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Localized Adjoint Method as a New Approach to Advection Dominated Flows

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ABSTRACT

Solution of advection-dominated transport problems by discrete interior methods is usually accomplished by employing some type of upstream weighting. Upwinded finite element formulations have also been developed. At present the authors are developing a procedure, based on Herrera's algebraic theory of boundary value problem, which systematically uses localized adjoint formulas. Here, the basic ideas of the method are explained. Also, the present state of development, as it applies to one and multi-dimensional steady-state and transient problem is revised.

INTRODUCTION

The numerical solution of the advective-difusive transport equation is a problem of great importance because many problems is science and engineering involve such mathematical model. The numerical treatment of advection dominated proceses is quite difficult. The procedures available 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 upstrea, weighting techniques, whose development is essentially ad-hoc.

An alternative and very promising approach has been introduced by Herrera [1-4]. In past work, this has been referred as "Optimal Test Function Method". However, from a technical point of view, it would be more appropriate to call such procedures "Localized Adjoint Methods". Also, in this manner, the method would be more clearly distinguised from other procedures. Thus, this is the terminology that will be adopted in what follows.

The starting point of localized adjoint methods is a rather simple and, as a matter of fact, old idea. Let $\mathcal{L}$ be a differential operator defined in a region Ω and let $\mathcal{L}^*$ be its formal adjoint. Then, when u and v satisfy suitable boundary conditions, Green's formula

$$\int_\Omega v\mathcal{L}u\,dx = \int_\Omega u\mathcal{L}^* v\,dx \qquad (1.1)$$

is satisfied. Equation (1.1) allows a convenient interpretation of the method of weighted residuals. Consider the problem of solving the equation

$$\mathcal{L}u = f_\Omega, \text{ in } \Omega \qquad (1.2)$$

subjected to homogeneous boundary conditions for which Green's formula (1.1) applies. In the method of weighted residuals, one usually considers a system of weighting (or test) functions $\{\varphi_1,\ldots,\varphi_N\}$. Then, one says that a function u' is an approximate solution of this problem when

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

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 the representation $u' = \sum a_\alpha \phi_\alpha$ of u in terms of the system $\{\phi_1,\ldots,\phi_N\}$ of base (or trial) functions. However, this representation is an artifice that bears no relation to the exact solution u.
The actual information about the exact solution contained in an approximate one, can be established making the following observations. From (1.2) it is clear that the exact solution u satisfies

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

Equations (1.3) and (1.4) together imply

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

or

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

by virtue of Green's formula (1.1). Consider the Hilbert space L^2, in which the inner productr of two functions u and v is given by $\int_\Omega uvdx$. Then, the system of equations (1.6) allows the following conclusion:
Any function u' whose projection, on the subspace spanned by the system of functions $\{\mathcal{L}^*\varphi_1,\ldots,\mathcal{L}^*\varphi\}$, coincides with that of the exact solution u, is an approximate solution. Indeed, this projection is <u>all the information</u> about the exact solution contained in 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 (1.1), but which are applicable even when the functions considered are not smooth. This is because in most applications weighting functions are localized (i.e., they have local support) and they usually violate the smoothness assumptions at the boundary of their support. Even more, the development of a theory spplicable 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 [1-4], recently developed an "algebraic theory of boundary value problems", in which the analysis of the information contained in an approximate solution 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

"Localized adjoint methods" consist in making systematic use of the resulting equations to analyse 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 recent years the authors have applied localized adjoint methods to advection diffusion equations. The numerical results indicate that this kind of methods possesses definite advantages over other procedures (5-8). Further improvements are expected to come from work presently under way, in which Herrera's theory is applied in space-time. The localized adjoint methods derived in this manner, clarify and perfect Eulerian Lagrangian procedures (9,10).

In what follows Herrera's (1-4) algebraic theory of boundary value problems is briefly explained. For a more detailed presentation and proofs of the results, the reader is referred to the original papers (1,2,4).

The general abstract boundary value problem to be considered corresponds to one with prescribed jumps and it is defined by the system of equations:

$$\langle Pu, v\rangle = \langle f, v\rangle \; ; \; \langle Bu, v\rangle = \langle g, v\rangle \; ; \; \langle Ju, v\rangle = \langle j, v\rangle \; \forall \; v \in D \qquad (2.1)$$

Where D is the linear space of admissible functions, P, B and J are bilinear functionals, while f, g and j are prescribed functionals (the data of the problem). Generally, the bilinear forms P, B and J are associated with the differential operator, the boundary values and the jumps accross discontinuities. When the sought solution is smooth, the prescribed jump j=0. Under the assumptions of the general theory, the three equations (2.1) are equivalent to the single variational formulation

$$\langle (P-B-J)u, v\rangle = \langle f - g - j, v\rangle \quad v \in D \qquad (2.2)$$

This variational formulation is said to be "the variational formulation in terms of the data of the problem", because Pu, Bu and Ju are prescribed.

Making use of the General Green's formula for operators in discontinuous fields (1.4)

$$\langle (P-B-J)u, v\rangle = \langle (Q-C-K)v, u\rangle \qquad (2.3)$$

the variational formulation (2.2) is transformed into

$$\langle (Q-C-K)\, v, u\rangle = \langle f-g-j, v\rangle \qquad (2.4)$$

This is said to be "the variational formulation in terms of the sought information", because $Q^{\bullet}u$ $C^{\bullet}u$ and $K^{\bullet}u$ are not prescribed. Generally, $Q^{\bullet}u$ supplies information at the interior of the region of definition of the problem, $C^{\bullet}u$ supplies information about the complementary boundary values, and $K^{\bullet}u$ yields the average of the solution (and derivatives) accross surfaces of discontinuity. Regarding the general Green's formula (2.3), it is assumed that the bilinear forms P and Q are formal adjoints, in the sense of the theory. The boundary bilinear forms B and C, can be constructed using arguments which are essentially standard. However, the construction of the operators J and K is not standard. The systematic manner supplied by Herrera's algebraic theory will be succintly explained now.

Let the region of definition of the problem Ω, be decomposed into two subregions Ω_I and Ω_{II} and assume the discontinuities of the trial and test functions can only occur on the common boundary Γ, separating Ω_I and Ω_{II}. Then, let the space of admissible functions be $D=D_I + D_{II}$, where D_I and D_{II} are linear spaces whose elements are functions defined in Ω_I and Ω_{II}, respectively.

After having constructed the operators B and C, two classes of functions, $S^{\ell}D$ and $S^{r}D$, are considered. Elementes belonging to S^{ℓ} will be said to be left smooth while those belonging to S^{r} will be said to be right-smooth. The classes S^{ℓ} and S^{r}, are taken to be conjugate subspaces; i.e.,

$$\langle (P-B)u, v\rangle = \langle (Q-C)u, v\rangle, \quad u\in S^{\ell} \;\&\; v \in S \qquad (2.5)$$

Given any element $u\in D$, write $u = \{u_I, u_{II}\}$ with $u_I \in D_I$ and $u_{II} \in D_{II}$. Define $u^{\ell} = \{u_I, u_{II}\}$ where $u_I^{\ell} \in D_I$ is left-smooth extension to Ω_I of $u_{II}\in D_{II}$, while $u_{II}^{\ell} \in D_{II}$ is the left-smooth extension to Ω_{II} of $u_I \in D_I$ the existence of such extensions is a fundamental hypothesis of the theory (see [1]). Then, it is possible to define

$$\overset{\bullet}{u}^{\ell} = (u^{\ell} + u)/2 \qquad (2.6a)$$

$$[u]^{\ell} = u^{\ell} - u \qquad (2.6b)$$

Equations (2.6) together, imply

$$u = \overset{\bullet}{u}^{\ell} - [u]^{\ell}/2 \qquad (2.7)$$

Observe that $u^{\ell} \in D$ and $[u]^{\ell} \in D$. These functions will be called the (abstract) average and jump, respectively, based on the left-smoothness criterium. Correspondingly, given any function $v\in D$, one considers the functions $v_I v_{II}$, v^{r}, $\overset{\bullet}{v}^{r}$ and $[v]^{r}$, which are defined replacing the left-smooth class of functions, by the right smooth class of functions.

By assumption, equation (2.5 holds whenever $u\in S^{\ell}$ and $v\in S^{r}$. However, $P-B \neq (Q-C)^{\bullet}$, in general. Thus, one defines

$$R = P - B - (Q - C)^{\bullet} \qquad (2.8)$$

In addition, the operators $R_I: D \longrightarrow D^*$ and $R_{II}: D \longrightarrow D^*$ are defined, for every $u = \{u_I, u_{II}\} \in D$, by

$$\langle R_I u, v\rangle = \langle Ru_I, v_I\rangle; \quad \langle R_{II} u, v\rangle = \langle Ru_{II}, v_{II}\rangle \qquad (2.9)$$

which hold for every $v=\{v_I, v_{II}\} \in D$. Using these operators, J and K are iven by [1]:

$$\langle Ju, v\rangle = \langle R_I [u]^1, v^r\rangle \qquad (2.10a)$$

and

$$\langle K^* u, v\rangle = \langle R_I \dot{u}^1, [v]^r\rangle \qquad (2.10b)$$

As a final remark, it is observed that the validity of equations (2.10) is pre served if R_I is replaced by R_{II} [1].

ADVECTION-DIFFUSION EQUATIONS

The methodology is applicable to steady state and time dependent problems in one and several dimensions.

A.- <u>One Dimensional Problems</u>. The steady state leads to ordinary differential equations, for which four algorithms were developed by Herrera et al. [3] They were derived by seeking nodal information only.

Algorithm 1.- The value of the function and its derivative;
Algorithm 2.- The value of the function only;
Algorithm 3.- The value of the derivative only;
Algorithm 4.- The function at some nodes and the derivative at some others.

For steady state the advection diffusion equation with linear sources is

$$\mathcal{L}u \equiv d\,(Ddu/dx)/dx - Vdu/dx + Ru = f_\Omega(x), \quad o \leq x \leq \ell \qquad (3.1)$$

and

$$\mathcal{L}^* v \equiv d(Ddv/dx)/dx - d(Vv)/dx + Rv \qquad (3.2)$$

The domain $[0,\ell]$ is divided into E subintervals or elements, not necessaryly equal, $[x_o, x_1], \ldots [x_{E-1}, x_E]$. In order to concentrate all the information at nodal points, test functions are required to satisfy $\mathcal{L}^*\varphi_{\alpha=0}$, locally. For algorithms 2 to 4, three-diagonal matrices are contained, while algorithm 1 yields tetra-diagonal matrices [3]. Thus far, two procedures have been employed for constructing the wieghting functions which satisfy the equation $\mathcal{L}^*\varphi_{\alpha=0}$ In [5] the (variable) coefficients of the equation were approximated by piece-wise polynomials, while in [6] polynomials were used to approximate the test functions, which were required to satisfy the equation $\mathcal{L}^*\varphi_{\alpha=0}$ at collocation points only. Using a semi-discretization approach,

the extension to time dependent problems is straightforward. For this case the advection-diffusion equation can be written as

$$\mathcal{L}u = \partial u/\partial t - f_{\Omega}(x,t) \qquad (3.3)$$

where $\mathcal{L}$ is differential operator in x, given by equation (3.1). Thus, in [7] the term $\partial u/\partial t$ was incorporated in the right-hand side of equation (3.1), at each time step, and the solution procedure for steady state problems was applied to the resulting equation.

B.- Problems in Several Dimensions. The results for advection dominated transport-diffusion problems, in several dimensions, have been presented in [8]. The procedure differs from that for one-dimensional problems, mainly, due to the fact that T-complete systems [11] are infinite in this case. Of course, only a finite number of test functions are used in actual applications, introducing a truncation error in this manner.

C.- Numerical Results. For one dimensional steady state problems the procedure yielded [5,6] very efficient and highly accurate algorithms, which advantageously compare with other algorithms.
For time dependent one-dimensional situations, only algorithms 1 and 2 were applied. These correspond to the use of fully discontinuous and C^0 weighting functions, respectively. Two test problems were treated to demonstrate the performance of the new method: the propagation of an initial step discontinuity and of a Gauss hill. The results and the efficiency of the procedure were compared with other methods, testing the effect of changing several parameters such as θ (in time), element Peclet number, as well as Courant number. The conclusion was reached that solutions obtained with this method are as least as good as those from the best available interior methods [7].
Similar conclusions were drawn in the case of two-dimensional problems. For details see [8]. In general, localized adjoint methods allow very effective treatment of boundary conditions, but this is specially noticeable for two-dimensional problems, due to its greater difficulty.

REFERENCES

[1] Herrera, I., "Unified approach to numerical methods", Part I, Num. Methods for Partial Differential Equations 1 (1), 25-44, 1985.

[2] Herrera, I., Ibid, Part 2, Num. Methods for Partial Differential Equations 1(3), 159-186, 1985.

[3] Herrera, I., Chargoy, L. and Alduncin, G. Ibid, Part 3, Num. Methods for Partial Differential Equations (4), 241-258, 1985.

[4] Herrera, I., "Unifying concepts in Applied Mathematics", Proc. G. Gail Symp., Laramie, 1985.

[5] Celia, M. A. and Herrera, I., "Solution of ordinary differential equations by a unified theory approach", Num. Methods for Partial Differential Equations, 3(2), 117-129, 1987.

[6] Herrera, I., "The algebraic theory approach for ordinary differential equations: highly accurate finite differences", Num. Methods for Partial Differential Equations, 3(3), 199-218, 1987.

[7] Celia, M.A.; Herrera, I; Bouloutas, E. and Kindred, J.S. "A New Numerical approach for the advective-diffusive transport equation", Num. Methods for Partial Differential Equations. 1988 (in press).

[8] Celia, M.A.; Bouloutas, E. and Herrera, I. "Application of Optimal Test Funtions Methods to Multi-dimensional Flow Problems. Proceedings 7th. International Conference, 1988.

[9] Herrera, I., Ewing, R.E.; Celia, M.A. and Russell, T. (to be published).

[10] Celia, M.A., Russell, T.; Herrera, I. and Ewing, R.E. (to be published).

[11] Herrera, I. Boundary Methods: An algebraic theory. Pitman, London, 1984.