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SHORT COMMUNICATION

A BRIEF NOTE ON UPWIND COLLOCATION

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SUMMARY

Upwind collocation on Hermite cubics is compared to orthogonal collocation with respect to effective diffusion. The one-dimensional constant coefficient advection–diffusion equation is employed to this end. The effective diffusion coefficient is determined exactly and is found to be dependent on the nodal solution values. The effective diffusion coefficients of three other upwinding schemes are also presented. Upwind collocation is found to have an effective diffusion coefficient like other upwinding schemes plus an extra term which may enhance or reduce the non-advective flux, depending on the problem solution and point location within the domain.

KEY WORDS Collocation Finite Element Method Upwind Schemes

INTRODUCTION

Upwinding schemes are commonly used in finite difference formulations for the numerical solution of hyperbolic and nearly-hyperbolic equations. In the past few years, upwinding schemes have been introduced into the methods of weighted residuals[1–4] and orthogonal collocation.[5–8] Inherent in upwinding schemes is an increase in numerical dissipation. This is exhibited by a decrease in the amplification ratio when compared to the spatially centred schemes they replace. Gresho and Lee[9] provide an incisive review and critique of the practice of upwinding.

The upwind collocation method has recently received considerable attention. Shapiro and Pinder[6] collocate asymmetric trial functions at Gauss–Legendre points whereas Allen and Pinder[7] use Hermite cubics as trial functions and collocate upwind of the Gauss–Legendre points. Allen[8] has provided an estimate of the increased dissipation of this scheme when applied to the model linear equation

$$\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x}-D\frac{\partial^2 c}{\partial x^2}=0 \quad \text{on } \Omega_{x,t} \tag{1}$$

The constants u and D are fluid velocity and diffusion coefficient, respectively, and $\Omega_{x,t}$ is the domain of interest in x and t.

The analysis by Allen was performed by determining a Galerkin finite element scheme equivalent to orthogonal collocation and then evaluating the error generated by inexact quadrature due to displacement of the Gauss points. He found that upwind collocation was

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equivalent to orthogonal collocation with the D replaced by (Allen's equation (3.7))

$$E \equiv D + \frac{\alpha}{2} u\,\Delta x + O(\alpha^2\,\Delta x^2) \tag{2}$$

where Δx is the element length and α is the displacement of the collocation point on the local element scale $[-1, 1]$. That is, if x_m is the orthogonal collocation point and x_m^* is the upwind collocation point, then $\alpha \equiv 2(x_m^* - x_m)/\Delta x$. DeBoor and Swartz[10] give error estimates for collocation on and off the Gauss–Legendre points which are $O(\Delta x^4)$ and $O(\Delta x^2)$, respectively, for Hermite cubics.

In this note the exact functional form of the effective diffusion coefficient, E, will be found rather than the approximate equation (2). This coefficient E, when inserted in the centred-in-space scheme for

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} - E\frac{\partial^2 c}{\partial x^2} = 0 \quad \text{on } \Omega_{x,t} \tag{1a}$$

will yield the same results as upwinding solutions to equation (1). Such an equivalence is desirable because it may then be possible to immediately study the upwind scheme using the von Neumann analysis of the centred (orthogonal collocation) scheme, as can be done for upwind difference methods.

UPWIND FINITE ELEMENT COLLOCATION ON HERMITE CUBICS

In this approach one requires that

$$\sum_{i=1}^{N}\left[\int_{\Omega_{xi}}\left(\frac{\partial \hat{c}_i}{\partial t} - D\frac{\partial^2 \hat{c}_i}{\partial x^2}\right)\delta(x-x_m)\,\mathrm{d}\Omega + \int_{\Omega_{xi}}\left(u\frac{\partial \hat{c}_i}{\partial x}\right)\delta(x-x_m^*)\,\mathrm{d}\Omega\right] = 0, \qquad m = 1, 2, \ldots, M \tag{3}$$

where N = number of non-overlapping finite elements
Ω_{xi} = x-domain of element i, $x \in [x_{i1}, x_{i2}]$
x_{i1}, x_{i2} = x-co-ordinates of left and right ends of element i
$\hat{c}_i(x, t)$ = approximating function for $c(x, t)$ on element i, given by

$$\hat{c}_i(x, t) = \sum_{j=1}^{2}\left[c_j(t)H_{0j}(x) + c_j'(t)H_{1j}(x)\right]$$

c_j = estimate of c at node j of element i
c_j' = estimate of $\partial c/\partial x$ at node j of element i
H_{nj} = Hermite cubic of nth type associated with node j of element i
x_m = orthogonal collocation points
x_m^* = upwind collocation points $= x_m - \alpha\,\Delta x/2$, $\alpha \geq 0$ for $u \geq 0$
m = integers $(1, 2, \ldots, M)$
M = the required number such that the system of equations, incorporating initial and boundary values, is determined.

Note that in equation (3) only the advection term is upwinded. The functional forms of the Hermite cubics are given in the Appendix.

We consider henceforth one term of the summation (3) and collocation points x_m and $x_m^* \in \Omega_{xi}$. The expansion for $\hat{c}_i$ is substituted into (3) and, when the Hermites are written in terms of the local coordinates $\xi \in [-1, 1]$, one obtains

$$\frac{dc_1(t)}{dt} H_{01}(\xi_m) + \frac{dc_2(t)}{dt} H_{02}(\xi_m) + \frac{dc_1'(t)}{dt} H_{11}(\xi_m) + \frac{dc_2'(t)}{dt} H_{12}(\xi_m)$$
$$- D\left(\frac{d\xi}{dx}\right)^2 \left[c_1(t) \frac{d^2 H_{01}}{d\xi^2}(\xi_m) + c_2(t) \frac{d^2 H_{02}}{d\xi^2}(\xi_m) + c_1'(t) \frac{d^2 H_{11}}{d\xi^2}(\xi_m) \right.$$
$$\left. + c_2'(t) \frac{d^2 H_{12}}{d\xi^2}(\xi_m) \right] + u\left(\frac{d\xi}{dx}\right)\left[c_1(t) \frac{dH_{01}}{d\xi}(\xi_m^*) + c_2(t) \frac{dH_{02}}{d\xi}(\xi_m^*) \right.$$
$$\left. + c_1'(t) \frac{dH_{11}}{d\xi}(\xi_m^*) + c_2'(t) \frac{dH_{12}}{d\xi}(\xi_m^*) \right] = 0 \tag{4}$$

Here m has the same meaning as in (3), ξ_m and ξ_m^* correspond to x_m and x_m^* in local co-ordinates, and (ξ_m) signifies 'evaluated at $\xi = \xi_m$.'

We now drop the subscript m for the collocation points, i.e. ξ will henceforth be equivalent to ξ_m of equation (4). Substituting the algebraic forms of the Hermites from equations (18)–(21) of the Appendix into (4) and noting that $\xi^* = \xi - \alpha$, we have

$$\frac{dc_1}{dt}[\tfrac{1}{4}(\xi-1)^2(\xi+2)] - \frac{dc_2}{dt}[\tfrac{1}{4}(\xi+1)^2(\xi-2)] + \frac{dc_1'}{dt}\left[\frac{\Delta x}{8}(\xi+1)(\xi-1)^2\right]$$
$$+ \frac{dc_2'}{dt}\left[\frac{\Delta x}{8}(\xi+1)^2(\xi-1)\right]$$
$$- \frac{4D}{\Delta x^2}\left[c_i \frac{3\xi}{2} - c_2 \frac{3\xi}{2} + c_1' \frac{\Delta x}{4}(3\xi-1) - c_2' \frac{\Delta x}{4}(3\xi+1)\right]$$
$$= -\frac{2u}{\Delta x}\left[\tfrac{3}{4}c_1(\xi^2-1) - \tfrac{3}{4}c_2(\xi^2-1) + c_1' \frac{\Delta x}{8}(3\xi^2-2\xi-1)\right.$$
$$\left. + c_2' \frac{\Delta x}{8}(3\xi^2+2\xi-1)\right] + \frac{2u}{\Delta x}\left[\tfrac{3}{4}c_1(2\alpha\xi-\alpha^2) - \tfrac{3}{4}c_2(2\alpha\xi-\alpha^2)\right.$$
$$\left. + c_1' \frac{\Delta x}{8}(6\alpha\xi - 2\alpha - 3\alpha^2) + c_2' \frac{\Delta x}{8}(6\alpha\xi + 2\alpha - 3\alpha^2)\right] \tag{5}$$

The first group on the right hand side of equation (5) corresponds to orthogonal collocation of the advection term of equation (2), and the final group is the overall change in the equation due to upwinding. Rearranging this last group of (5), one obtains

$$-\frac{2u}{\Delta x}\left[\tfrac{3}{4}c_1(2\alpha\xi-\alpha^2) - \tfrac{3}{4}c_2(2\alpha\xi-\alpha^2) + c_1' \frac{\Delta x}{8}(6\alpha\xi-2\alpha-3\alpha^2)\right.$$
$$\left. + c_2' \frac{\Delta x}{8}(6\alpha\xi+2\alpha-3\alpha^2)\right]$$
$$= -\frac{2u}{\Delta x}\alpha\left[\tfrac{3}{2}c_1\xi - \tfrac{3}{2}c_2\xi + c_1' \frac{\Delta x}{4}(3\xi-1) + c_2' \frac{\Delta x}{4}(3\xi+1)\right]$$
$$+ \frac{2u}{\Delta x}\alpha^2\left[\tfrac{3}{4}c_1 - \tfrac{3}{4}c_2 + \tfrac{3}{8}c_1' \Delta x + \tfrac{3}{8}c_2' \Delta x\right]$$
$$\equiv -\frac{2u}{\Delta x}\alpha[A] + \frac{2u}{\Delta x}\alpha^2[B] \tag{6}$$

Substituting the result (6) into (5) and noting that the group $[A]$ appears multiplying $4D/\Delta x^2$ in equation (5), we determine that the effective diffusion for this scheme is

$$E = D + \frac{\alpha}{2} u \, \Delta x - \frac{3\alpha^2}{2} u \, \Delta x \frac{(c_1 - c_2) + \frac{\Delta x}{2}(c_1' + c_2')}{6\xi(c_1 - c_2) + \Delta x(3\xi - 1)c_1' + \Delta x(3\xi + 1)c_2'} \tag{7}$$

The result of Allen[8] for the leading term in α, our equation (2), is therefore confirmed.

The most interesting aspect of the result (7) is the last term (in α^2), which shows that the effective diffusion depends on the nodal solution values c_i and c_i'. As such, the von Neumann method of analysis can be applicable only for a linearized case. The non-linear term will be more closely examined later.

OTHER UPWINDING METHODS

To gain additional perspective on the effective diffusion coefficient determined above, we discuss briefly three other upwinding methods: finite differences, finite elements with asymmetric weighting, and Galerkin finite elements with inaccurate quadrature. Discussions of upwind finite differences pervade the literature; see for example pp. 502–505 of Reference 11. The linear finite element Galerkin approximation to equation (1) can be upwinded by applying asymmetric weighting functions[2,12] to the advective term and using the symmetric trial functions to weight all other terms. Alternatively, the integrals of the advection term arising from a linear Bubnov–Galerkin scheme can be inexactly evaluated by moving the Gauss quadrature points away from the zeros of the associated Legendre polynomial, thus achieving the upwinding.[4,13] Artificial diffusion is introduced by each of these methods, leading to the expression for effective diffusion

$$E = D + \frac{\alpha}{2} u \, \Delta x \tag{8}$$

which is a widely known result.

DISCUSSION

Upwind finite difference methods and weighted residual methods (linear bases) lead to identical values of effective diffusion, E. The diffusion D is augmented in each case by

$$\frac{\alpha}{2} u \, \Delta x \tag{9}$$

resulting from upwinding alone. Effects of any other numerical techniques (e.g. time stepping) are not included. That all of these methods lead to identical effective diffusion coefficients should not come as a total surprise, since the upwind weighted residual schemes were motivated by the upwind difference scheme for this particular model equation, equation (1).

Upwind collocation on Hermite cubics generates a component of numerical diffusion identical to equation (9), plus an extra component. This new term, proportional to α^2, was shown by equation (7) to depend on the solution, c_i and c_i'. Let us re-examine the artificial diffusion due to this method. Multiplying the artificial component of the effective diffusion,

$E-D$, of equation (7) by $-4[A]/\Delta x^2$, which appears in equation (6), and rearranging we have

$$-\frac{4}{\Delta x^2}\left(\frac{\alpha}{2}u\,\Delta x\right)\left[\tfrac{3}{2}c_1\xi-\tfrac{3}{2}c_2\xi+c_1'\frac{\Delta x}{4}(3\xi-1)+c_2'\frac{\Delta x}{4}(3\xi+1)\right]$$

$$+(\alpha^2 u)\frac{12}{\Delta x}\left[\frac{c_1-c_2}{2}+\frac{c_1'+c_2'}{2}\frac{\Delta x}{2}\right] \quad (10)$$

The first group of (10) is seen to be a diffusion-like group

$$-\int_{\Omega_{xi}}\left(\frac{\alpha}{2}u\,\Delta x\frac{\partial^2 c}{\partial x^2}\right)\delta(x-x_m)\,\mathrm{d}\Omega \quad (11)$$

Now look at the second group of equation (10), which we rewrite

$$-6\alpha^2 u\left[\frac{c_2-c_1}{\Delta x}-\frac{c_1'+c_2'}{2}\right] \quad (12)$$

The second diagonal (fourth order) Padé approximant is

$$c_1-c_2+\frac{\Delta x}{2}\left[\left(\frac{\partial c}{\partial x}\right)_1+\left(\frac{\partial c}{\partial x}\right)_2\right]=\frac{\Delta x^2}{12}\left[\left(\frac{\partial^2 c}{\partial x^2}\right)_2-\left(\frac{\partial^2 c}{\partial x^2}\right)_1\right]+O(\Delta x^4) \quad (13)$$

Multiplying by $6\alpha^2 u/\Delta x$ we obtain

$$-6\alpha^2 u\left[\frac{c_2-c_1}{\Delta x}-\frac{c_1'+c_2'}{2}\right]=\frac{\alpha^2 u\,\Delta x}{2}\left[\left(\frac{\partial^2 c}{\partial x^2}\right)_2-\left(\frac{\partial^2 c}{\partial x^2}\right)_1\right]+O(\Delta x^3) \quad (14)$$

But, recognizing that

$$\left[\left(\frac{\partial^2 c}{\partial x^2}\right)_2-\left(\frac{\partial^2 c}{\partial x^2}\right)_1\right]\Big/\Delta x=\frac{\partial^3 c}{\partial x^3}+O(\Delta x) \quad (15)$$

we find that upwind collocation on Hermite cubics has thus added the terms

$$-\frac{\alpha}{2}u\,\Delta x\frac{\partial^2 c}{\partial x^2}+\frac{\alpha^2}{2}u\,\Delta x^2\frac{\partial^3 c}{\partial x^3}+O(\Delta x^3) \quad (16)$$

to the left side of equation (1), which confirms Allen's order estimate, equation (2). Equation (16) shows that upwind collocation leads to both artificially diffusive and dispersive terms, as indicated by the second and third order derivatives in (16), respectively. It should be recalled that α is determined for each collocation point, so a slightly different equation is being solved by the orthogonal collocation method on Hermite cubics at each collocation point.

CONCLUSIONS

(1) The effective diffusion engendered in upwind collocation on Hermite cubics is dependent on the numerical solution of the model equation, i.e. it is non-linear.

(2) The effects of upwind collocation on Hermite cubics, equation (16), can be decomposed into the sum of two parts. The first part is identical to the numerical dispersion arising from other frequently used upwinding methods, equation (9).

(3) The remaining part of the numerical effects of upwind collocation on Hermite cubics is of order $(\alpha^2\,\Delta x^2)$ and is proportional to $\partial^3 c/\partial x^3$.

(4) Both dissipation and dispersion will be generated by upwind collocation, as implied in equation (16).

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APPENDIX: HERMITE CUBICS ON $x \in [a, b]$

The Hermite cubic is a simple osculation polynomial. When interpolating in one-dimension, the values of the function and its first derivative at two points separated by a distance Δx are required. The interpolate is written

$$c(x) \approx \hat{c}(x) = \sum_{i=1}^{2} [c_i H_{0i}(x) + c_i' H_{1i}(x)] \tag{17}$$

where $x \in [a, b]$, c_i and c_i' are coefficients, and H_{0i} and H_{1i} are Hermite cubics of the zeroth and first kind. These cubics are given by

$$H_{01}(x) = \tfrac{1}{4}(\xi - 1)^2(\xi + 2) = \tfrac{1}{4}(\xi^3 - 3\xi + 2) \tag{18}$$

$$H_{02}(x) = -\tfrac{1}{4}(\xi + 1)^2(\xi - 2) = -\tfrac{1}{4}(\xi^3 - 3\xi - 2) \tag{19}$$

$$H_{11}(x) = \frac{\Delta x}{8}(\xi + 1)(\xi - 1)^2 = \frac{\Delta x}{8}(\xi^3 - \xi^2 - \xi + 1) \tag{20}$$

$$H_{12}(x) = \frac{\Delta x}{8}(\xi + 1)^2(\xi - 1) = \frac{\Delta x}{8}(\xi^3 + \xi^2 - \xi - 1) \tag{21}$$

with

$$\xi \equiv [2x - (a + b)]/\Delta x, \quad \text{i.e.} \quad \xi \in [-1, 1] \quad \text{and} \quad \Delta x \equiv b - a.$$

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