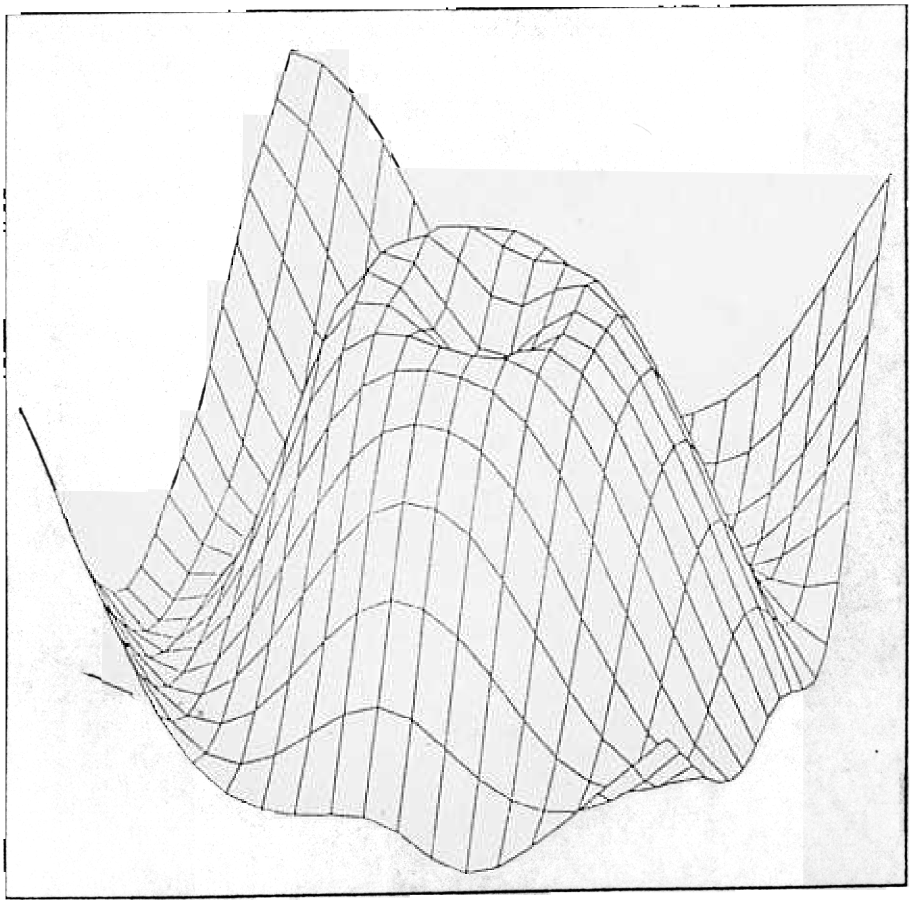
# ADVANCES IN COMPUTER METHODS FOR PARTIAL DIFFERENTIAL EQUATIONS - VII



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# ELLAM PROCEDURES FOR ADVECTION DOMINATED TRANSPORT

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## 1. INTRODUCTION

The Localized Adjoint Method (LAM) is a new and promising methodology for discretizing partial differential equations which has been introduced by I. Herrera. It is based on Herrera's Algebraic Theory of Boundary Value Problems [1-5], as it is explained in a companion paper [6]. Applications have successively been made to ordinary differential equations, for which highly accurate algorithms were developed [4,7-9], multidimensional steady state problems [10], and optimal spatial methods for advection-diffusion equations [11-18]. More recently, the development of generalizations of Characteristic Methods, known as Eulerian-Lagrangian Localized Adjoint Method (ELLAM), was initiated [19,20]. Already many specific applications have been made [21-26].

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) Time truncation error dominates the solutions, (ii) 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. However, other Eulerian methods can be developed that perform better than OSM approximations [27-29], although they still suffer from severe Courant number limitations.

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. Furthermore, because the spatial and temporal dimensions are coupled through the characteristic tracking, the influence of time truncation error is greatly reduced. 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. These functions locally satisfy the homogeneous adjoint equation within each element. The method so obtained is the Eulerian-Lagrangian Localized Adjoint Method (ELLAM) [19,20]. The ELLAM approach, in addition to providing a unification of characteristic methods (CM's), supplies a systematic framework for incorporating boundary conditions in $CM$ approximations. Any type of boundary conditions can be accommodated in a mass conservative manner. This seems to be the first complete treatment of boundary conditions in Eulerian-Lagrangian methods, that leads to a conservative scheme for the general transport equations [19].

Up to now two different classes of test functions have been used in ELLAM: bilinear functions (Bilinear-ELLAM) [19,20,30,31] which are defined as "chapeau" functions at level time $t^{n+1}$, and constant along characteristic curves. 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 (Cell-ELLAM), is under investigation [32,33]. In this paper these approaches are briefly explained.discussion of the relative merits of these approaches, is presented.

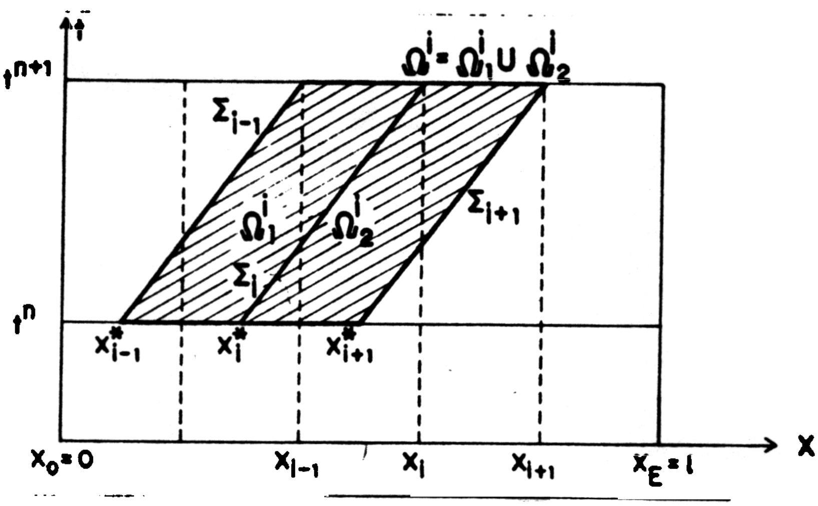


FIGURE 1. Decomposition of $\Omega$ into the subregions $\Omega^i$, $i = 1,$ $E$.

The following properties of the ELLAM Cells method are worth mentioning: it is directly applicable to the case of variable coefficients; the formulation is simpler than the Bilinear-ELLAM, both in the interior and at the boundaries. This is especially relevant in complicated problems, such as Petroleum Engineering.

## 2. Advection-Diffusion Equation

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

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

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

subject to initial conditions

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

and suitable boundary conditions, at $x = 0$ and $l$. Here, it is assumed that $V > 0$. The following development accommodates any combination of boundary conditions. The manner in which the region $\Omega$ and the initial conditions were chosen in Eqs. (2.1) and (2.2), is convenient when applying a step by step solution procedure. Observe that in this case the adjoint operator $\mathcal{L}^*$ is:

$$\mathcal{L}^* w \equiv -\frac{\partial w}{\partial t} - \frac{\partial}{\partial x}\left(D\frac{\partial w}{\partial x}\right) - V\frac{\partial w}{\partial x} + Rw. \tag{2.3}$$

It will be useful to decompose the boundary $\partial\Omega$ into $\partial_0\Omega, \partial_l\Omega, \partial_n\Omega$ and $\partial_{n+1}\Omega$, which are defined as the subsets of $\Omega$ for which $(x,t)$ satisfies $x = 0, x = l, t = t^n$ and $t = t^{n+1}$, respectively. The initial conditions, given by Eq. (2.2), are to be satisfied at $\partial_n\Omega$ and the boundary conditions pertain to $\partial_0\Omega \cup \partial_l\Omega$. These latter conditions can be of Dirichlet ($u = u_\partial$), Neumann ($D\frac{\partial u}{\partial x}\mathrm{n} = q$) or Robin type, or a combination of them. Here, it is understood that $\mathrm{n} = 1$ at $x = l$ and $\mathrm{n} = -1$ at $x = 0$. For the time being, only Dirichlet conditions will be considered, although the methodology accommodates any of them.

In addition, a partition of $[0,l]$ is introduced and the region $\Omega$ is decomposed into a collection of subregions $\Omega^1, \ldots, \Omega^E$, each one associated with the node of the same subindex, as shown in Fig. 1. These subregions are limited by space-time curves $\Sigma_\alpha$ whose positions at any time $t$ ($t^n \leq t \leq t^{n+1}$) are given by the functions $\sigma_\alpha(t)$ and it will be assumed that discontinuities exclusively occur on these lines. Thus for the general notation introduced in [6], in this volume, $\Sigma = \cup\Sigma_\alpha$ in this case. Clearly, the velocity of propagation $V_\Sigma$ of each one of these lines is $d\sigma_\alpha/dt$.

The bilinear function $C(w,u)$ is defined by:

$$C(w,u) = -uw \text{ on } \partial_{n+1}\Omega, \qquad C(w,u) \equiv 0 \text{ on } \partial_n\Omega, \tag{2.4a}$$

$$C(w,u) = w\left(D\frac{\partial u}{\partial x} - Vu\right)\mathbf{n} \text{ on } \partial_0\Omega \cup \partial_l\Omega. \tag{2.4b}$$

When the boundary conditions are Neumann, this definition must be modified to be:

$$C(w,u) = -u\left(D\frac{\partial w}{\partial x} + Vw\right)\mathbf{n}$$

or if the flux $(D\frac{\partial u}{\partial x} - Vu)\mathbf{n}$ $(= F)$ is prescribed:

$$C(w,u) = -uD\frac{\partial w}{\partial x}\mathbf{n}.$$

While the function $\mathcal{K}(w,u)$ is equal to the sum:

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

with $\mathcal{K}^0$ and $\mathcal{K}^1$ defined by:

$$\mathcal{K}^0(w,u) = (1+V_\Sigma^2)^{-1/2}\dot{u}\left\{\left[D\frac{\partial w}{\partial x}\right] + (V - V_\Sigma)[w]\right\};$$

$$\mathcal{K}^1(w,u) = -(1+V_\Sigma^2)^{-1/2}[w]D\overline{\dot{\frac{\partial u}{\partial x}}} \tag{2.6b}$$

where $[u] = u_+ - u_-$, $\dot{u} = (u_+ + u_-)/2$ and $u_+$, $u_-$ represent the limits of $u$ as $\Sigma$ is approached from the positive and negative sides, respectively. In what follows, the positive side of $\Sigma$ is defined to be the one towards which the vector $\mathbf{N}$, perpendicular to $\Sigma$, points to. The direction of this vector is chosen arbitrarily.

Observe that $C^*(u,\cdot) \equiv 0$ on $\partial_n\Omega$, no information is sought at $t = t^n$, which is natural for an initial value problem. Observe also that $\mathcal{K}^0$ and $\mathcal{K}^1$ are defined so that are associated with the value of the sought solution $u$ and with the derivative of the sought solution $\partial u/\partial x$, respectively.

LAM procedures use "Herrera's variational formulation in terms of the sought information", as is explained in [6]. For this case it is:

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

where $D_2$ is a suitable set of weighting functions,

$$\langle Q^*u, w\rangle = \int_\Omega u\mathcal{L}^*w\,d\mu,$$

$$\langle C^*u, w\rangle = \int_{\partial_{n+1}} C(w,u)dx + \int_{t^n}^{t^{n+1}} \{C(w,u)\}_{x=l}\,dt + \int_{t^n}^{t^{n+1}} \{C(w,u)\}_{x=0}\,dt,$$

$$\langle K^*u, w\rangle = \int_\Sigma \mathcal{K}(w,u)\,d\mu = \sum_\alpha \int_{\Sigma_\alpha} \mathcal{K}(w,u)\,d\mu \tag{2.8c}$$

and

$$\langle f, w\rangle = \int_\Omega wf_\Omega\,d\mu; \quad \langle g, w\rangle = \int_{\partial\Omega} g_\partial(w)\,d\mu; \quad \langle j, w\rangle = \int_\Sigma j_\Sigma(w)\,d\mu. \tag{2.9}$$

Here, $d\mu$ is used to denote the element of area (space-time) in $\Omega$ and of length in any of the space-time curves which constitute $\Sigma$. The functions $g_\partial$ and $j_\Sigma$ are defined by means of the boundary and jump conditions, respectively, as explained in [6].

It is convenient to decompose the bilinear functional $K^*$ into the contributions which stem from $\Sigma_\alpha$, for $\alpha = 1, \ldots, E$. If we define

$$\langle K_\alpha^* u, w\rangle = \int_{\Sigma_\alpha}\left\{\dot{u}\left[D\frac{\partial w}{\partial x}\right] - [w]D\overline{\dot{\frac{\partial u}{\partial x}}} - (V - V_\Sigma)\dot{u}\right\}_\alpha dt,$$

where, the subindex $\Sigma_\alpha$ means that the line integral is to be carried out on $\Sigma_\alpha$ (note that $dt = (1+V_\Sigma^2)d\mu$), then

$$K^* = \sum_{\alpha=1}^{E} K_\alpha^*. \quad (\text{:}$$

The linear functionals $Q^*u, C^*u$ and $K^*u$, supply information about the sought solution at points in the interior of the region $\Omega$, the complementary boundary values at $\partial\Omega$ and the generalized averages of the solution at $\Sigma$, respectively.

It is convenient, also, to decompose the bilinear functional $C^*$ into the contributions from $\partial_n\Omega, \partial_{n+1}\Omega, \partial_0\Omega$, and $\partial_l\Omega$. In this manner one can write:

$$C^* = C^*_{n+1} + C^*_0 + C^*_l, \tag{2.12}$$

where

$$\langle C^*_{n+1}u, w\rangle = -\int_0^l (uw)_{t=t^{n+1}}\,dx, \tag{2.13a}$$

$$\langle C^*_0 u, w\rangle = -\int_{t^n}^{t^{n+1}} w\left\{\left(D\frac{\partial u}{\partial x} - Vu\right)\right\}_{x=0} dt, \qquad \langle C^*_l u, w\rangle = -\int_{t^n}^{t^{n+1}} w\left\{\left(D\frac{\partial u}{\partial x} - Vu\right)\right\}_{x=l} dt. \tag{2.13b}$$

The functionals (2.9) for equation (2.1) are: $\langle j, w\rangle \equiv 0$ and $g$, defined by $g = g_n + g_0 + g_l$, with

$$\langle g_n, w\rangle = -\int_0^l u^n w(t^n)\,dx,$$

$$\langle g_0, w\rangle = -\int_{t^n}^{t^{n+1}} \left\{uD\frac{\partial w}{\partial x}\right\}_{x=0} dt, \qquad \langle g_l, w\rangle = -\int_{t^n}^{t^{n+1}} \left\{uD\frac{\partial w}{\partial x}\right\}_{x=l} dt.$$

The "variational formulation in terms of the sought information" for the transient advection-diffusion equation in space-time is obtained by substituting (2.3) to (2.6) in (2.7). This formulation supplies a firm basis for analyzing the information that is contained in an approximate one. In particular it yields guidelines for developing weighting functions which concentrate the information in a desired manner. A possibility is to eliminate all the information in the interior of each one of the subregions $\Omega^i$ $(i = 1, \ldots, E)$.

In this later case:

$$\mathcal{L}^*w \equiv -\frac{\partial w}{\partial t} - \frac{\partial}{\partial x}\left(D\frac{\partial w}{\partial x}\right) - V\frac{\partial w}{\partial x} + Rw = 0, \text{ in } \Omega \tag{2.15}$$

and Eq. (2.7) becomes $\langle (C^* + K^*)u, w\rangle = \langle g - f, w\rangle$. Different choices of test functions that satisfy (2.15), lead to different classes of approximations, including optimal spatial methods and general characteristic methods [20]. The classification of numerical methods into OSM and CM, can be related to the speed of propagation of discontinuity lines. If time independent solutions of Eq. (2.15) are chosen, as weighting functions, then $V_\Sigma = 0$, necessarily, and one is led to optimal spatial methods, to which several papers have been devoted, using the LAM approach [12-18]. On the other hand, if the lines $\Sigma_j$, satisfy $V_\Sigma = V$, characteristic methods are obtained. Eulerian Lagrangian Localized Adjoint Methods (ELLAM) use this latter approach [19,20,30–33]

An important advantage of the ELLAM approach, is due to its ability to deal with boundary conditions, effectively. By inspection of Eq. (2.4$b$), it is seen that weighting functions which eliminate the information at lateral boundary of $\Omega$, (i.e., $C(w^i, \cdot) = 0$), must fulfill:

$$w^i = 0, \text{ on } x = 0 \text{ and } x =$$

When the support of $w^i$ does not intersect lateral boundaries, condition (2.15) is automatically fulfilled. When this is not the case, to satisfy (2.15), special functions for each type of boundary condition must be constructed, although the construction of these test functions may be complicated, in general.

Quite satisfactory results in the treatment of boundary conditions have been reported, even without the use of the specialized test functions mentioned above. Indeed it has been concluded the ELLAM approach provides a systematic and consistent methodology for proper incorporation of boundary conditions. This allowed to construct an overall approximation that possesses the conservative property, thereby assuring conservation of mass in the numerical solution [19].

For the implementation of ELLAM procedures two different classes of test functions have been used up to now: bilinear functions (Bilinear-ELLAM) [19,20,30,31], and more recently constant weights [32,33], which yield an ELLAM "cells" or "control volume" method.

## 3. Bilinear-ELLAM

This approach was first presented by the ELLAM Group in [19,20]. 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 [34]).

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:

$$w^i(x,t) = \begin{cases} \dfrac{x - x_{i-1}}{\Delta x} + V\dfrac{t^{n+1} - t}{\Delta x}, & (x,t) \in \Omega_1^i \\[2ex] \dfrac{x_{i+1} - x}{\Delta x} + V\dfrac{t^{n+1} - t}{\Delta x} & (x,t) \in \Omega_2^i \\[2ex] 0 & \text{all other } (x,t) \end{cases}$$

where $\Omega_1^i$ and $\Omega_2^i$ 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.; $[dw/dx] \neq 0$). In view of Eqs. (2.6), it is clear that for this choice, $\mathcal{K}^1(w,u)$ vanishes identically while

$$\mathcal{K}^0(w^i, u) = (1 + V_\Sigma^2)^{-1/2} \dot{u} \left[ D\frac{\partial w^i}{\partial x} \right]$$

This latter expression does not vanish on three lines of discontinuity, at most: $\Sigma_{i-1}$, $\Sigma_i$ and $\Sigma_{i+1}$. Thus

$$\langle K^* u, w^i \rangle = \sum_{j=i-1}^{i+1} \langle K_j^* u, w^i \rangle$$

The jumps are

$$\left[\frac{\partial w}{\partial x}\right]_{i-1} = \frac{1}{\Delta x}; \quad \left[\frac{\partial w}{\partial x}\right]_{i} = \frac{-2}{\Delta x}; \quad \left[\frac{\partial w}{\partial x}\right]_{i+1} = \frac{1}{\Delta x}. \qquad (3.4)$$

When the region $\Omega^i$ does not intersect the lateral boundaries, the boundary terms (2.4b) and (2.13b) vanish and the variational principle in terms of the sought information (2.7), reduces to $\langle (C_{n+1}^* + K^*)u, w \rangle = \langle g_n - f, w^i \rangle$:

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

$$= \int_{x_{i-1}^*}^{x_{i+1}^*} u(x,t^n) w^i(x,t^n)\, dx + \int_\Omega f_\Omega w^i\, dx dt, \qquad (3.5)$$

where the unknowns have been collected in the left-hand member of the equation while the data is included in the right one. Recall that $\sigma_i(t)$ is describing the characteristic curve $\Sigma_i$, so that the integrals where they appear are integrals along the characteristics.

Notice that the unknown function $u(x,t)$ has not yet been approximated by any specific functional form. The integrals that appear in this equation may in fact be approximated in many different ways. Different approximations of these integrals lead to different CM algorithms reported in the literature. In all of these, the integrals are approximated in terms of nodal values of $u$ at the discrete time levels $t^n$ and $t^{n+1}$, so that the unknowns in the equation ultimately correspond to nodal values at time $t^{n+1}$. 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 (MMOC) of Douglas and Russell [35]. Further details of the derivations are given in [19].

When a region $\Omega^i$ intersects the inflow boundary, several cases can occur. As an example, we discuss the case illustrated in Fig. 2. Then, the equation $\langle (C_{n+1}^* + K^*)u, w \rangle = \langle g_n - f, w^i \rangle$, becomes:

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

$$+ \int_{t_{i+1}^*}^{t_{i-1}^*} w^i \left\{ D\frac{\partial u}{\partial x}(0,t) - Vu(0,t) \right\} dt = \frac{D}{\Delta x}\left\{ \int_{t_i^*}^{t_{i-1}^*} u(0,t)\, dt - \int_{t_{i+1}^*}^{t_i^*} u(0,t) dt \right\} + \int_\Omega f_\Omega w^i\, dx dt$$

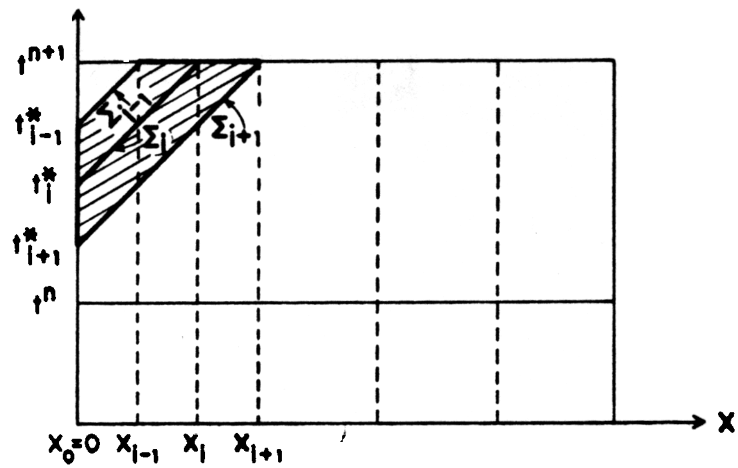


FIGURE 2. Case when the support of the bilinear weighting function $w^i$ intersects the inflow boundary.

The integrals along characteristics appearing in Eq. (3.6), can again be evaluated by means of a fully implicit approximation. However, approximation of the last term in the left side of Eq. (3.6) must be handled with special care, to obtain an algorithm with satisfactory properties. If we simply discretize the unknown diffusive boundary flux along the time direction, the discretization will be unsatisfactory for large Courant number $Cu = V\Delta t/\Delta x$, 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. The remaining part of that integral, can be approximated as it is indicated next:

$$\int_{t^*_{i+1}}^{t^*_{i-1}} w^i D\frac{\partial u}{\partial x}(0,t)\,dt = \frac{D}{V}\int_{x_{i-1}}^{x_{i+1}} w^i\frac{\partial u}{\partial x}(x,t^{n+1})\,dx + O(\Delta t^2) \tag{3.7}$$

Approximations similar to (3.7) were proposed by Russell [30], although the derivation presented here, is more direct, and have been used satisfactorily in numerical applications [19,30,31]. Recently, Wang et al. [31], have carried out an error analysis of several approximations of this kind. Neumann and flux boundary conditions, prescribed in the inflow boundary, can be handled in a similar fashion [19,30,31].

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 $\Sigma_E$, 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 in the outflow boundary, it can be obtained applying procedures which amount essentially to post-processing.

Neumann or flux conditions, imposed in the outflow boundary, are more complicated to deal with (see [19]), when this approach is used. This is in contrast with the method ELLAM cells (or control volume), which is explained in Section 4.

## 4. ELLAM Cells

Keeping the same notation as in the last Section, a notation which is fairly usual for the cells method is introduced. Writing $x_{i+1/2} = x_i + \Delta x/2$, the subintervals $[x_{i-1/2}, x_{i+1/2}]$ (with $i = 1,\ldots,E-1$), $[x_0, x_{1/2}]$ and $[x_{E-1/2}, x_E]$, will be the "cells", while the points $\{x_0,\ldots,x_E\}$ will be the cell "centers". Notice that the first and the last cells are half-length. Assuming $R \equiv 0$, in Eq. (2.1), the test functions to be used, regardless of whether the coefficients are constant or variable, are:

$$w^i(x,t) = \begin{cases} 1, & \text{if } (x,t)\in\Omega^i \\ 0, & \text{if } (x,t)\notin\Omega^i \end{cases} \tag{4.1}$$

where the regions $\Omega^i$ are limited by the curves $\Sigma_{i-1/2}, \Sigma_{i+1/2}$ ($i = 1,\ldots,E-1$) and the boundaries of the space-time region $\Omega$, as illustrated in Fig. 3.

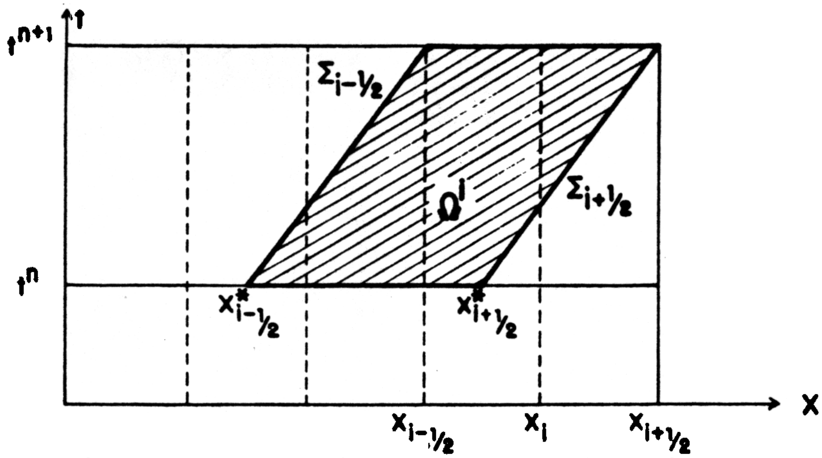


FIGURE 3. Space-time support of the weighting function $w^i$ for the method of cells.

For this case the weighting functions have continuous normal derivative everywhere, although the function it self is discontinuous on the "characteristic" curves $\Sigma$, passing through the boundaries of the cells. Therfore $\mathcal{K}^0(w,u) \equiv 0$, by virtue of Eq. (2.6a), and all the information that is gathered on $\Sigma$, concerns the first derivative of the solution, exclusively. In addition $V_\Sigma = V$.

When the subregion $\Omega^i$ does not intersect the lateral boundaries of the entire region $\Omega$, $\mathcal{K}^1(w^i,u)$ does not vanish identically in two lines of discontinuity, at most: $\Sigma_{i-1/2}$ and $\Sigma_{i+1/2}$. There:

$$[w]_{\Sigma_{i-1/2}} = 1; \qquad [w]_{\Sigma_{i+1/2}} = -1. \tag{4.2}$$

Replacing Eqs. (4.2) into (2.6b), it is obtained

$$\mathcal{K}^1(w,u)_{\Sigma_{i\pm1/2}} = \pm(1+V^2)^{-1/2}\frac{\partial u}{\partial x}. \tag{4.3}$$

Hence, the variational principle in terms of the sought information $\langle (C^*_{n+1} + K^*)u, w\rangle = \langle g_n - f, w^i\rangle$, becomes:

$$\int_{x_{i-1/2}}^{x_{i+1/2}} u(x,t^{n+1})\,dx + \int_{t^n}^{t^{n+1}} D\frac{\partial u}{\partial x}(\sigma_{i-1/2}(t),t)\,dt - \int_{t^n}^{t^{n+1}} D\frac{\partial u}{\partial x}(\sigma_{i+1/2}(t),t)\,dt$$

$$= \int_{x^*_{i-1/2}}^{x^*_{i+1/2}} u(x,t^n)\,dx + \int_\Omega f_\Omega\,dx\,dt. \tag{4.4}$$

where the unknowns have been collected in the left-hand member of the equation, while the data was left in the right one.

Eq. (4.4) is similar to (3.5). In it, the unknown function has not yet been approximated by any specific functional form and the integrals that appear there can be approximated in many different ways. As in Section 3, different approximations of these integrals lead to different algorithms. To be specific, the integrals over characteristics will be approximated by means of a fully implicit approximation. Thus:

$$\int_{t^n}^{t^{n+1}} D\frac{\partial u}{\partial x}(\sigma_{i-1/2}(t),t)\,dt - \int_{t^n}^{t^{n+1}} D\frac{\partial u}{\partial x}(\sigma_{i+1/2}(t),t)\,dt = \left\{\left(D\frac{\partial u}{\partial x}\right)^{n+1}_{i-1/2} - \left(D\frac{\partial u}{\partial x}\right)^{n+1}_{i+1/2}\right\}\Delta t \tag{4.5}$$

Regarding the integral of $u$ at time $t^{n+1}$, there are also several possibilities for approximating it. The simplest is

$$\int_{x_{i-1/2}}^{x_{i+1/2}} u(x,t^{n+1})\,dx = u_i^{n+1}\Delta x + O(\Delta x^3) \tag{4.6}$$

However, the numerical experiments carried out thus far, indicate that the use of Eq. (4.6), produces too much numerical diffusion. A more refined option is:

$$\int_{x_{i-1/2}}^{x_{i+1/2}} u(x,t^{n+1})\,dx = \left(\frac{u_{i+1} + u_{i-1} + 22u_i}{24}\right)\Delta x + O(\Delta x^5) \tag{4.7}$$

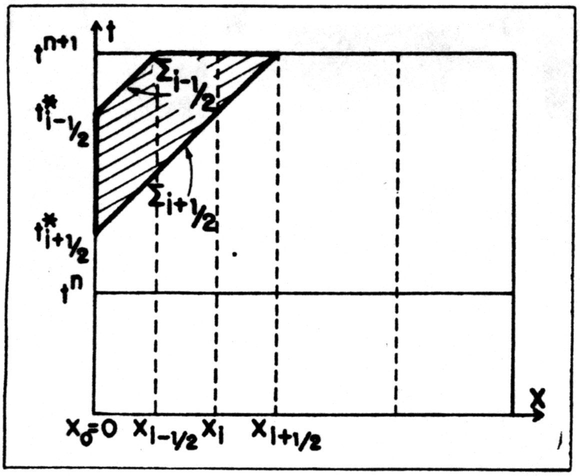


FIGURE 4. Case when the support of the weighting function $w^i$ for the cells method intersects the inflow boundary.

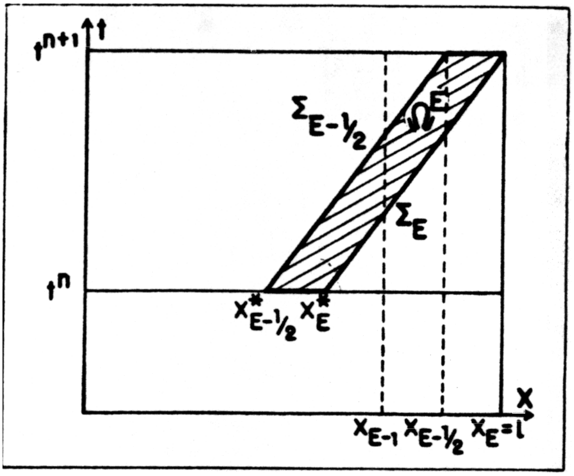


FIGURE 5. Space-time support of the weighting function $w^E$ for Neumann and flux conditions at the inflow boundary.

When the region $\Omega^i$ intersects the inflow boundary, procedures similar to those described in Section 3, must be applied. As an example, consider the equation associated with node $x_i$, illustrated in Fig. 4. This is:

$$\int_{x_{i-1/2}}^{x_{i+1/2}} u(x,t^{n+1})\,dx + D\left\{\int_{t^*_{i-1/2}}^{t^{n+1}} \frac{\partial u}{\partial x}(\sigma_{i-1/2}(t),t)\,dt - \int_{t^*_{i+1/2}}^{t^{n+1}} \frac{\partial u}{\partial x}(\sigma_{i+1/2}(t),t)\,dt\right\}$$
$$+ \int_{t^*_{i+1/2}}^{t^*_{i-1/2}} \left\{D\frac{\partial u}{\partial x}(0,t) - Vu(0,t)\right\} dt = \int_{\Omega} f_\Omega\,dx\,dt. \quad (4.8)$$

Observe that for this case (Dirichlet data), $\langle g_0 + g_l, w^i\rangle \equiv 0$ by virtue of Eq. (2.14b), since $\partial w^i/\partial x \equiv 0$. The treatment of the integral over the boundary $x = 0$ requires some care. As was the case for Eq. (3.6), the crossing of characteristic curves must be avoided when approximating such integral. The term containing $u(0,t)$ is known and can be transposed to the right-hand side of the equation. The remaining one, can be approximated in essentially the same manner that was done for Eq. (3.6); i.e.

$$\int_{t^*_{i+1/2}}^{t^*_{i-1/2}} D\frac{\partial u}{\partial x}(0,t)\,dt = \frac{D}{V}\int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial u}{\partial x}(x,t^{n+1})\,dx + O(\Delta t^2) \quad (4.9)$$

Although the discussion here has been restricted to Dirichlet boundary conditions, similar procedures can be applied to Neumann and flux conditions.

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 an interval neighboring $x_E = l$. Also, the system of equations that is obtained in the manner explained above, is closed, because $u_E^{n+1}$ is datum.

To treat outflow Neumann or flux conditions, it is necessary to incorporate $u_E^{n+1}$, as an additional unknown. To this end, it is convenient to add one more weighting function, whose support $\Omega_E$ is half the size of the other ones, as illustrated in Fig. 5, to close the system of equations.

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