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LOCALIZED ADJOINT METHOD: AN OVERVIEW

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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, was unrelated. More recently, it has been recognized that there are many relations between them and that it is desirable to develop foundations common to all of 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".

The Localized Adjoint Method (LAM) is a new and promising methodology for discretizing partial differential equations, which was proposed by the author [4] and is based on Herrera's Algebraic Theory of Boundary Value Problems [1-5]. Applications have successively been made to ordinary differential equations, for which highly accurate and efficient algorithms were developed [4,6-8], multidimensional steady state problems [9] and optimal spatial methods for advection-diffusion equations [10-18]. More recently, generalizations of Characteristic Methods known as Eulerian-Lagrangian Localized Adjoint Method (ELLAM), were developed [19,20] and many specific applications have already been made [21-28]. Related work and additional applications are underway (see [29], for additional references).

In this paper the Localized Adjoint Method is briefly explained and some of the ideas are illustrated by means of simple examples. In a companion paper, presented in this meeting [29], ELLAM procedures, which have been quite successful for treating advection dominated transport, are discussed.

2. LOCALIZED ADJOINT METHOD

In the construction of approximate solutions there are two processes, equally important but different, that should be clearly distinguished [20]. 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 [20] (see also Section 4).

The fact that the two above mentioned processes have considerable independence, 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. Localized Adjoint Method is a methodology I have proposed [2-4], to carry out such analysis and develop new algorithms using the insight so gained.

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.

In the Localized Adjoint Method, the information about the exact solution contained in an approximate one, is exhibited applying Herrera's Algebraic Theory of Boundary Value Problems. This approach is more direct than the Theory of Distributions. It is also more appropriate to carry out the analysis, when localized weighting functions are used, as is the case in most numerical methods. In this respect, the Algebraic Theory allows simultaneous use of discontinuous trial and test functions, something which is not possible when the Theory of Distributions is applied.

3. 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

$$\mathcal{L}u = f_{\Omega}, \quad \text{in } \Omega \tag{3.1}$$

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. The definition of formal adjoint requires that a differential operator \mathcal{L} and its formal adjoint \mathcal{L}^* , satisfy the condition that $w\mathcal{L}u - u\mathcal{L}^*w$ be a divergence; i.e.:

$$w\mathcal{L}u - u\mathcal{L}^*w = \nabla \cdot \{\underline{\mathcal{D}}(u, w)\}$$
(3.2)

for a suitable vector-valued bilinear function $\underline{\mathcal{D}}(u, w)$. Integration of (3.2) over Ω and application of generalized divergence theorem [30], yield:

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

where

$$\mathcal{R}_{\partial}(u,w) = \underline{\mathcal{D}}(u,w) \cdot \underline{n} \quad \text{and} \quad \mathcal{R}_{\Sigma}(u,w) = -[\underline{\mathcal{D}}(u,w)] \cdot \underline{n}$$
(3.4)

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 <u>n</u>, 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 [31] and they can be obtained decomposing the bilinear function \mathcal{R}_{∂} . Indicating, as it is usual, transposes of bilinears forms by means of a star, the general form of such decomposition is:

$$\mathcal{R}_{\partial}(u,w) \equiv \underline{\mathcal{D}}(u,w) \cdot \underline{n} = \mathcal{B}(u,w) - \mathcal{C}^{*}(u,w)$$
(3.5)

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 $\mathcal{C}^{*}(u, w)$ can only be evaluated after the problem has been solved and is called the "complementary boundary values" [20].

In a similar fashion, convenient formulations of boundary value problems with prescribed jumps, requires constructing Green's formulas in discontinuous fields. For the case when the coefficients of \mathcal{L} are continuous (discontinuous coefficients have been treated previously [4]), the corresponding decomposition is easy to obtain and it stems from the algebraic identity:

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

where for every function u,

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

while u_+ and u_- stand for the limits of u on the positive and negative sides, respectively. It yields

$$\mathcal{R}_{\Sigma}(u,w) = \mathcal{J}(u,w) - \mathcal{K}^{*}(u,w)$$
(3.8)

with

$$\mathcal{J}(u,w) = -\underline{\mathcal{D}}([u], \dot{w}) \cdot \underline{n}$$

$$\mathcal{K}(w,u) = \underline{\mathcal{D}}(\dot{u}, [w]) \cdot \underline{n}$$
(3.9a)

Generally, the jump $\mathcal{J}(u, w)$ is prescribed, while $\mathcal{K}^{\bullet}(u, w)$ are 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 Equation (3.1), together with

$$\mathcal{B}(u,\cdot) = g_{\partial}$$
 and $\mathcal{J}(u,\cdot) = j_{\partial}$

Introducing the notation

$$\langle Pu, w \rangle = \int_{\Omega} w \mathcal{L}u \, dx;$$
 $\langle Q^*u, w \rangle = \int_{\Omega} u \mathcal{L}^*w \, dx$ (3.11a)

$$\langle Bu, w \rangle = \int_{\partial \Omega} B(u, w) dx;$$
 $\langle C^*u, w \rangle = \int_{\partial \Omega} C(w, u) dx$ (3.11b)

$$\langle Ju, w \rangle = \int_{\Sigma} \mathcal{J}(u, w) dx$$
 and $\langle K^*u, w \rangle = \int_{\Sigma} \mathcal{K}(w, u) dx$ (3.11c)

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

$$\langle f, w \rangle = \int_{\Omega} w f_{\Omega} dx; \quad \langle g, w \rangle = \int_{\partial \Omega} g_{\partial}(w) dx; \quad \langle j, w \rangle = \int_{\Sigma} j_{\Sigma}(w) dx; \quad (3.12)$$

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

....

$$\langle (Q^* - C^* - K^*)u, w \rangle = \langle f - g - j, w \rangle \forall w \in D_2$$
(3.13)

The linear functionals $Q^{\bullet}u$, $C^{\bullet}u$ and $K^{\bullet}u$, 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 Eqs. (3.11) and will be illustrated in the examples that follow.

In view of (3.13), when the method of weighted residuals is applied, an approximate solution $\hat{u} \in D_1$, satisfies:

$$\langle (Q^* - C^* - K^*)\hat{u}, w^{\alpha} \rangle = \langle f - g - j, w^{\alpha} \rangle, \qquad \alpha = 1, \dots, N$$
(3.14)

Since the exact solution satisfies (3.13), it is clear that:

$$\langle (Q^* - C^* - K^*)\hat{u}, w^\alpha \rangle = \langle (Q^* - C^* - K^*)u, w^\alpha \rangle, \qquad \alpha = 1, \dots, N$$
(3.15)

Eqs. (3.15), can be applied to analyze the information about the exact solution that is contained in an approximate one and have been used extensively in the development of the Localized Adjoint Method.

4. DISCUSSION

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 the averages K^*u , into averages of the function, the first derivative, etc. This is achieved writing K^* as the sum of operators K^{0*}, K^{1*}, \ldots , each one containing the information about the average of the derivative of the corresponding order. Such decomposition is induced when $K^*(u, w)$ is decomposed point-wise, into the sum of bilinear functions $K^{0*}(u, w), K^{1*}(u, w), \ldots$, each one containing the corresponding information point-wise. Similarly, J will be written as the sum of operators J^0, J^1, \ldots , 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:

$$K = \sum_{i} K^{i}; \qquad J = \sum_{i} J^{i}; \qquad \mathcal{K} = \sum_{i} \mathcal{K}^{i}; \qquad \mathcal{J} = \sum_{i} \mathcal{J}^{i}$$
(4.1)

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

$$\mathcal{L}u \equiv -\frac{d}{dx} \left(D\frac{du}{dx} - Vu \right) + Ru = f_{\Omega}, \quad \text{in } \Omega \equiv [0, l]$$
(4.2a)

Attention will be restricted to the case when D and V are continuous, in which case the smoothness conditions implied by conservation of mass and Fickian diffusion are:

$$[u] = 0$$
 and $\left[\frac{\partial u}{\partial x}\right] = 0$, on Σ (4.2b)

by virtue of the assumed continuity of V and D.

A partition $\{0 = x_0, x_1, \dots, x_{E-1}, x_E = l\}$ is introduced, which is assumed to be uniform; i.e., $x_{\alpha} - x_{\alpha-1} = h$ is independent of α . It will be further assumed, that trial and test functions may have jump discontinuities at internal nodes, only. This corresponds to taking $\Sigma = \{x_1, \dots, x_{E-1}\}$, in the general framework presented in Section 2. On Σ , the choice $\underline{n} = 1$ is convenient, because in this manner the positive side of Σ is the side that is determined by the sense of the *x*-axis. Boundary conditions satisfied at 0 and *l*, can be Dirichlet, Neumann or Robin boundary conditions, but they are left unspecified, since the following developments accommodate any of them.

The formal adjoint of the operator \mathcal{L} , as defined by (4.2a), is:

$$\mathcal{L}^{\bullet}w \equiv -\frac{d}{dx}\left(D\frac{dw}{dx}\right) - V\frac{dw}{dx} + Rw$$
(4.3)

Therefore:

$$w\mathcal{L}u - u\mathcal{L}^*w \equiv \frac{d}{dx}\left\{u\left(D\frac{dw}{dx} + Vw\right) - wD\frac{du}{dx}\right\}$$
(4.4)

and

$$\underline{\mathcal{D}}(u,w) \equiv u \left(D \frac{dw}{dx} + Vw \right) - w D \frac{du}{dx}$$
(4.5)

Application of Eqs. (3.9), yields:

$$\mathcal{J}^{0}(u,w) = -[u]\left(D\frac{\dot{d}w}{dx} + V\dot{w}\right); \qquad \qquad \mathcal{J}^{1}(u,w) = \dot{w}D\left[\frac{du}{dx}\right] \qquad (4.6a)$$

$$\mathcal{K}^{0}(w,u) = \dot{u} \left[D \frac{dw}{dx} + Vw \right]; \qquad \qquad \mathcal{K}^{1}(w,u) = -[w] D \frac{\dot{du}}{dx} \qquad (4.6b)$$

from which $\mathcal J$ and $\mathcal K$ are obtained by means of Eqs. (4.1). In Eqs. (4.6), 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:

$$\mathcal{B}(u,w) = u \left(D \frac{dw}{dx} + Vw \right) \underline{n}; \qquad \mathcal{C}(w,u) = w D \frac{du}{dx} \underline{n}$$
(4.7)

for Dirichlet data,

$$\mathcal{B}(u,w) = -wD\frac{du}{dx}\underline{n}; \qquad \mathcal{C}(w,u) = -u\left(D\frac{dw}{dx} + Vw\right)\underline{n}$$
(4.8)

for Neumann data and

$$\mathcal{B}(u,w) = -w \left(D \frac{du}{dx} - Vu \right) \underline{n}; \qquad \mathcal{C}(w,u) = -u D \frac{dw}{dx} \underline{n}$$
(4.9)

when total flux is prescribed.

For ordinary differential equations it is easy to construct algorithms which concentrate all the information at internal nodes [5]. The conditions to be satisfied by weighting functions are: $\mathcal{L}^* w \equiv 0$ and $\mathcal{C}(w, \cdot) \equiv 0$. This latter requirement implies the boundary conditions:

$$w = 0; \qquad D\frac{dw}{dx} + Vw = 0; \qquad D\frac{dw}{dx} = 0$$
(4.10)

to be satisfied wherever Dirichlet, Neumann or flux conditions are prescribed for the sought solution. The actual construction of such weighting functions is very efficient when collocation is used [6]. 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 Eq. (4.6b).

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

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

$$(4.11)$$

These are C^0 test functions; for them the system of equations (3.15) reduces to:

$$\langle K^* u, w^{\alpha} \rangle = \langle K^* \hat{u}, w^{\alpha} \rangle, \qquad \alpha = 1, \dots, N$$

$$(4.12)$$

When the system of test functions $\{w^1, \ldots, w^N\}$ is TH-complete, Eqs. (4.12) imply that $K^*\hat{u} = K^*u$, which in the present case is equivalent to

$$\hat{u}(x_j) = u(x_j), \qquad j = 1, \dots, E-1$$
 (4.13)

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 [32], where a rigorous discussion of this question in an abstract setting was presented, allowing considerable 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 [33].

Observe that Eqs. (4.13) 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, Eqs. (4.13) 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 internal 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:

$$\hat{u}(x) = U_0 \Phi^0 + U_E \Phi^E + \sum_{j=1}^{E-1} U_j \Phi^j(x).$$
(4.14)

TH-complete systems which satisfy (4.11) have dimension E-1 [33]. Let us apply the system of equations (3.14), using the weighting functions $\{w^1, \ldots, w^{E-1}\}$, where $\{w^1, \ldots, w^{E-1}\}$ is a TH-complete system. Then any solution of the resulting system has the property:

$$U_j = u(x_j), \qquad j = 1, \dots, E-1$$

by virtue of (4.13). Thus, the exact values are predicted correctly, independently of the base functions used.

5. THE METHOD OF CELLS

Let us consider Eq. (4.2a), in the case $R \equiv 0$. Keeping the same partition as before, let us denote by $x_{i+1/2}$ (i = 0, ..., E-1), the middle point of the intervals $[x_i, x_{i+1}]$. The decomposition of \mathcal{K} :

$$\mathcal{K}(w,u) = \mathcal{K}^{0}(w,u) + \mathcal{K}^{\mathcal{F}}(w,u)$$
(5.1)

where

$$\mathcal{K}^{\mathbf{0}}(w,u) = \dot{u} \left[D \frac{dw}{dx} \right]; \qquad \mathcal{K}^{\mathcal{F}}(w,u) = -[w] \left(D \frac{\overline{du}}{dx} - Vu \right)$$
(5.2)

will be used in the sequel. Define the system of weighting functions $\{w^1, \ldots, w^{E-1}\}$, as the characteristic functions of each one of the subintervals $[x_{\alpha-1/2}, x_{\alpha+1/2}]$; i.e.,

$$w^{\alpha}(x) = \begin{cases} 1, & x_{\alpha-1/2} < x < x_{\alpha+1/2} \\ 0, & \text{elsewhere} \end{cases}$$

Then $\mathcal{L}^* w^{\alpha} = 0$ and

$$K^{0}(w,u) = 0 \quad \text{while} \quad K^{\mathcal{F}}(w,u) = \left(D\frac{du}{dx} - Vu\right)_{\alpha+1/2} - \left(D\frac{du}{dx} - Vu\right)_{\alpha-1/2}$$

so that Eqs. (3.15) become

$$\langle K^* \hat{u}, w^{\alpha} \rangle = \langle K^* u, w^{\alpha} \rangle, \qquad \alpha = 1, \dots, E-1$$
 (5.5)

In this case the system of weighting functions is not TH-complete and the equality $K^*\hat{u} = K^*u$, does not follow. However, the information supplied by the system of weighted equations, is concentrated at the internal nodes and refers to the total flux $D\frac{du}{dx}$ - Vu. Such system of equations contains E unknowns $\left(D\frac{du}{dx} - Vu\right)_{\alpha+1/2}$, for $\alpha = 0, \dots, E-1$; and E-1 equations. Thus, further processing is required to obtain a system having a unique solution. This depends

and E = 1 equations. Thus, turner processing is required to obtain a system having a unique solution. This depends on the boundary conditions to be satisfied. For Dirichlet boundary conditions, it is standard to use the relations

$$\left(D\frac{du}{dx} - Vu\right)_{\alpha+1/2} = D\frac{\hat{u}_{\alpha+1} - \hat{u}_{\alpha}}{h} - V\frac{\hat{u}_{\alpha+1} + \hat{u}_{\alpha}}{2} + O(h^2)$$
(5.6)

to replace the E unknowns fluxes by only E - 1 unknown values of the solution at the internal nodes (\hat{u}_{α} , $\alpha = 1, \ldots, E - 1$). In this manner, an E by E system of equations is obtained. The author's Algebraic Theory of Boundary Value Problems yields the same system of equations, if the trial function (4.14) is used, while U_0 and U_E are set to be equal to the prescribed boundary values.

On the other hand, if the Dirichlet condition is replaced by a flux condition on the left boundary, a TH-complete system of weighting functions is obtained, if the system defined by Eq. (5.3) is supplemented with the characteristic function of the interval $[x_0, x_{1/2}]$. Observe that due to Eq. (4.9), no additional unknown is introduced by this weighting function. In this latter case, any approximate solution will yield the exact values of the flux at the inter-element boundaries. In particular, if the nodal values of the approximate solution are introduced by means of Eq. (5.6), the identity

$$\left(D\frac{du}{dx} - Vu\right)_{\alpha+1/2} \equiv D\frac{\hat{u}_{\alpha+1} - \hat{u}_{\alpha}}{h} - V\frac{\hat{u}_{\alpha+1} + \hat{u}_{\alpha}}{2}$$
(5.7)

will hold, because the fluxes at the inter-element boundaries are predicted exactly by the approximate solution. This is in spite of the fact that in this case, the values of the solution at the cell centers are predicted to order h^2 , only.

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