Finite Elements in Fluids

New trends and applications

Part II

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FINITE ELEMENTS IN FLUIDS
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APPLICATION OF LAM TO ADVECTION DOMINATED TRANSPORT

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ABSTRACT. Two very effective Eulerian-Lagrangian approaches to treat advection-dominated transport, have been developed in the general framework of the Localized Adjoint Method: Bilinear ELLAM (BELLAM) and ELLAM-Cells (CELLAM). In this paper, they are explained and discussed briefly.

1. INTRODUCTION

The numerical solution of the advective-diffusive transport equation is a problem of great importance because many problems in science and engineering involve such mathematical models. When the process is advection dominated the problem is especially difficult. The methods available derive from two main approaches: Eulerian and Lagrangian, or Eulerian-Lagrangian, when such approaches are combined.

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 ($Cu \equiv V\Delta t/\Delta x$) 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. In addition, other Eulerian methods can be developed that perform better than OSM approximations, although they still suffer from severe Courant number limitations. In [1], a review of this class of methods and characteristics methods that were available previous to the development of Eulerian-Lagrangian Localized Adjoint Methods, was presented.

Lagrangian procedures profit from the structure of characteristic curves, treating the advective component by a characteristic tracking algorithm (a Lagrangian frame of reference), and the diffusive step is treated separately using a more standard spatial approximation. These methods have the significant advantage that Courant number restrictions of Eulerian methods are alleviated because of the Lagrangian nature of the advection step. When the procedure is purely Lagrangian, a moving grid has to be used, but the grid is fixed when the approach is Eulerian-Lagrangian, as in the Modified Method of Characteristics (MMOC).

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 [1–7]. These functions locally satisfy the homogeneous adjoint equation within each element. The method so obtained is the Eulerian-Lagrangian Localized Adjoint Method (ELLAM), whose theoretical basis was explained at some length in [2]. This framework is quite wide and in addition to providing a unification of characteristic methods (CM's), supplies a systematic procedure for incorporating boundary conditions in CM approximations. Complete treatments of boundary conditions in Eulerian-Lagrangian methods are feasible, and the resulting algorithms are mass conservative, when this frame work is used.

The theoretical framework of ELLAM [2] can be implemented in many different manners. Up to now two different classes of test functions have been used in ELLAM. In [1], bilinear functions which are defined as the "chapeau" functions at level time t_{n+1} and constant along characteristic curves, were applied and in this manner the first complete treatment of boundary conditions in Eulerian-Lagrangian methods was developed, which leaded to a conservative scheme for the general transport equations.

In addition, the application of test functions which are defined as box functions at level t_{n+1}, and which are also constant along characteristic curves, has been carried out independently in [3,4], under the name of FVELLAM, where some numerical difficulties were encountered and in [5–7], under the name of ELLAM Cells (CELLAM), where such numerical difficulties were overcome. In this paper, a brief description of these procedures and a discussion of their relative merits, is presented.

2. Bilinear ELLAM (BELLAM)

In what follows, we consider the one-dimensional transient advection-diffusion equation in conservation form:

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

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

subject to initial conditions

$$u(x,t_n) = u^n(x),$$

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 were chosen in Eqs. (2.1) and (2.2), is convenient when applying a step by step solution procedure. This approach was first presented in a sequence of two papers ([1] and [2]). For simplicity only the case of constant coefficients will be explained here, although the case of variable coefficients has already been implemented (see for example [8]). For simplicity, we proceed in an ad-hoc manner, but a more systematic exposition placing the procedures discussed in this article in the general frame-work of the Localized Adjoint Method (LAM), is given in this same volume [9] (see also [2]).

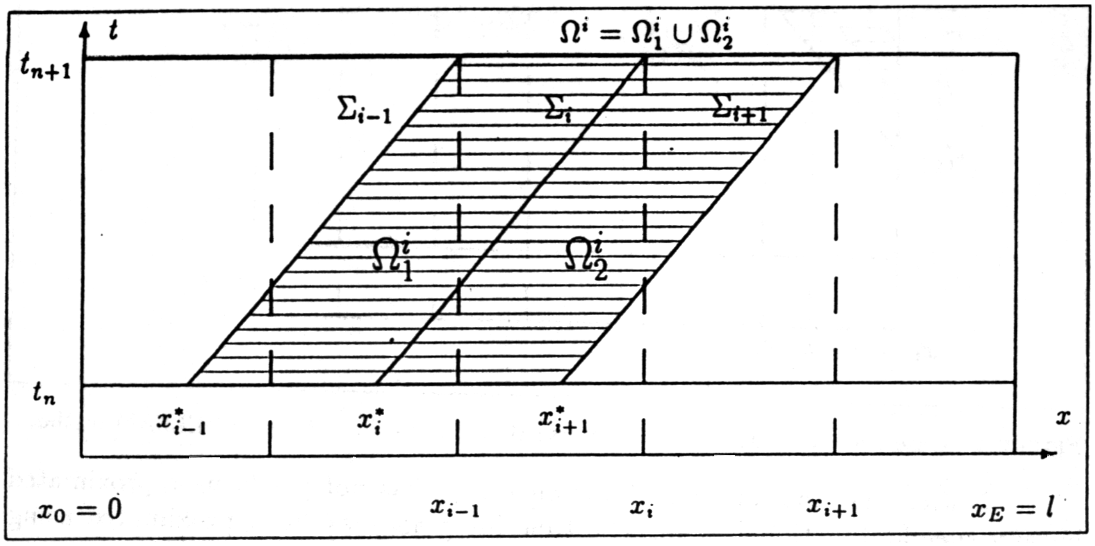


FIGURE Space-time support of w^i for BELLAM method

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

$$w^i(x,t) = \begin{cases} \dfrac{x - x_{i-1}}{\Delta x} + V\dfrac{t_{n+1} - t}{\Delta x} & (x,t) \in \Omega^i_1, \\[2ex] \dfrac{x_{i+1} - x}{\Delta x} + V\dfrac{t_{n+1} - t}{\Delta x} & (x,t) \in \Omega^i_2, \\[2ex] 0, & \text{all other } (x,t), \end{cases}$$

where Ω^i_1 and Ω^i_2 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

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

2.1 Discretization in the interior of Ω

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

$$\int_{x_{i-1}}^{x_{i+1}} u(x, t_{n+1}) w^i(x, t_{n+1})\, dx \quad \frac{D}{\Delta x}\left\{ \int_{t_n}^{t_{n+1}} u(\sigma_{i-1}(t), t)\, dt \right.$$

$$\left. 2\int_{t_n}^{t_{n+1}} u(\sigma_i(t), t)\, dt + \int_{t_n}^{t_{n+1}} u(\sigma_{i+1}(t), t)\, dt \right\}$$

$$\int_{x^*_{i-1}}^{x^*_{i+1}} u(x, t_n) w^i(x, t_n)\, dx + \int_{\Omega} f_{\Omega} w^i\, dx\, dt,$$

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).

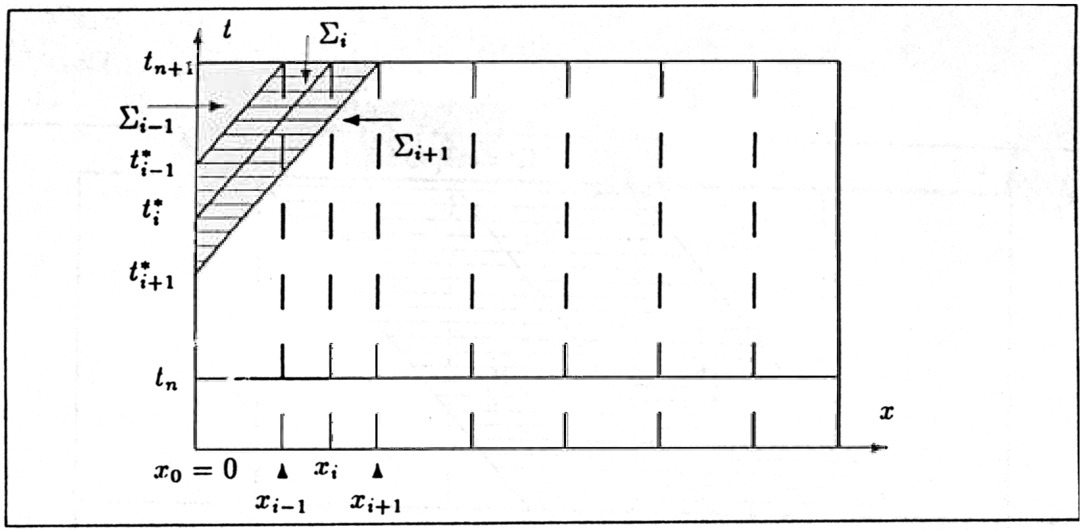


FIGURE 2. Case when the support of w^i intersects the inflow boundary for BELLAM methd

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 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. 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 (see [1]).

2.2 Boundary conditions

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_i, it is obtained:

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

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

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

The integrals along characteristics appearing in Eq. (2.6) can again be evaluated by means of a fully implicit approximation. However, it must be mentioned that 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 3, where a derivation satisfying such conditions is carried out for CELLAM (a more detailed exposition is given in [7]).

The last term in the left-hand side of Eq. (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 [5], is equivalent to:

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

However, this approximation, 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 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. ELLAM CELLS

This method was presented originally in [5] and [7] (see also [6]). To explain this method and conform with notations that are standard for the method of cells, it is convenient to modify slightly the notation. A partition

$$\{x_1, x_{3/2}, x_{5/2}, \quad , x_{E-1/2}, x_E\}$$

is introduced, which induces a partition of Ω into subregions $\{\Omega^1, \Omega^2, \dots, \Omega^E\}$, if for each $i = 2, \dots, E$, 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

$$x_{i+1/2} - x_{i-1/2} = h, \quad \text{for} \quad i = 2, \quad , E-1, \quad x_{3/2} - x_1 = h/2, \quad x_E - x_{E-1/2} = h/2 \qquad (3.1)$$

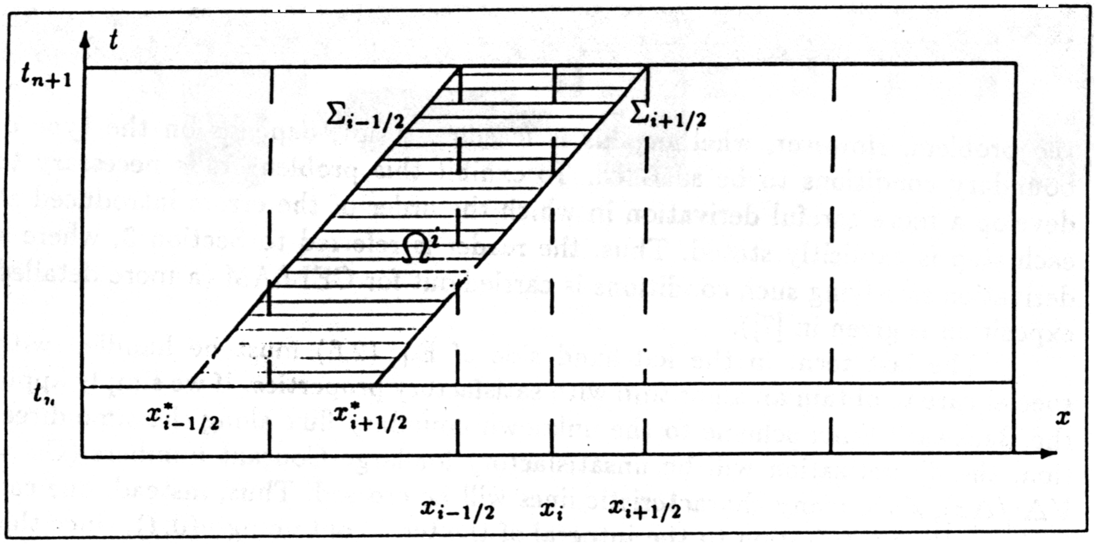


FIGURE 3. Space-time support of w^i for CELLAM method

A system of constant weighting functions is applied. These are the characteristic functions of the subregions that constitute this partition. Actually, not all of them are required. The system of weighting function that was applied in [7] is:

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

3.1 Discretization in the interior of Ω

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

$$\int_{x_{\alpha-1}}^{x_{\alpha+1}} u^{n+1}\,dx + \int_{t_n}^{t_{n+1}} \left(D\frac{\partial u}{\partial x}\right)_{\Sigma_{\alpha+1/2}} dt \; - \int_{t_n}^{t_{n+1}} \left(D\frac{\partial u}{\partial x}\right)_{\Sigma_{\alpha-1/2}} dt = \int_{x^*_{\alpha-1}}^{x^*_{\alpha+}} u^n\,dx \qquad (3.3)$$

Equation (3.3) and a modified version of it designed to incorporate terms contributed by the boundary when Ω^α intersects the time-axis, is the starting point of the numerical treatment. Observe that

$$\int_{x_{\alpha-1}}^{x_{\alpha+1}} u^{n+1}\,dx - \int_{x^*_{\alpha-1}}^{x^*_{\alpha+1}} u^n\,dx = O(hk) \qquad (3.4a)$$

and

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

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 Eqs. (3.4), 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 (3.3) *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 [7], the processing of such information had as its goal, 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. (3.3), the integrals from t_n to t_{n+1}, were firstly approximated in a fully implicit manner (i.e., by a one-step Backward-Euler approximation at t_{n+1}). Thus

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

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

For a uniform spacing and constant coefficients, a central difference approximation scheme is applied, which yields:

$$\left\{ \left(\frac{\partial u^{n+1}}{\partial x}\right)_{\alpha+1/2} \quad \left(\frac{\partial u^{n+1}}{\partial x}\right)_{\alpha-1/2} \right\} k = \frac{u_{\alpha+1} + u_{\alpha-1} - 2u_\alpha}{h} k + O(h^3k) \quad (3.6)$$

The extension of this formula to the case of a non-uniform partition, can be done in a similar manner. However, the order of the error associated with such an approximation is reduced by one and the overall error in (3.6) 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 time levels of the time discretization at nodes. Thus, all the approximations in space have to be carried out with special care. A special feature of the approximations that were used in [7], is that no assumption was made about the shape of the solution.

The first integral in (3.3) is approximated by

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

and only the second order derivative requires a numerical approximation, since the information is being concentrated in the "cell centers". To get a tri-diagonal structure for the matrix, it is convenient to use three-point approximations only. In the case of a "uniform partition", a central difference approximation yields

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

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 (3.8), 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. (3.3) was approximated using an approach similar to (3.7); 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.

3.2 Boundary conditions

The numerical approximations presented thus far, 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. In connection with the numerical treatment of boundary conditions, numerical diffusion is due to a large extent, to the fact that characteristics do not cross the boundaries of the spatial region Ω_x, at times levels belonging to the partition of the time interval. Thus, just as in the interior of the spatial region, the approximations in space have to be performed with special care to minimize numerical diffusion, when dealing with the boundary conditions, it is the time integrals that have to be treated with special care. This is specially true for an inflow boundary, by two reasons at least. Firstly, the information that is supplied at an inflow boundary has a larger effect on the solution than that which is supplied at an outflow boundary, since the former is transmitted to the interior of the spatial region by advection and diffusion, while the latter is only transmitted by diffusion. Secondly, 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.

In [7], it was pointed out that to some extent 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 accuracy. However, when the total flux is prescribed or when considering boundary conditions of Neuman type, this was not the case. This was discussed in [7], in connection with total flux conditions and the argument presented there is explained here.

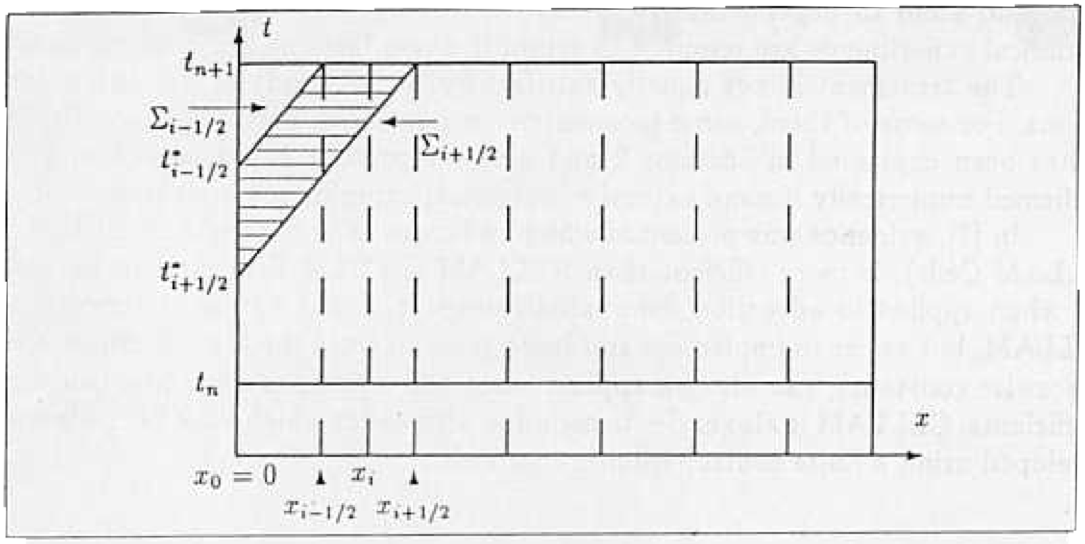
Assume that total flux conditions are being considered and that Ω^α intersects the inflow boundary, as illustrated in Fig. 4. Then, the weighted equation is [7]:

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

$$\int_{t^*_{\alpha+1/2}}^{t^*_{\alpha-1/2}} \left(D\frac{\partial u}{\partial x}\right)_{\Sigma_{\alpha+1/2}} dt = \int_{t^*_{\alpha+1/2}}^{t^*_{\alpha-1/2}} F(t)\,dt \quad (3.9)$$

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

Since $F(t)$ is a datum, the corresponding integral offers no special difficulty in being approximated to any desired order of accuracy. The first two integrals, which also occur in the left-hand side Eq. (3.3), can be treated in the manner that was explained when the "discretization in the interior of Ω", was discussed.



IGURE 4. Case when the support of w^i intersects the inflow boundary for CELLAM method.

However, the last integral of the same side of the equation, is not amenable to be approximated to the order of accuracy that is required. If a translation in any direction is a applied to the expression under the integral sign, for its evaluation, this must be done without crossing characteristic curves, in order to preserve the advantages of characteristic methods [7]. A translation along the characteristic curve $\Sigma_{\alpha+1/2}$, yields

$$\int_{t^*_{\alpha+1/2}}^{t^*_{\alpha-1/2}} \left(D\frac{\partial u}{\partial x}\right)_{\Sigma_{\alpha+1/2}} dt = (t^*_{\alpha-1/2} - t^*_{\alpha+1/2})\left(D\frac{\partial u^{n+1}}{\partial x}\right)_{\alpha+1/2} + O(k^2 \quad (3.10)$$

which is not of the required precision.

Developing algorithms which overcome the shortcoming of the approximation (3.10), would be considerably more elaborate. For example, one could construct weighting functions satisfying suitable boundary conditions, using the guidelines of the general theory of the Localized Adjoint Method [2]. However, thus far this has not been required. The inconsistency of the order approximation which is introduced when Eq. (3.10) is used, has not been manifested in the results of the numerical experiments that have been carried out up to now.

4. Discussion and conclusions

The problem of treating numerically advection-diffusion problems when advection is dominant has been a challenging problem for a long time. A natural goal of the research efforts that have taken place in this area is to develop algorithms whose efficiency is independent of the Courant number, independently of the boundary conditions that are imposed. A very important step forward was given with the development of characteristic methods, specially the modified method of characteristics [10–12]. However, the inability of those methods to treat the boundary conditions systematically had been a very limitative factor in their applications.

Localized Adjoint Method [2], when combined with the method of characteristics, has lead to the development of Eulerian-Lagrangian Localized Method (ELLAM) which has permitted a systematic treatment of boundary conditions and the development of mass conservative algorithms [1–7]. The numerical evic presented in [1] and [7] indicate that the algorithms develop in this framewor essentially independent of the magnitude of the Courant number (the integer of it) and seem to depend mainly on its fractionary part. However, additi numerical experiments are required to establish these facts on a more firm b

The treatment is not equally satisfactory for all kinds of boundary ditions. For some of them, some inconsistencies have been detected theoretic as has been explained in Sections 2 and 3 of the present paper, which ma confirmed numerically if more extensive numerical experiments are carried ou

In [7], evidence was presented which indicates that the method CELI (ELLAM-Cells), is more efficient than BELLAM (ELLAM-Bilinear). In par lar, when applied to advection dominated transport, CELLAM is as accurat BELLAM, but easier to implement and more general, since the test functions (piecewise constant), can also be applied when the equations have non-cons coefficients. CELLAM is also easier to combine with codes which have been alr developed using a finite control-volume approach.

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