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Advances on the Numerical Simulation of Steep Fronts

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Summary

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. These are usually based on Petrov-Galerkin formulations. More recently the author has proposed a procedure which produces optimal test functions using approximate solutions of the adjoint equation. Advantages of this method are: a) no arbitrary parameters appear in their definitions, b) the functions vary continuously with the coefficients of the equations, c) the definition of weighting functions results from a systematic and mathematically sound formulation and d) rapidly convergent and accurate solutions are obtained. The only procedure with comparable efficiency is the version of Petrov-Galerkin due to Hughes and Brooks. In this paper a comparison of test functions for these methods is carried out and conclusions drawn from such comparison.

Introduction

The numerical solution of the advective-diffusive transport equation is a problem of great importance because many problems in science and engineering have mathematical representations characterized by sharp fronts. This happens when the process is advection dominated, in which case its numerical treatment is very difficult. Considerable work has been expended in developing discretization formulae for this kind of problems [1-3]. Most have focused on upstream weighting techniques. A fundamental criticism to these methods is the essentially ad-hoc nature of their development. This is manifested through the presence of an arbitrary parameter, the choice of which has to be decided by the analyst. An alternative and very promising approach has been introduced by the author [4-9]. In the past several researchers [2,3], when developing test functions, have considered them optimal when they yield exact values at the nodes. More generally, the author has proposed to consider a system of weighting functions optimal when they yield exact values at inter-element boundaries for arbitrary excitation terms. When this is done, this criterium of optimality reduces to the notion of T(Trefftz)-completeness which has been introduced by the author [4].Herrera's approach consists in using optimal test functions (OTF) systematically.

Numerical comparisons have been carried out between the results obtained using the author's method and other procedures [9]. In general, it was found that the OTF method yields more satisfactory results. The only procedure whose results were very close, is the Petrov-Galerkin method of Hughes and Brooks [3]. In this paper Herrera's OTF method is described. Then, a comparison between the test functions used in these two methods is carried out. They are shown to be quite similar up to fairly large values of the element Peclet number. The optimal test functions used in the author's approach are derived via the solution of the adjoint differential equation. The test functions of Hughes and Brooks are derived in a relatively ad-hoc manner and using very different considerations. However, they turn out to be good approximations of the solutions of the adjoint differential equation (OTF), except for very large values of the element Peclet number or when the source terms are large. This explains the good preformance of Hughes' approach. There are three situations in which the advantages of the author's approach are clear: for large Peclet numbers, when the source term is strong (in a sense which is made clear in the section of conclusions) and when higher order algorithms are required.

Herrera's OTF Method

Let us introduce the approximation for one-dimensional steady-state transport equation with sources, given by

$$\mathcal{L} u \equiv \frac{d}{dx} \left(D \frac{du}{dx}\right) - V\frac{du}{dx} + Ru = f_\Omega(x), \quad 0 \le x \le \ell \tag{1}$$

$$u(0) = g_0 \tag{2a}$$

$$u(\ell) = g_\ell \tag{2b}$$

first type boundary conditions are chosen for convenience of presentation only. The numerical procedure has been implemented for general differential equations and general boundary conditions [6-8].

The domain $[0,\ell]$ is divided into E subintervals, or elements (not necessarily equal), $\{[x_0,x_1], [x_1,x_2],\ldots,[x_{E-1},x_E]\}$, where $x_0=0$ and $x_E=\ell$. This yields E+1 nodal points $\{x_0,x_1,\ldots,x_E\}$.

We adopt the representation

$$u(0) = \sum_{i=0}^{E} U_i \, \phi_i(x) \tag{3}$$

where U_i are the nodal values of $u(x)$. A test function $w(x)$ will be taken localized in the union of two neighboring subintervals $[x_{j-1},x_j]$ and $[x_j,x_{j+1}]$, where x_j is any interior node (Fig. 1). In addition, the test function w satisfies

$$w(x_{j-1})=0 \tag{4a}$$

$$w(x_{j+1})=0 \tag{4b}$$

$$w(x_j-) = w(x_j+) \tag{4c}$$

condition (4c) states that the limits from the right and form the left agree at the node x_j;i.e. w is continuous at node x_j. However, generally, the derivative of the test function w will have a jump discontinuity at x_j (Fig. 1).

Multiplying $\mathcal{L}u$ by w, integrating from x_{j-1} to x_{j+1}, and applying "generalized Gauss Theorem" for functions with jump discontinuities (see, for example [10]), it is obtained.

$$\int_{x_{j-1}}^{x_{j+1}} w\mathcal{L}u dx = -\left[uD\frac{dw}{dx}\right]_{x_{j-1}}^{x_{j+1}} + \left[\!\left[uD\frac{dw}{dx}\right]\!\right]_{x_j} + \int_{x_{j-1}}^{x_{j+1}} u\mathcal{L}^* w dx \tag{5}$$

Here, the "jump" $[\![\;]\!]$, is defined by

$$\left[\!\left[uD\frac{dw}{dx}\right]\!\right]_{x_j} = u_j(x_j+)D\frac{dw}{dx}(x_j+) - u(x_j-)D\frac{dw}{dx}(x_j-) \tag{6}$$

while the adjoint operator $\mathcal{L}^*$ is defined by

$$\mathcal{L}^* w \equiv \frac{d}{dx}\left(D\frac{dw}{dx}\right) + \frac{d}{dx}(Vw) + Rw \tag{7}$$

In the author's procedure, the optimal test function w satisfies $\mathcal{L}^* w=0$. In this case, combining (5) with (1), it is obtained

$$A_{j-}U_{j-1}+A_jU_j+A_{j+}U_{j+1} = \int_{x_{j-1}}^{x_{j+1}} wf_\Omega dx \tag{8}$$

where

$$A_{j-}=\left(D\frac{dw}{dx}\right)_{x_{j-1}};\quad A_j=\left[\!\left[D\frac{dw}{dx}\right]\!\right]_{x_j};\quad A_{j+1}=-\left(D\frac{dw}{dx}\right)_{x_{j+1}} \tag{9}$$

When equation (8) is applied at each one of the interior nodes (i.e., $j=1,\ldots,E-1$), the unknown values $(U_1,\ldots,U_{E-1})$ of the solution there, can be obtained from the resulting system of $E-1$ equations. Before closing this Section, we observe that the optimal test function w used in (8), may be thought as defined throughout the whole interval $[0,\ell]$, if its value is identically zero outside $[x_{j-1},x_{j+1}]$. In view of equations (4), such test function is continuous on $[0,\ell]$ but its derivative has jumped discontinuities at interior nodes.

Comparison with Petrov-Galerkin

The procedure explained before has been applied to advection dominated problems using semi-discretization [9]. The results so obtained are quite satisfactory, being oscillation free, to a large extent. The only method whose results are close for a large range of Peclet numbers is the Petrov-Galerkin version of Hughes and Brooks [3]. After a more careful analysis it was found that this is due to the fact that the weighting functions used in both methods are close to each other.

Hughes' test function is

$$w = \phi + \tfrac{1}{2}[(\coth\alpha) - 1/\alpha]\, V\frac{d\phi}{dx} \tag{10}$$

where ϕ is a basis function and $\alpha = Vh/2$ is the element Peclet number. In Figs. 2 and 3 the test functions for both methods are compared.

In Fig. 3, we have introduced a non-dimensional measure of the strength of the source term

$$\rho = 4\frac{RD}{V^2} \tag{11}$$

From inspection of these figures we conclude that Hughes' test functions yield good approximations except when Peclet number is large, specially if the source strength ρ is not small. An additional point must be made in connection with this comparison, in Herrera's procedure it is possible to produce solutions of any desired order of accuracy [7], something which is not possible when using Hughes' approach.

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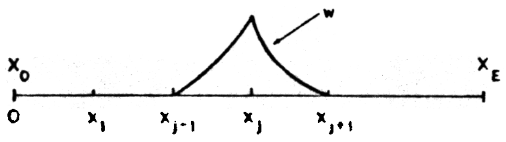

Fiq A typical test function.

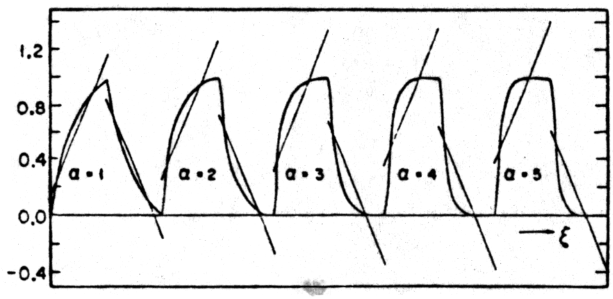

Fig. 2 Comparison of Hughes test function with Herrera's optimal test function. Straight-lines are Hughes and α is the element Peclet number.

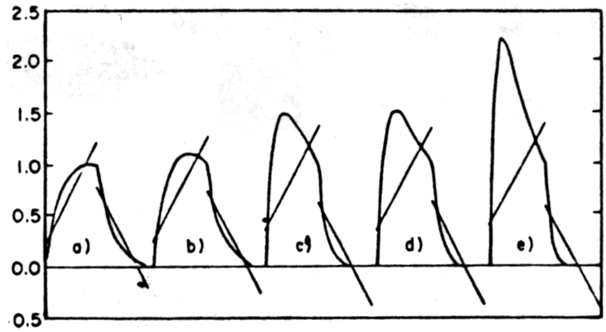

Fig. 3 Comparison of Hughes test function for a) ρ=.44, α=1.5; b) ρ=.55, α=1.9; c) ρ=.064, α=3.95; d) ρ=.36, α= 4; e) ρ=.36, α=6. 2α is the element Peclet number.