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ADVANCES IN THE NUMERICAL SIMULATION OF STEEP FRONTS

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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 problems, is revised.

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 semi-discretization approach have been based on upstream 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 appropiate to call such procedures "Localized Adjoint Methods". Also, in this manner the method would be more clearly distinguished 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 (see, e.g., [5]). Let $\mathcal{L}$ be a differential operator defined in region Ω and let $\mathcal{L}^*$ be its formal adjoint. Then, when u and v satisfy

suitable boundary conditions, Green's formula

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

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

$$\mathcal{L}u = f_{\Omega}, \text{ in } \Omega \tag{1.2}$$

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

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

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 $u' = \Sigma a_{\alpha}\phi_{\alpha}$ 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

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

Equations (1.3) and (1.4) together imply

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

or

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

by virtue of Green's formula (1.1). Consider the Hilbert space L^2, 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 conclusion:

Any function u', whose projection on the subspace spanned by the system of functions $\{\mathcal{L}^*\varphi_1, \ldots \mathcal{L}^*\varphi_N\}$, coincides with that of the exact solution u, is an approximate solution. Indeed, this projection is all the information 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 usually violate the smoothness assumptions at the boundary of their supprot. Even more, the development of a theory applicable to carry out the analysis when both base and test functions are fully discontinuous, was 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).

2.- LOCALIZED ADJOINT METHODS

"Localized adjoint methods" consist in making systematic use of the resulting equations 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 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-Lagragian procedures [9,10].

3.- ADVECTION-DIFFUSION EQUATIONS

The methodology has been applied to steady state and time dependent problems in one and several dimensions [5-8].

A.- One Dimensional Problems.- 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

$$\mathcal{L}u \equiv d(Ddu/dx)/dx - Vdu/dx + Ru = f_\Omega(x),\ 0 \leq x \leq \ell \qquad (3.1)$$

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 necessarily equal, $[x_0,x_1],\ldots,[x_{E-1},x_E]$. 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 obtained, while algorithm 1 yields tetra-diagonal matrices [3]. Thus far, two procedures have been employed for constructing the weighting functions wich 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 those previously available.

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 these proceedings. In general, localized adjoint methods allow very effective treatment of boundary conditions, but this is specially noticiable for two-dimensional problems, due to its greater difficulty.

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A QUICK Finite Element

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Abstract

Petrov-Galerkin finite elements corresponding to higher order upwind finite difference schemes, including the QUICK scheme, for convection dominated problems are introduced and demonstrated. These elements are developed using either trial or test functions which are extended to higher polynomial degrees by including nodes external to the element under consideration. In simple one dimensional situations, the finite elements are shown to reproduce second and third order finite difference approximations for the convective term, an unaffected (second order) diffusion term and a consistent upwind mass term. A two dimensional driven cavity fluid flow (stream function-vorticity formulation) solution at a Reynolds Number of 1000 is also presented.

1. Introduction

Numerical solutions of convection dominated problems have long suffered from the instability of centered or Bubnov-Galerkin representations of the convection terms. In order to obtain stable solutions, some form of upwinding, whether of the finite differences, or of the finite volume interpolations, or of the test functions in a Petrov-Galerkin finite element method, is usually employed. In effect, an artificial or numerical diffusion, in the form of a first order, second derivative, truncation error is introduced. With a consistent finite element technique or with careful blending of upwind and centered forms, this additional error may be negated in combination with other error terms present. Extraordinarily accurate and even exact results are possible in particular situations.

In finite volume formulations of the fluid flow and transport equations, quadratic upwind interpolation [1] of convected quantities has provided an alternative means of stabilizing solutions without introducing numerical diffusion. In finite difference methods second or third order upwind differences have been used to similar effect [2,3]. In either case the discrete equations contain terms from more upstream nodes than downstream nodes. While such methods do not eliminate the "wiggles", their magnitude is limited and their presence is confined to regions of very steep gradients [4]. Accuracy in smooth regions of the solution is generally enhanced [4,5].