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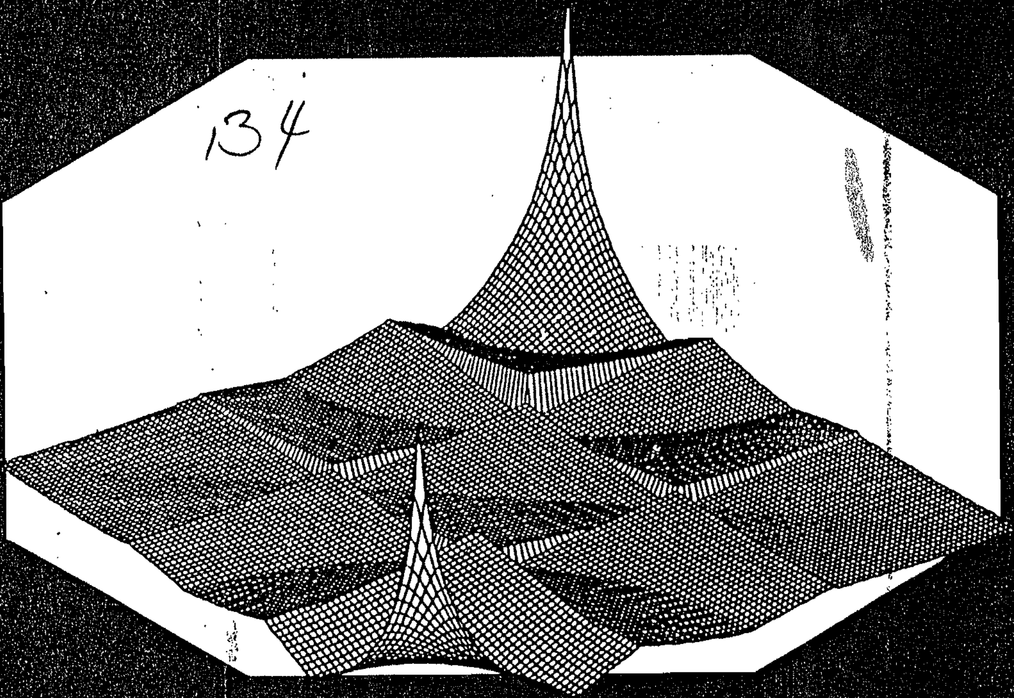

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Localized Adjoint Method: Topics for Further Research and some Contributions

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ABSTRACT

Localized Adjoint Method (LAM), is a new and promising methodology for discretizing partial differential equations, based on the author's Algebraic Theory of Boundary Value Problems, which has been successfully applied to ordinary and partial differential equations. Recently, a sequence of two papers was devoted to applying Localized Adjoint Method (LAM), in space-time, to problems of advective diffusive transport. The resulting methodology, called Eulerian-Lagrangian localized adjoint method (ELLAM), yields a general formulation that subsumes many characteristic methods (CM). The LAM constitutes a general and powerful framework for investigating and comparing a wide variety of numerical methods, and supplies insights to innovate them. However, further research should be carried out in many points. This paper indicates some of such points and anounces results recently obtained.

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 it is desirable to develop [illegible] all of them. In this spirit the author ped the Algebraic Theory of Boundary Value Problems [1-5] has led to what is at present known as the "Localized Adjoint ı".

.'he Localized Adjoint Method (LAM) is a new and promising ıology for discretizing partial differential equations, which ;ed on Herrera's Algebraic Theory of Boundary Value Problems Applications have successively been made to ordinary ential equations, for which highly accurate algorithms were ped [4,6-8], multidimensional steady state problems [9] and ıl spatial methods for advection-diffusion equations [10-18]. recently, in a pair of articles [19,20] generalizations of :teristic Methods that we refer to as Eulerian-Lagrangian zed Adjoint Method (ELLAM), were provided by the ELLAM Group Celia, R.E. Ewing, T.F. Russell and the author). Related work been published separately [21-25] and some more specific ations have already been made [26-31].

in the conclusions of the second of the ELLAM articles [20], a ıl discussion of the ELLAM methodology, and to some extent of .AM itself, was presented. In particular, a more complete e of the possibilities that should be explored and the :ms that must be tackled, in order to make of ELLAM a more ive modeling tool, was established. It was recognized that the framework has been demonstrated to be very suitable for ıting specialized test functions. The effect that different ary and continuity (or smoothness) conditions, satisfied by 'unctions, have on approximate solutions was clearly exhibited. the LAM framework leads in a natural manner to a definition of le unknowns for a given problem. For example, when developing umerical implementation of ELLAM in [19], it became apparent in some cases it was necessary to introduce the total flux as lditional unknown at the boundaries, in spite of the fact that ıain goal was to predict the value of the function at time t^{n+1}. .s also demonstrated that in the LAM approach it is possible to simultaneously, discontinuous trial and test functions, which ther approaches is not. The generality of the theory was corroborated, once more, by applying it to systems of equations and deriving Mixed Methods.

However, there are many points that should be studied in more depth. For example, among the theoretical questions which are open, one can mention that Herrera's Algebraic Theory of Boundary Value Problems, imply a kind of operator extensions of great generality (the "algebraic extensions"). Using them fully discontinuous trial and test functions can be applied simultaneously, which is not possible when standard theory of distributions is used. However, in this respect it is desirable to establish more clearly the relation between the algebraic extensions and the theory of distributions. Another theoretical question that should be tackled, refers to the concept of TH-complete systems of test functions. This concept was originally introduced by the author and extensively studied for symmetric operators [1,32], but the corresponding development for non-symmetric operators is wanting.

Among the more numerical aspects, there also many questions that should studied further. For example, very effective numerical procedures were developed for ordinary differential equations [6], but an extensive comparison of the efficiency of such procedures has not been carried out thus far. Also, we need to develop more efficient procedures for the construction and application of test functions which satisfy boundary conditions required in the numerical implementations. We need a more extensive study of both the theory and implementation of ELLAM techniques for variable coefficients particularly in multidimensional applications. Implementation of boundary conditions for variable-coefficient problems in multiple dimensions is also an important problem. Even in the one-dimensional case and in spite of the important progress that has already been made [19.20], several points remain open, in this respect. In addition, the treatment of nonlinear problems deserves further study. Since the unknown variables appear in nonlinear coefficients of the problem that are usually evaluated in the interior of mesh blocks via numerical quadrature, greater attention must be placed on the full approximation theoretic properties of the trial functions in these applications. The potential of local refinement in both space and time holds enormous potential for ELLAM and is the object of ongoing research.

Finally, we want to emphasize that LAM forms a general and powerful framework for investigating and comparing a wide variety of numerical methods. The framework motivates different choices of test functions to approximate different properties of the unknowns or even different unknowns, such as fluxes. The general theory is expanding to provide more insight. In addition, the ELLAM methods appear to have enormous flexibility and potential for treating general advection-diffusion-reaction problems.

2. THE CRITERIUM OF TH-COMPLETENESS

The discussion concerns functional-valued operators such as $R:D_1 \longrightarrow D_2^{*}$, which are linear, and their transposes $(R^{*}:D_2 \longrightarrow D_1^{*})$. Here, D_1 and D_2 are two linear spaces, the spaces of trial and test functions, respectively, in which no further structure is assumed. We write $\langle Ru,w\rangle = \langle R^{*}w,u\rangle$ for the associated bilinear functional, whenever $u \in D_1$ and $w \in D_2$. We underline auxiliary concepts whose definitions can be found in other papers [2,5,33,34].

Definitions 2.1.- Consider an operator $R:D_1 \longrightarrow D_2^{*}$ and an ordered pair of linear subspaces $\{I_1, I_2\}$, with $I_1 \subset D_1$ & $I_2 \subset D_2$. Such pair is said to be conjugate for R, when

$$u \in I_1 \ \&\ w \in I_2 \Longrightarrow \langle Ru,w\rangle = 0 \qquad (2.1)$$

Definition 2.2.- Let $\{I_1, I_2\}$, be a pair of subspaces ($I_1 \subset D_1$ and $I_2 \subset D_2$), conjugate for R. Then, a subset $\mathcal{E} \subset I_2$, is said to be TH-complete for I_1, when for every $u \in D_1$, one has:

$$\langle Ru,w\rangle = 0 \ \forall\ w \in \mathcal{E} \Longrightarrow u \in I_1 \qquad (2.2)$$

Theorem 2.1.- Let R, R_1 and R_2, be functional-valued operators and assume $R = R_1 + R_2$. Define the pairs of linear subspaces $\{I_{11}, I_{22}\}$ and $\{I_{12}, I_{21}\}$, by:

$$I_{11} = N_{R_2} \subset D_1 \qquad I_{22} = N_{R_1^{*}} \subset D_2 \qquad (2.3a)$$

$$I_{12} = N_{R_1} \subset D_1 \qquad I_{21} = N_{R_2^{*}} \subset D_2 \qquad (2.3b)$$

Then

a) Each of the pairs $\{I_{11}, I_{22}\}$ and $\{I_{12}, I_{21}\}$, are conjugate with respect to R.

When in addition, R_1^* & R_2^* can be varied independently, one has:

b) I_{22} is TH-complete for I_{11}

c) I_{21} is TH-complete for I_{12}

Definiton 2.3 (ABSTRACT FORMULATION OF PROBLEMS WITH JUMPS).- Let the operators $P:D_1 \longrightarrow D_2^*$, $B:D_1 \longrightarrow D_2^*$, $J:D_1 \longrightarrow D_2^*$, $Q:D_2 \longrightarrow D_1^*$, $C:D_2 \longrightarrow D_1^*$ and $K:D_2 \longrightarrow D_1^*$, satisfy Green-Herrera formula [2,20]:

$$P - B - J = Q^* - C^* - K^* \qquad (2.4)$$

An abstract formulation of boundary value problems with prescribed jumps is the following:

Given U_Ω, U_∂ and U_Σ, belonging to D_1, define $f=PU_\Omega$, $g=BU_\partial$ and $j=JU_\Sigma$, the problem is to find $u \in D_1$, such that

$$Pu = f; \; Bu = g \; \& \; Ju = j \qquad (2.5)$$

Theorem 2.2.- Let the operators $C':D_1 \longrightarrow D_2^*$; $C'':D_1 \longrightarrow D_2^*$; $K':D_1 \longrightarrow D_2^*$; $K'':D_1 \longrightarrow D_2^*$; be such that: $C=C'+C''$ and $K=K'+K''$. Assume:

a).- $u \in D_1$ is a solution of the boundary value problem with prescribed jumps;

b).- $B+J$ is a boundary operator for P, while B and J are disjoint;

c).- $Q-C'-K'$ and $C''+K''$ can be varied independently, while $(C'')^*$ and $(K'')^*$ are disjoint.

Then:

A).- The system of equations (2.5), is equivalent to the single equation:

$$(P-B-J)u = f-g-j \qquad (2.6)$$

B).- $\{N_{(C''+K'')^*}, N_{Q-C'-K'}\}$ is a conjugate pair for $P-B-J$;

C).- $N_{Q-C'-K'}$ is TH-complete for $N_{(C''+K'')^*}$;

D).- If $\mathcal{E} \subset N_{Q-C'-K'}$ is TH-complete for $N_{(C''+K'')^*}$, then for any $\hat{u} \in D_1$, one has:

$$\langle (C''^* + K''^*)\hat{u}, w \rangle = \langle g+j-f, w \rangle \; \forall w \in \mathcal{E} \implies C''^*\hat{u} = C''^*u \text{ and } K''^*\hat{u} = K''^*u \qquad (2.7)$$

Remark.- Also, the assumption that $Q-C'-K'$ and $C''+K''$ can be varied independently, is tantamount to assume existence of solution of the homogeneous "adjoint problem":

Given any $W \in D_2$, *find a* $w \in D_2$ *such that*

$$(Q-C'-K')w = (Q-C'-K')W, \text{ while } (C''+K'')w = 0 \qquad (2.8)$$

Also, when $\hat{u} \in D_1$, is an approximate solution, the relations $C''^{*}\hat{u} = C''^{*}u$ and $K''^{*}\hat{u} = K''^{*}u$, imply, depending on the choice of C" and K", that some complementary boundary values, and values of the solution and its derivatives are predicted exactly at the interelement boundaries Σ, even if the approximate solution is fully discontinuous. For specific applications of this result, the reader is referred to previous work, already cited (in particular, see [20] for an extensive discussion of this point, in connection with ordinary differential equations).

3. APPLICATION TO DIFFERENTIAL EQUATIONS

The manner in which differential equations, including systems of such equations, are incorporated in the general setting of the author's Algebraic Theory of Boundary Value Problems has been explained in several previous papers (see for example [20]). In the brief explanation here presented, we follow a procedure introduced in [33], in which Sobolev spaces are used locally.

Consider a region Ω and for simplicity, assume the spaces of trial and test functions, defined in Ω, are the same linear space: D (i.e., $D=D_1=D_2$). Assume further, that functions belonging to D 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 would be the union of all the interelement boundaries. To be specific, consider a linear differential operator $\mathcal{L}$ of order m and assume $\{\Omega_1,\dots,\Omega_E\}$ is a partition of Ω. More precisely, $\{\Omega_1,\dots,\Omega_E\}$ is a collection of disjoint open regions (the "elements") of Ω, such that Ω is contained in the closure of the union of $\{\Omega_1,\dots,\Omega_E\}$. Then, one can define $D=H^m(\Omega_1)\oplus\dots\oplus H^m(\Omega_E)$, where $H^m(\Omega_i)$ is the Sobolev space of order m, defined in Ω_i. In this case $\Sigma=\Omega-(\Omega_1\cup\dots\cup\Omega_E)$.

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.:

$$w\mathcal{L}u-u\mathcal{L}^*w = \nabla\cdot\{\underline{\mathcal{D}}(u,w)\} \qquad (3.1)$$

for a suitable vector-valued bilinear function $\underline{\mathcal{D}}(u,w)$. Then, one defines bilinear functions $\mathcal{B}(u,w)$ and $\mathcal{C}(w,u)$ on $\partial\Omega$ (see [35]), such that

$$\mathcal{B}(u,w) - \mathcal{C}^{*}(u,w)=\underline{\mathcal{D}}(u,w)\cdot\underline{n} \qquad (3.2)$$

where, as it is usual, transposes of bilinear forms are denoted by means of a star. A basic property required of $\mathcal{B}(u,w)$ is that for any u which satisfies the prescribed boundary and initial conditions, $\mathcal{B}(u,w)$ is a well-defined linear function of w, independent of the particular choice of u.

Similarly, one defines on Σ the bilinear functions $\mathcal{J}(u,w)$ and $\mathcal{K}(w,u)$, by

$$\mathcal{J}(u,w) = -\underline{\mathcal{D}}([u],\dot{w})\cdot\underline{n}, \quad \mathcal{K}(w,u) = \mathcal{D}(u,[w])\cdot\underline{n} \qquad (3.3)$$

where

$$[u]= u_{+} - u_{-}, \qquad \dot{u} = (u_{+} + u_{-})/2 \qquad (3.4)$$

An important property of the bilinear function $\mathcal{J}(u,w)$ is that, when the jump of u is specified, it defines a unique linear function of w. Consider the

initial-boundary value problem with prescribed jumps

$$\mathcal{L}u = f_{\Omega}, \quad \text{in } \Omega_{i}, \text{ for } i=1,\dots,E \qquad (3.5a)$$

where $f_{\Omega}\in H^{0}(\Omega)$, together with

$$\mathcal{B}(u,\cdot) = g_{\partial}, \qquad \text{on } \partial\Omega \qquad (3.5b)$$

and

$$\mathcal{J}(u,\cdot) = j_{\partial}, \qquad \text{on } \Sigma \qquad (3.5c)$$

Here, g_{∂} and j_{∂} are the linear functions defined by the (initial and) boundary and jump conditions, respectively (see [20]). Then, introducing the notation

$$\langle Pu,w\rangle = \sum_{i} \int_{\Omega_i} w\mathcal{L}u\,dx; \qquad \langle Q^{*}u,w\rangle = \sum_{i} \int_{\Omega_i} u\mathcal{L}^{*}w\,dx \qquad (3.6a)$$

$$\langle Bu,w\rangle = \int_{\partial\Omega}\mathcal{B}(u,w)dx; \qquad \langle C^{*}u,w\rangle = \int_{\partial\Omega}\mathcal{C}(w,u)dx \qquad (3.6b)$$

$$\langle Ju,w\rangle = \int_{\Sigma}\mathcal{J}(u,w)dx \quad \text{and} \quad \langle K^{*}u,w\rangle = \int_{\Sigma}\mathcal{K}(w,u)dx \qquad (3.6c)$$

the problem can be formulated by means of Equ. (2.6) and the results of Section 2 can be applied. In particular, and depending on the choice of K", Equ. (2.7) implies that if a TH-complete system of weighting functions is used, the average of an approximate solution, yields an exact prediction of the values of the solution on the interelement boundaries Σ. Applications and illustrations of these facts, were given in [4,6,7,20].

4. THE ALGEBRAIC EXTENSIONS

As already mentioned, the operators $\mathcal{L}$ and $\mathcal{L}^*$ are understood in a distributional sense, and since they are of order *m*, both $\int_{\Omega_i} w\mathcal{L}u dx$ and $\int_{\Omega_i} u\mathcal{L}^* w dx$ are well defined for every $i=1,\ldots,E$. However, $D \subset H^0(\Omega)$, but the relation $D \subset H^1(\Omega)$ does not hold and when $u \in D$, one can only grant that $\mathcal{L}u \in H^{-m}(\Omega)$ and $\mathcal{L}^* w \in H^{-m}(\Omega)$. Thus, $\int_\Omega w\mathcal{L}u dx$ and $\int_\Omega u\mathcal{L}^* w dx$ are not well defined for every $u \in D$ and $w \in D$. This Section is devoted to present extensions $\hat{\mathcal{L}}$ and $\hat{\mathcal{L}}^*$ (the "algebraic extensions"), of $\mathcal{L}$ and $\mathcal{L}^*$, respectively, for which $\int_\Omega w\hat{\mathcal{L}}u dx$ and $\int_\Omega u\hat{\mathcal{L}}^* w dx$ are well defined for every $u \in D$ and $w \in D$.

The "algebraic extension" $\hat{\mathcal{L}}$ corresponding to the distributional operator $\mathcal{L}$, is defined to be the bilinear functional P-J. More precisely, $\hat{\mathcal{L}}$ is defined by:

$$\int_\Omega w\hat{\mathcal{L}}u dx = \langle (P-J)u,w\rangle \qquad (4.1)$$

which holds whenever $u \in D$ and $w \in D$. Similarly, the algebraic extension corresponding to $\hat{\mathcal{L}}^*$ is defined to be the bilinear functional Q^*-K^*; i.e.:

$$\int_\Omega u\hat{\mathcal{L}}^* w dx = \langle (Q-K)^* u,w\rangle \qquad (4.2)$$

which also holds when both u and w belong to D. These operator extensions satisfy Green-Herrera formula [20]:

$$\int_\Omega w\hat{\mathcal{L}}u dx - \int_\Omega u\hat{\mathcal{L}}^* w dx = \langle (B-C^*)u,w\rangle \qquad (4.3)$$

which holds whenever $u \in D$ and $w \in D$. This exhibits $\hat{\mathcal{L}}^*$ as the formal adjoint of $\hat{\mathcal{L}}$. In a previous paper [33], it was shown that $\hat{\mathcal{L}}$ and $\hat{\mathcal{L}}^*$ are indeed extensions of the distributional operators $\mathcal{L}$ and $\mathcal{L}^*$, respectively, and examples of the application of the algebraic extensions were given. The fact that $\hat{\mathcal{L}}$ is indeed an extension of $\mathcal{L}$, means that

$$\int_\Omega w\hat{\mathcal{L}}u dx = \int_\Omega w\mathcal{L}u dx \qquad (4.4)$$

whenever the latter integral is defined.

As a first illustration, let us consider the operator $\mathcal{L}$ and its algebraic extension, in the case when the distributional operator

$\mathcal{L}$=d/dx, the region $\Omega = (-1,1)$ and the partition of Ω is made of two subintervals: $\Omega_1 = (-1,0)$ and $\Omega_2 = (0,1)$. Then $\mathcal{L}^* = -d/dx$, while $\mathcal{D}(u,w) = uw$. Let the function u be essentially a Heaviside step function ($u=0$ for $-1<x<0$; and $u=1$ for $0\le x<1$), while w is taken having different degrees of smoothness.

Case A.- $w\in H^1(\Omega)$, so that w is continuous.

i) In this case:

$$\int_{-1}^{1} w\mathcal{L}u\,dx = \int_{-1}^{1} u\mathcal{L}^* w\,dx + (uw)\Big|_{-1}^{1} = -\int_0^1 \frac{dw}{dx}\,dx + w(1) = w(0). \qquad (4.5a)$$

This result is standard. In essence, it corresponds to $\mathcal{L}u$ being a Dirac's Delta Function.

ii) Using the fact that $\mathcal{D}(u,w) = uw$, it is seen that

$$\int_{-1}^{1} w\hat{\mathcal{L}}u\,dx = \sum_i \int_{\Omega_i} w\mathcal{L}u\,dx + (\dot{w}[u])_{x=0} = w(0) \qquad (4.5b)$$

since $[u]_{x=0}=1$, while $\dot{w}(0)=w(0)$, because w is continuous. Thus, Equ. (4.4) is verified for this case.

Case B.- w has a jump discontinuity at $x=0$, so that $w\in D$ but $w\notin H^1(\Omega)$.

i) $\int_{-1}^{1} w\mathcal{L}u\,dx$ is not defined.

ii) $\int_{-1}^{1} w\hat{\mathcal{L}}u\,dx$ is well defined and it is still given by (4.4b), except that $\dot{w}(0)\neq w(0)$, so that

$$\int_{-1}^{1} w\hat{\mathcal{L}}u\,dx = \dot{w}(0) \qquad (4.6)$$

where it is recalled that $\dot{w}(0)=(w(0+)+w(0-))/2$.

As a second illustration, replace d/dx by d^2/dx^2, in the previous example. Then $\mathcal{L}^* = \mathcal{L}$, while $\mathcal{D}(u,w) = w\frac{du}{dx} - u\frac{dw}{dx}$ and proceeding as before:

Case A.- $w\in H^2(\Omega)$, so that w is continuous, with continuous first order derivative.

i) In this case:

$$\int_{-1}^{1} w\mathcal{L}u\,dx = \int_{-1}^{1} u\mathcal{L}^* w\,dx + (wu'-uw')\Big|_{-1}^{1} = \int_0^1 w''\,dx - w'(1) = -w'(0) \qquad (4.7a)$$

where u' and w' stand for the derivatives of u and w, respectively. This is a standard case. In essence, this result corresponds to u'' being the derivative of Dirac's Delta Function, when u is a Heaviside step function.

ii) Using the fact that $\mathcal{D}(u,w) = wu'-uw'$, it is seen that:

$$\int_{-1}^{1} w\hat{\mathcal{L}}u\,dx = \sum_i \int_{\Omega_i} w\mathcal{L}u\,dx + (\dot{w}[u'] - \dot{w}'[u])_{x=0} = -w'(0) \qquad (4.7b)$$

where the fact that $\dot{w}'(0)=w'(0)$, because w' is continuous, has been used. Again, Equs. (4.7) agree with Equ. (4.4).

Case B.- w' has a jump discontinuity at $x=0$, so that $w \in D$ but $w \notin H^2(\Omega)$.

i) $\int_{-1}^{1} w\mathcal{L}u\,dx$ is not defined.

ii) $\int_{-1}^{1} w\hat{\mathcal{L}}u\,dx$ is well defined and it is still given by (4.6b), except that $\dot{w}'(0) \neq w'(0)$, so that

$$\int_{-1}^{1} w\hat{\mathcal{L}}u\,dx = -\dot{w}'(0) \qquad (4.8)$$

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