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ELLAM: AN EFFECTIVE TOOL FOR MODELLING SHARP FRONTS IN QUANTITATIVE ISOTOPIC HYDROLOGY

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Abstract

The main topic of study of Quantitative Isotopic Hydrology is the transport of isotopes by water flowing in a porous medium, and their interactions. The mathematical models of such processes are based in the advection-diffusion equation or systems of such equations. Until recently, effective mass conservative algorithms capable of modeling advection-dominated transport were lacking. However, many of the difficulties encountered previously have been overcome by ELLAM methods, recently developed by the author and coworkers. Here, the different implementations of ELLAM methods that exist at present, are presented and evaluated, with the purpose of making them more readible available to the scientific community working in Quantitative Isotopic Hydrology.

1. INTRODUCTION

The numerical solution of the advection-diffusion equation, is a problem of great importance in the study of transport of solutes by a liquid phase. A particular case of this general problem, is the study of the transport of a tracer by water flowing in a porous medium. The central problem of Quantitative Isotopic Hydrology, is precisely this problem.

The numerical treatment of the advection-diffusion equation, when advection is dominant, has been a challenging problem for a long time, specially if sharp fronts are present. A feature that is required from algorithms in order to be able to model effectively advection dominated transport, is that its performance be independent of the Courant number, to a large extent. Another feature which is essential, specially in Quantitative Isotopic Hydrology, is that the algorithms be mass-conservative, even when significant boundary behavior is present.

A general class of methods that has been quite successful and is being applied extensively, is the Eulerian-Lagrangian Localized Adjoint Method (ELLAM)[1-20]. One important feature of ELLAM methods, is that they are the only characteristic methods thus far developed, that are mass conservative. This property enhances

further the potential applications of ELLAM methods to mathematical models of Quantitative Isotopic Hydrology.

This paper is devoted to explain and discuss the ELLAM methodology with the intention of making it more readily available to the scientific community working in Quantitative Isotopic Hydrology. In addition, a brief critical comparison of the different ELLAM implementations that have been developed, is made.

The methods available to treat the advective-diffusive transport equation, are usually classified into: Eulerian, Lagrangian and Eulerian-Lagrangian. A method is called Eulerian, when the spatial grid is kept fixed in time. It is called Lagrangian or characteristic method, when the time derivatives are discretized following the motion of the fluid particles and it is called Eulerian-Lagrangian, when the fluid particles are tracked, but the spatial grid is kept fixed through time.

When applied to advection dominated transport, the salient features of approximations which derive from an Eulerian approach, may be summarized as follows: (i) The time truncation error dominates the solutions, (ii) The solutions are characterized by significant numerical diffusion and some phase errors, (iii) The Courant number ($Cu \equiv \frac{V\Delta t}{\Delta x}$) is generally restricted to be less than one, and sometimes much less than one. Among such procedures, one may distinguish Optimal Spatial Methods (OSM), in which an accurate solution of the spatial problem is developed.

Other Eulerian methods seek to cancel the errors introduced by the time discretization with the errors produced by the spatial discretization (see, for exmple [21-24]). Some of such methods actually improve to some extent, the inconvenient features of Eulerian methods in general, mentioned above. However, they still suffer from severe Courant number limitations [ ].

In Lagrangian methods in general, the problem is solved step by step in time. The process of obtaining the solution at the new time level from the solution at the previous one, in turn, is carried out in two teps: one in which fluid particles are tracked and a second one in which a purely spatial elliptic problem is solved. This latter step is frequently called the "diffusive step", because the elliptic character of the problem is induced by the presence of diffusion (usually Fickian).

Methods which are purely Lagrangian carry out the particle tracking forward in time. This introduces distorsions of the spatial

grid, which complicate the implementation of the diffusive step and lead to inacuracies of the solution. In Eulerian-Lagrangian approaches the grid is kept fixed at all times, avoiding in this manner the grid distorsions. To this end, the particles are tracked backwards in time. Thus, such procedures profit from the structure of characteristic curves when carrying out the time-discretization, but in addition they profit of having kept fixed the spatial grid, when carrying out the diffusive step. Eulerian-Lagrangian methods have the significant advantage that Courant number restrictions of Eulerian methods are overcome to a large extent, since the advection term is eliminated from the elliptic problems to be solved at each time step.

On the other hand, the Localized Adjoint Method (LAM) is a methodology for discretizing partial differential equations which was introduced by the author [25-30]. This procedure is based on Herrera's Algebraic Theory of Boundary Value Problems [31-35] (also [25]). Applications have successively been made to ordinary differential equations, for which highly accurate algorithms were developed [25-27], multidimensional steady state problems [28] and optimal spatial methods for advection-diffusion equations [29-30].

Recently, Localized Adjoint Method (LAM) has been applied in space-time, in an Eulerian-Lagrangian manner to problems of advective-diffusive transport, using specialized test functions [1-3,7-9]. These functions locally satisfy the homogeneous adjoint equation within each element. The general methodology so obtained is the Eulerian-Lagrangian Localized Adjoint Method (ELLAM).

Like characteristic methods in general [36-43], ELLAM methods have the advantage that Courant number restrictions of purely Eulerian methods are removed to a large extent, but in addition they present other important advantages. Until ELLAM was developed, characteristic methods had had three kinds of limitations: inability to rigorously treat boundary fluxes when characteristics intersect inflow or outflow boundaries, inability to ensure mass conservation and the introduction of numerical dispersion for some methods, due to low order interpolation or integration [44].

On the other hand, the general framework of ELLAM, as has been presented in [2] (see also [6]), is quite wide. In contrast to other characteristic methods, ELLAM allows systematic treatments of boundary conditions and the resulting algorithms are mass

conservative [1]. In addition, it provides a unification of characteristic methods (CM's).

The general methodology of ELLAM [2], can be implemented in many different manners. Up to now two kinds of implementations have been developed. They derive from the application of two different classes of test functions. In [1], bilinear functions which are defined as "chapeau" functions at level time t^{n+1} and constant along characteristic curves, were applied and in this manner the first mass conservative Eulerian-Lagrangian scheme for the general transport equations, was developed. This method is referred to as BELLAM [7].

An alternative manner of implementing ELLAM, is to use test functions which are piece-wise constant, and are advected with the transport velocity of the problem. In [7,8], under the title of "ELLAM Cells" (CELLAM), a very effective implementation of ELLAM using this kind of test functions, has been developed. CELLAM has the advantages of ELLAM methods described above, but in addition it ensures local mass conservation and yields algorithms which are more convenient for existing solute-transport codes which are based on finite differences. Thus far, the numerical performance of CELLAM has been slightly better than that of BELLAM [7-9]. Also, the simplicity of the implementation of the method, is appealing.

In passing, we mention that an implementation (FVELLAM) using similar test functions was intended in [45], but the authors reported numerical difficulties which severely limit the applicability of their results.

2. BILINEAR ELLAM (BELLAM)

This approach was first presented in a sequence of two papers [1,2]. Consider the one-dimensional transient advection-diffusion equation in conservative form:

$$\mathcal{L}u \equiv \frac{\partial u}{\partial t} - \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x} - Vu\right) + Ru = f_\Omega(x,t), \quad \text{in } \Omega \tag{2.1}$$

$$x \in \Omega_x = [0, l]$$
$$t \in \Omega_t = [t^n, t^{n+1}]$$
$$(x,t) \in \Omega = \Omega_x \times \Omega_t$$

subject to initial conditions

$$u(x, t^n) = u^n(x), \tag{2.2}$$

and suitable boundary conditions, at x=0 and l. The following development accommodates any combination of boundary conditions. The

manner in which the region Ω and the initial conditions are chosen in Eqs. (2.1) and (2.2), is suitable for applying a step by step solution procedure.

To make the exposition more readable, only the case of constant coefficients will be explained here, although variable coefficients have already been treated (see for example [11]). For simplicity, we proceed in an ad-hoc manner. More systematic expositions placing the procedures discussed in this article in the general frame-work of the Localized Adjoint Method (LAM), are given in [2] and [5].

For the case when the coefficients of Eq. (2.1) are constant, the source term vanishes (R≡0) and the partition is uniform, the test functions used are:

$$w^i(x,t) = \begin{cases} \dfrac{x-x_{i-1}}{\Delta x} + V\dfrac{t^{n+1}-t}{\Delta x}, & (x,t)\in\Omega_1^i \\ \dfrac{x_{i+1}-x}{\Delta x} + V\dfrac{t^{n+1}-t}{\Delta x}, & (x,t)\in\Omega_2^i \\ 0, \quad \text{all other } (x,t) \end{cases} \tag{2.3}$$

where Ω_1^i and Ω_2^i are as is shown in Fig.1. Such weighting functions satisfy $\mathcal{L}^* w^i = 0$ and are continuous (i.e $[w]=0$), but have discontinuous first derivatives (i.e.; $[dw/dx]\neq 0$). The jumps are

$$\left[\frac{\partial w}{\partial x}\right]_{i-1} = \frac{1}{\Delta x}\ ; \quad \left[\frac{\partial w}{\partial x}\right]_{i} = \frac{-2}{\Delta x}; \quad \left[\frac{\partial w}{\partial x}\right]_{i+1} = \frac{1}{\Delta x}. \tag{2.4}$$

DISCRETIZATION IN THE INTERIOR OF Ω

When the region Ω^i does not intersect the lateral boundaries, integration over Ω^i, yields

$$\int_{x_{i-1}}^{x_{i+1}} u(x,t^{n+1})w^i(x,t^{n+1})dx - \frac{D}{\Delta x}\left\{\int_{t^n}^{t^{n+1}} u(\sigma_{i-1}(t),t)dt - 2\int_{t^n}^{t^{n+1}} u(\sigma_i(t),t)dt + \int_{t^n}^{t^{n+1}} u(\sigma_{i+1}(t),t)dt\right\}$$
$$= \int_{x_{i-1}^*}^{x_{i+1}^*} u(x,t^n)w^i(x,t^n)dx + \int_\Omega f_\Omega w^i dxdt, \tag{2.5}$$

where the unknowns have been collected in the left-hand member of the equation while the data is included in the right one. In Eq. (2.5), it is assumed that $x=\sigma_i(t)$ is the characteristic curve passing through x_i at time t_{n+1} (Fig. 1).

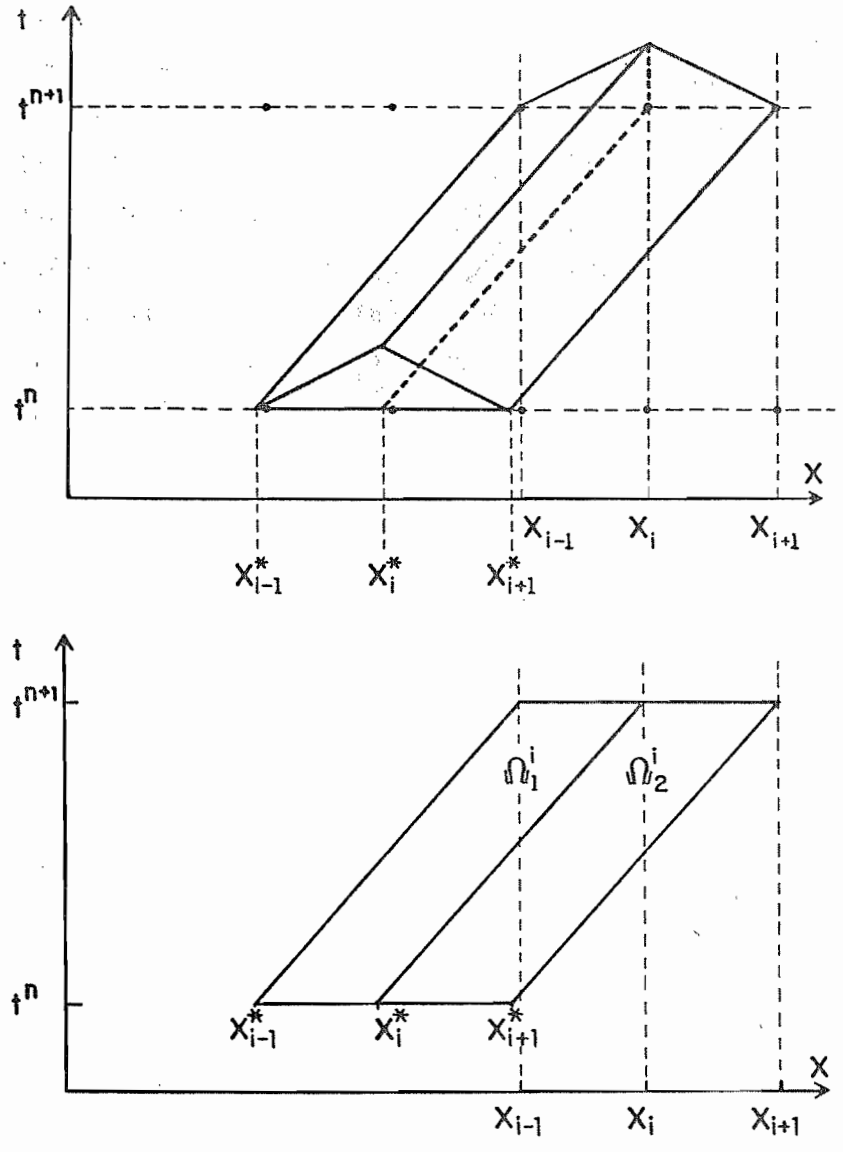

Figure 1.- Test functions used in BELLAM.

Notice that the unknown function u(x,t) has not yet been approximated by any specific functional form. The time integrals may be approximated using a Backward-Euler (fully implicit) scheme. Then the spatial integrals that appear in Eq. (2.5), may be approximated in many different ways, using the nodal values of u at the discrete time levels t^n and t^{n+1}, exclusively, so that the unknowns in the equation ultimately correspond to nodal values at time t^{n+1}. Different approximations of these integrals lead to different CM algorithms reported in the literature [1]. For example, piecewise linear spatial interpolation of u at time levels t^n and t^{n+1}, coupled with a one-point (at $t=t^{n+1}$) fully implicit approximation to the temporal integral, leads to the modified method of characteristics of Douglas and Russell [40].

When a region Ω^i intersects the inflow boundary, several cases can occur. As an example, we discuss the case illustrated in Fig. 2. Then, integrating Eq. (2.1) over the region Ω_1, it is obtained:

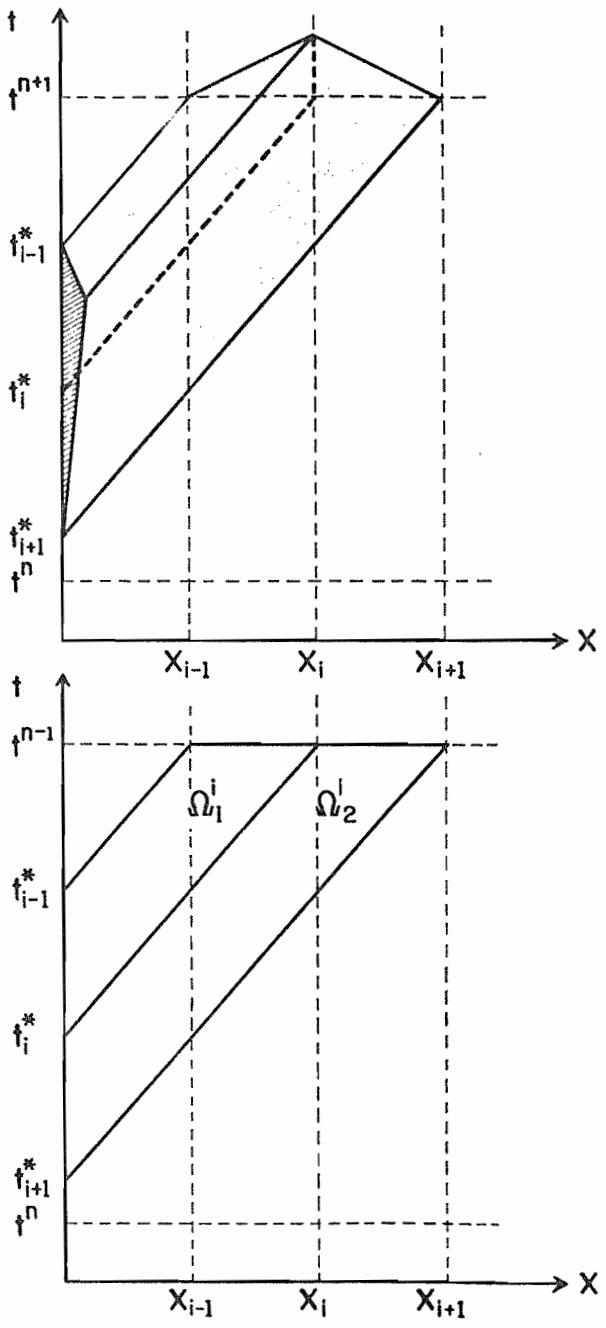

Figure 2.- Case when the domain of the test functions intesects the inflow boundary (BELLAM).

$$\int_{x_{i-1}}^{x_{i+1}} u(x,t^{n+1})w^i(x,t^{n+1})dx - \frac{D}{\Delta x}\left\{\int_{t^*_{i-1}}^{t^{n+1}} u(\sigma_{i-1}(t),t)dt - 2\int_{t^*_i}^{t^{n+1}} u(\sigma_i(t),t)dt\right.$$

$$\left. + \int_{t^*_{i+1}}^{t^{n+1}} u(\sigma_{i+1}(t),t)dt\right\} + \int_{t^*_{i+1}}^{t^*_{i-1}} w^i\left\{D\frac{\partial u}{\partial x}(0,t) - Vu(0,t)\right\}dt =$$

$$\frac{D}{\Delta x}\left\{\int_{t^*_i}^{t^*_{i-1}} u(0,t)dt - \int_{t^*_{i+1}}^{t^*_i} u(0,t)dt\right\} + \int_\Omega f_\Omega w^i dxdt \qquad (2.6)$$

The integrals along characteristics appearing in Equ. (2.6), can again be evaluated by means of a fully implicit approximation.

However, the fact that each of these three integrals has a different length, introduces problems for achieving consistency in the order of accuracy of the approximations, for some classes of boundary conditions, at least. Suitable combinations of the integrals just mentioned, with the last integral of the left-hand side of Eq. (2.6), may overcome the problem. However, whether this is feasible or not, depends on the type of boundary conditions to be satisfied. To exhibit this problem, it is necessary to develop a more careful derivation in which the order of the errors introduced at each step, is explicitly stated. Thus, the reader is referred to Section 5, where a more careful derivation of a similar equation is presented for CELLAM.

The last term in the left-hand side of Equ. (2.6) must be handled with special care, to obtain an algorithm with satisfactory properties. If we simply apply the Backward-Euler scheme to the unknown boundary flux along the time direction, the discretization will be unsatisfactory for large Courant numbers ($Cu=V\Delta t/\Delta x$), since many characteristic lines will be crossed. Thus, instead, one can evaluate the contribution to the integral of the term containing $u(0,t)$, since this is Dirichlet data, and transpose it to the right side of the equation. In [1], the remaining part of the integral was approximated in a way which, as indicated in [8], is equivalent to:

$$\int_{t^*_{i+1}}^{t^*_{i-1}} w^i D\frac{\partial u}{\partial x}(0,t)dt \cong \frac{D}{V}\int_{x_{i-1}}^{x_{i+1}} w^i\frac{\partial u}{\partial x}(x,t^{n+1})dx \qquad (2.7)$$

This approximation however, as pointed out in [7], is not necessarily consistent with the order of approximation that is required in the formulation: $O(\Delta x\Delta t^2)$. This latter order of

approximation can be achieved, using relations similar to Eq. (2.7), only if the expressions under the integrals, are suitably combined with the integrals along characteristics present in Eq. (2.6), and this is possible, as has been already been mentioned, only for some kinds of boundary conditions [7].

For outflow boundary conditions of Dirichlet type, the outflow boundary contributions vanish for all the test functions. This is due to the fact that all the weighting functions vanish in the characteristic Σ_E, which passes through (x_E, t^{n+1}), and beyond it. Also, the system of equations that is obtained in the manner explained above, is closed, because u_E^{n+1} is datum. If additional information is desired at the outflow boundary, it can be obtained applying procedures which amount essentially to post-processing [1].

3. SOME REMARKS ON DISCRETE METHODS

There are two basic tasks that every numerical method for partial differential equations has to accomplish [2,6,7]:

i).- Gathering information about the sought solution; and

ii).- Interpolating or, more generally, processing such information.

These two processes are distinct, although in many numerical methods they are not differentiated clearly. In procedures which are derived from the method of weighted residuals, the information about the exact solution that is gathered, is determined mainly by the weighting functions used. Since this information does not determine uniquely the sought solution, some procedure for extending it is required, in order to fill the gaps of information and exhibit at the end, a unique approximate solution.

Different methods of solution follow different strategies for accomplishing this latter task of extending the information that is available. In general, interpolation and extrapolation procedures are applied. For example, in finite element methods some basis functions are chosen and the approximate solution is assumed to be a superposition of such functions. In this case, the information about the exact solution which is gathered by the weighting functions, is interpolated in a manner which is determined by the family of basis functions chosen.

Clearly, it is not convenient to carry out the process of extending the information blindly, ignoring what is the actual information that is available. However, this is what is usually

done. On the contrary, it is advantageous to make use of the insight gained when the available information has been identified, since the selection of the best procedure for extending it, is strongly dependent on the information that is at hand.

Due to these facts, in recent works [6,7] the author has advocated an approach for developing numerical methods, in which the processes i) and ii) are clearly separated. Firstly, the information about the sought solution that is at hand, is identified and secondly, using that insight, a procedure for extending such information is defined.

Herrera's Algebraic Theory of Boundary Value Problems [25,31-35], which permits localizing the adjoint, has shown to be quite suitable for identifying the information contained in approximate solutions. The use of this theory has clear advantages over other options, such as the standard theory of distributions, because of two reasons at least: the use of the algebraic theory permits the localization of the adjoint, and the simultaneous use of discontinuous trial and test functions is feasible. Then, depending on the information that is identified, interpolation procedures suitable for handling it efficiently, are selected and applied. This is what should be properly called Localized Adjoint Method. The introduction of basis functions is not required and, even more, their use is inconvenient in some cases. In [7] and [8], this approach was applied quite successfully to derive CELLAM.

4 ELLAM CELLS (CELLAM)

This method was presented originally in [7] and [8] (see also [9]). The notations adopted conform with those which are usual for cell approaches. A partition $\{x_1, x_{3/2}, x_{5/2}, \ldots, x_{E-1/2}, x_E\}$, is introduced, which induces a partition of Ω into subregions $\{\Omega^1, \Omega^2, \ldots, \Omega^E\}$, if for each $i=2,\ldots,E-1$, Ω^i is defined as the subregion of Ω, limited by the characteristic curves $\Sigma_{i-1/2}$ and $\Sigma_{i+1/2}$ (see Fig.3), while Ω^1 is that part of Ω which lies to the left of $\Sigma_{3/2}$ and Ω^E is the subregion of Ω which lies to right of $\Omega_{E-1/2}$. The subregions of the partition are called "cells" and they are said to be "uniform" when

$$x_{i+1/2}-x_{i-1/2} = h, \text{ for } i=2,\ldots,E-1;\ x_{3/2}-x_1=h/2, x_E-x_{E-1/2}=h/2 \quad (4.1)$$

A system of constant weighting functions is applied. These are the characteristic functions of the subregions that constitute this

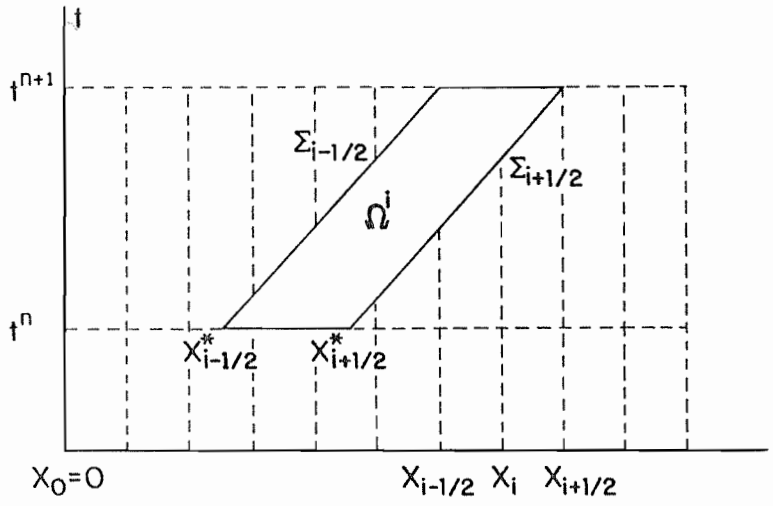

Figure 3.- Test functions used in CELLAM.

partition. Actually, not all of them are required. The system of weighting functions applied to derive CELLAM [7], is:

$$w^{\alpha}(x,t) = \begin{cases} 1, & \text{if } (x,t)\in\Omega^{\alpha} \\ 0, & \text{if } (x,t)\notin\Omega^{\alpha} \end{cases}, \quad \alpha=2,\ldots,E-1, \qquad (4.2)$$

DISCRETIZATION IN THE INTERIOR OF Ω

In the case when Ω^{α} does not intersect the lateral boundaries of the region $\Omega=[0,1]X[t_n,t_{n+1}]$, integration of Eq. (2.1) over Ω^{α}, yields:

$$\int_{x_{\alpha-1}}^{x_{\alpha+1}} u^{n+1}dx + \int_{t_n}^{t_{n+1}} (D\frac{\partial u}{\partial x})_{\Sigma_{\alpha+1/2}} dt - \int_{t_n}^{t_{n+1}} (D\frac{\partial u}{\partial x})_{\Sigma_{\alpha-1/2}} dt$$

$$= \int_{x^*_{\alpha-1}}^{x^*_{\alpha+1}} u^n dx \qquad (4.3)$$

Equation (4.3) and a modified version of it designed to incorporate boundary terms when the lateral boundaries of Ω are intersected by Ω^{α}, is the starting point of the numerical treatment. Observe that

$$\int_{x_{\alpha-1}}^{x_{\alpha+1}} u^{n+1}dx - \int_{x^*_{\alpha-1}}^{x^*_{\alpha+1}} u^n dx = O(hk) \qquad (4.4a)$$

and

$$\int_{t_n}^{t_{n+1}} (D\frac{\partial u}{\partial x})_{\Sigma_{\alpha+1/2}} dt - \int_{t_n}^{t_{n+1}} (D\frac{\partial u}{\partial x})_{\Sigma_{\alpha-1/2}} dt = O(hk) \qquad (4.4b)$$

where $h = \max(h_{i+1/2}-h_{i-1/2})$ and $k = t_{n+1}-t_n$. Thus, in the developments it is required that integrals such as those appearing in Equs. (4.4), be evaluated to a precision of $O(hk^2)$, at least. It will be assumed that $h \approx k$, so that $O(hk^2)=O(h^2k)=O(k^3)=O(h^3)$.

Equation (4.3) supplies information about the sought solution in the interval $[x_{\alpha-1/2}, x_{\alpha+1/2}]$ at time t_{n+1} and about its x-derivative on the characteristics $\Sigma_{\alpha-1/2}$ and $\Sigma_{\alpha+1/2}$. In the CELLAM approach [7], the goal of the information processing is to concentrate all of it, in the value of the solution at the "cell center" x_α, at time $t=t_{n+1}$. To this end, in Eq. (4.3), the integrals from t_n to t_{n+1}, are firstly approximated in a fully implicit manner (i.e., by a one-step Backward-Euler approximation at t_{n+1}). Thus

$$\int_{t_n}^{t_{n+1}} \left\{ \left(D\frac{\partial u}{\partial x}\right)_{\Sigma_{\alpha+1/2}} - \left(D\frac{\partial u}{\partial x}\right)_{\Sigma_{\alpha-1/2}} \right\} dt =$$

$$\left\{ \left(D\frac{\partial u^{n+1}}{\partial x}\right)_{\alpha+1/2} - \left(D\frac{\partial u^{n+1}}{\partial x}\right)_{\alpha-1/2} \right\} k + O(hk^2) \qquad (4.5)$$

For a uniform spacing and constant coefficients, a central difference approximation yields:

$$\left\{ \left(\frac{\partial u^{n+1}}{\partial x}\right)_{\alpha+1/2} - \left(\frac{\partial u^{n+1}}{\partial x}\right)_{\alpha-1/2} \right\} k = \frac{u_{\alpha+1}^{n+1} + u_{\alpha-1}^{n+1} - 2u_\alpha^{n+1}}{h} k + O(h^3k) \qquad (4.6)$$

The extension of this formula to the case of a non-uniform partition, can be done in a similar manner. However, the order of precision is reduced by one and the overall error in (4.6), becomes $O(h^2k)$.

In characteristic methods, most of the numerical diffusion is due to the interpolations in space, which are required because in general, characteristics do not cross the t_n time level at nodes. Thus, all the approximations in space have to be carried out with special care. A special feature of the approximations used in the derivation of CELLAM [7], is that no assumption is made about the shape of the solution.

The first integral in (4.3), is approximated by

$$\int_{x_{\alpha-1}}^{x_{\alpha+1}} u^{n+1} dx = u_\alpha^{n+1} h_\alpha + \frac{1}{24}\left(\frac{\partial^2 u^{n+1}}{\partial x^2}\right)_\alpha h_\alpha^3 + O(h^5) \qquad (4.7)$$

and only the second order derivative requires a numerical approximation, since the information is being concentrated in the "cell centers". To get a tridiagonal structure for the matrix, it

is necessary to use three-point approximations only. In the case of a "uniform partition", a central difference approximation yields

$$\int_{x_{\alpha-1}}^{x_{\alpha+1}} u^{n+1} dx = \left(\frac{u_{\alpha+1}^{n+1} + u_{\alpha-1}^{n+1} + 22u_{\alpha}^{n+1}}{24} \right) h + O(h^5) \qquad (4.8)$$

If the partition is non-uniform, the approximation to the second order derivative by a three-point scheme is only first order, and the error in the evaluation of the integral in (4.8), is only order four.

There is greater freedom for the choice of the approximations to be used in the evaluation of the integrals at time t_n, since they do not affect the structure of matrix of the final system of algebraic equations. In [7], the integral appearing in the right-hand side of Eq. (4.3) was approximated using an approach similar to the one used for deriving Equ. (4.7); i.e., integrating the Taylor series expansion of u^n around the mid-point 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 three and one, respectively. This yields an approximation which is fourth order in h.

5. BOUNDARY CONDITIONS

The numerical approximations presented thus far, apply only when the subregion $\Omega^{\alpha} \subset \Omega$ does not intersect the lateral boundaries $\partial_o \Omega \cup \partial_\ell \Omega$, of the region Ω. When this is not the case, boundary conditions must be included. This Section is devoted to presenting the CELLAM procedures for dealing with them.

In Eulerian-Lagrangian approaches, the analyst does not have control of the discretization at an inflow boundary, since it is completely determined by the spatial discretization. However, the situation in this respect is a little better at an outflow boundary. Thus, when dealing with boundary conditions, specially at an inflow boundary, numerical diffusion is due to a large extent, to the fact that characteristics do not cross the boundaries of the space-time region Ω, at times levels belonging to the partition of the time interval. Thus, just as in the interior of the spatial region, the approximatinos in space have to be performed with special care to minimize numerical diffusion, when dealing with boundary conditions the time integrals on the boundaries have to be treated with special care.

There is an additional reason which enhances this effect at an inflow boundary. The information that is supplied at an inflow boundary has a larger effect on the solution than that coming from an outflow boundary, specially in the case of advection-dominated transport, because the former is transmitted to the interior of the spatial region by advection and diffusion, while the latter is only transmitted by diffusion.

In [7], it was pointed out that in some cases, it is more difficult to achieve the desired degree of accuracy in the integrals with respect to time at the boundary, than in the integrals with respect to x, at the different time levels. For Dirichlet boundary conditions, the different terms occur in a combination which is suitable for obtaining the desired degree of accuray. However, when the total flux is prescribed or when considering boundary conditions of Neuman type, this is not the case [7].

A.- Dirichlet Conditions

For this case, we use E-2 test functions; namely, those associated with subregions $\Omega^2,\ldots,\Omega^{E-1}$. In particular, no test function is applied on the first subregion (Ω^1) or on the last one (Ω^E). See Fig. 4.

Inflow Boundary

Dirichlet 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.

Assume Ω^α intersects the inflow boundary, as illustrated in Fig. 4. Then

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

$$\int_{t^*_{\alpha+1/2}}^{t^*_{\alpha-1/2}} \left\{ (D\frac{\partial u}{\partial x})_{\Sigma_{\alpha+1/2}} - (D\frac{\partial u}{\partial x})_{x=0} \right\} dt - \int_{t^*_{\alpha+1/2}}^{t^*_{\alpha-1/2}} Vu(0,t)\,dt \qquad (5.1)$$

The first two integrals of the right-hand member are like those appearing in Equs. (4.8) and (4.5), and can be handled similarly. In addition, the last one in this equation is easy to deal with, since u(0,t) is the prescribed boundary value. The third integral, however, requires a special treatment.

Firstly, observe that $(D\frac{\partial u}{\partial x})_{\Sigma_{\alpha+1/2}} - (D\frac{\partial u}{\partial x})_{x=0}$ is $O(h)$. Thus, for any $x\in[x_{\alpha-1/2}, x_{\alpha+1/2}]$, one has

$$(D\frac{\partial u}{\partial x})(x_{\Sigma_{\alpha+1/2}}(t^*), t^*) - (D\frac{\partial u}{\partial x})(0, t^*) = D\frac{\partial u^{n+1}}{\partial x}(x_{\alpha+1/2}) - D\frac{\partial u^{n+1}}{\partial x}(x) + O(hk) \quad (5.2)$$

where, for brevity, we have written t^* instead of $t^*(x)$. The approximation implied by Equ. (5.2), has the property that the values of the functions involved, at time t^*, are approximated by their values at time t_{n+1}, on the same characteristic. In this manner, crossing of characteristics is avoided. Such property is important in order to preserve the advantages of characteristic methods.

Equ. (5.2), can be used to obtain

$$\int_{t^*_{\alpha+1/2}}^{t^*_{\alpha-1/2}} \left\{ (D\frac{\partial u}{\partial x})_{\Sigma_{\alpha+1/2}} - (D\frac{\partial u}{\partial x})_{x=0} \right\} dt = (t^*_{\alpha-1/2} - t^*_{\alpha+1/2})(D\frac{\partial u^{n+1}}{\partial x})_{\alpha+1/2} +$$

$$\int_{x_{\alpha-1/2}}^{x_{\alpha+1/2}} D\frac{\partial u^{n+1}}{\partial x}(x)\frac{dt^*}{dx}(x)dx + O(hk^2) \quad (5.3)$$

As an illustration of the numerical implementation for this equation, we explain the case of constant coefficients. In this case

$$t^*(x) = t_{n+1} - \frac{x}{V} \quad (5.4)$$

so that

$$\frac{dt^*}{dx} = -\frac{1}{V} \quad (5.5)$$

and Equ. (5.3), becomes

$$\int_{t^*_{\alpha+1/2}}^{t^*_{\alpha-1/2}} \left\{ (D\frac{\partial u}{\partial x})_{\Sigma_{\alpha+1/2}} - (D\frac{\partial u}{\partial x})_{x=0} \right\} dt = \frac{x_{\alpha+1/2} - x_{\alpha-1/2}}{V}(D\frac{\partial u^{n+1}}{\partial x})_{\alpha+1/2} -$$

$$\frac{D}{V}(u^{n+1}_{\alpha+1/2} - u^{n+1}_{\alpha-1/2}) + O(hk^2) \quad (5.6)$$

In Equ. (5.6), the derivative $\partial u^{n+1}/\partial x$ at $x_{\alpha+1/2}$ ($\alpha=2,\ldots,E-1$), must be approximated to order $O(h^2)$, to be consistent with the order of approximation. For a non-uniform mesh, this requires a three-point scheme.

For $\alpha=2$, the boundary value u_1^{n+1}, occurs in equations such as (4.6) and (4.8), and it must be required that at each time level, u_1^{n+1} be equal to the prescribed boundary value. This is the indirect manner of imposing the boundary conditions that we referred to at the beginning of this section.

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 $x=l$. 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; i.e., introducing them instead of u_E^{n+1} in approximations such as (4.6) and (4.8).

B.- Flux Conditions

For this case, we use E test functions. Thus, the test functions associated with regions Ω^1 and Ω^E, which were omitted when dealing with Dirichlet boundary conditions, are applied when dealing with this kind of boundary condition, and the values of u^{n+1} at zero and at l are treated as unknowns.

Inflow Boundary

Fig. 4, illustrates a case in which Ω^α intersects the inflow boundary. For flux boundary conditions, it is more convenient to write Equ. (5.1) in the form:

$$\int_{\Omega^\alpha} \mathcal{L}u\,d\sigma = \int_{x_{\alpha-1/2}}^{x_{\alpha+1/2}} u^{n+1}dx - \int_{t^*_{\alpha-1/2}}^{t_{n+1}} \left\{ (D\frac{\partial u}{\partial x})_{\Sigma_{\alpha+1/2}} - (D\frac{\partial u}{\partial x})_{\Sigma_{\alpha-1/2}} \right\} dt -$$

$$\int_{t^*_{\alpha+1/2}}^{t^*_{\alpha-1/2}} (D\frac{\partial u}{\partial x})_{\Sigma_{\alpha+1/2}}\,dt - \int_{t^*_{\alpha+1/2}}^{t^*_{\alpha-1/2}} F(t)dt \qquad (5.7)$$

Here, $F \equiv (Vu - D\frac{\partial u}{\partial x})_{x=0}$, is prescribed.

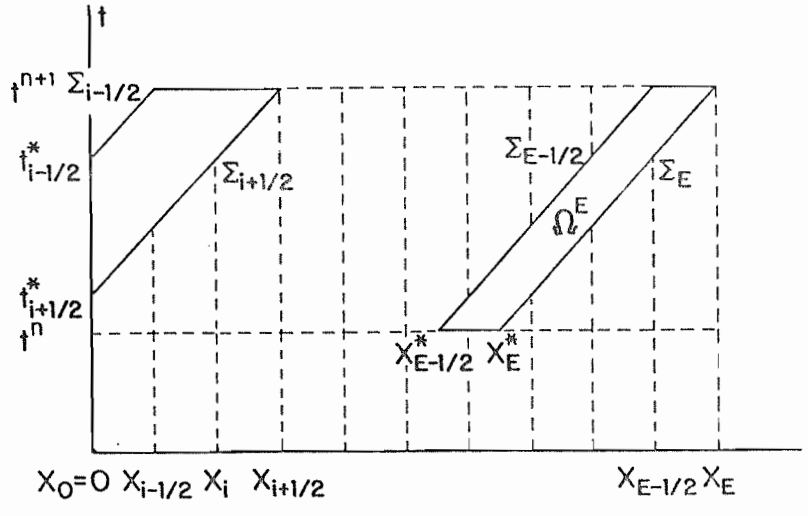

Figure 4.- Cases when the domain of the test functions intersects the lateral boundaries (CELLAM).

Since F(t) is a datum, the corresponding integral offers no special difficulty in being approximated to any desired order of accuracy. The other integrals can be treated in a manner similar to what was done in the case of Dirichlet conditions. The approximation

$$\int_{t^*_{\alpha+1/2}}^{t^*_{\alpha-1/2}} (D\frac{\partial u}{\partial x})_{\Sigma_{\alpha+1/2}} dt \cong (t^*_{\alpha-1/2} - t^*_{\alpha+1/2})(D\frac{\partial u^{n+1}}{\partial x})_{\alpha+1/2} \qquad (5.8)$$

is similar to one used in Equ. (5.3). However, the term $(D\frac{\partial u}{\partial x})_{x=0}$ which appears in Equ. (5.3), is missing here, because it was incorporated in the flux F. Due to this fact, approximation (5.8) is only $O(k^2)$, which is not consistent with the order of approximation that has been used in all other terms.

However, such a shortcoming has not been manifested in the numerical applications, which use Equ. (5.8). In particular, all the numerical experiments reported in this article, use this approximation. The development of an algorithm fully consistent with the order of accuracy that was set at the beginning of our discussion, would require a procedure, considerably more elaborate, which would not be justified at this point.

In addition, it must be mentioned that when the support of a weighting function intersects any of the corners of the domain Ω, the treatment presented requires slight modifications, whose details we leave out. At the inflow boundary, this happens for two test functions. One is w^1 and there is one more, whose support intersects the corner $(0, t_n)$, as shown in Fig. 4.

Outflow Boundary

The only weighting function whose support intersects the outflow boundary is w^E. Applying it, we get

$$\int_{\Omega^E} \mathcal{L}u\,d\sigma = \int_{x_{E-1/2}}^{l} u^{n+1}dx - \int_{x^*_{E-1/2}}^{l} u^n dx - \int_{t_n}^{t_{n+1}} F(t)dt + \int_{t_n}^{t_{n+1}} (D\frac{\partial u}{\partial x})_{\Sigma_{E-1/2}} dt \qquad (5.9)$$

Using three points approximations, one can evaluate the first two integrals of the right-hand side of this equation to $O(h^4)$. The third one offers no difficulty, since F(t) are data. Finally, an approximating procedure analogous to Equ. (5.8), can be applied to the last integral. However, the comments that were made immediately after Equ. (5.8), apply here too.

6 NUMERICAL COMPARISONS

The efficiencies of the BELLAM and CELLAM procedures have been compared. In [7], numerical examples that involve significant boundary behavior were solved, using these two methods. The results obtained there, are described next. The following change in the notation is noticed: In this Section, instead of taking the spatial region to be the interval $[0,1]$, as we did in the theoretical discussions, we set $\Omega_x=[a,b]$.

Consider an advancing Gaussian hill that may cross an inflow or an outflow boundary. Its general expression is

$$u_a(x,t) = \frac{1}{(1+4\pi Dt)^{1/2}}\exp\left(\frac{-\pi(x-Vt)^2}{1+4\pi Dt}\right) \qquad (6.1)$$

and the initial and boundary conditions are chosen in such a way that the exact solution of the problem is (6.1). Thus, the initial conditions are

$$u_I(x) = \exp(-\pi x^2) \qquad (6.2)$$

while the boundary conditions are

$$u(a,t) = u_a(a,t) \qquad (6.3a)$$

and

$$u(b,t) = u_a(b,t) \qquad (6.3b)$$

whenever Dirichlet conditions are considered. In addition, they are

$$\left(Vu - D\frac{\partial u}{\partial x}\right)(a,t) = \left(Vu_a - D\frac{\partial u_a}{\partial x}\right)(a,t) \qquad (6.4a)$$

and

$$\left(Vu - D\frac{\partial u}{\partial x}\right)(b,t) = \left(Vu_a - D\frac{\partial u_a}{\partial x}\right)(b,t) \qquad (6.4b)$$

whenever total flux boundary conditions are considered. In the numerical examples, only Dirichlet and total flux boundary conditions will be treated.

Several combinations of initial and boundary conditions are prescribed for Equ. (2.1), but in such a manner that for any of them the exact solution is given by Equ. (6.1). Also, domains considered were: $I=[2^1/_3,9]$, $O=[-3,2^1/_3]$ and $N=[-3,9]$. For them, the pulse crosses an inflow boundary, an outflow boundary and neither, respectively.

A. Comparison based on the Euclidean Norm

As explained in previous sections, in the CELLAM method the information about the sought solution is concentrated exclusively in the cell-centers and no base functions are used. This implies that no assumptions are made about the shape of the solution. This is in

contrast with other ELLAM procedures, in which the shape of the solution is assumed [1].

One consequence of this way of handling the information, is that some of the standard procedures for measuring the errors of approximate solutions, are not appropriate. In [1], for example, in which bilinear basis functions were used (the space of such functions, which are piece-wise linear and continuous in Ω_x, will be denoted be $\mathcal{S}$), the L^2 error of the approximate solution that BELLAM yields (and such approximate solution necessarily belongs to $\mathcal{S}$), was compared with the L^2 error of the projection of the exact solution on $\mathcal{S}$. This ratio is necessarily greater or equal to one, because of the minimal property of the projection.

When all the information is concentrated at the cell-centers, the best we can do is to obtain the exact values at those points. This, however, does not define a function of the space $\mathcal{S}$, and a direct comparison using the L^2 norm, is not possible. Of course, one could try to use linear interpolation of the approximate values at the cell-centers, to associate an element of $\mathcal{S}$ to the approximate solution. However, if one proceeds in that manner, even the optimal solution (i.e., that whose values at the cell-centers are the exact values) would give an L^2 error that in general, will be greater than that of the projection, again because of the minimal property of the projection. To illustrate this fact and its importance in the different cases tested, Table 1 compares the L^2 error of the linear interpolation, when the values at the cell-centers are the exact ones, with the error of the projection of the exact solution, on $\mathcal{S}$. It can be seen that in all cases, the L^2 error of the linear

Table 1. Comparison of L^2 errors between the projection of the exact solution on the space of piecewise linear functions and the function of this space, whose values are exact at the nodes ("interpolation").

DOMAIN	ΔX	ERROR PROJECTION	ERROR INTERPOLATION
N	0.267	0.715E-02	0.159E-01
N	0.053	0.265E-03	0.646E-03
I	0.267	0.715E-02	0.159E-01
I	0.053	0.265E-03	0.646E-03
O	0.267	0.497E-02	0.102E-01
O	0.053	0.177E-03	0.429E-03

interpolation of the exact values, is at least twice that of the projection on $\mathcal{S}$. Thus, if this measure of the error is used, one would not be able to discriminate between different methods on the basis of performance.

Before leaving this point, we would like to remark that when the information about the exact solution consists of the exact values at the cell centers exclusively, the extension of this information to the entire interval can be done in manners which are more efficient than using linear interpolation. For example, one could use a high order interpolation procedure, or solve a local problem (this is a kind of post-processing), to mention just a few of the possibilities for processing such information.

Therefore, a norm that directly compares the values at the cell centers was used to compare the errors of the different methods. The norm chosen was the "average Euclidean norm"

$$\|u-\hat{u}\| = \left(\frac{1}{E} \sum_{1}^{E} (u_i - \hat{u}_i)^2 \right)^{1/2}$$

Here, u_i are the values of the exact solution at the cell centers, while $\hat{u}_i$ are those of the approximate one.

Table 2 summarizes the numerical results. As in [1], the final time $t_f=0.5$, Δx is taken to be $4/15 \cong 0.267$ ($Pe=26\frac{2}{3}$) and $\Delta x=\frac{4}{75} \cong 0.0533$ ($Pe=5\frac{1}{3}$). For $\Delta x=\frac{4}{15}$, $\Delta t=0.25$ was used ($Cu=9\frac{3}{8}$). For $\Delta x=4/75$, the values 0.25, 0.05 and 0.01 of Δt, were used, which correspond to $Cu=46\frac{7}{8}$, $9\frac{3}{8}$ and $1\frac{1}{7}$, respectively. The integrals involving initial or boundary conditions were evaluated using Gauss-Kronrod rules to a high degree of precision. In Table 2, the Euclidean errors associated with the approximate solutions that were derived using CELLAM are compared with those obtained with BELLAM [1]. In all cases the errors listed correspond to the final time $t_f=0.5$.

TABLE 2. Comparison of errors between ELLAM-Cells and Bilineal-ELLAM

Run	DOM	Bound.Cond IN	Bound.Cond OUT	Δx	Δt	Euclidean Error Cells	Euclidean Error Bilineal	Maximun Value Cells	Maximun Value Bilin	Maximun Value Exact
1	N	D	F	0.267	0.25	0.501E-02	0.652E-02	0.804	0.813	0.784
2	N	D	F	0.053	0.25	0.442E-02	0.446E-02	0.803	0.803	0.784
3	N	D	F	0.053	0.05	0.103E-02	0.105E-02	0.788	0.788	0.784
4	N	D	F	0.053	0.01	0.353E-03	0.265E-03	0.785	0.785	0.784
5	I	D	F	0.267	0.25	0.315E-02	0.695E-02	0.791	0.806	0.784
6	I	D	F	0.053	0.25	0.276E-02	0.289E-02	0.793	0.793	0.784
7	I	D	F	0.053	0.05	0.727E-03	0.822E-03	0.786	0.786	0.784
8	I	D	F	0.053	0.01	0.232E-03	0.289E-03	0.784	0.785	0.784
9	I	F	F	0.267	0.25	0.302E-02	0.684E-02	0.791	0.807	0.784
10	I	F	F	0.053	0.25	0.275E-02	0.287E-02	0.793	0.793	0.784
11	I	F	F	0.053	0.05	0.718E-03	0.821E-03	0.786	0.786	0.784
12	I	F	F	0.053	0.01	0.247E-03	0.293E-03	0.784	0.785	0.784
13	O	D	D	0.267	0.25	0.298E-02	0.452E-02	0.816	0.816	0.816
14	O	D	D	0.053	0.25	0.258E-02	0.262E-02	0.816	0.816	0.816
15	O	D	D	0.053	0.05	0.557E-03	0.614E-03	0.816	0.816	0.816
16	O	D	D	0.053	0.01	0.264E-03	0.202E-03	0.816	0.816	0.816

In general terms, one may conclude that in these examples, CELLAM performed slightly better than BELLAM. Runs 1 to 4 do not involve significant boundary contributions. When this is the case, BELLAM and the Modified Method of Characteristics (MMOC), become identical [1]. From the results shown in Table 2, it follows that in the examples treated, CELLAM is slightly more precise than MMOC. On the other hand, when the boundary contributions are important, MMOC is considerably less accurate than CELLAM and BELLAM.

B. Comparison Based on the Maximum Value

In [1], the maximum of the numerical solution was compared with the maximum of the exact solution. Thus, for completeness, the same comparison is made here and the results are also illustrated in Table 2. Inspecting this table, it is seen that also when the performance is judged according to this criterium, the results obtained with CELLAM are at least as good as BELLAM.

Observe that when the domain is $O=[-3,2\frac{1}{3}]$, the maximum of the Gaussian distribution (6.1) has already crossed the outflow boundary of the spatial domain, so that when the boundary conditions are of Dirichlet type, the maximum values of the approximate and the exact solutions are equal. Hence, this comparison is not informative in those cases.

7 DISCUSSION AND CONCLUSIONS

The central subject of Quantitative Isotopic Hydrology, consists in studying the transport of tracers by water flowing in a porous medium and the interactions that take place between the solid matrix and the solutes. The corresponding mathematical models, derive from the advection-diffusion equation. The numerical solution of this equation, is a problem of great importance in many other scientific and technical fields, as well and it is being the subject of intensive research.

The numerical treatment of the advection-diffusion equation when advection is dominant, has been a challenging problem for a long time, specially if a sharp front is present. A feature that is required from algorithms in order to be able to model effectively advection dominated transport, is that its performance be independent of the Courant number, to a large extent. Another feature which is essential, specially in Quantitative Isotopic Hydrology, is that the algorithms be mass-conservative, even when significant boundary behavior is present.

It has been recognized that in order for the performance of an algorithm to be independent of the Courant number, it is necessary to incorporate in its formulation the structure of characteristic lines. Methods which are based in the characteristic structure of the differential equations, are known as "characteristic" or "Lagrangian" methods. Until recently, characteristic methods had had three important limitations: inability to ensure mass conservation, inability to treat boundary fluxes effectively and the introduction of numerical dispersion, due to low order interpolation or integration.

With the developmenmt by the author and coworkers, of Eulerian-Lagrangian Localized Adjoint Methods (ELLAM), which are based in the general LAM methodology introduced by the author, the limitations of characteristic methods mentioned above, have been overcome to a large extent.

The ELLAM approach can be implemented in several manners. Up to now two such implementations have been developed: BELLAM and CELLAM. Evidence has been presented, which indicates that CELLAM is at least as accurate as BELLAM and in some cases, more accurate. In addition, CELLAM is easier to implement and more general, since it is applicable to the general advection-diffusion equation with non-constant coefficients.

Here BELLAM and CELLAM have been explained and discussed, making them more readibly available to the scientific community which works in Quantitative Isotopic Hydrology.

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