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Localized Adjoint Methods in Water Resources Problems

I. Herrera

Instituto de Geofisica, UNAM, Apdo. Postal 22-582, 14000 México DF, México

ABSTRACT

Lacalized Adjoint Method is a new methodology of wide applicability, based on the author's Green's formulas for discontinuous fields. Here it is presented in connection with transport diffusion problems for which the Eulerian-Lagrangian Localized Adjoint Method (ELLAM) has been formulated by the LAM group (M.A. Celia, R.E. Ewing and T.F. Russell, in addition to the author). The ELLAM development unifies characteristic methods, treats boundary conditions systematically, yielding conservative schemes.

1. INTRODUCTION

The numerical solution of the advective-diffusive transport equation is a problem of great importance because many problems in science and engineering involve such mathematical model. The numerical treatment of advection dominated processes 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 up-stream weighting techniques, whose development is essentially ad-hoc.

An alternative and very promising approach has been introduced by Herrera [1-5] and coworkers. In past work, this has been referred as "Optimal Test Functions 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 distinguished from other procedures. Hence, this is the terminology that has been adopted more recently [6,7].

The starting point of localized adjoint methods is a very simple idea. Let $\mathcal{L}$ be a differential operator that will be applied to functions 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

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

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, a function u' is said to be an approximate solution of this problem when

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

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

The following observations permit establishing the actual relation that exists between an approximate solution and the exact one and derive the actual information about the exact solution which is contained in an approximate one. From (1.2), it is clear that the exact solution u, satisfies

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

Equations (1.3) and (1.4) together imply

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

or

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

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

> *A function u' is an approximate solution if and only if, its projection on the space spanned by the system of functions* $\{\mathcal{L}^*\varphi_1,\ldots,\mathcal{L}^*\varphi_N\}$, *coincides with that of the exact solution u. As a matter of fact, this is* all the information *about the exact solution contained in an approximate one.*

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

The very simple and precise result just presented clarifies much the nature of approximate solutions and it would be desirable to apply it, in a systematic manner, to analyze discrete methods. For this purpose it is necessary to have available Green's formulas similar to (1.1), but that can be applied even when the functions considered are not smooth, since in most numerical applications the weighting functions are localized (i.e., they have local support) and they usually do not satisfy the smoothness requirements at the boundary of their support. Even more, the development of a theory applicable to carry out the analysis when both base and test functions are fully discontinuous, is most desirable since standard theory of distributions is not applicable to that case.

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

"Localized adjoint methods (LAM)", which are presently being developed by the LAM group (M.A Celia, R.E. Ewing, I. Herrera and T.F. Russell), consist in making systematic use of that theory to analyze the information contained in approximate solutions. Since the quality of the results obtained with a numerical method depends, in an important manner, on the weighting functions used, one of the main goals of localized adjoint methods, thus far, has consisted in developing improved weighting functions. In this paper the LAM methodology is explained in connection with transport diffusion problems.

2. GREEN-HERRERA'S FORMULAS FOR TRANSPORT-DIFFUSION EQUATIONS

The general abstract boundary value problem considered by the theory is formulated in a linear space of functions D and corresponds to one with prescribed jumps. It is defined by the system of equations:

$$Pu = f; \qquad Bu = g; \qquad Ju = j \qquad (2.1)$$

where P, B and J are functional valued operators, while $f \in D$, $g \in D^*$ and $j \in D^*$ are prescribed functionals (the data of the problem). Here, D^* is the algebraic dual of D (i.e. D^* is the space of linear functionnals defined on D). The general theory supplies a systematic procedure for deriving the operators P, B and J, as well as Q, C and K, to be introduced later on. Their definitions depend on the differential operator, the boundary conditions and smoothness conditions considered. The linear functionals f, g and j, are determined by the data of the problem; in particular, when the sought solution is smooth, the prescribed jump j=0.

The bilinear functionals B and J are constructed so that they are boundary operators for P, which are fully disjoint [2,5]. In this case the system of equations (2.1) is equivalent to the single equation

$$(P - B - J)u = f - g - j \qquad (2.2)$$

This equation is a variational formulation of the problem, as can be verified observing that (2.2) is equivalent to

$$\langle (P - B - J)u, v \rangle = \langle f - g - j, v \rangle \quad \forall \ v \in D \qquad (2.3)$$

This is said to be "the variational formulation in terms of the data of the problem", because according to (2.1) Pu, Bu and Ju are prescribed.

Making use of the Herrera's general Green formula for operators in discontinuous fields [2,5]

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

the variational formulation (2.3) is transformed into

$$\langle (Q^* - C^* - K^*)u, v \rangle = \langle f - g - j, v \rangle \ \forall \ v \in D \qquad (2.5)$$

Where for any bilinear functional, the star refers to the corresponding transposed bilinear functional. Formulation (2.5) is said to be "the variational formulation in terms of the sought information", because Q^*u, C^*u and K^*u are not prescribed. Generally, Q^*u, C^*u and K^*u supply information about the sought solution at the interior of the region of definition of the problem, the complementary boundary values and the average of the solution (and its derivatives) across interelement boundaries (where the base and test functions chosen may have jump discontinuities), respectively.

Making use of the variational formulation in terms of the sought information, the arguments that lead to the formulation of

Localized Adjoint Methods, constitute a mere repetition of those presented in the Introduction. Given a system of weighting functions $\{\varphi_1,\ldots,\varphi_N\}\subset D$, an approximate solution is again any function $u'\in D$ which satifies

$$<(Q^*-C^*-K^*)u',\varphi_\alpha> = <f-g-J,\varphi_\alpha> \ , \ \alpha=1,\ldots,N \quad (2.6)$$

Clearly, equation (2.6) implies

$$<(Q^*-C^*-K^*)u',\varphi_\alpha> = <(Q^*-C^*-K^*)u,\varphi_\alpha>, \ \alpha=1,\ldots,N \quad (2.7)$$

since an exact solution also satisfies (2.6). Equation (2.7), is the basis for the analysis of the information contained in an approximate solution and constitutes the foundation of Localized Adjoint Methods. In particular, when the test functions are chosen satisfying the adjoint differential equation ($Q\varphi_\alpha=0$), the information is concentrated at the nodes (K^*u) and complementary boundary values (C^*u), exclusively.

3. EULERIAN-LAGRANGIAN LOCALIZED ADJOINT METHOD (ELLAM)

LAM procedure was applied by the LAM group [6,7] to the one-dimensional transient advection-diffusion equation

$$\mathcal{L}u \equiv \frac{\partial u}{\partial t} + V\frac{\partial u}{\partial x} - D\frac{\partial^2 u}{\partial x^2} = f_\Omega(x,t) \ ; \quad (x,t)\in\Omega_{x,t} \quad (3.1)$$

subjected to the initial and boundary conditions:

$$u(x,0)=u_I(x) \quad (3.2a)$$

$$u(0,t)=u_0(t) \text{ and } \partial u/\partial x(l,t)=q_l(t) \quad (3.2b)$$

Here, $\Omega_{x,t}$ is the space-time rectangle $[0,l]X[0,T]$.

For any function v, the adjoint operator

$$\mathcal{L}^*v \equiv -\frac{\partial v}{\partial t} - \frac{\partial}{\partial x}(Vv) - D\frac{\partial^2 v}{\partial x^2} \ ; \quad (x,t)\in\Omega_{x,t} \quad (3.3)$$

satisfies

$$v\mathcal{L}u - u\mathcal{L}^*v \equiv \frac{\partial}{\partial t}(uv) + \frac{\partial}{\partial x}\left(vVu+D(u\frac{\partial v}{\partial x} - v\frac{\partial u}{\partial x})\right) \quad (3.4)$$

which is a divergence form in space-time. Integrating (3.4) in the region $\Omega_{x,t}$ and applying a generalized version of divergence theorem [8], which is applicable to functions with jump discontinuities, it is obtained

$$\int_{\Omega x,t}\{v\mathcal{L}u - u\mathcal{L}^*v\}dxdt \equiv \int_0^T\{(Vv+D\frac{\partial v}{\partial x})u - vD\frac{\partial u}{\partial x}\}\Big|_0^l dt + \int_0^l uv\Big|_0^T dx$$

$$- \int_\Sigma[\{(V-V_\Sigma)v+D\frac{\partial v}{\partial x})\}u - vD\frac{\partial u}{\partial x}\ ]dt \quad (3.5)$$

where Σ includes all the curves where jump discontinuities can occur and for any function w, the notation [w] denotes the jump in

w across Σ:

$$[w] = w_+ - w_- \qquad (3.6)$$

As it is usual when formulating initial-boundary value problems in a weak manner, a bilinear form $\langle Pu, v\rangle$ is introduced weighting the differential operator $\mathcal{L}u$ with the function v. In a similar fashion the bilinear form $\langle Qv, u\rangle \equiv \langle Q^* u, v\rangle$ is defined weighting $\mathcal{L}^* v$ with the function u. Thus

$$\langle Pu, v\rangle \equiv \int_{\Omega x,t} v\mathcal{L}u\,dx\,dt \qquad \text{while} \qquad \langle Q^* u, v\rangle \equiv \int_{\Omega x,t} u\mathcal{L}^* v\,dx\,dt \quad (3.7)$$

To accomodate the boundary and initial conditions (3.2) the operators B and C are defined by

$$\langle Bu, v\rangle = -\int_0^T \{(Vv + D\frac{\partial v}{\partial x})u\}_0 dt + \int_0^1 (uv)_0 dx - \int_0^T (vD\frac{\partial u}{\partial x})_1 dt \qquad (3.8a)$$

and

$$\langle C^* u, v\rangle = -\int_0^T (vD\frac{\partial u}{\partial x})_0 dt - \int_0^1 (uv)_T dx - \int_0^T \{(Vv + D\frac{\partial v}{\partial x})u\}_1 dt \qquad (3.8b)$$

so that $\langle (B-C^*)u, v\rangle$ includes all the boundary terms appearing in (3.5). The definition of the bilinear forms J and K depends on the smoothness conditions to be satisfied by the sought solution u. Usually for transport diffusion problems physical requirements impose the conservation of mass condition, which implies continuity of u and $\partial u/\partial x$, unless the equation coefficients are discontinuous. For these smoothness conditions the general theory of the author [2,5] yields

$$\langle Ju, v\rangle = -\int_\Sigma \{((V-V_\Sigma)\bar{v} + D\overline{\frac{\partial v}{\partial x}})[u] - \bar{v}D[\frac{\partial u}{\partial x}]\}dt \qquad (3.9a))$$

and

$$\langle K^* u, v\rangle = \int_\Sigma \{((V-V_\Sigma)[v] + D[\frac{\partial v}{\partial x}])\bar{u} - [v]D\overline{\frac{\partial u}{\partial x}}\}dt \qquad (3.9b)$$

where the jump [ ] is taken as in (3.6), while for any function w, $\bar{w}$ is the average across Σ, defined by:

$$\bar{w} \equiv (w_+ + w_-)/2 \qquad (3.10)$$

In view of (3.5), one has

$$\langle (P-B-J)u, v\rangle = \langle (Q^*-C^*-K^*)u, v\rangle \qquad (3.11)$$

which is Green-Herrera formula (2.4), as it applies to the transport diffusion equation. The weak variational formulation in terms of the data of the boundary value problem, with specified jumps, is now given by (2.3)

$$\langle (P-B-J)u, v\rangle = \langle f-g-j, v\rangle \qquad \forall\, v\in D \qquad (3.12)$$

where f, g and j are linear functionals defined in terms of the data of the problem. They are such that f=Pu, g=Bu and j=Ju when u is a solution of the problem. Thus

$$\langle f, v\rangle \equiv \int_\Omega v f_\Omega dxdt \qquad \forall\, v\in D \qquad (3.13a)$$

$$\langle g, v\rangle = -\int_0^T \{(Vv + D\frac{\partial v}{\partial x})\}_0 u_0 dt - \int_0^T (vD)_1 q_1 dt - \int_0^1 (v)_0 u_1 dx \qquad (3.13b)$$

while j is the identically zero functional, when a smooth solution is sought. The variational formulation in terms of the sought information is given by (2.5):

$$\langle (Q^* - C^* - K^*)u, v\rangle = \langle f - g - j, v\rangle \quad \forall\, v\in D \qquad (3.14)$$

Equation (3.14) can be applied to analyze the information contained in approximate solutions. In this manner a generalization of Characteristic Methods, called Eulerian-Lagrangian Localized Adjoint Method (ELLAM), has been developed by the author in collaboration with Celia, Ewing and Russell [6,7].

3. GENERAL COMMENTS AND CONCLUSIONS

Many numerical methods use characteristic analysis to accomodate the advective component of transport. Such Characteristic Methods include Eulerian-Lagrangian Methods (ELM) [9-11], Modified Method of Characteristics (MMOC) [12,13], and operator splitting methods [14,15]. The ELLAM approximations provide a systematic framework for development of Characteristic Methods for numerical approximation of advective-diffusive transport equations. The Localized Adjoint Method (LAM) procedures lead naturally to the definition of special space-time test functions that produce the generalized CM approximations. The resulting set of approximating equations subsumes many of the CM approximations proposed in the literature. It therefore unifies these methods. In addition, the development inherently provides a systematic procedure for proper incorporation of all types of boundary conditions in a mass conservative manner.

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