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Localized Adjoint Method as a Boundary Method

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1.- INTRODUCTION

Three of the most powerful numerical methods for partial differential equations are finite elements, finite differences and boundary element methods. The foundations of each one of these methodologies, as originally formulated, were unrelated. More recently, it has been recognized that there are many relations between them. In this spirit, the author developed his Algebraic Theory of Boundary Value Problems [1-5] which has led to what is at present known as the "Localized Adjoint Method".

In the construction of approximate solutions there are two processes, equally important but different, that should be clearly distinguished [6]. They are:

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. The information about the exact solution that is gathered, is determined mainly by the weighting functions, while the manner in which it is interpolated depends on the base functions chosen. Examples have been given for which these processes are not only independent but, they do not need to be carried out simultaneously [6].

This, by the way, exhibit some of the severe limitations associated with methods, such as the Galerkin method, in which base and test functions are required to be the same. The conditions that test functions must satisfy in order to be effective for gathering information are, in general, quite different to those that must be satisfied by base functions, in order to be effective interpolators. The questions posed by the above comments are very complex and to explore them in all its generality is quite difficult. A first step is to have a procedure for exhibiting the information about the exact solution, contained in an approximate one. The usefulness of this insight is two-fold: firstly, it can be used to develop weighting functions which concentrate such information in a desired manner and secondly, such knowledge permits interpolating or, more generally, processing the available information more effectively.

Localized Adjoint Method is a methodology I have proposed [2-5], for carrying out such analysis and for developing improved algorithms. When this approach is used, the information about the exact solution contained in an approximate one, is exhibited applying Herrera's Algebraic Theory of Boundary Value Problems. This procedure is more direct than applying the Theory of Distributions, mainly because the sought information is expressed in terms of localized inner products, which permit a more direct physical interpretation. Also, the author's Algebraic Theory allows simultaneous use of discontinuous trial and test functions.

From the start, Herrera's Algebraic Theory of Boundary Value Problems has had a close connection with Boundary Methods. As a matter of fact, its development was motivated by theoretical needs that were encountered in the development of Trefftz Method [7]. For symmetric operators, a full account of the theory was given in book form [1]. Later on, it was extended to non-symmetric operators [2-5].

Applications have successively been made to ordinary differential equations, for which highly accurate and efficient algorithms were developed [4,8-10], multidimensional steady state problems [11] and optimal spatial methods for advection-diffusion equations [12-20]. More recently, generalizations of Characteristic Methods known as Eulerian-Lagrangian Localized Adjoint Method (ELLAM), were developed [21,6]. ELLAM allows a very systematic treatment of boundary conditions and this permitted to obtain the first characteristic algorithms possessing the mass-conservation property. Many specific applications have already been made [22-29] and related work and additional applications are underway [30].

In all these applications, the algorithms that have been developed concentrate the information in the interelement boundaries. In order to achieve this, the weighting functions w^{α}, are required to satisfy the adjoint equation: $\mathcal{L}^{*} w^{\alpha}=0$. When this is done, the resulting procedure is a generalized boundary method.

In this paper the Localized Adjoint Method is briefly explained and some of the ideas are illustrated by means of simple examples.

2. VARIATIONAL FORMULATION IN TERMS OF THE SOUGHT INFORMATION

Consider a region Ω and the linear spaces D_1 and D_2 of trial and test functions defined in Ω, respectively. Assume further, that functions belonging to D_1 and D_2 may have jump discontinuities across some internal boundaries whose union will be denoted by Σ.

For example, in applications of the theory to finite element methods, the set Σ could be the union of all the interelement boundaries. In this setting the general boundary value problem to be considered is one with prescribed jumps, across Σ. The differential equation is

$$\mathcal{L}u = f_{\Omega}, \qquad \text{in } \Omega \qquad (2.1)$$

where Ω may be a purely spatial region or more generally, it may be a space-time region. Certain boundary and jump conditions are specified on the boundary $\partial\Omega$ of Ω and on Σ, respectively. When Ω is a space-time region, such conditions generally include initial conditions. In the literature on mathematical modeling of macroscopic physical systems, there are many examples of initial-boundary value problems with prescribed jumps.

When $\mathcal{L}^*$ is the adjoint of $\mathcal{L}$, one has:

$$w\mathcal{L}u - u\mathcal{L}^* w = \nabla \cdot (\underline{\mathcal{D}}(u,w)) \qquad (2.2)$$

for a suitable vector-valued bilinear function $\underline{\mathcal{D}}(u,w)$. Integration of (2.2) over Ω and application of generalized divergence theorem [31], yield:

$$\int_{\Omega}(w\mathcal{L}u - u\mathcal{L}^* w)dx = \int_{\partial\Omega} \mathcal{R}_{\partial}(u,w)\, dx + \int_{\Sigma} \mathcal{R}_{\Sigma}(u,w)\, dx \qquad (2.3)$$

where

$$\mathcal{R}_{\partial}(u,w) = \underline{\mathcal{D}}(u,w)\cdot\underline{n} \quad \text{and} \quad \mathcal{R}_{\Sigma}(u,w) = -[\underline{\mathcal{D}}(u,w)]\cdot\underline{n} \qquad (2.4)$$

Here, the square brackets stand for the "jumps" across Σ of the function contained inside; i.e., limit on the positive side minus limit on the negative one. Here, as in what follows, the positive side of Σ is chosen arbitrarily and then the unit normal vector $\underline{n}$, is taken pointing towards the positive side of Σ. Observe that generally, $\mathcal{L}u$ will not be defined on Σ, since there u and its derivatives may be discontinuous. Thus, in this article, it is understood that integrals over Ω are carried out excluding Σ.

In the general theory of partial differential equations, Green's formulas are used extensively [32] and they can be obtained introducing suitable decompositions of the bilinear function $\mathcal{R}_{\partial}$. Indicating, as it is usual, transposes of bilinears forms by means of a star, the general form of such decompositions is:

$$\mathcal{R}_{\partial}(u,w) \equiv \underline{\mathcal{D}}(u,w)\cdot\underline{n} = \mathcal{B}(u,w) - \mathcal{C}^*(u,w) \qquad (2.5)$$

where $\mathcal{B}(u,w)$ and $\mathcal{C}(w,u)$ are two bilinear functions. In general, $\mathcal{B}(u,w)$ is associated with the prescribed boundary values, while

$\overset{*}{\mathscr{C}}(u,w)$ can only be evaluated after the problem has been solved and is called the "complementary boundary values" [6].

Green's formulas for problems with prescribed jumps, stem from the algebraic identity:

$$\left[\mathscr{D}(u,w)\right] = \underline{\mathscr{D}}([u],\dot{w}) + \underline{\mathscr{D}}(\dot{u},[w]) \qquad (2.6)$$

which holds when the coefficients of $\mathscr{L}$ are continuous (for discontinuous coefficients see [4]), and where for every function u:

$$[u] = u_+ - u_- , \qquad \dot{u} = (u_+ + u_-)/2 \qquad (2.7)$$

while u_+ and u_- stand for the limits of u on the positive and negative sides, respectively. Equ. (2.6), yields

$$\mathscr{R}_\Sigma(u,w) = \mathscr{J}(u,w) - \overset{*}{\mathscr{K}}(u,w) \qquad (2.8)$$

with

$$\mathscr{J}(u,w) = -\underline{\mathscr{D}}([u],\dot{w})\cdot\underline{n} \qquad (2.9a)$$

$$\mathscr{K}(w,u) = \underline{\mathscr{D}}(\dot{u},[w])\cdot\underline{n} \qquad (2.9b)$$

Generally, the jump $\mathscr{J}(u,w)$ is prescribed, while $\overset{*}{\mathscr{K}}(u,w)$ is part of the sought information and can only be evaluated after the initial-boundary value problem has been solved and certain information about the average of the solution and its derivatives on Σ, is known. Such information, is called the "generalized averages".

The initial-boundary value problem with prescribed jumps, can be formulated point-wise, by means of the equation (2.1), together with

$$\mathscr{B}(u,\cdot) = g_\partial, \text{ on } \partial\Omega \qquad (2.10a)$$

and

$$\mathscr{J}(u,\cdot) = j_\partial, \text{ on } \Sigma \qquad (2.10b)$$

Introducing the notation

$$\langle Pu,w\rangle = \int_\Omega w\mathscr{L}u\,dx; \qquad \langle \overset{*}{Q}u,w\rangle = \int_\Omega u\overset{*}{\mathscr{L}}w\,dx \qquad (2.11a)$$

$$\langle Bu,w\rangle = \int_{\partial\Omega}\mathscr{B}(u,w)dx; \qquad \langle \overset{*}{C}u,w\rangle = \int_{\partial\Omega}\mathscr{C}(w,u)dx \qquad (2.11b)$$

$$\langle Ju,w\rangle = \int_\Sigma \mathscr{J}(u,w)dx \quad \text{and} \quad \langle \overset{*}{K}u,w\rangle = \int_\Sigma \mathscr{K}(w,u)dx \qquad (2.11c)$$

and defining the linear functionals f, g, $j \in D_2^*$ by means of:

$$\langle f,w\rangle = \int_\Omega w f_\Omega dx; \quad \langle g,w\rangle = \int_{\partial\Omega} g_\partial(w)dx \;; \quad \langle j,w\rangle = \int_\Sigma j_\Sigma(w)dx; \quad (2.12)$$

"Herrera's variational formulation in terms of the sought information", is written as

$$\langle (Q^* - C^* - K^*)u,w\rangle = \langle f - g - j,w\rangle \;\forall\; w \in D_2 \qquad (2.13)$$

The linear functionals Q^*u, C^*u and K^*u, supply information about the sought solution at points in the interior of the region Ω, the complementary boundary values at $\partial\Omega$ and the generalized averages of the solution at Σ, respectively, as can be verified by inspection of Equs. (2.11) and will be illustrated in the examples that follow.

In view of (2.13), when the method of weighted residuals is applied, an approximate solution $\hat{u} \in D_1$, satisfies:

$$\langle (Q^* - C^* - K^*)\hat{u},w^\alpha\rangle = \langle f-g-j,w^\alpha\rangle \;,\; \alpha=1,\ldots,N \quad (2.14)$$

Since the exact solution satisfies (2.13), it is clear that:

$$\langle (Q^* - C^* - K^*)\hat{u},w^\alpha\rangle = \langle (Q^* - C^* - K^*)u,w^\alpha\rangle, \; \alpha=1,\ldots,N \quad (2.15)$$

Equs. (2.15), can be used to analyze the information about the exact solution that is contained in an approximate one and have been applied extensevily in the development of the Localized Adjoint Method.

3. ORDINARY DIFFERENTIAL EQUATIONS

As has already been mentioned, K^*u supplies information about the average of the solution and its derivatives across the surface Σ of discontinuity. Such information can be classified further. In particular, it is useful to decompose K^*u into the averages of the function, the first derivative etc. This is achieved writing K^* as the sum of operators K^{0*}, K^{1*},..., each one containing the information, about the average of the derivative of the corresponding order. Such decomposition is induced when $\mathcal{K}^*(u,w)$ is decomposed point-wise, into the sum of bilinear functions $\mathcal{K}^{0*}(u,w)$, $\mathcal{K}^{1*}(u,w)$,..., each one containing the corresponding information point-wise. Similarly, J will be written as the sum of operators J^0, J^1,..., each one of them containing the jump of the derivative of corresponding order and $\mathcal{J}(u,w)$ will be the sum of $\mathcal{J}^0(u,w)$, $\mathcal{J}^1(u,w)$, etc. When this is done:

$$K=\sum_l K^l; \qquad J=\sum_l J^l; \quad \mathcal{K}=\sum_l \mathcal{K}^l; \qquad \mathcal{J}=\sum_l \mathcal{J}^l \qquad (3.1)$$

A physical situation that the general ordinary differential equation of second order mimics, is transport in the presence of advection, diffusion and linear sources, as is the case when chemical reactions take place, and a notation related with such processes will be adopted. Thus, the general equation to be considered, is:

$$\mathcal{L}u \equiv -\frac{d}{dx}\left(D\frac{du}{dx} - Vu\right) + Ru = f_{\Omega}, \text{ in } \Omega \equiv [0,l] \tag{3.2a}$$

subject to the smoothness conditions

$$[u] = 0 \quad \text{and} \quad \left[\frac{\partial u}{\partial x}\right] = 0, \qquad \text{on } \Sigma \tag{3.2b}$$

A uniform partition $\{0=x_0,\ x_1,\ldots,\ x_{E-1},\ x_E=l\}$ is introduced, with $x_\alpha - x_{\alpha-1} = h$. It will be further assumed, that trial and test functions may have jump discontinuities at internal nodes, so that $\Sigma = \{x_1,\ldots,x_{E-1}\}$, in the general framework of Section 2. On Σ, $\underline{n}=1$ is chosen. Boundary conditions satisfied at 0 and l, can be Dirichlet, Neumann or Robin boundary conditions, but they are left unspecified.

The formal adjoint of the operator $\mathcal{L}$, is:

$$\mathcal{L}^{*}w \equiv -\frac{d}{dx}\left(D\frac{dw}{dx}\right) - V\frac{dw}{dx} + Rw \tag{3.3}$$

Therefore:

$$w\mathcal{L}u - u\mathcal{L}^{*}w \equiv \frac{d}{dx}\left(u\left(D\frac{dw}{dx} + Vw\right) - wD\frac{du}{dx}\right) \tag{3.4}$$

and

$$\underline{\mathcal{D}}\ (u,w) \equiv u\left(D\frac{dw}{dx} + Vw\right) - wD\frac{du}{dx} \tag{3.5}$$

Application of Equs. (2.9), yields:

$$\mathcal{J}^{0}(u,w) = -[u]\left(D\overline{\frac{dw}{dx}} + V\dot{w}\right); \qquad \mathcal{J}^{1}(u,w) = \dot{w}D\left[\frac{du}{dx}\right] \tag{3.6a}$$

$$\mathcal{K}^{0}\ (w,u) = \dot{u}\left[D\frac{dw}{dx} + Vw\right]; \qquad \mathcal{K}^{1}(w,u) = -[w]D\dot{\overline{\frac{du}{dx}}} \tag{3.6b}$$

from which $\mathcal{J}$ and $\mathcal{K}$ are obtained by means of Equs. (3.1). In Equs. (3.6), as wherever deemed necessary, a bar is used to make clear that the dot on top refers to the whole expression covered by the bar.

The definitions of the bilinear functions $\mathcal{B}(u,w)$ and $\mathcal{C}(w,u)$, depend on the type of boundary conditions to be satisfied. They may be taken as:

$$\mathcal{B}(u,w) = u\ \left(D\frac{dw}{dx} + Vw\right)\underline{n}; \qquad \mathcal{C}(w,u) = w\ D\frac{du}{dx}\underline{n} \tag{3.7}$$

for Dirichlet data,

$$\mathcal{B}(u,w) = -w\, D\frac{du}{dx}\underline{n};\ \mathcal{C}(w,u) = -u\, (D\frac{dw}{dx} + Vw)\underline{n} \qquad (3.8)$$

for Neumann data and

$$\mathcal{B}(u,w) = -w\, (D\frac{du}{dx} - Vu)\underline{n}; \qquad \mathcal{C}(w,u) = -u\, D\frac{dw}{dx}\underline{n} \qquad (3.9)$$

when total flux is prescribed.

For ordinary differential equations it is easy to construct algorithms which concentrate all the information at internal nodes [4]. The conditions to be satisfied by weighting functions are: $\mathcal{L}^* w \equiv 0$ and $\mathcal{C}(w,\cdot) \equiv 0$. These latter conditions are:

$$w=0; \qquad D\frac{dw}{dx} + Vw = 0; \qquad D\frac{dw}{dx} = 0 \qquad (3.10)$$

which hold wherever Dirichlet, Neuman or flux conditions are prescribed for the sought solution. The actual construction of such weighting functions is very efficient when collocation is used [8]. In the case of algorithms for which approximate solutions contain information about the exact solution at internal nodes, exclusively, the information about the first derivative must be removed. This is achieved if $\mathcal{K}^1(w,\cdot)=0$, at internal nodes. Thus, the weighting functions must satisfy the additional condition $[w]=0$, by virtue of Equ. (3.6b).

In summary, the weighting functions that concentrate all the information in the values of the sought solution at internal nodes satisfy

$$\mathcal{L}^* w = 0,\ \text{on}\ \Omega; \quad \mathcal{C}(w,\cdot)=0,\ \text{on}\ \partial\Omega=\{0,l\}; \ [w]=0,\ \text{on}\ \Sigma \qquad (3.11)$$

These are C^0 test functions; for them the system of equations (2.15) reduces to:

$$\langle K^* u, w^\alpha \rangle = \langle K^* \hat{u}, w^\alpha \rangle,\ \alpha=1,\ldots,N \qquad (3.12)$$

When the system of test functions $\{w^1,\ldots,w^N\}$ is TH-complete, Equs. (3.12) imply that $K^*\hat{u}=K^*u$, which in the present case is equivalent to

$$\dot{\hat{u}}(x_j) = u(x_j),\ j=1,\ldots,E-1 \qquad (3.13)$$

where u(x), is the exact solution. Thus, the values of the sought solution are predicted exactly at internal nodes.

Here, as in what follows, the concept of TH-completeness is used. This concept was introduced by Herrera in [1,33], where a rigorous discussion of this question in an abstract setting was presented, allowing considerble generality, since the conclusions that were obtained, are independent of the order of the differential equations and the number of independent variables involved. However, that discussion refers to symmetric operators and recent results for non-symmetric ones, can be found in [34].

Observe that Equs. (3.13) hold independently of the base functions used, because when deriving them, nothing was assumed about such functions. Therefore, when the system of weighting functions is TH-complete, Equs. (3.13) hold even if the system of test functions are fully discontinuous, or they violate the prescribed boundary conditions.

Let $\{\Phi^0, \Phi^1, \ldots, \Phi^E\}$ be a system of base functions which, for the time being, are assumed to be continuous (but whose derivatives may have jump discontinuities at iternal nodes), such that (for every $\alpha=1,\ldots,E$) $w^\alpha=1$ at node x_α, while it vanishes at every other node. For the case when the prescribed boundary conditions are non-homogeneous, a suitable representation of the approximate solution is:

$$\hat{u}(x) = U_0\Phi^0 + U_E\Phi^E + \sum_{j=1}^{E-1} U_j\Phi^j(x) \qquad (3.14)$$

TH-complete systems which satisfy (3.11) have dimension E-1 [34]. Let us apply the system of equations (3.14), using a TH-complete system $\{w^1, \ldots, w^{E-1}\}$ of weighting functions. Then any solution of the resulting system has the property:

$$U_j = u(x_j), \; j=1,\ldots,E-1 \qquad (3.15)$$

by virtue of (3.13). Thus, the exact values are predicted correctly, independently of the base functions used. ndeed, discontinuous functions $\Phi^j(x)$ can be used in (3.14) and Equs. (3.13) hold, anyway.

4. ADVECTION-DIFFUSION EQUATION

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

$$\mathcal{L}u \equiv \frac{\partial u}{\partial t} - \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x} - Vu\right) + Ru = f_\Omega(x,t), \text{ in } \Omega \qquad (4.1)$$

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

subject to initial conditions

$$u(x,t^n) = u^n(x), \qquad (4.2)$$

and suitable boundary conditions, at x=0 and l. In this case, the adjoint operator $\mathcal{L}^*$ is:

$$\mathcal{L}^* w \equiv -\frac{\partial w}{\partial t} - \frac{\partial}{\partial x}\left(D\frac{\partial w}{\partial x}\right) - V\frac{\partial w}{\partial x} + Rw \qquad (4.3)$$

It will be useful to decompose the boundary $\partial\Omega$ into $\partial_o\Omega$, $\partial_l\Omega$, $\partial_n\Omega$ and $\partial_{n+1}\Omega$, which are defined as the subsets of Ω for which (x,t) satisfies $x=0$, $x=l$, $t=t^n$ and $t=t^{n+1}$, respectively (Fig.1a). The initial conditions, given by Eq. (4.2), are to be satisfied at $\partial_n\Omega$ and the boundary conditions pertain to $\partial_o\Omega\cup\partial_l\Omega$. These latter conditions can be of Dirichlet ($u=u_\partial$), Neumann ($D\frac{\partial u}{\partial x}\underline{n}=q$) or Robin type, or a combination of them. Here, it is understood that $\underline{n}=1$ at $x=l$ and $\underline{n}=-1$ at $x=0$. For definitness, for the time being, only Dirichlet conditions will be considered, although the general methodology accommodates any of them [6].

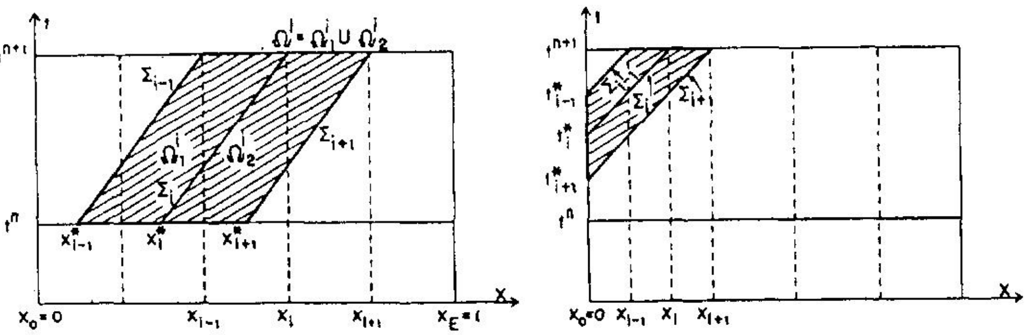

Figure 1.- a) Decomposition of Ω into the subregions Ω^i, $i = 1,\ldots E$.
b) Case when the support of the bilinear weighting function w^i intersects the inflow boundary.

In addition, a partition $\{x_0,x_1,\ldots,x_E\}$ of $[0,l]$ is introduced and the region Ω 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.1a. These subregions are limited by space-time curves Σ_α ($\alpha=1,\ldots,E$), whose positions at any time t ($t^n\le t\le t^{n+1}$) are given by the functions $\sigma_\alpha(t)$ and it will be assumed that discontinuities occur on these lines, exclusively. Thus for the general notation introduced in Section 2, $\Sigma=\cup\Sigma_\alpha$ in this case. Clearly, the velocity of propagation V_Σ of each one of these lines is $d\sigma_\alpha/dt$. Also, the unit normal vector to Σ, of the general theory, is a space-time vector which will be written as: $\underline{N}=(1+V_\Sigma)^{-1/2}(\underline{n},1)$, where $\underline{n}$ is a unit vector in space [6].

The bilinear functions $\mathcal{B}(u,w)$ and $\mathcal{C}(w,u)$ are defined by:

$$\mathcal{B}(u,w) \equiv 0, \qquad \mathcal{C}(w,u) = -uw \text{ on } \partial_{n+1}\Omega \qquad (4.4a)$$

$$\mathcal{B}(u,w) = -uw, \qquad \mathcal{C}(w,u) \equiv 0 \text{ on } \partial_n\Omega \qquad (4.4b)$$

$$\mathcal{B}(u,w)\ u\ D\frac{\partial w}{\partial x}, \qquad \mathcal{C}(w,u) = w\left(D\frac{\partial u}{\partial x} - Vu\right)\underline{n} \quad \text{on } \partial_0\Omega \cup \partial_l\Omega. \qquad (4.4c)$$

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

$$\mathcal{K}(w,u)=\mathcal{K}^0(w,u) + \mathcal{K}^1(w,u), \qquad (4.5)$$

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

$$\mathcal{K}^0(w,u) = (1+V_\Sigma^2)^{-1/2}\dot{u}\{[D\frac{\partial w}{\partial x}] + (V - V_\Sigma)[w]\}; \qquad (4.6a)$$

$$\mathcal{K}^1(w,u) = -(1+V_\Sigma^2)^{-1/2}[w]D\overline{\frac{\partial u}{\partial x}}^{\bullet} . \qquad (4.6b)$$

Observe that $\mathcal{C}^*(u,\cdot)\equiv 0$ on $\partial_n\Omega$, so that no information is sought at $t=t^n$, as is usually the case for an initial value problem.

LAM procedures use "Herrera's variational formulation in terms of the sought information", as was explained in Section

2. For this case, it is:

$$\langle (Q^* - C^* - K^*)u,w\rangle = \langle f - g - j,w\rangle \ \forall\ w\in D_2, \qquad (4.7)$$

where D_2 is a suitable set of weighting functions,

$$\langle (Q^*u,w\rangle = \int_\Omega u\mathcal{L}^* w d\mu \qquad (4.8a)$$

$$\langle C^*u,w\rangle = \int_{\partial_{n+1}} \mathcal{C}(w,u)dx + \int\{\mathcal{C}(w,u)\}_{x=l}dt + \int\{\mathcal{C}(w,u)\}_{x=0}dt, \qquad (4.8b)$$

$$\langle K^*u,w\rangle = \int_\Sigma \mathcal{K}(w,u)d\mu = \sum_\alpha \int_{\Sigma_\alpha} \mathcal{K}(w,u)d\mu \qquad (4.8c)$$

and

$$\langle f,w\rangle = \int_\Omega wf_\Omega d\mu;\ \langle g,w\rangle = \int_{\partial\Omega} g_\partial(w)d\mu\ ;\ \langle j,w\rangle = \int_\Sigma j_\Sigma(w)d\mu. \qquad (4.9)$$

Here, $d\mu$ is used to denote the element of area (space-time) in Ω and of length, in the case of line integrals.

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

$$\langle K_\alpha^* u,w\rangle = \int_{\Sigma_\alpha}\left\{\dot{u}\left[D\frac{\partial w}{\partial x}\right] - [w]\left(D\overline{\frac{\partial u}{\partial x}}^{\bullet} - (V - V_\Sigma)\dot{u}\right)\right\}_\alpha dt, \qquad (4.10)$$

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

$$K^* = \sum_{\alpha=1}^{E} K_\alpha^*. \qquad (4.11)$$

The bilinear functional C^* can be written in terms of the contributions coming from $\partial_n\Omega$, $\partial_{n+1}\Omega$, $\partial_0\Omega$, and $\partial_l\Omega$. In this manner one can write:

$$C^* = C^*_{n+1} + C^*_0 + C^*_l, \qquad (4.12)$$

where

$$\langle C^*_{n+1}u,w\rangle = -\int_0^l (uw)_{t=t^{n+1}} dx \qquad (4.13a)$$

$$\langle C^*_0 u,w\rangle = -\int\left\{w\left(D\frac{\partial u}{\partial x} - Vu\right)\right\}_{x=0} dt \qquad (4.13b)$$

$$\langle C^*_l u,w\rangle = \int\left\{w\left(D\frac{\partial u}{\partial x} - Vu\right)\right\}_{x=l} dt \qquad (4.13c)$$

Define

$$\langle g_n,w\rangle = -\int_0^l u^n w(t^n)dx; \qquad (4.14a)$$

$$\langle g_D,w\rangle = \int_{\partial_D\Omega} u_\partial D\frac{\partial w}{\partial x}\,\underline{n}dt \quad \langle g_N,w\rangle = -\int_{\partial_N\Omega} wq\,\underline{n}dt; \qquad (4.14b)$$

$$\langle g_F,w\rangle = -\int_{\partial_F\Omega} wF\,\underline{n}dt, \qquad (4.14c)$$

Using Equs. (2.12), it is seen that $g=g_n+g_D+g_N+g_F$. Also, $\langle j,w\rangle\equiv 0$.

5. ELLAM PROCEDURES FOR ADVECTION-DIFFUSION EQUATIONS

Two ELLAM approaches that have been used thus far, for advection dominated transport are presented in this Section.

The first one ("bilinear ELLAM"), applies bilinear ("chapeau") test functions [21]. For the case of constant coefficients, such functions are:

$$w^i(x,t) = \begin{cases} \dfrac{x-x_{i-1}}{\Delta x} + V\dfrac{t^{n+1}-t}{\Delta x}, & (x,t)\in\Omega^i_1 \\ \dfrac{x_{i+1}-x}{\Delta x} + V\dfrac{t^{n+1}-t}{\Delta x}, & (x,t)\in\Omega^i_2 \\ 0, & \text{all other } (x,t) \end{cases} \qquad (5.1)$$

where Ω^i_1 and Ω^i_2 are as shown in Fig.1a. They 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. (4.6), it is clear that $\mathcal{K}^1(w,u)$ vanishes identically, while

$$\mathcal{K}^0(w^i,u) = (1+V_\Sigma^2)^{-1/2}\dot{u}\left[D\frac{\partial w^i}{\partial x}\right]. \qquad (5.2)$$

This latter expression does not vanish on three lines of discontinuity, at most: Σ_{l-1}, Σ_l and Σ_{l+1}. There:

$$\left[\frac{\partial w}{\partial x}\right]_{l-1} = \frac{1}{\Delta x}\ ;\quad \left[\frac{\partial w}{\partial x}\right]_{l} = \frac{-2}{\Delta x};\quad \left[\frac{\partial w}{\partial x}\right]_{l+1} = \frac{1}{\Delta x}. \tag{5.3}$$

When the region Ω^l does not intersect the lateral boundaries, the boundary terms (4.4c–e) and (4.13b) vanish and the variational principle in terms of the sought information (4.7), reduces to $\langle C^*_{n+1}+K^*)u,w\rangle=\langle g_n-f,w^l\rangle$; i.e.:

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

$$= \int_{x^*_{l-1}}^{x^*_{l+1}} u(x,t^n)w^l(x,t^n)dx + \int_\Omega f_\Omega w^l dxdt, \tag{5.4}$$

where the unknowns have been collected in the left-hand member of the equation.

Notice that the unknown function u(x,t) has not yet been approximated by any specific functional form. As a matter of fact, LAM procedures do not require assuming any specific form for u and 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]. See [21] for additional details.

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

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

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

$$\frac{D}{\Delta x}\left\{\int_{t_l^*}^{t_{l-1}^*} u(0,t)dt - \int_{t_{l+1}^*}^{t_l^*} u(0,t)dt\right\} + \int_{\Omega} f_{\Omega} w^l dxdt \qquad (5.5)$$

The integrals along characteristics appearing in Equ. (5.5), can again be evaluated by means of a fully implicit approximation. However, approximation of the last term in the left side of Equ. (5.5) 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. 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:

$$\int_{t_{l+1}^*}^{t_{l-1}^*} w^l D\frac{\partial u}{\partial x}(0,t)dt = \frac{D}{V}\int_{x_{l-1}}^{x_{l+1}} w^l\frac{\partial u}{\partial x}(x,t^{n+1})dx + O(\Delta t^2) \qquad (5.6)$$

The use of this approximation yields satisfactory results [21] and this has been corroborated by an error analysis recently carried out [35]. Neumann or flux conditions, imposed in the outflow boundary, are more complicated to deal with (see [21]). However, such boundary conditions are easy to treat when a control-volume procedure is used, as it is explained next.

The second procedure ("ELLAM Cells"), is a control-volume method applied in an Eulerian-Lagragian manner [30]. Firstly, modifications in the notation which are usual for the method of cells, will be introduced. Writing $x_{l+1/2} \equiv x_l + \Delta x/2$, the subintervals $[x_{l-1/2}, x_{l+1/2}]$, $[x_0, x_{1/2}]$ 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 of half-length. Assuming $R\equiv 0$, in Equ. (4.1), the test functions to be used, regardless of whether the coefficients are constant or not, are:

$$w(x,t)= \begin{cases} 1, & \text{if } (x,t)\in\Omega^l \\ 0, & \text{if } (x,t)\notin\Omega^l \end{cases} \qquad (5.7)$$

where the subregions Ω^l are limited by the curves $\Sigma_{l-1/2}$, $\Sigma_{l+1/2}$ and the boundaries of the space-time region Ω, as illustrated in Fig. 2a.

For this case the weighting functions have discontinuities in the "characteristic" curves Σ, although the first derivatives are continuous. Also, the velocity of propagation of such discontinuities is $V_\Sigma=V$, so that $\mathcal{K}^0(w,u)\equiv 0$, by virtue of Eq. (4.6a), and the information that is gathered on Σ, concerns the first derivative of the solution, exclusively.

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

$$\left[\frac{\partial w}{\partial x}\right]_{\Sigma_{i-1/2}} = 1; \quad \left[\frac{\partial w}{\partial x}\right]_{\Sigma_{i+1/2}} = -1. \tag{5.8}$$

Replacing Equs. (5.8) into (4.6b), yields:

$$\mathcal{K}^i(w,u)_{\Sigma i\pm 1/2} = \pm\,(1+V^2)^{-1/2}\,\frac{\partial u}{\partial x} \tag{5.9}$$

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

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

$$= \int_{x^*_{i-1/2}}^{x^*_{i+1/2}} u(x,t^n)dx + \int_\Omega f_\Omega dxdt. \tag{5.10}$$

Equ. (5.10) is similar to (5.4); in it, the unknown function has not been, and will not be, approximated by any specific functional form and the integrals that appear there can be approximated in many different ways. As in the case when the test functions were bilinear, different approximations of these integrals lead to different algorithms. To be specific, the case when the integrals over characteristics are approximated by means of a fully implicit approximation, is here discussed [30]. Thus:

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

$$\left\{\left(D\partial u/\partial x\right)^{n+1}_{i-1/2} - \left(D\partial u/\partial x\right)^{n+1}_{i+1/2}\right\}\Delta t \tag{5.11}$$

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

$$\int_{x_{i-1/2}}^{x_{i+1/2}} u(x,t^{n+1})dx = u_i^{n+1}\Delta x + O(\Delta x^3) \tag{5.12}$$

However, this is not consistent with the order of approximation at which other terms are treated and to obtain satisfactory numerical results, it is necessary to use a more refined option, such as [30]:

$$\int_{x_{i-1/2}}^{x_{i+1/2}} u(x,t^{n+1})dx = \frac{u_{i+1}^{n+1} + u_{i-1}^{n+1} - 22u_i^{n+1}}{24} + O(\Delta x^5) \tag{5.13}$$

When the region Ω^i intersects the inflow boundary, procedures similar to those that were described for bilinear ELLAM must be applied [30]. For outflow boundary conditions of Dirichlet type, the out-flow 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 Newmann or flux conditions, it is necessary to incorporate u_E^{n+1}, as an additional unknown, and to add one more weighting function, in order to close the system of equations. The support Ω_E, of such weighting function is half the size of the other ones, as illustrated in Fig. 4.

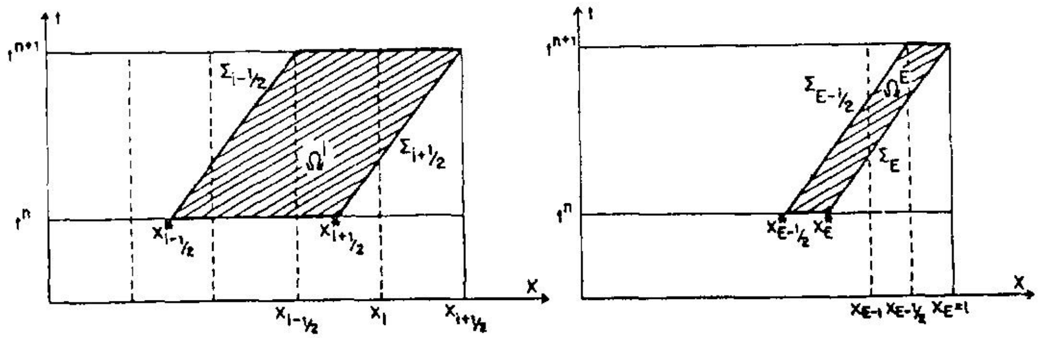

Figure 2a.- Space-time support of the wighting function w^i for the method of cells. b).- Space-time support of the weighting functions W^E for Neuman and flux conditions at the inflow boundary.

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A Non-Nodal Collocation Procedure in Three-Dimensional Elasticity

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ABSTRACT

A non-nodal collocation procedure to consider traction discontinuities in boundary element method (BEM) analysis of three-dimensional elasticity problems is discussed here. The numerical implementation for triangular boundary elements and numerical results for two applications are presented.

INTRODUCTION

Boundary element method (BEM) computer codes must include adequate techniques to deal with traction discontinuities, otherwise over refined meshes may be required in the neighbourhood of regions where such discontinuities occur (or are expected to occur). Over refinement, besides being expensive may not give accurate results.

A technique to overcome this difficulty, which does not require implementation of any special computational procedure, is that proposed by Brebbia[1] who employed in the neighbourhood of points of discontinuity, two nodes (in two-dimensional analyses) close to each other but not linked by elements. This scheme was used for a short period, being abandoned in favour of more rigorous techniques.

The first rigorous general procedure to deal with traction discontinuities was developed by Chaudonneret[2], for two-dimensional elasticity. Two extra equations for points where tractions could be discontinous were obtained from the assumption that the stress tensor be uniquely defined, together with the condition of invariance of trace of the strain tensor. Thus it was possible to consider extra unknowns, that appear when discontinuity of surface tractions is considered. An equivalent procedure for potential analysis has been proposed by Alarcon et alii[3] who obtained extra equations from the condition of uniqueness of the flux vector at corners.

The procedure most widely used now days is that proposed by Patterson and Sheikh[4], in which collocation points and functional nodes are dislocated towards the interior of any element whose extreme nodes are located at points where surface traction

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