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Edited by:

C. Taylor and K. Morgan
University College of Swansea, Swansea, U.K.

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Vol. 2

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NUMERICAL METHODS IN FLUIDS

PREFACE

This second volume in the series of texts devoted to recent advances in the numerical solution of flow problems follows on from the first successful text printed in 1980. Again each chapter is devoted to a specific area of research and the contributors have developed and adequately referenced recent aspects of the topic being considered. It is evident that considerable advances are apparent in all areas of research associated with flow problems and, hopefully, further developments will evolve from ideas projected in this book.

In each chapter the authors introduce each topic, providing adequate referencing, and develop the application of the proposed technique to specific problems. In common with the first volume, these range from potential flow to those where turbulence phenomena dominate. The advocated techniques are demonstrated by specific application, and, where necessary, most authors indicate the limitations of these by direct comparison with other numerical models or experimental results.

The editors wish to express their thanks to the authors and the advisory panel in making this publication possible.

Finally, the editors wish to state that views expressed and conclusions drawn in the text are solely those of the contributing authors.

C. TAYLOR

K. MORGAN

CONTENTS

CHAPTER 1

A SURVEY OF FINITE DIFFERENCES WITH UPWINDING FOR NUMERICAL MODELLING OF THE INCOMPRESSIBLE CONVECTIVE DIFFUSION EQUATION

B.P. Leonard

City University of New York, College of Staten Island

ABSTRACT

Central difference methods, although excellent for problems dominated by even-ordered spatial derivatives, have been plagued by unphysical oscillations or computational non-convergence when applied to the first-derivative convection term in fluid mechanics. This has led to the development of a variety of non-centered upstream-shifted convective differencing schemes, the general philosophy of which is often known as "upwinding." Although smooth and computationally docile solutions can be achieved by upwinding, it is often at the direct expense of accuracy. This is true even in the case of so-called "optimally weighted" upwind schemes unless they have been carefully generalized in a consistent manner. As the present analysis will show, a misinformed application of finite differences with (certain types of) upwinding can lead to unacceptable inaccuracies without any indication that gross errors have been committed. It will also be shown, however, that a straight-forward upstream-shifted third-order convective differencing scheme automatically combines inherent stability and accuracy, and is algorithmically consistent with (standard) second-order diffusive differencing. Slight problems in thin boundary layers can be resolved (accurately) by introducing alternate interpolation functions into the basic third-order technique.

INTRODUCTION

Finite difference methods have been very successful when applied to physical problems such as diffusion and wave motion, for which the governing differential equations involve dominant second-order spatial derivatives. The same is true for solid mechanics problems in which spatial fourth derivatives are dominant. For all these problems, classical (second-order) central differencing is entirely adequate in terms of accuracy, stability and algorithmic simplicity. Thus it seems natural to try to apply similar methods to the first derivative convection term in fluid mechanics problems. Unfortunately, central-difference methods for convection are usually plagued by unphysical oscillations or explosive nonconvergence -- a well known (but poorly understood) phenomenon. A popular "remedy" for this has been the use of first-order upstream-shifted convective differencing (Roache, 1976), which gives very smooth and computationally docile results. It is now generally recognized, however, that the "artificial diffusion" associated with this so-called "full upwinding" method severely corrupts the solution (Leonard, 1978). Recently, "partial upwinding" techniques (based on a weighted combination of first- and second-order differences, or the equivalent in terms of a finite element formulation) have been strongly advocated (Heinrich & Zienkiewicz, 1979), the degree of upwinding being based on the exact solution of a specialized model problem (Raithby & Torrance, 1974; Heinrich *et al.*, 1977). There has been a tendency to apply these so-called optimal upwinding methods to more general problems with the assumption (or hope!) that high accuracy is being achieved. However, under even only moderately high convection conditions, optimal upwinding reverts to full (first-order) upwinding, and to the extent that the particular problem differs from the model problem on which the technique is based, accuracy is severely impaired by the artificial diffusion thereby introduced. Optimal upwinding methods can be generalized, and this has recently been done within the framework of finite element techniques (Hughes & Brooks, 1979; Brooks & Hughes, 1980). It is clear that similar techniques could be developed in terms of finite differences; however, this type of generalization is not pursued here. Rather, an algorithmically straight-forward *third*-order finite difference method is introduced which possesses inherent stability and is of high accuracy. Sharp boundary-layer regions can then be accurately resolved without numerical oscillations by introducing an adjusted interpolation scheme -- specifically, the three-point quadratic interpolation of the standard third-order method is partially replaced by (an approximation to) a three-point exponential interpolation in appropriate regions. The relative weighting between quadratic and exponential interpolation is determined by local shape characteristics of the solution itself, leading to excellent accuracy throughout all flow regimes.

The model incompressible convective diffusion equation

$$\frac{\partial \phi}{\partial t} = - u \frac{\partial \phi}{\partial x} + \Gamma \frac{\partial^2 \phi}{\partial x^2} + S \qquad (1)$$

is useful for the study of computational methods in fluid mechanics. The equation is nominally one-dimensional; however, it is important to recognize that it is appropriate to a much wider class of flow situations because other transport terms not written explicitly in Equation (1) can be considered to be contained in S (in addition to explicit source terms). The necessity of including an effective source term in a model equation cannot be over-emphasized. One of the problems with so-called optimal upwinding is that, until recently (Brooks & Hughes, 1980) it was based on an exact *steady-state* solution of Equation (1) with $S \equiv 0$. It is not surprising that early forms of optimal upwinding break down under unsteady conditions (Gresho & Lee) or when there is an effective source term due either to actual sources or to cross-grid transport (Hughes & Brooks, 1979) in multi-dimensional flow.

For studying the relative merits of spatial differencing techniques, Equation (1) can be rewritten in a nominally steady (one-dimensional) form as

$$u \frac{\partial \phi}{\partial x} = \Gamma \frac{\partial^2 \phi}{\partial x^2} + S^* \qquad (2)$$

where $S^* = S - \partial\phi/\partial t$. In a real (unsteady, multi-dimensional, compressible, turbulent) flow simulation, at any instant of time and at a given (y,z) location (line), all effects not represented in the first two terms of Equation (2) can be lumped into $S^*(x)$. Although the study of variable coefficients is obviously important, the *essential* qualities of spatial finite difference methods can be studied by assuming u and Γ to be constants. This is the philosophy behind the model test problem studied here, using a simple specified source term $S^*(x)$.

In the next section, a number of spatial finite difference operators are analyzed in terms of their Taylor series expansions (as an indication of accuracy) and with respect to a property called "feedback sensitivity" (which determines whether an algorithm has inherent damping, is neutral, or is actually unstable). It will be shown, for example, that one of the main problems with central differencing (of *any* order) is a total lack of feedback sensitivity when applied to derivatives of *odd* order. Thus, there is no inherent damping of oscillatory perturbations. By contrast, non-centered convective differencing schemes always have a non-zero feedback sensitivity, and this can be made negative (thereby guaranteeing inherent damping) by choosing an upwind bias. Until recently, most upwinding strategies have been based on first-order difference schemes or modifications thereof, with some preliminary flirtations with second-order upwinding (Hodge *et al*, 1979). Unfortunately, such schemes tend to have low accuracy; but, because they produce plausible looking (i.e. "wiggle"-free) results, they have remained very popular in spite of their known (and often ignored) shortcomings. An alternative philosophy, based on a simple third-order upwind scheme, is advocated in the present analysis. As will be seen, the third-order convective differencing scheme is a logical extension of second-order central differencing for diffusion -- both are exact for a cubic polynomial. For reference, a centered fourth-order scheme is also briefly discussed.

The remainder of the paper forms a comparative review of several spatial differencing schemes as applied to a model test problem for which exact solutions are also given. The oscillatory nature of second-order central differencing is made quite apparent. The intolerable artificial diffusion of both first-order (hybrid) *and* so-called optimal schemes is demonstrated. The high accuracy and strong inherent damping characteristics of the third-order scheme are immediately clear, although the polynomial interpolation scheme is still unable to resolve sharp boundary layers without (a few) wiggles. Finally, the "exponentially adjusted" third-order scheme is seen to give results which are graphically almost indistinguishable from the exact solution over the complete range of Péclet numbers, from pure diffusion to pure convection.

ANALYSIS OF FINITE-DIFFERENCE OPERATORS

The diffusion term

By far the most popular finite-difference approximation to the diffusion term in Equation (1) involves the second central difference. Using classical Taylor series analysis, this can be written

$$\Gamma\left[\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2}\right] = \Gamma\left[\left(\frac{\partial^2\phi}{\partial x^2}\right)_i + \frac{1}{12}\phi_i^{(iv)}\Delta x^2 + \ldots\right] \quad (3)$$

The discretization error is proportional to Δx^2; thus this operator is known as being "second-order accurate." Note that the coefficient of Δx^2 involves a fourth-derivative term, so that the discretization is an exact representation of the second derivative (at the point i) for a *cubic* polynomial. This means, in particular, that in a solution using this operator (assuming all other terms are at least as accurate), local truncation error is proportional to Δx^4. This operator combines high formal accuracy with algorithmic simplicity. It also possesses another attractive property: *negative feedback sensitivity* -- as will now be demonstrated.

Feedback sensitivity

In order to understand the concept of feedback sensitivity, assume that a numerical simulation of Equation (1) has been made and consider the evolution of the central node value, ϕ_i:

$$\frac{\partial \phi_i}{\partial t} = \mathrm{RHS} \tag{4}$$

where RHS represents the numerically modelled terms on the right-hand side. In general, RHS will involve some dependence on ϕ_i; thus, the evolution of perturbations in ϕ_i can be studied by taking the variation of Equation (4) with respect to ϕ_i, giving

$$\frac{\partial \delta\phi_i}{\partial t} = \frac{\partial \mathrm{RHS}}{\partial \phi_i} \delta\phi_i \tag{5}$$

which has a formal solution

$$\delta\phi_i = \exp[\int \Sigma \, \partial t] \tag{6}$$

where the *feedback sensitivity* is given by

$$\Sigma = \frac{\partial \mathrm{RHS}}{\partial \phi_i} \tag{7}$$

Clearly, a positive feedback sensitivity would lead to exponential growth of any perturbations and is therefore undesirable. If $\Sigma = 0$, there is no inherent feedback, the algorithm has neutral sensitivity and (certain types of) perturbations can be superimposed on the solution without affecting the RHS -- the algorithm is insensitive to these errors and no automatic corrective action is taken. This type of neutral sensitivity is often associated with temporal and spatial oscillations (i.e. wiggles!). It is directly analogous to the oscillatory nature of marginal stability in dynamic systems. Negative feedback sensitivity, on the other hand, assures that corrective action will automatically be taken by the algorithm to damp out random fluctuations. This is clearly a highly desirable property of any numerical algorithm.

In the case of the diffusion operator given by Equation (3) it is clear that

$$\Sigma = -2\Gamma/\Delta x^2 \tag{8}$$

and since Γ is physically always positive, the operator has negative feedback sensitivity giving it good inherent damping properties. Note that if a *computed* diffusion coefficient itself takes on an erroneous negative value, the consequent positive feedback then indicated by Equation (8) usually guarantees that computational diaster will follow rapidly.

Other diffusion operators

It is interesting to compare other second-order finite-difference operators for diffusion which may not be quite so well known (for reasons that will become obvious). Consider, for example

$$\Gamma\left[\frac{\phi_{i+2}-\phi_{i+1}-\phi_{i-1}+\phi_{i-2}}{3\Delta x^2}\right] = \Gamma\left[\left(\frac{\partial^2\phi}{\partial x^2}\right)_i + \frac{5}{12}\phi_i^{(iv)}\Delta x^2 + \ldots\right] \qquad (9)$$

Superficially, the Taylor expansion is not unlike that of Equation (3): the second-order discretization error has a fourth-derivative coefficient (which is zero for a cubic); the only obvious difference is the numerical factor. However, in this case, ϕ_i does not appear in the operator and so the feedback sensitivity is

$$\Sigma \equiv 0 \qquad (10)$$

-- there is no corrective feedback! In fact, solutions using this operator are susceptible to unphysical parasitic oscillations (of wavelength $3\Delta x$), clearly an undesirable characteristic.

An even less desirable diffusion operator can be formed as follows

$$\Gamma\left[\frac{\phi_{i+2} - 2\phi_{i+1} + 2\phi_i - 2\phi_{i-1} + \phi_{i-2}}{2\Delta x^2}\right] =$$

$$\Gamma\left[\left(\frac{\partial^2\phi}{\partial x^2}\right)_i + \frac{7}{12}\phi_i^{(iv)}\Delta x^2 + \ldots\right] \qquad (11)$$

which again has a Taylor series expansion superficially similar to Equations (9) or (3). But, for this operator, the feedback sensitivity is *positive*:

$$\Sigma = \Gamma/\Delta x^2 \qquad (12)$$

-- an algorithm using this operator would be inherently *unstable*!

There are many other practical finite-difference operators for diffusion. For obvious reasons, the fourth-order central-difference form

$$\Gamma\left[\frac{-\phi_{i+2} + 16\,\phi_{i+1} - 30\,\phi_i + 16\,\phi_{i-1} - \phi_{i-2}}{12\,\Delta x^2}\right]$$

$$= \Gamma\left[\left(\frac{\partial^2\phi}{\partial x^2}\right)_i - \frac{1}{90}\,\phi_i^{(vi)}\Delta x^4 + \ldots\right] \qquad (13)$$

is very popular. Note that the operator is exact for a quintic polynomial; thus, local truncation error is $O(\Delta x^6)$. The feedback sensitivity is negative:

$$\Sigma = -\,5\Gamma/2\Delta x^2 \qquad (14)$$

and similar to (slightly stronger than) that of the standard second-order operator given by Equation (8).

Modelling the convection term

When one considers the success of second-order central differencing for diffusion, it is natural to consider using a similar operator for the first-derivative convection term in Equation (1). This would be

$$-\,u\left[\frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}\right] = -\,u\left[\left(\frac{\partial\phi}{\partial x}\right)_i + \frac{1}{6}\,\phi_i'''\Delta x^2 + \ldots\right] \qquad (15)$$

which has the same formal order of discretization error as that of Equation (3); note, however, that this convective operator is exact only for a quadratic polynomial, giving a formal local truncation error $O(\Delta x^3)$. As should by now be immediately obvious, this convective operator has *neutral* feedback sensitivity, $\Sigma \equiv 0$. And this is essentially the major problem with this operator. As will be seen, neutral feedback sensitivity is a characteristic common to all *central* difference methods (of any order) when applied to *odd*-order derivatives.

When second-order central differencing is used for both convection and diffusion in modelling Equation (1), negative feedback sensitivity is dependent entirely on the diffusion term. Under high convection conditions, this is relatively very weak and the solution is susceptible to both temporal and spatial unphysical oscillations. The nondimensional parameter which represents the relative ratio of modelled convection and diffusion terms is the generalized grid Péclet number

$$P_\Delta = u\Delta x/\Gamma \qquad (16)$$

Typically, for second-order central differencing, when $P_\Delta \lesssim 2$, the negative feedback sensitivity of the diffusion operator is strong enough to damp out potential wiggles. But to the extent that P_Δ exceeds 2, the damping becomes relatively weaker and weaker, and in the high-convection regime the wiggles may corrupt large regions of the flow domain.

The problems associated with central-differencing's neutral feedback sensitivity are not cured by going to higher-order *central* methods. For example, the fourth-order central-difference operator for convection is

$$- u \left[\frac{-\phi_{i+2} + 8\phi_{i+1} - 8\phi_{i-1} + \phi_{i-2}}{12\Delta x} \right]$$

$$= - u \left[\left(\frac{\partial \phi}{\partial x} \right)_i - \frac{1}{4} \phi_i^{(v)} \Delta x^4 + \ldots \right] \tag{17}$$

Although this has high formal accuracy, there is no ϕ_i term in the operator, and $\Sigma \equiv 0$. Once again there is the possibility of wiggles under high-convection conditions, although the amount of physical diffusion needed to dampen wiggles is smaller than that for the second-order case.

Note that the corresponding operator for the third derivative

$$\frac{\phi_{i+2} - 2\phi_{i+1} + 2\phi_{i-1} - \phi_{i-2}}{2\Delta x^3} = \left(\frac{\partial^3 \phi}{\partial x^3} \right)_i + \frac{1}{4} \phi_i^{(v)} \Delta x^2 + \ldots \tag{18}$$

also has neutral feedback sensitivity. A little reflection will reveal that this must be a common property of all *central* difference methods when modelling *odd*-order derivatives.

The upwinding strategy

First-order upwinding Early "remedies" for central-differencing's problems with convection involved a strategy of using the one-sided first difference, usually with "physical plausibility" arguments to determine which direction should be favoured for taking the difference (e.g. see Roache, 1976). Instead of making *a priori* judgements as to the appropriateness of the direction, consider both first differences of the convection term:

$$- u \left[\frac{\phi_i - \phi_{i-1}}{\Delta x} \right] = - u \left[\left(\frac{\partial \phi}{\partial x} \right)_i - \frac{1}{2} \phi_i'' \Delta x + \ldots \right] \tag{19}$$

and

$$- u\left[\frac{\phi_{i+1} - \phi_i}{\Delta x}\right] = - u\left[\left(\frac{\partial\phi}{\partial x}\right)_i + \frac{1}{2}\,\phi_i''\Delta x + \ldots\right] \tag{20}$$

Note that the leading discretization error is equivalent to a physical diffusion term (i.e. a second derivative) with an effective diffusion coefficient of

$$\Gamma_{num} = \pm\, u\Delta x/2 \tag{21}$$

Thus, by choosing Equation (19) when $u > 0$ and (20) when $u < 0$, the discretization error terms are always stabilizing. This, of course, is the "upwinding" strategy. The same conclusion is reached by studying the feedback sensitivity,

$$\Sigma = \mp\, u/\Delta x \tag{22}$$

which is always negative if upwinding is used.

In fact, by combining Equations (19) and (20), first-order upwinding can be written in terms of central-difference operators (regardless of the sign of u) as

$$- u\left[\frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}\right] + |u|\left[\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{2\Delta x}\right]$$
$$= - u\left[\left(\frac{\partial\phi}{\partial x}\right)_i + \frac{1}{2}|u|\phi_i''\Delta x + \ldots\right] \tag{23}$$

from which it is immediately clear that

$$\Gamma_{num} = |u|\Delta x/2 \tag{24}$$

and

$$\Sigma = - |u|/\Delta x \tag{25}$$

Although at first sight the negative feedback sensitivity of first-order upwinding seems quite attractive in comparison with central differencing's total lack, it must be remembered that the equation being modelled is the convective *diffusion* equation and that by using first-order upwinding for convection a "false diffusion" term is automatically added which will corrupt the modelling of the physical diffusion term unless

$$\Gamma_{num} \ll \Gamma \tag{26}$$

which, from Equations (16) and (21), is the same as requiring

$$P_\Delta << 1 \tag{27}$$

-- a much more stringent requirement than the $P_\Delta \lesssim 2$ condition needed for (non-wiggly) computations using second-order central differencing. There have been arguments in the literature to the effect that first-order upwinding actually becomes more accurate for very *large* values of P_Δ (Spalding, 1972; Raithby, 1976). However, as is shown quite dramatically in the next section, such arguments are entirely fallacial, being based on the results of a degenerate test problem which has virtually no relevance to most practical flow situations.

It is now generally acknowledged among most professional computational fluid dynamicists that the false diffusion introduced by first-order upwinding renders this method unacceptable for practical purposes. To overcome these difficulties, essentially two different types of philosophy have developed, which might be categorized as "partial first-order upwinding" (a weighted mixture with second-order central differencing) and "higher-order upwinding." Unfortunately, most partial upwinding methods revert to full first-order upwinding under (even only moderately) high convection conditions (e.g. $P_\Delta \gtrsim 5$). The real problem is that such methods have been widely advertised as being highly accurate under such conditions, whereas they certainly are not! Once again, the fallacy stems from the degenerate test problem mentioned earlier. One would have to take great care to generalize a finite-difference method based on partial first-order upwinding to take account of the unsteady effects, cross-grid transport, and explicit source terms, all of which are missing in currently popular techniques. So far, this has apparently not been done, although progress is being made in the corresponding development of finite-*element* methods (Brooks & Hughes, 1980).

Second-order upwinding With respect to higher-order upwind schemes, there has been tentative interest in a second-order full upwind scheme, for which the convective term is written (Hodge *et al.*, 1979)

$$- u \left[\frac{3\phi_i - 4\phi_{i-1} + \phi_{i-2}}{2\Delta x} \right]$$

$$= - u \left[\left(\frac{\partial \phi}{\partial x} \right)_i - \frac{1}{3} \phi_i''' \Delta x^2 + \frac{1}{4} \phi_i^{(iv)} \Delta x^3 + \dots \right] \tag{27}$$

for $u > 0$, and