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CHAPTER 6

Localized Adjoint Methods: A New Discretization Methodology

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ABSTRACT. Localized Adjoint Method is a new and promising methodology of wide applicability, based on Herrera's Algebraic Theory of Boundary Value Problems. Thus, the general theory is briefly explained and then its application is illustrated with transport diffusion problems for which the Eulerian-Lagrangian Localized Adjoint Method (ELLAM) has been formulated by the LAM group (M.A.Celia, R.E. Ewing and T.F. Russell, in addition to the author). The ELLAM development unifies characteristic methods, treats boundary conditions systematically, yielding conservative schemes.

1. INTRODUCTION. The Localized Adjoint Method (LAM) is a new and promising methodology for discretizing partial differential equations which has been introduced by Herrera [1-7] and coworkers, and which is being applied to a wide range of problems [8-19]. The basic algebraic theory was developed by Herrera et. al. in [1-5] and then appplied to develop highly accurate algorithms for ordinary differential equations in [4, 8, 9]. Celia et. al. [12] developed efficient algorthms for multi-dimensional steady state problems as well as one-dimensional advection-dispersion problems [10, 11]. More recently, the LAM group (M.A. Celia, R.E. Ewing, I. Herrera and T.F. Russell) developed the Eulerian-Langrangian Localized Adjoint Method (ELLAM) [6, 7, 17, 18]. Multiphase flow simulation has been dealt with by Herrera and Ewing [13] and Ewing and Celia [14]. Contaminant transport has been considered by Celia et. al. [11, 16, 17]. Multi-dimensional nested grids are being developed by Neuman [19]. In the present article the general methodology is briefly explained, introducing new explicit formulas for the case when the coefficients of the differential operators are continuous. The application of the procedures are illustrated with the transport diffusion equations [6, 7].

The numerical solution of the advective-diffusive transport equation

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is a problem of great importance because many problems in science and engineering involve such mathematical model. The numerical treatment of derive from two main approaches: standard semidiscretization and Eulerian-Lagrangian. The main distinguishing feature of the latter is the use of characteristics to carry out the discretization in time. Most formulas that have been developed using a standard semidiscretization approach have been based on up-stream weighting techniques, whose development is essentially ad-hoc. This is in contrast with LAM approach which is very systematic.

There is a point on terminology, that must be mentioned. In some past work "Localized Adjoint Methods" were called "Optimal Test Function Methods", and it has been only more recently that the new terminology has been used, since it is more precise and also, it more clearly distinguishes this method from other procedures.

The starting point of Localized Adjoint Methods is a very simple but fundamental question. What is the relation between an approximate solution and the exact one. To be more precise, we proceed to give an answer to this question in a very simple situation. Consider the problem of solving the equation

$$\mathcal{L}u = f_\Omega , \qquad \text{in} \quad \Omega \qquad (1.1)$$

subjected to homogeneous boundary conditions for which Green's formula

$$\int_\Omega v\mathcal{L}u\,dx = \int_\Omega u\mathcal{L}^* v\,dx \qquad (1.2)$$

applies, when $\mathcal{L}^*$ is the formal adjoint of $\mathcal{L}$. In the method of weighted residuals, one usually considers a system of weighting (or test) functions $\{w_1,\ldots,w_N\}$. Then, a function u' is said to be an approximate solution of this problem when

$$\int_\Omega(\mathcal{L}u' - f_\Omega)w_\alpha dx = 0 , \qquad \alpha = 1,\ldots,N. \qquad (1.3)$$

Generally, the system of N equations (1.3) has many solutions, but in order to obtain a system possessing a unique solution, it is customary to introduce a representation $u' = \Sigma A_\alpha \phi_\alpha$ of the approximate solution in terms of the system $\{\phi_1,\ldots,\phi_N\}$ of base (or trial) functions. However, this representation is an artifice that bears little relation with the exact solution u.

The following observations permit establishing the actual relation that exists between an approximate solution and the exact one and derive the actual information about the exact solution which is contained in an approximate one. From (1.1), it is clear that the exact solution u, satisfies

$$\int_\Omega(\mathcal{L}u - f_\Omega)w_\alpha dx = 0, \qquad \alpha = 1,\ldots,N. \qquad (1.4)$$

Equations (1.3) and (1.4) together imply

$$\int_\Omega w_\alpha \mathcal{L}u'\,dx = \int_\Omega w_\alpha \mathcal{L}u\,dx \qquad \alpha = 1,\ldots,N. \qquad (1.5)$$

or

$$\int_\Omega u'\mathcal{L}^* w_\alpha dx = \int_\Omega u\mathcal{L}^* w_\alpha dx \qquad \alpha = 1,\ldots,N. \qquad (1.6)$$

by virtue of Green's formula (1.1). Consider the Hilbert space L^2, of square integrable functions and in which the inner product of two functions, u and v, is given by $\int_\Omega uv\,dx$. Then, the system of equations (1.6) allows the following interpretation:

A function u' is an approximate solution if and only if, its projection on the space spanned by the system of functions $(\mathcal{L}^* w_1,\ldots,\mathcal{L}^* w_N)$, *coincides with that of the exact solution u.*

As a matter of fact, this is all the information *about the exact solution contained in an approximate one.*

In this light, the representation $u' = \Sigma A_\alpha \phi_\alpha$ can be interpreted as a procedure for extrapolating the actual information contained in the approximate solution.

The very simple and precise result just presented clarifies much the nature of approximate solutions and it would be desirable to apply it, in a systematic manner, to analyze discrete methods. For this purpose it is necessary to have available Green's formulas similar to (1.2), but that can be applied even when the functions considered are not smooth, since in most numerical applications the weighting functions are localized (i.e., they have local support) and they usually do not satisfy the smoothness requirements at the boundary of their support. Even more, the development of a theory applicable to carry out the analysis when both base and test functions are fully discontinuous, is most desirable since standard theory of distributions is not applicable to that case.

Herrera [1-5], recently developed an "algebraic theory of boundary value problems" with precisely that property; that is, in which the analysis can be carried out when both trial and test functions are fully discontinuous. Such setting is ideal for localizing the adjoint equation (1.6).

"Localized adjoint methods (LAM)", in whose development the LAM group (M.A Celia, R.E. Ewing, I. Herrera and T.F. Russell) has been working and it is being applied at present to many problems [8-19], consist in making systematic use of that theory to analyze the information contained in approximate solutions. Since the quality of the results obtained with a numerical method depends, in an important manner, on the weighting functions used, one of the main goals of localized adjoint methods, thus far, has consisted in developing improved weighting functions. In this paper the LAM methodology is explained in connection with transport diffusion problems.

2. GREEN-HERRERA FORMULAS. The main ingredients of the author's Algebraic Theory of (initial) boundary value problems are

i).- General Green-Herrera formulas, for differential operators in discontinuous fields; and

ii).- The operator extension (purely algebraic) induced by such formulas.

For simplicity, attention will be restricted to the case when the differential operators possess continuous coefficients, but such formulas have been developed for the general case of differential operators with discontinuous coefficients [2,4,20]. By definition, a differential operator and its formal adjoint $\mathcal{L}^*$, satisfy

$$v\mathcal{L}u - u\mathcal{L}^* v = \nabla\cdot(\underline{\mathcal{D}}(u,v)) \qquad (2.1)$$

where $\underline{\mathcal{D}}(u,v)$ is a vector-valued bilinear function, defined at every point of the region Ω. When considering time-dependent problems, Ω will be a region in space-time. Generally, Ω will be divided in many subregions (the elements), in each of which weighting and test functions will be assumed to

be sufficiently differentiable for the operators to be well defined in its interior. The union of the interelement boundaries will be denoted by Σ. Trial and test functions will be taken from two linear spaces D_1 and D_2, and they together with their derivatives may have jump discontinuities across Σ.

Integration of equation (2.1) and application of generalized divergence (Gauss) theorem [21], yields:

$$\int_\Omega (v\mathcal{L}u - u\mathcal{L}^* v)dx = \int_{\partial\Omega} \underline{\mathcal{D}}(u,v)\cdot\underline{n}\, dx - \int_\Sigma [\underline{\mathcal{D}}(u,v)]\cdot\underline{n}\, dx \qquad (2.2)$$

Generally, $\mathcal{L}u$ as well as $\mathcal{L}^* v$ may not be defined on Σ, where the functions may be discontinuous. Thus, here as in what follows, integrals over Ω are carried out excluding Σ and differential operators are understood in an elementary sense and not in a distributional sense. In equation (2.2), the square brackets stand for the "jumps" across Σ of the function contained inside; i.e. value on the plus side minus value in the minus side (the plus side is defined as that one towards which the unit normal on Σ points to).

Green-Herrera formulas are obtained by carrying out suitable decompositions of the bilinear functions $\underline{\mathcal{D}}(u,v)\cdot\underline{n}$ on the boundary $\partial\Omega$ of Ω and of $-[\underline{\mathcal{D}}(u,v)]\cdot\underline{n}$ on the interelemnt boundaries Σ. The decomposition of $\underline{\mathcal{D}}(u,v)\cdot\underline{n}$ is standard (see, for example, Lions and Magenes [22]) and leads to the definition of two bilinear functions $\mathcal{B}(u,v)$ and $\mathcal{C}(v,u)$ such that

$$\underline{\mathcal{D}}(u,v)\cdot\underline{n} = \mathcal{B}(u,v) - \mathcal{C}(v,u) \qquad (2.3)$$

whose definitions depend on the type of boundary and initial conditions, which are prescribed. The function $\mathcal{B}(u,v)$ is such that, when considering boundary (initial) value problems, for any u which satisfies the prescribed boundary conditions, $\mathcal{B}(u,v)$ is a well-defined linear function of v, independent of the particular choice of u. This linear function will be denoted by g_∂ (thus, its value for any given function v, will be $g_\partial(v)$).

The decomposition of $-[\underline{\mathcal{D}}(u,v)]\cdot\underline{n}$ is easily carried out using the identity

$$[\underline{\mathcal{D}}(u,v)] = \underline{\mathcal{D}}_+(u,v) - \underline{\mathcal{D}}_-(u,v) = \underline{\mathcal{D}}(u_+,v_+) - \underline{\mathcal{D}}(u_-,v_-) \qquad (2.4)$$

which holds when the differential operators have continuous coefficients. Let the average $\dot{u}$ of any function u be defined by

$$\dot{u} = (u_+ + u_-)/2 \qquad (2.5)$$

Then it is easy to verify that

$$u_+ = \dot{u} + \tfrac{1}{2}[u]\ ; \qquad u_- = \dot{u} - \tfrac{1}{2}[u] \qquad (2.6)$$

which allows writing

$$\underline{\mathcal{D}}(u_+,v_+) = \underline{\mathcal{D}}(\dot{u},\dot{v}) + \tfrac{1}{2}\underline{\mathcal{D}}(\dot{u},[v]) + \tfrac{1}{2}\underline{\mathcal{D}}([u],\dot{v}) + \tfrac{1}{4}\underline{\mathcal{D}}([u],[v]) \qquad (2.7a)$$

$$\underline{\mathcal{D}}(u_-,v_-) = \underline{\mathcal{D}}(\dot{u},\dot{v}) - \tfrac{1}{2}\underline{\mathcal{D}}(\dot{u},[v]) - \tfrac{1}{2}\underline{\mathcal{D}}([u],\dot{v}) + \tfrac{1}{4}\underline{\mathcal{D}}([u],[v]) \qquad (2.7b)$$

Equations (2.4) and (2.7) together, yield

$$[\underline{\mathcal{D}}(u,v)] = \underline{\mathcal{D}}(\dot{u},[v]) + \underline{\mathcal{D}}([u],\dot{v}) \qquad (2.8)$$

Defining

$$\mathcal{J}(u,v) \equiv -\underline{\mathcal{D}}([u],\dot{v})\cdot\underline{n} \qquad \mathcal{K}(v,u) \equiv \underline{\mathcal{D}}(\dot{u},[v])\cdot\underline{n} \qquad (2.9)$$

it is clear that

$$-[\underline{\mathcal{D}}(u,v)]\cdot\underline{n} = \mathcal{J}(u,v) - \mathcal{K}(v,u) \qquad (2.10)$$

This is the desired decomposition of the bilinear function $-[\underline{\mathcal{D}}(u,v)]\cdot\underline{n}$. The basic properties which lead to this choice of $\mathcal{J}$ and $\mathcal{K}$, have been developed more thoroughly in the author's algebraic theory [2]. In particular, at a given point of Σ, [u] and u, can be varied independently. When [u] takes a given value, $\mathcal{J}(u,v)$ is a well defined functional of v, independent of the specific choice of u. In connection with boundary (initial) value problems with prescribed jumps, the linear function of v which is obtained when $\mathcal{J}(u,v)$ is evaluated keeping [u] equal to the prescribed jumps, will be denoted by j_∂ (thus, its value for any given v, will be $j_\partial(v)$).

At this point it is convenient to introduce the following bilinear functionals:

$$\langle Pu,v\rangle \equiv \int_\Omega v\mathcal{L}u\,dx\ ; \quad \langle Qv,u\rangle \equiv \langle Q^* u,v\rangle \equiv \int_\Omega u\mathcal{L}^* v\,dx \qquad (2.11a)$$

$$\langle Bu,v\rangle \equiv \int_{\partial\Omega}\mathcal{B}(u,v)dx;\ \langle C^* u,v\rangle \equiv \int_{\partial\Omega}\mathcal{C}(u,v)dx \qquad (2.11b)$$

$$\langle Ju,v\rangle \equiv \int_\Sigma\mathcal{J}(u,v)dx;\ \text{and}\ \langle K^* u,v\rangle \equiv \int_\Sigma\mathcal{K}(v,u)dx \qquad (2.11c)$$

By means of these definitions, using (2.3) and (2.10), equation (2.2) becomes

$$P - Q^* = B - C^* + J - K^* \qquad (2.12)$$

This is <u>Green-Herrera formula for operators in discontinuous fields</u> [2,5]. It can be applied when both trial and test functions are discontinuous, something which is not possible when using standard theory of distributions.

Rearranging (2.12), it is possible to write

$$P - B - J = Q^* - C^* - K^* \qquad (2.13)$$

The left-hand side of equation (2.13) can be interpreted as an extension of the differential operator $\mathcal{L}$, which was originally defined for differentiable functions only, to fully discontinuous functions. Indeed:

> *The differential operator $\mathcal{L}$, when applied to a smooth function* u *which stisfies homogeneous boundary conditions, yields the linear functional* Pu. *However, when applied to a fully discontinuous function* u, *which does not satisfy homogeneous boundary conditions, it yields the linear functional* (P-B-J)u.

The general boundary (initial) value problem to be considered is one with prescribed jumps. The differential equation is

$$\mathcal{L}u = f_\Omega \qquad \text{in } \Omega \qquad (2.14)$$

In addition, some boundary conditions (and initial conditions) are specified on $\partial\Omega$, while jump conditions are specified at Σ. When modelling continuous systems, such jump conditions stem from basic conservation or, more generally, balance laws of continuous mechanics [20].

Using the bilinear functionals thus far introduced, such boundary (initial) value problem with prescribed jumps, can be formulated variationally as

$$\langle Pu,v\rangle = \langle f,v\rangle;\ \langle Bu,v\rangle = \langle g,v\rangle;\ \langle Ju,v\rangle = \langle j,v\rangle\ \forall\ v\in D_2 \qquad (2.15)$$

where f, g and j, are linear functionals defined by

$$\langle f,v\rangle = \int_\Omega v f_\Omega dx \; ; \; \langle g,v\rangle = \int_{\partial\Omega} g_\partial(v)dx \; ; \; \langle j,v\rangle = \int_\Sigma j_\partial(v)\, dx \quad (2.16)$$

All they can evaluated using the data of the problem.

Generally, the bilinear functionals J and B, are boundary operators for P, which are fully disjoint (For the definitions of the concepts that have been underlined here, the reader is referred to the author's original papers [2,5]. Further details can also be found in those publications). When this is the case, the system of equations (2.15), is equivalent to the single variational equation

$$\langle (P - B - J)u,v\rangle = \langle f - g - j,v\rangle \qquad \forall\, v\in D_2 \quad (2.17)$$

This is said to be "the variational formulation in terms of the data of the problem", becuase Pu, Bu and Ju are prescribed. Making use of Green-Herrera formula (2.13), the variational formulation (2.17) is transformed into

$$\langle (Q^* - C^* - K^*)u,v\rangle = \langle f - g - j,v\rangle \;\forall\; v\in D_2 \qquad (2.18)$$

This is said to be "the variational formulation in terms of the sought information", because Q^*u, C^*u and K^*u are not prescribed. It can be seen, by virtue of equations (2.11), that Q^*u, C^*u and K^*u supply information about the sought solution at the interior of the region Ω (where the problem is defined), the complementary boundary values at $\partial\Omega$ and the average of the solution (and its derivatives) across the surfaces Σ of discontinuity.

Making use of the variational formulation in terms of the sought information, the arguments that lead to the formulation of Localized Adjoint Methods, constitute a mere repetition of those presented in the Introduction. Given a system of weighting functions $\{w_1,\ldots,w_N\}\subset D_2$, an approximate solution is again any function $u'\in D_1$ which satisfies

$$\langle (Q^* - C^* - K^*)u', w_\alpha\rangle = \langle f-g-j, w_\alpha\rangle \;,\; \alpha=1,\ldots,N \quad (2.19)$$

Clearly, this equation together with (2.18) implies

$$\langle (Q^* - C^* - K^*)u', w_\alpha\rangle = \langle (Q^* - C^* - K^*)u, w_\alpha\rangle,\; \alpha=1,\ldots,N \quad (2.20)$$

since an exact solution also satisfies (2.19). Equation (2.20), is the basis for the analysis of the information contained in an approximate solution and constitutes the starting point of Localized Adjoint Methods.

3. EULERIAN-LAGRANGIAN LAM. When applying the methods of Section 2 to time dependent problems, it will be necessary to consider a region Ω in space-time. Also, the surface Σ on which discontinuities can occur, will be a surface in space-time and a suitable notation will be required. The set of points of Ω whose time value is t, will be denoted by $\Omega(t)$ and correspondingly, $\Sigma(t)$ stands for the set of points of Σ whose time value is t. Space-time vectors $\underline{M}$ will be written as pairs:

$$\underline{M} = (\underline{m}\,,\, m_t) \qquad (3.1)$$

where $\underline{m}$ is the vector made by its spatial components and while m_t corresponds to its temporal component. Let the $\underline{V}_\Sigma$ be the vectorial velocity of the surface of discontinuity $\Sigma(t)$. This is a space vector which can be written as

$$\underline{V}_\Sigma = V_\Sigma \underline{n} \qquad (3.2)$$

where $\underline{n}$ is the unit normal vector to $\Sigma(t)$. Generally, V_Σ can be positive or negative, depending on the sense of motion of $\Sigma(t)$ and the choice of $\underline{n}$.

3.1.- **One Dimensional ELLAM.**- For this case, $\underline{n}$ can be chosen as equal to one and this will be done in what follows. Observe that the space-time vector $(V_\Sigma,1)$ is tangent to Σ. Using this fact, it is easy to see that a space-time unit normal vector $\underline{N}$ to Σ, is given by

$$\underline{N} = (1+V_\Sigma^2)^{-1/2}(1, -V_\Sigma) \qquad (3.3)$$

Consider the one-dimensional transient advection-diffusion equation subject to appropiate initial and boundary conditions

$$\mathcal{L}u \equiv \frac{\partial u}{\partial t} + V\frac{\partial u}{\partial x} - D\frac{\partial^2 u}{\partial x^2} = f_\Omega(x,t), \text{ in } \Omega \qquad (3.4)$$

$$u(x,0) = u_I(x), \qquad \text{on } \partial_I\Omega \equiv \Omega(0) \qquad (3.5a)$$

$$u(0,t) = u_o(t), \qquad \text{on } \partial_o\Omega \qquad (3.5b)$$

$$\frac{\partial u}{\partial x}(l,t) = q_l(t), \qquad \text{on } \partial_l\Omega \qquad (3.5c)$$

Here, the space-time region $\Omega=\Omega_x X\Omega_t$, with $\Omega_x=[0,l]$ and $\Omega_t=[0,T]$. In addition, $\partial_o\Omega$ and $\partial_l\Omega$ are the subsets of Ω for $x=0$ and $x=l$, respectively. First and second type boundary conditions are assumed for demonstration purposes only; the following development accomodates any combination of boundary conditions.

The adjoint operator is

$$\mathcal{L}^* w \equiv -\frac{\partial w}{\partial t} - \frac{\partial}{\partial x}(Vw) - D\frac{\partial^2 w}{\partial x^2} \qquad (3.6)$$

and $\underline{\mathcal{D}}(u,v)$ as defined by (2.5) is

$$\underline{\mathcal{D}}(u,w) \equiv \left\{uD\frac{\partial w}{\partial x} - w\left(D\frac{\partial u}{\partial x} - Vu\right), uw\right\} \qquad (3.7)$$

Therefore

$$-[\underline{\mathcal{D}}(u,w)]\cdot\underline{N} = -(1+V_\Sigma^2)^{-1/2}\left[uD\frac{\partial w}{\partial x} - w\left(D\frac{\partial u}{\partial x} - (V-V_\Sigma)u\right)\right] \qquad (3.8)$$

Assuming that the physical process which equation (3.4) mimics is that of transport with Fickian diffusion, of a solute whose concentration is u, in a free fluid moving with velocity V, the smoothness conditions implied by mass balance are

$$\left[u(V - V_\Sigma) - D\frac{\partial u}{\partial x}\right] = 0, \qquad \text{on } \Sigma \qquad (3.9a)$$

In addition, Fickian diffusion implies

$$[u] = 0, \qquad \text{on } \Sigma \qquad (3.9b)$$

When the coefficients V and D are continuous, equations (3.9) are satisfied, if and only if, u and its spatial derivative are continuous across Σ. Application of equation (2.9) yields

$$\mathcal{J}(u,w) = -(1+V_\Sigma^2)^{-1/2}\left\{[u]D\overline{\frac{\partial w}{\partial x}} - \dot{w}\left(D\left[\frac{\partial u}{\partial x}\right] - (V-V_\Sigma)[u]\right)\right\} \qquad (3.11a)$$

$$\mathcal{K}(w,u) = (1+V_\Sigma^2)^{-1/2}\{\dot{u}\left[D\frac{\partial w}{\partial x}\right] - [w]\left(\overline{D\frac{\partial u}{\partial x}} - (V - V_\Sigma)\dot{u}\right)\} \qquad (3.11b)$$

It is clear now that $J_\Sigma(v)\equiv 0$ on Σ, since the sought solution is required to satisfy the condition $[u]=\left[\frac{\partial u}{\partial x}\right]\equiv 0$ on Σ.

The bilinear functions $\mathcal{C}(u,w)$ and $\mathcal{B}(u,w)$, to be defined on the boundary, must be constructed taking into account the kind of boundary conditions to be satisfied. For the kind of boundary conditions given by equations (3.5), they are

$$\mathcal{B}(u,w) = u\left(D\frac{\partial w}{\partial x} + V\,w\right), \quad \mathcal{C}(w,u) = wD\frac{\partial u}{\partial x}, \quad \text{on } \partial_o\Omega \qquad (3.12a)$$

$$\mathcal{B}(u,w) = -\,wD\frac{\partial u}{\partial x}, \quad \mathcal{C}(w,u) = -u\left(D\frac{\partial w}{\partial x} + V\,w\right), \quad \text{on } \partial_l\Omega \qquad (3.12b)$$

$$\mathcal{B}(u,w) = -uw \quad \text{on } \partial_I\Omega \qquad (3.12c)$$

$$\mathcal{C}(w,u) = -uw \quad \text{on } \partial_T\Omega \qquad (3.12d)$$

where $\partial_T\Omega\equiv\Omega(T)$. Observe that the decomposition of $\underline{\mathcal{D}}(u,v)\cdot\underline{N}$ in $\Omega(0)\cup\Omega(T)$ does not have a point-wise character. This reflects the fact that this is an initial-value problem. From (3.5) and (3.12), it follows that

$$g_\partial(w) = u_o\left(D\frac{\partial w}{\partial x} + V\,w\right) \quad \text{on } \partial_o\Omega \qquad (3.13a)$$

$$g_\partial(w) = -\,wDq_l \quad \text{on } \partial_l\Omega \qquad (3.13b)$$

$$g_\partial(w) = -u_I w \quad \text{on } \partial_I\Omega \qquad (3.13c)$$

The expressions for the bilinear functionals B, C, J and K, are obtained integrating $\mathcal{B}$, $\mathcal{C}$, $\mathcal{J}$ and $\mathcal{K}$, on the boundary and on Σ. Asuming that Σ is the union of the set of curves $\{\Sigma_1, \Sigma_2, \ldots, \Sigma_E\}$ in space-time (Fig.1),

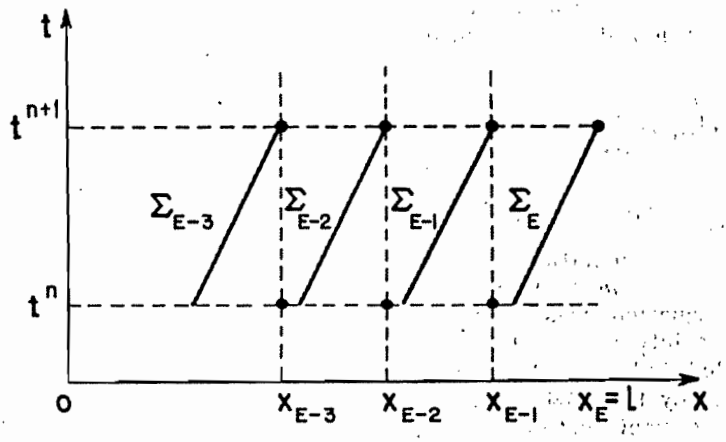

Figure 1.- The surface of discontinuity Σ.

the expressions for J and K^* are the summ of the contributions of each one of these curves. Thus, one can write

$$J = \sum_{\alpha=1}^{E} J_\alpha \quad \text{and} \quad K^* = \sum_{\alpha=1}^{E} K^*_\alpha \qquad (3.14)$$

where

$$\langle J_\alpha u,w\rangle = \int_0^T \{[u]D\overline{\frac{\partial w}{\partial x}} - \dot{w}\left(D\left[\frac{\partial u}{\partial x}\right] - (V - V_\Sigma)[u]\right)\}_\alpha dt \qquad (3.15a)$$

$$\langle K_\alpha^* u,w\rangle = \int_0^T \{\dot{u}\left[D\frac{\partial w}{\partial x}\right] - [w]\left(D\overline{\frac{\partial u}{\partial x}} - (V - V_\Sigma)\dot{u}\right)\}_\alpha dt \qquad (3.15b)$$

Here, the subindex α means that the value of the integrand is taken on Σ_α. To obtain equations (3.14), use has been made of the fact that, on each Σ_α, the element of time dt, is $(1+V_\Sigma^2)^{-1/2}$ times the length element in space-time.

In a similar fashion, it is convenient to decompose the bilinear functionals B and C^* into the contributions which stem from $\partial_I\Omega$, $\partial_T\Omega$, $\partial_o\Omega$ and $\partial_l\Omega$. The corresponding expressions are:

$$B = B_I + B_o + B_l \quad \text{and} \quad C^* = C_T^* + C_o^* + C_l^* \qquad (3.16)$$

In view of (3.12), it is clear that

$$\langle B_o u,w\rangle = \int_o^T \{u\left(D\frac{\partial w}{\partial x} + V\, w\right)\}_{x=o} dt;\ \langle B_l u,w\rangle = -\int_o^T \{wD\frac{\partial u}{\partial x}\}_{x=l} dt \qquad (3.17a)$$

$$\langle B_I u,w\rangle = -\int_o^l (uw)_{t=o} dx;\ \langle C_T^* u,w\rangle = -\int_o^l (uw)_{t=T} dx \qquad (3.17b)$$

$$\langle C_o^* u,w\rangle = \int_o^T (wD\frac{\partial u}{\partial x})_{x=o} dt;\ \langle C_l^* u,w\rangle = -\int_o^T \{u\left(D\frac{\partial w}{\partial x} + V\, w\right)\}_{x=l} dt \qquad (3.17c)$$

To complete the formulation of the problem, it remains to define the linear functionals f, g, and j. The first one is given by (2.16), while the latter one is zero, because the sought solution together with its normal derivative is required to be continuous. On the other hand, one can write $g=g_I+g_o+g_l$, with

$$\langle g_o,w\rangle = \int_o^T \{u_o\left(D\frac{\partial w}{\partial x} + V\, w\right)\}_{x=o} dt;\ \langle g_l,w\rangle = -\int_o^T (wDq_l)_{x=l} dt \qquad (3.18a)$$

$$\langle g_I,w\rangle = -\int_o^l (u_I w)_{t=o} dx; \qquad (3.18b)$$

The variational formulation in terms of the data of the problem is now given by (2.17), while that in terms of the sought information is given by (2.18). This equation was applied to analyze the information contained in approximate solutions. In this manner a generalization of Characteristic Methods, called Eulerian- Lagragian Localized Adjoint Methods (ELLAM), has been developed by the LAM group [6,7].

Many numerical methods use characteristic analysis to accomodate the advective component of transport. Such Characteristic Methods include Eulerian-Lagrangian Methods (ELM) [9-11], Modified Method of Characteristics (MMOC) [12,13], and operator splitting methods [14,15]. The ELLAM approximations provide a systematic framework for development of Characteristic Methods for numerical approximation of advective-diffusive transport equations. The Localized Adjoint Method (LAM) procedures lead naturally to the definition of special space-time test functions that produce the generalized CM approximations. The resulting set of approximating equations subsumes many of the CM approximations proposed in

the literature. It therefore unifies these methods. In addition, the development inherently provides a systematic procedure for proper incorporation of all types of boundary conditions in a mass conservative manner.

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