Generalized Eulerian - Lagrangian Method of Cells for Contaminant Migration and Comparison with other methods

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ABSTRACT

Eulerian - Lagrangian Localized Adjoint Method (ELLAM), based on Herrera's algebraic theory of boundary value problems, offer the advantages of Eulerian - Lagrangian method (ELM) in the numerical treatment of Advection-Dominated Flows, while also conserving mass and handling general boundary conditions. In this paper a generalized ELLAM method of cells is presented, in which the test functions are piecewise constant, and are advected with the transport velocity. It goes along lines presented previously by Herrera & Herrera and subsumes many specific methods based on combined Lagrangian and Eulerian approaches so-called characteristics methods (CM). Optimal weighting and interpolating functions are used simultaneously. Comparison with other methods are made.

1.- Introduction

Advection-diffusion transport equations are important in many branches of engineering and applied science. These equations are characterized by a nondissipative (hyperbolic) advective transport component and a dissipative (parabolic) diffusive component. When diffusion is the dominant process, virtually all numerical solution procedures perform well. However, when advection is the dominant transport process, most numerical procedures exhibit some combination of excessive nonphysical oscillations and excessive numerical diffusion. In terms of results of numerical solutions, numerical dispersion gives the appearance of an artificial, grid-dependent increase in physical dispersion. Numerical oscillation, common in second-order schemes, is manifested by overshoot and undershoot about the true solution. Both of those problems can be resolved by the use of refined space and time grids; however, the added computational effort needed to reach the required degree of refinement commonly makes a simulation intractable for most computers.

Recent developments have generally been along one of two approaches: Eulerian or Characteristic. For advection-dominated problems, Eulerian methods generally require small time steps for reasons of accuracy, and tend to be ineffective because of the strong influence of the time derivative. The second approach (Characteristic methods), solve separately for the advective and dispersive components of the ADE. Advection is solved on a Lagrangian-type grid by tracking along characteristics on the velocity field. Dispersion is solved on an Eulerian spatial grid. Many approaches to characteristic methods have appeared in the literature under a variety of names, including Eulerian-Lagrangian methods (Neuman[11]), method of characteristics (Konikow[10]), modified method of characteristics (Douglas[5]; Russell[3]), an operator-splitting methods (Espedal[4]). These methods have the significant advantage that Courant number restrictions of purely Eulerian methods are alleviated because of the Lagrangian nature of the advection step. Problems with characteristic methods, in general, arise in three areas: inability to rigorously treat boundary fluxes when characteristics intersect inflow or outflow boundaries, inability to ensure conservation of mass, and the introduction of numerical dispersion, for some methods, due to low-order interpolation or integration (Healy[5]).

This paper presents details of development and implementation of a generalized Eulerian-Lagrangian method of cells (Herrera[9]). This method, is a general characteristic-based numerical solution procedure that applies to a variety of transport equations. In this approach, finite differences and boundary elements are incorpored in a new "algebraic theory". Details of the ELLAM approach have been presented by Celia[1,2], Herrera[8], Healy[5], and Wang[12]. The present paper begins by reviewing the LAM procedure, including discussion of the general approach as well as specific formulations that have been developed to date. This is followed by the specific space-time LAM formulation that naturally leads to a generalized Eulerian-Lagrangian method of the cells. Finally, a discussion of several additional topics is presented.

2.- Preliminary Notions

Considering a region Ω and the linear spaces D_1 and D_2 of trial and test functions defined in Ω (space-time region). Assume further that functions belonging to D_1 and D_2 may have jump discontinuities across some internal boundaries whose union will be denoted by Σ. According to Herrera's theory, the definition of a formal disjoint requires that a differential operator $\mathcal{L}$ and its formal adjoint $\mathcal{L}^*$ satisfy the condition that $w\,\mathcal{L}\,u - u\,\mathcal{L}^*\,w$ be a divergence, i.e.,

$$w\,\mathcal{L}\,u - u\,\mathcal{L}^*\,w = \nabla \cdot \{\underline{\mathcal{Q}}(u, w)\}, \tag{1}$$

for suitable vector-valued bilinear function $\underline{\mathcal{Q}}(u, w)$. Integration of Eq. (1) over Ω and application of the generalized divergence theorem (Herrera[6]) yields

$$\int_\Omega \{w\,\mathcal{L}\,u - u\,\mathcal{L}^*\,w\}dx = \int_{\partial\Omega} \mathcal{R}_\partial(w, u)\,dx + \int_\Sigma \mathcal{R}_\Sigma(w, u)\,dx, \tag{2}$$

$$\text{with} \quad \mathcal{R}_\partial(u, w) = \underline{\mathcal{Q}}(u, w)\cdot\underline{n} \quad \text{and} \quad \mathcal{R}_\Sigma(u, w) = -\left[\underline{\mathcal{Q}}(u, w)\right]\cdot\underline{n}, \tag{3}$$

$\partial\,\Omega$ and Σ are boundary and jump conditions specified on the boundary of Ω. A decomposition of the bilinear function $\mathcal{R}_\partial$ is

$$\mathcal{R}_\partial(u, w) = \underline{\mathcal{Q}}(u, w)\cdot\underline{n} = \mathcal{B}(u, w) - \mathcal{C}^*(u, w), \tag{4}$$

where $\mathcal{B}(u, w)$ and $\mathcal{C}(w, u) = \mathcal{C}^*(u, w)$ are two bilinear functions. When considering initial-boundary value problems, the definitions of these bilinear forms depend on the type of boundary and initial conditions to be prescribed. A basic property required of $\mathcal{B}(u, w)$ is that for any u that satisfies the prescribed boundary and initial conditions, $\mathcal{B}(u, w)$ is a well-defined linear function of w, independent of the particular choice of u.

In a similar fashion, convenient formulations of boundary value problems with prescribed jumps requires constructing Green's formulas in discontinuous fields. This can be done by introducing a general decomposition of the bilinear function $\mathcal{R}_\Sigma(u, w)$ whose definition is pointwise. The general theory includes the treatment of differential operators with discontinuous coefficients (Herrera[6]). If continuous coefficients are considered, such decomposition is easy to obtain, and it stems from the algebraic identity:

$$\left[\underline{\mathcal{Q}}(u,w)\right] = \underline{\mathcal{Q}}\left([u], \dot{w}\right) + \underline{\mathcal{Q}}\left(\dot{u}, [w]\right), \tag{5}$$

where

$$[u] = u_+ - u_-, \qquad \dot{u} = (u_+ + u_-)/2. \tag{6}$$

The decomposition is obtained by combining the second of Eqs. (3) with (5):

$$\mathcal{R}_\Sigma(u, w) = \mathcal{J}(u, w) - \mathcal{K}^*(u, w), \tag{7}$$

with $$\mathcal{J}(u, w) = - \underline{\mathcal{D}}([u], \dot{w}) \cdot \underline{n}, \tag{8}$$

$$\mathcal{K}^*(u, w) = \mathcal{K}(w, u) = \underline{\mathcal{D}}(\dot{u}, [w]) \quad \underline{n}. \tag{9}$$

On the other hand, Eq. (2) can be written as

$$\langle P u, w\rangle - \langle Q^* u, w\rangle = \langle B u, w\rangle - \langle C^* u, w\rangle + \langle J u, w\rangle - \langle K^* u, w\rangle.$$

This is an identity between bilinear forms and can be written more briefly as

$$P - B - J = Q^* - C^* - K^*. \qquad (\ )$$

In order to associate a variational formulation with this problem, define the linear functionals $f, g, j \in D2^*$ by means of

$$\langle f, w\rangle = \int_\Omega w f_\Omega \, dx, \ \langle g, w\rangle = \int_{\partial\Omega} g_\Omega (w) \, dx, \ \langle j, w\rangle = \int_\Sigma j_\Sigma (w) \, dx. \tag{12}$$

Then a variational formulation of the initial-boundary value problem with prescribed jumps is

$$P u = f, \qquad B u = g, \qquad J u = j.$$

The bilinear functional J just constructed, as well as B, are boundary operators for P, which are fully disjoint. When this is the case, the system of equations (12) is equivalent to the single variational equation

$$\langle (P - B - J) u, \mathrm{w}\rangle = \langle f - g - j, w\rangle \qquad \forall w \in D_2. \tag{14}$$

This is said to be "the variational formulation in terms of the data of the problem," because Pu, Bu, and Ju are prescribed. Making use of formula (11), the variational formulation (14) is transformed into

$$\langle (Q^* - C^* - K^*) u, w\rangle = \langle f - g - j, w\rangle \qquad \forall w \in D_2 \tag{15}$$

This is said to be "the variational formulation in terms of the sought information," because Q^*u, C^*u, *and* K^*u are not prescribed. The variational formulation (14) and (15) are equivalent by virtue of the identity (11). The linear functionals Q^*u, C^*u, *and* K^*u supply information about the sought solution at points in the interior of the region Ω, the complementary boundary values at $\partial\,\Omega$, and the generalized averages of the solution at Σ, respectively.

Since the exact solution satisfies (15) it must be that

$$\langle (Q^* - C^* - K^*) \hat{u}, w^\alpha\rangle = \langle (Q^* - C^* - K^*) u, w^\alpha\rangle \quad \alpha = \qquad , N, \tag{16}$$

Eq. (16) can be used to analyze the information about the exact solution that is contained in an approximate one. In localized adjoint methods, these observations have been used as a framework for selecting more convenient test functions.

3.- Fundamentals of ELLAM Cells

To illustrate the underlying concept of ELLAM, consider the following transport equation in conservative form for subsurface contaminants, subject to boundary conditions at $x = 0$ and ℓ, and to initial conditions

$$\mathcal{L}u \equiv \frac{\partial u}{\partial t} - \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x} - Vu\right) + Ru = f_\Omega(x,t) \qquad \text{in } \Omega,$$
$$u\left(x,t^n\right) = u^n(x). \tag{18}$$

The adjoint operator is

$$\mathcal{L}^* \equiv -\frac{\partial w}{\partial t} - \frac{\partial}{\partial x}\left(D\frac{\partial w}{\partial x}\right) - V\frac{\partial w}{\partial x} + Rw$$

For the case when the coefficients of Eq. (17) are constant, the source term vanishes ($R = 0$). The partition is defined uniform, and the test functions used in ELLAM cells are piecewise constant in space (Herrera[8]). This typical C^{-1} test function is shown in figure 1. Notice that the piecewise linear test functions are defined in a "corner-centered" grid while the piecewise constant functions are defined on a block-centered grid.

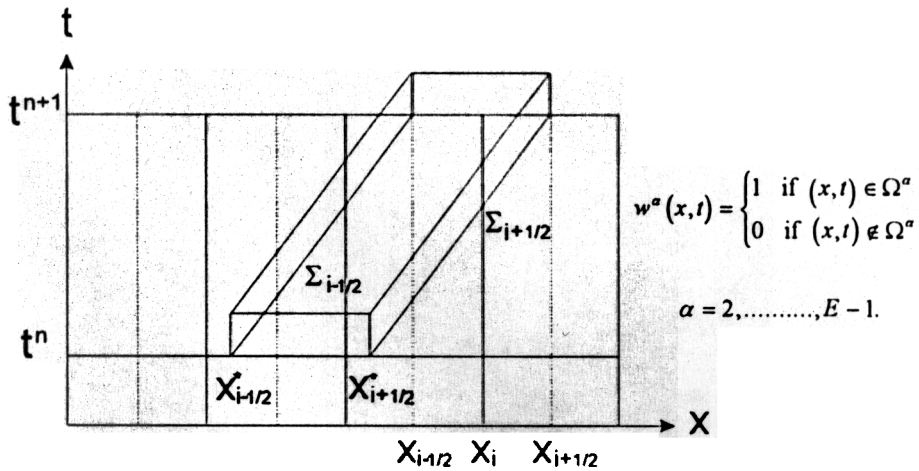

Figure 1. Partition of the region Ω and piecewise constant test function.

The bilinear function $\mathcal{K}(w,u)$ is associated with the values of u and its first-order derivative on Σ, and can be written as

$$\mathcal{K}(w,u) = \mathcal{K}^0(w,u) + \mathcal{K}^1(w,u).$$

A partition $\{x_1, x_{3/2}, x_{5/2},\ldots,x_{E-1/2},x_E\}$ into E subintervals of the interval $(0, \ell)$ is introduced, for which $x_1 = 0$ and $x_E = \ell$. The points

$$x_i = (x_{i-1/2} + x_{i+1/2})/2, \qquad i = 2, \quad , E -$$

will be referred to as the "cell centers." Notice that x_1 and x_E are boundary points of $(0,\ell)$ and they are not midpoints of any of the subintervals. Furthermore, using the fact that $V_\Sigma \equiv V$, one obtains $\mathcal{K}^0(w,u) = 0$, so that

$$\mathcal{K}(w,u) \equiv \mathcal{K}^1(w,u) = \pm\left(1+V^2\right)^{-1/2} D\frac{\partial u}{\partial x} \quad \text{on } \Sigma_{\alpha \pm 1/2}.$$

For any $\alpha = 2,..., E\text{-}1$, Ω does not intersect the lateral boundary $x = \ell$, because it has been assumed that $V > 0$ and $V\Sigma = V$. If in addition, Ω^α does not intersect the boundary $x = 0$, then $\mathcal{C}(w,u)$ vanishes everywhere, except at the interval of $\partial_{n+1}\,\Omega$ (i.e., $t = t_{n+1}$), where $x_{\alpha-1} < x < x_{\alpha+1}$. There $\mathcal{C}(w,u) = -u$. Taking all this into account, the variational principle (Eq. 2) becomes

$$\int_{x_{\alpha-1/2}}^{x_{\alpha+1/2}} u^{n+1} dx + \int_{t^n}^{t^{n+1}} \left(D\frac{\partial u}{\partial x}\right)_{\Sigma_{\alpha+1/2}} dt - \int_{t^n}^{t^{n+1}} \left(D\frac{\partial u}{\partial x}\right)_{\Sigma_\alpha} dt = \int_{x_{\alpha-1/2}^*}^{x_{\alpha+1/2}^*} u^n dx.$$

The integrals from t^n to t^{n+1} will be approximated in a fully implicit manner, by a one-step backward Euler approximation. The firsts integral in space is approximated by a central difference approximation, and the second integral in space is approximated integrating the Taylor expansion of u^n around the midpoint of the interval $[x_{\alpha-1}^*, x_{\alpha+1}^*]$. However, since such point is not a cell center, u^n is not known there and an interpolation must be used to evaluate it. Using three-point formulas, u^n and its second-order derivative can be evaluated to orders there and one, respectively.

The numerical approximations presented thus for apply only when the subregion $\Omega^\alpha \subset \Omega$ does not intersect the lateral boundaries $\partial_0\Omega \cup \partial_\ell\,\Omega$, of the region Ω. When this is not the case, boundary conditions must be included. For Dirichlet conditions, we use E-2 test functions, namely, those associated with subregions $\Omega^2,..., \Omega^{E-1}$. In particular, no test function is applied on the first subregion (Ω^1) or on the last one (Ω^E). For inflow boundary, conditions are incorporated in the numerical equations in two manners: directly, through the boundary terms and indirectly, imposing the condition that, in the numerical approximations, some of the variables take the prescribed boundary values. For outflow boundary, observe that the last test function to be applied is w^{E-1}. The support of this test function is Ω^{E-1}, which does not intersect the lateral boundary $x = \ell$. Thus, none of the boundary terms involving the outflow boundary occur in the numerical equations and the prescribed boundary values are incorporated in the numerical equations in an indirect manner exclusively, imposing the condition u_E^{n+1} in approximations.

4.- Discussion and conclusions

In this paper, localized adjoint method has been applied in space-time to problems of advective-diffusive transport. The approach is based on space-time discretizations in which the test functions are piecewise constant, and are advected with the transport velocity of the problem. The resulting method is referred to as the ELLAM cells, and whose basic ingredients consist of (a) identifying the information about the sought solution contained in the approximate one; and (b) using this insight to choose the interpolation procedure. This approach, in addition to providing a unification of Characteristic Methods (CM), supplies a systematic framework for incorporation of boundary conditions in CM approximations. Any type of boundary conditions can be accommodated in a mass conservative manner.

Two test problems were treated to demonstrate the performance of the new method: the propagation of an initial step discontinuity and of a Gauss hill. The results and the efficiency of the procedure were compared with other methods, testing the effect of changing several parameters such as θ (in time), element Peclet number, as well as Courant number. The drawn conclusion was that solutions obtained with this method are as least as good as those from the best available interior methods (Celia[1], Herrera[6,7]).

However, we need a more extensive study of both the theory and implementation of ELLAM techniques for variable coefficients particularly in multidimensional applications. Implementation of boundary conditions for variable-coefficients problems in multiple dimensions is also an important problem. Even in the one-dimensional case and in spite of the important progress that has already been made (Celia[1], Herrera[7]), several points remain open in this respect. In addition, the treatment of nonlinear problems deserves further study. Since the unknown variables appear in multilinear coefficients of the problem that are usually evaluated in the interior at mesh blocks via numerical quadrature, greater attention must be placed on the full approximation theoretic properties of the trial functions in these applications. The potential at local refinement in both space and time holds enormous potential for ELLAM an is the object of ongoing research.

Finally we want to emphasize that LAM forms a general and powerful framework for investigating and comparing a wide variety of numerical methods. The framework motivates different properties of the unknowns or even different unknowns, such as fluxes. The general theory is expanding to provide more insight. In addition, the ELLAM methods appear to have enormous flexibility and potential for treating general advection-diffusion-reaction problems.

Key words: Contaminant Transport, Advection-Dominated Flows, ELLAM-cells

Acknowledgments

This research was supported in part by the Autonomous University of the State of Mexico, and by the Institute of Geophysics of the National University of Mexico.

REFERENCES

Celia, M.A., T.F. Russell, I. Herrera, and R.E. Ewing, 1990. "An Eulerian-Lagrangian Localized adjoint method for the Advection-Diffusion Equation," *Adv. Water Res.* 13, 187.

2 Celia, M.A. 1994. Eulerian-Lagrangian Localized Adjoint Methods for Contaminant simulations. A. Peters et al. (eds.). *Computational Methods in Water Resources X*, Heidelberg. 207-216.

3 Douglas, J., Jr., AND T.F. Russell. 1982. 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, 871-885.

4 Espedal, M.S., and R.E. Ewing. 1987. Characteristic Petrov-Galerkin subdomain methods for two-phase immiscible flow. *Comput. Methods Appl. Mech. Eng.*, 64, 113-136.

5 Healy, R.W., and T.F. Russell. 1993. A finite-volume Eulerian-Lagrangian Localized Adjoint Method for solution of the Advection-Dispersion equation. *Water Resour. Res.*, Vol 29, No 7, pp. 2399-2413.

6 Herrera, I, L. Chargoy, and G. Aldulcin. 1985. "Unified formulation of numerical methods. Part III. Finite differences and ordinary differential equations," *Numer. Methods Partial Different. Equ.* 1. 241.

7 Herrera, I. 1987. The algebraic theory approach for ordinary differential equations: Highly accurate finite differences. *Numer. Methods Partial Different. Equ.* 3, 199-218.

8 Herrera, I., R.E. Ewing, M.A. Celia, and T.F. Russell. 1993. Eulerian-Lagrangian Localized Adjoint Method: The theorical Framework. *Numer. Methods Partial Different. Equ.* 9, 431-457.

9 Herrera, G., and I. Herrera. 1993. Eulerian- Lagrangian Method of Cell Based on Localized Adjoint Method. *Numer. Methods Partial Different. Equ.* 10, 205-223.

10 Konikow, L.F., and J.D. Bredehoeft. 1978. Computer model of two-dimensional solute transport and dispersion in groundwater, in *Techniques of Water-Resource Investigations*, Book 7, Chapter C2, 90 pp., US Geological Survey, Washington, DC.

11 Neuman, S.P. 1984. Adaptive Eulerian-Lagrangian finite-element method for advection-dispersion, *Int. J. Numer. Methods Eng.*, 20, 321-337.

12 Wang, H., and R.E. Ewing. 1994. Optimal-Order Convergence rates for Eulerian-Lagrangian Localized Adjoint Methods for Reactive Transport and Contamination in Groundwater. *Numer. Methods Partial Different. Equ.* 11, 1-31.