the source term. We comment on the use of numerically computed velocity fields below. The space–time boundary can be partitioned into inflow and outflow boundary

$$\begin{aligned} &\Pi^{(\mathrm{I})} = \{(\mathbf{x},t) \in \partial\Omega \times T : \mathbf{v}(\mathbf{x},t) \cdot \mathbf{n} \leqslant 0\}, \\ &\Pi^{(\mathrm{O})} = (\partial\Omega \times T) \backslash \Pi^{(\mathrm{I})}. \end{aligned} \tag{2}$$

Eq. (1) is augmented with the following boundary conditions