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ACCURATE NUMERICAL SIMULATION OF ADVECTION USING LARGE TIME STEPS

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SUMMARY

This paper describes a technique for achieving accurate numerical simulations of advective transport at large Courant numbers using large time steps. The scheme is called ULTIMATE DISCUS and it implements Leonard's universal flux limiter and QUICKEST algorithms within a semi-Lagrangian treatment of advection. This enables the scheme to achieve monotonic solutions, mass conservation and, most importantly, high accuracy without any limit on the time step (or Courant number).

The results of numerical experiments of advection over a fixed distance show that the accuracy of the method increases with increasing spatial resolution and generally increases (but in a non-trivial manner) with increasing Courant number. Accuracy is exact at all integer values of Courant number; for Courant numbers increasing between zero and one, accuracy improves rapidly and monotonically; for other integer–integer ranges of Courant number there is a minimum of accuracy close to the mid-range value. This behaviour is explained in terms of the known accuracy of the QUICKSET algorithm as a function of Courant number and the reducing number of interpolative steps required in the simulations as the Courant number increases. The use of the flux limiter is shown to remove non-physical oscillations from the solution, but at the price of a few per cent reduction in global accuracy caused by increased suppression of peak values.

KEY WORDS: semi-Lagrangian; advection; accuracy

INTRODUCTION

This paper focuses on the modelling of pure advection at high Courant numbers using what could best be described as a hybrid scheme, in the sense that it combines the advantages of three basic techniques which have been available for many years in more than one area of computational fluid dynamics (CFD). Although the authors' application area is concerned with pollutant transport in rivers and coastal waters, the methods described here will find application in other areas of CFD, since the difficulties of accurately modelling advection-dominated flows are all pervasive throughout the CFD community.

The numerical scheme to be described is called ULTIMATE DISCUS and it includes elements from the method of characteristics, control volume discretization and flux limiting. The original non-

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flux-limiting version of the method, DISCUS (Domain of Influence Search for Convective Unconditional Stability), was recently reported.[1] That paper showed the potential of the basic method for accurate advection calculations at Courant numbers greater than one, but excluded detailed background information. Without the flux limiter, solutions from the scheme developed wiggles (unphysical grid-scale oscillations) in areas of rapid changes in gradient of the advected variable, as would be expected. Inclusion of the flux limiter eliminates the wiggles, but there is a price to pay.

ULTIMATE DISCUS is closely related to the so-called Eulerian–Lagrangian or semi-Lagrangian schemes which have been appearing in the literature for some years and is essentially the same as the flux-based modified method of characteristics (FBMMOC) advocated by Roache,[2] the main difference being the use of Leonard's QUICKEST scheme[3] together with his universal flux limiter[4,5] instead of van Leer's MUSCL algorithm.[6]

The essential ingredients of semi-Lagrangian advection calculations[7] are that the advected variable is tracked along characteristics (fluid trajectories) and results are obtained on a regular mesh by following only those characteristics which terminate at the mesh grid points. Since in general the characteristics do not begin at mesh grid points, some interpolation of the advected variable is required. The strength of the method lies in its unconditional stability at all Courant numbers; its weaknesses are that mass conservation and monotonic profiles are not guaranteed. These can be remedied, however, by casting the scheme in a conservative flux-based form[2] and implementing a shape-preserving algorithm. Usually the latter works by automatically limiting the calculations (using monotonicity-based constraints),[4] but recent work[8] shows that the same effect can be achieved by using a shape-preserving integral reconstruction technique when interpolating the advected variable.

In common with previous work by the authors,[9] the paper presents practical accuracy norms for the scheme, which illustrate the way in which its accuracy depends on spatial resolution and Courant number. The significant divergence from previously accepted wisdom allowed by schemes such as DISCUS, which benefit from acknowledging the physical nature of advection, is that accuracy tends to increase as the time step increases. Moreover, there is no limit to the magnitude of the time step. These are important features and indicate crucial advantages over Eulerian schemes which are limited to relatively small time steps either on stability grounds (so-called explicit schemes) or an accuracy grounds (so-called implicit schemes). Hence the computing time required by DISCUS for extensive advection simulations is greatly reduced. Moreover, use of a conservative control volume discretization ensures mass conservation. For many years it has been the accuracy of the modelling of advection which has restricted the development of numerical models of pollutant transport and water quality in rivers, estuaries and coastal regions. The advent of schemes like DISCUS suggests it will be the commonly used second-order-accurate modelling of the diffusion terms which will be the limiting factor in the future.

The aims of the paper, therefore are (a) to present a derivation of the DISCUS algorithm, (b) to describe the inclusion of a flux limiter (i.e. the ULTIMATE DISCUS scheme) and (c) to present and interpret results from numerical simulations of the original and flux-limited algorithms for a range of spatial resolutions and Courant numbers. Throughout, we limit the discussion to the case of one-dimensional pure advection under a steady, spatially uniform velocity field solved on a uniform computational grid. The authors are currently extending the method for use in more complex and arguably more practically useful situations, such as non-uniform velocity fields and in the presence of physical diffusion. To paraphrase Leonard (one of the pioneers in advection modelling), however, it is pointless to complicate the issues before we have demonstrated that we can adequately solve simple linear advection problems, a significant embarrassment of many codes being that they are unable to resolve unsteady, one-dimensional advection at constant velocity with an acceptable accuracy.

THE DISCUS AND ULTIMATE DISCUS ALGORITHMS

One-dimensional pure advection is described by the equation

$$\partial C/\partial t + \partial(UC)/\partial x = 0, \tag{1}$$

where U is the advecting velocity, C is the advected variable, t is time and x is the spatial co-ordinate.

Figure 1 shows the space–time computational plane used for the numerical solution of equation (1), assuming a positive velocity field acting to the right. It is assumed that all values of C are known at the grid points at the present time level (n) and we wish to calculate all the values of C at the grid points at the future time level ($n+1$). The broken line is a characteristic along which information propagates across the computational plane. Moreover, the advected variable is constant along a characteristic and its slope is the reciprocal of the velocity. Because of the uniform velocity field, all the characteristics are parallel. Focusing on just grid point i, it is evident that

$$C(i, n+1) = C(f, n), \tag{2}$$

where f is the foot of the characteristic which terminates at grid point i at the future time level. Equation (2) is the essential ingredient of a semi-Lagrangian scheme and it ensures that the transfer of information is in sympathy with the physical process of advection. Clearly, because f does not coincide with a grid point, recourse to interpolation is necessary in the evaluation of $C(f, n)$. The accuracy of any such characteristic-based numerical scheme is crucially dependent on the interpolation method used.

It is easy to show, but perhaps not well known, that the Courant number may be evaluated from the slope of the characteristic,

$$\text{slope of characteristic} = 1/U, \tag{3a}$$

and from Figure 1,

$$\text{slope of characteristic} = \Delta t/(1+\alpha)\Delta x. \tag{3b}$$

Combining these two equations gives

$$\text{Courant number } N1 = U\Delta t/\Delta x = 1+\alpha. \tag{4}$$

It should be clear that α is a fractional distance step and that it takes values between zero and one. It can also be interpreted as a fractional Courant number; other workers use the term remnant Courant number.[8] Figure 1, therefore, only applies for Courant numbers between one and two, but the extension to other Courant number ranges is straightforward.

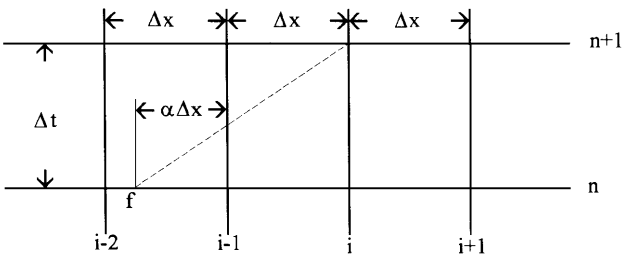

Figure 1. Space–time computational plane

Consider now Figure 2, which shows part of the computational plane in greater detail. In particular the time step has been split such that the characteristic terminating at grid point i passes through grid point $i-1$ at the fractional time step τ. In the ULTIMATE DISCUS scheme the evaluation of $C(i, n+1)$ is undertaken as a three-step procedure: firstly, a control volume discretization over the partial time step $\tau\Delta t$ to evaluate $C(i-1, n+\tau)$; secondly, the application of a flux limiter to this evaluation; thirdly, point-to-point transfer of the flux-limited value of C along the characteristic for the partial time step $(1-\tau)\Delta t$. In the simpler DISCUS algorithm the flux limiter is omitted.

Step 1

With regard to Figure 2, L and R indicate the location of the left-hand (LH) and right-hand (RH) faces of the control volume centred about grid point $i-1$. The usual conservative control-volume-based discretization of equation (1) is given by

$$C(i-1, n+\tau) - C(i-1, n) = \frac{\tau\Delta t}{\Delta x}[F(L, n) - F(R, n)], \tag{5}$$

where F represents the flux of the advected variable ($= UC$) at the control volume face. Strictly, the terms on the left-hand side (LHS) of equation (5) are control volume average values rather than nodal values and the fluxes on the right-hand side (RHS) are time step average values. Leonard[4] discusses the implications of this and shows that in the uniform velocity case equation (5) is valid if the face values are defined appropriately.

An alternative way of writing equation (5) is

$$C(i-1, n+\tau) - C(i-1, n) = \frac{1}{\Delta x}[\tilde{F}(L) - \tilde{F}(R)], \tag{6}$$

where $\tilde{F}$ is a time-integrated flux. The RHS of equation (5) or (6) simply represents the difference in mass of the advected variable entering and leaving the control volume during the partial time step. The time-integrated flux terms are written more formally as

$$\tilde{F}(L) = \int_t^{t+\tau\Delta t} F(L)\,\mathrm{d}T, \qquad \tilde{F}(R) = \int_t^{t+\tau\Delta t} F(R)\,\mathrm{d}T, \tag{7a, b}$$

where T is a dummy time variable used solely to undertake the integration. In principle the integrals in equations (7a) and (7b) can be evaluated using any numerical integration technique.

Figure 3 shows an expanded view of the lower partial time step shown in Figure 2 and allows a physical explanation of the time-integrated fluxes to be appreciated. With reference to the LH face, the foot (g) of the broken characteristic tracked back from the LH face at time $n+\tau$ indicates the extent of the spatial domain from which the time-integrated flux should be calculated. Any part of the

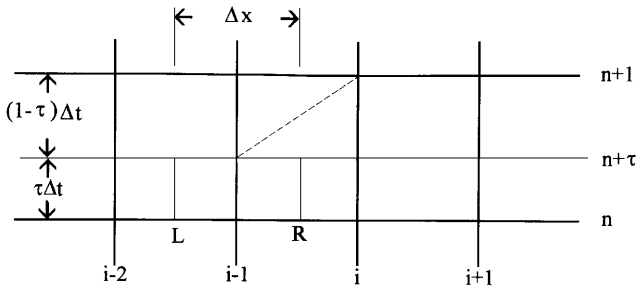

Figure 2. Detail of computational plane around grid point $i-1$

spatial profile of C further upstream of (to the left of) g at time n will not pass through the control volume's LH face during the partial time step. Equally, any part of the spatial profile of C further downstream of L at time n cannot influence the flux through the LH face, since it has already passed through it. Hence we could replace the time integrals of flux (equations (7a) and (7b)) with the following spatial integrals of C (the velocity cancelling and X being a dummy spatial integration variable):

$$\tilde{F}(L) = \int_g^L C \, \mathrm{d}X, \qquad \tilde{F}(R) = \int_h^R C \, \mathrm{d}X. \tag{8a, b}$$

Roache[2] recommends approximating the time integrals in terms of the fluxes passing through the control volume faces at the centre of the partial time step, i.e. as the product of the value of C at the foot of the characteristic (shown as a bold line in Figure 3) terminating at the face at time $n + \tau/2$, the velocity and the partial time step. Hence

$$\tilde{F}(L) \approx C(\#_L, n) U \tau \Delta t, \qquad \tilde{F}(R) \approx C(\#_R, n) U \tau \Delta t. \tag{9a, b}$$

Clearly, these reduce to approximations of the spatial integrals by replacing the product $U\tau\Delta t$ by $\alpha\Delta x$. Hence equation (6) may be written as

$$C(i-1, n+\tau) - C(i-1, n) = \alpha[C(\#_L, n) - C(\#_R, n)]. \tag{10}$$

Note that the adoption of Roache's approximation implies a linear variation in C over the distance $\alpha\Delta x$, i.e. second-order accuracy. From a consideration of the slope of the characteristics it is evident that α is simply the Courant number associated with the calculation described by equation (10) and is defined as

$$\alpha = U\tau\Delta t/\Delta x. \tag{11}$$

In view of equation (4), which defines the Courant number $N1$ for the complete time step, it is possible, and indeed more convenient, to regard α as a fractional Courant number given by (for the particular case under consideration)

$$\alpha = N1 - 1. \tag{12}$$

It is easy to show that equations (11) and (12) are consistent with each other. Note that α can also be interpreted as an interpolation parameter used in evaluating $C(\#_L, n)$ and $C(\#_R, n)$ from the grid point values of C.

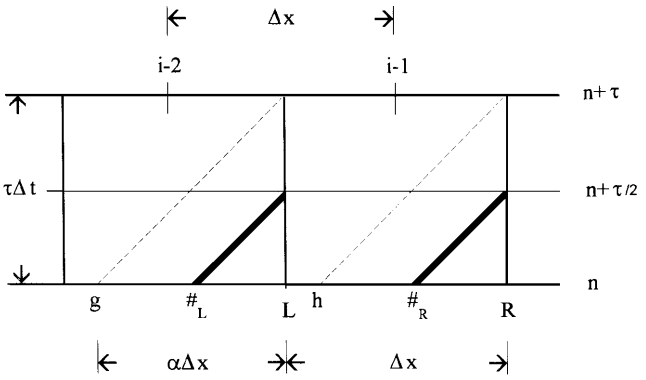

Figure 3. Expanded view of computational plane for control volume centred at grid point $i - 1$

Numerous methods are available for estimating $C(\#_L, n)$ and $C(\#_R, n)$. Undoubtedly, one of the best schemes is Leonard's QUICKEST algorithm.[3,4] This scheme gives a time step average estimate for the face values of the advected variable (i.e. exactly what we require, although it is probably not always appreciated that the QUICKEST estimates are indeed equivalent to $C(\#_L, n)$ and $C(\#_R, n)$) and is of third-order accuracy in time and space while remaining computationally efficient. Recent work[9,10] confirms the promise of the scheme and it is also recommended by Roache as a likely alternative to the combined upstream and Lax–Wendroff method used in his FBMMOC method. Interestingly, the scheme has been derived in a number of different ways[4,11–13] to that originally given by Leonard.[3] As a final note, it is well known[3] that exactly the same algebraic expression for $C(i-1, n+\tau)$ would be obtained if it were calculated from upstream-biased cubic interpolation at time level n followed by point-to-point transfer along the characteristic terminating at grid point $i-1$ at time level $n+\tau$. The difference in philosophy between the two approaches, however, is not merely numerical semantics, because only by using a control volume discretization can the next step of the scheme be implemented.[2]

Step 2

A number of workers[2,4,10] discuss the performance of flux limiters for suppressing unphysical oscillations (wiggles) generated in areas of rapid changes in gradient of the advected variable. Van Leer's MUSCL scheme and Leonard's ULTIMATE scheme appear to have the edge and we have adopted the latter. The reader is recommended to consult Reference 4 for details of the method. Briefly, however, the method applies constraints to a calculated control volume face value of the advected variable such that values which would cause non-monotonicity are replaced with ones which preserve monotonicity. It should be recognized that flux limiters are not a universal panacea: yes, they remove unphysical oscillations from numerical results, but they can also have side-effects, resulting in profiles of the advected variable becoming distorted in a variety of ways. When ULTIMATE is combined with QUICKEST, the effects are reminiscent of the presence of excessive numerical diffusion with peak values being attenuated and profile widths being artificially increased (this is illustrated in the results shown later).

Leonard[4] and Leonard and Niknafs[5] describe a method for increasing the accuracy of the basic ULTIMATE QUICKEST scheme in regions of physical extrema while retaining the suppression of wiggles in the vicinity of rapid changes in gradient of the advected variable. By using a high enough order of accuracy approximation of the control volume face values, the resulting adaptive algorithm reduces numerical diffusion to minimal levels and offers the prospect of very accurate simulations at Courant numbers less than one. After consulting the next section, readers will see that the incorporation of this refinement within ULTIMATE DISCUS would extend this promise to all Courant numbers. We have refrained from doing this here, however, since we wish first to illustrate the enhanced accuracy obtainable by using ULTIMATE DISCUS as opposed to using ULTIMATE QUICKEST, i.e. by extending the use of the basic third-order-accurate scheme for use with large time steps.

Step 3

With reference to Figure 2 it is clear that point-to-point transfer along the characteristic for the upper partial time step gives

$$C(i, n+1) = C(i-1, n+\tau). \tag{13}$$

Combining the above steps into a single-stage algorithm gives the ULTIMATE DISCUS scheme for Courant numbers between one and two as

$$C(i, n+1) = C(i-1, n) + \alpha[C(L, *) - C(R, *)], \tag{14}$$

where an asterisk indicates flux-limited, time step average values of C evaluated using the ULTIMATE QUICKEST scheme. The scheme is easily generalized to any Courant number, since all that this alters is the location of the cell for which the control volume discretization is required: the larger the Courant number, the further upstream this cell is located. Roache[2] refers to this cell as the core cell. In all cases the fractional Courant number lies between zero and one. Indeed, when it equals zero or one, i.e. when the Courant number for the complete time step is an integer, the scheme gives exact point-to-point transfer. Hence the general ULTIMATE DISCUS scheme is

$$C(i, n+1) = C(i-p, n) + \alpha[C(i-p-\tfrac{1}{2}, *) - C(i-p+\tfrac{1}{2}, *)], \tag{15}$$

where $p(=\mathrm{INT}(N1))$ is the truncated integer value of the Courant number $N1$ and $\alpha = N1 - p$. The use of $\frac{1}{2}$ in the spatial indices indicates a control volume face.

The most important feature of this algorithm is that it recognizes and benefits from the characteristic nature of advection. The values of the advected variable which most heavily influence the unknown value $C(i, n+1)$ are those at time level n which are close to the foot of the characteristic back-tracked from $C(i, n+1)$. This is the bedrock of the DISCUS method. Only by using information from this part of the computational plane can a highly accurate solution be obtained. The ability of this scheme to work at any Courant number should now be clear, since the only effect that the Courant number has is to alter the slope of the characteristic in the third step of the procedure, i.e. to determine the number of cells between the *i*th cell and the core cell. The numerical algorithm is unconditionally stable because the fractional Courant number is always less than one.

Although it may not be obvious, the algorithm is essentially the same as the FBMMOC method described by Roache.[2] Equation (15) appears more compact than the expressions given by Roache for two reasons. Firstly, Roache does not give his algorithm in as condensed a form as possible. In contrast with equation (11) of Roache's paper, equation (15) recognizes that contributions to the conservation of the advected variable from cells located between the core cell and the *i*th cell cancel when the expressions for the time-integrated fluxes for both face values are substituted into the control volume discretization. Indeed, some of the terms which cancel reflect the fact that when the Courant number is high, part of the advected profile will pass through both faces of the control volume during a time step.

Secondly, Roache allows for a spatially varying velocity field while equation (15) does not, although it is easily generalized to do so by using a local fractional Courant number for each control volume face[2,4] (note, however, that the flux limiter may need refining). In a similar way the recognition of the upstream movement of the core cell implied by the reduced grid point index in *all* the terms on the RHS of equation (15) automatically ensures that the algorithm is consistent with Roache's 'correct' as opposed to his 'incorrect' or 'naive' method. His 'naive' method is equivalent to the first term on the RHS of equation (15) being $C(i, n)$, which as he points out leads to erroneous results when the Courant number is greater than one.

NUMERICAL EXPERIMENTS

A series of numerical experiments were undertaken with DISCUS and ULTIMATE DISCUS in order to enumerate their accuracy and to illustrate the effect of their errors on spatial profiles of C. Each experiment consisted of simulating the one-dimensional pure advection of a Gaussian profile of the advected variable by a uniform velocity field. Simulations were undertaken for Courant number $N1$

between 0·1 and 22·5 and for two spatial resolutions $N3$ (7·76, 15·52) defined as $4\sigma/\Delta x$, where σ is the standard deviation of the Gaussian. The smaller $N3$-value is equivalent to a standard deviation of $1{\cdot}94\Delta x$ as used by Leonard and Niknafs.[5] The velocity and distance travelled by the profile were the same in each experiment (1 m s^{-1} and 36 km respectively). The Courant number was varied by changing the time step and hence the number of time steps required to advect the profile the required distance varied with Courant number. $N3$ was varied by changing the standard deviation of the initial profile. A number of simple error norms were evaluated by comparing the computed profile at the end of the calculations with the analytical solution. Clearly, in the absence of physical diffusion the Gaussian profile undergoes pure translation with no change in shape (or variance). Note that other profile shapes, e.g. rectangular, sine-squared or semielliptical functions, would be sterner tests for the algorithms.

DISCUSSION OF RESULTS

Figures 4 and 5 show the percentage error in the peak value of the advected Gaussian at the end of the experiment as a function of Courant number and spatial resolution for both DISCUS and ULTIMATE DISCUS. Figure 4 shows values at or close to Courant numbers of 0·5, 1·5, 2·5, . . . , 9·5, 10·5, 16·5 and 22·5 and illustrates how the accuracy of both schemes tends to increase with increasing Courant number and with increasing spatial resolution. Clearly, most of the improvement in accuracy (at constant $N3$) occurs for Courant numbers increasing up to 10, beyond which the accuracy tends to remain approximately constant. It is also evident that DISCUS is always more accurate than ULTIMATE DISCUS. Figure 4 gives a superficial view of the variation in accuracy with Courant number, however, as illustrated in Figure 5, which shows some results at a greater Courant number resolution. Here, for Courant numbers between one and three the accuracy of both schemes is seen to vary in a systematic way between integer values of Courant number, with a local minimum of accuracy (maximum of error) occurring close to, but not necessarily at, the mid-range value. Clearly, the analytical solution is simulated exactly at integer values of Courant number, as expected. There is no reason to doubt that similar patterns exist for all integer–integer ranges of Courant number. The

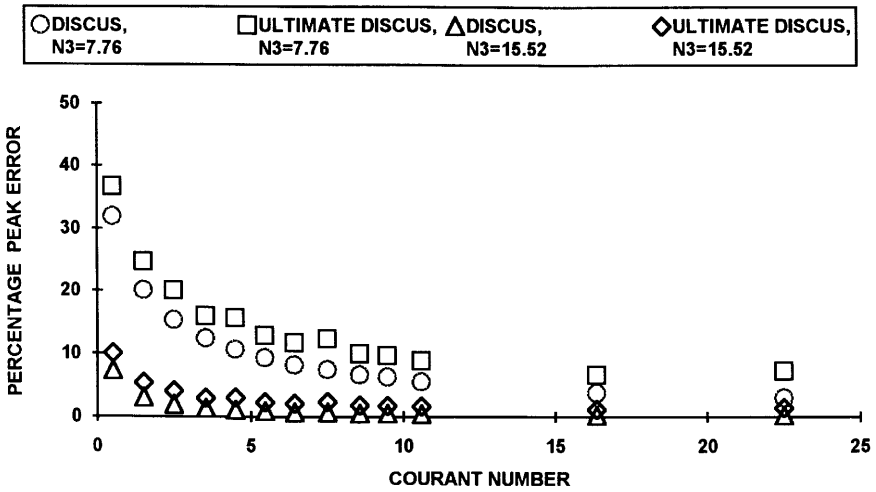

Figure 4. Accuracy of numerical schemes as a function of Courant number

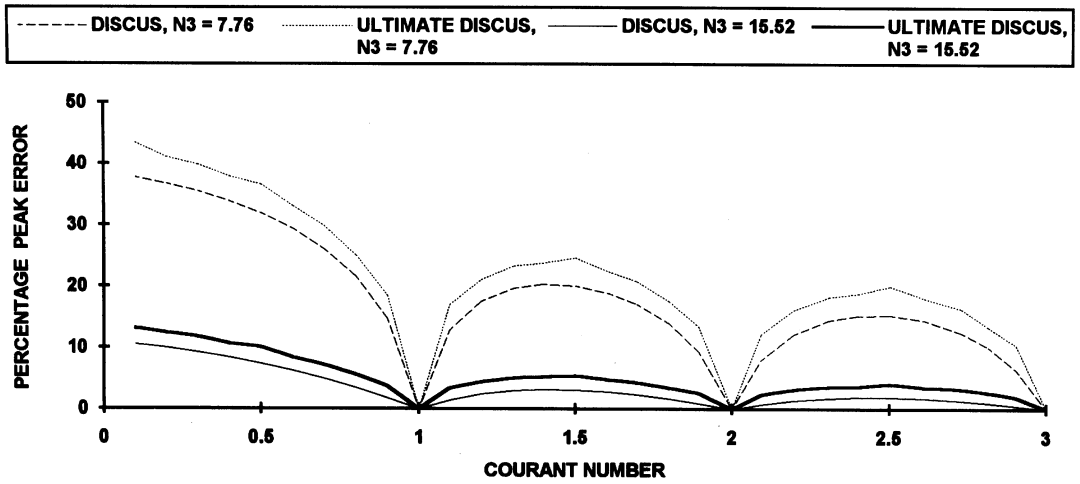

Figure 5. Detail of variation in accuracy of numerical schemes for Courant numbers between zero and three

obvious exception is between zero and one, where accuracy increases monotonically with increasing Courant number. Again it is clear that DISCUS is always more accurate than ULTIMATE DISCUS.

These accuracy plots require careful interpretation. A von Neumann stability analysis of the QUICKEST scheme for pure advection[3] reveals that for a constant spatial resolution its amplification factor varies with Courant number in the range from zero to one in a symmetrical manner, with a minimum occurring when the Courant number is 0·5 and unity occurring when the Courant number is zero or one. Now the amplification factor is a measure of the error per time step of the scheme, so that if the QUICKEST scheme were run at Courant numbers of 0·2 and 0·8 for the same number of time steps, we would expect exactly the same values for any error norms evaluated (and, indeed, this is what we find). The results reported here appear not to show this, however, only because of the way in which the Courant number was varied, which involved increasing the time step and necessarily decreasing the number of time steps required to advect the test profile the same distance in each experiment.

For example, a Courant number of 0·2 utilized 900 time steps of length 40 s, while a Courant number of 0·8 utilized 200 time steps of length 18 s. Hence the total error at the end of the two simulations ought not to be the same: the error in the simulation using the greatest number of time steps is expected to be greater and this is borne out by Figure 5. The accuracy of the DISCUS scheme (which uses the QUICKEST algorithm at all Courant numbers) for a constant spatial resolution is wholly controlled by the fractional Courant number α, so that the error per time step is the same not only for Courant numbers of 0·2 and 0·8 but also for 1·2, 1·8, 2·2, 2·8, etc.

This argument explains the variation in percentage peak error illustrated by the results. In particular it explains: the monotonically decreasing accuracy as the Courant number reduces from one to zero; why in each other integer–integer Courant number range the accuracy distribution is slightly skewed towards the lower end of the range rather than being symmetrical; and why there is a general increase in accuracy as the Courant number increases as shown in Figure 4. The behaviour of the accuracy of the ULTIMATE DISCUS scheme mirrors that of DISCUS closely, because only occasionally does the flux limiter require the face value obtained using QUICKEST to be modified.

These results also show how important it is for modellers to known what each other mean by accuracy. Clearly, there is a big difference between accuracy per calculated time step and accuracy

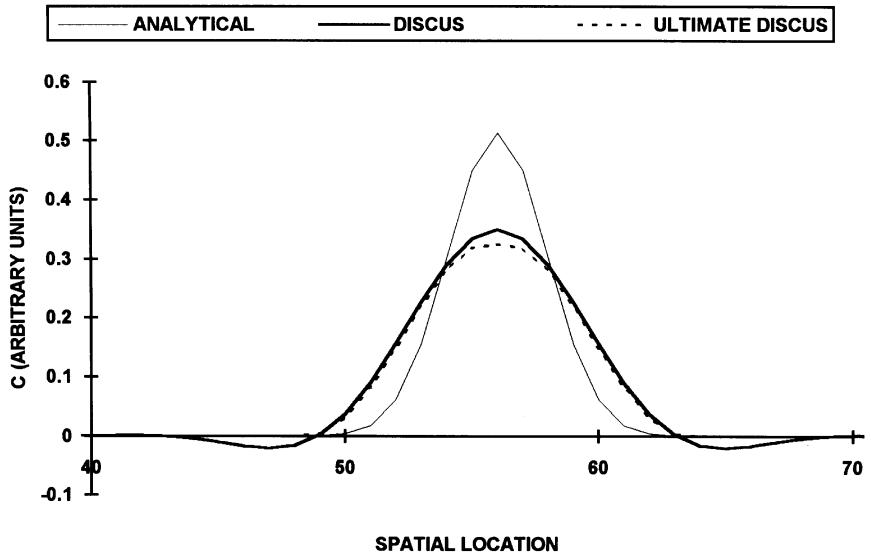

Figure 6(a). Analytical and numerical solutions; Courant number $N1 = 0{\cdot}5$, spatial resolution $N3 = 7{\cdot}76$

achieved over a specified advection distance. Similarly, quoting numerically obtained accuracy as a function of Courant number is not enough—details of the manner in which the Courant number was varied are needed for the results to be properly interpreted.

Figures 4 and 5 also show the improved accuracy of both schemes as the spatial resolution is increased. Significant reductions in the percentage peak error are achieved at all non-integer Courant numbers by doubling the spatial resolution. Clearly, further improvements in accuracy are expected at

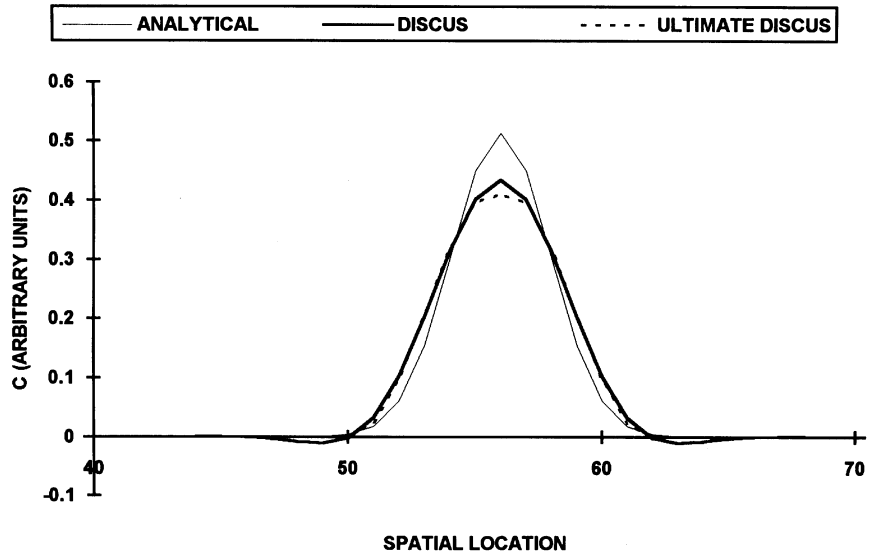

Figure 6(b). Analytical and numerical solutions; Courant number $N1 = 2{\cdot}5$, spatial resolution $N3 = 7{\cdot}76$

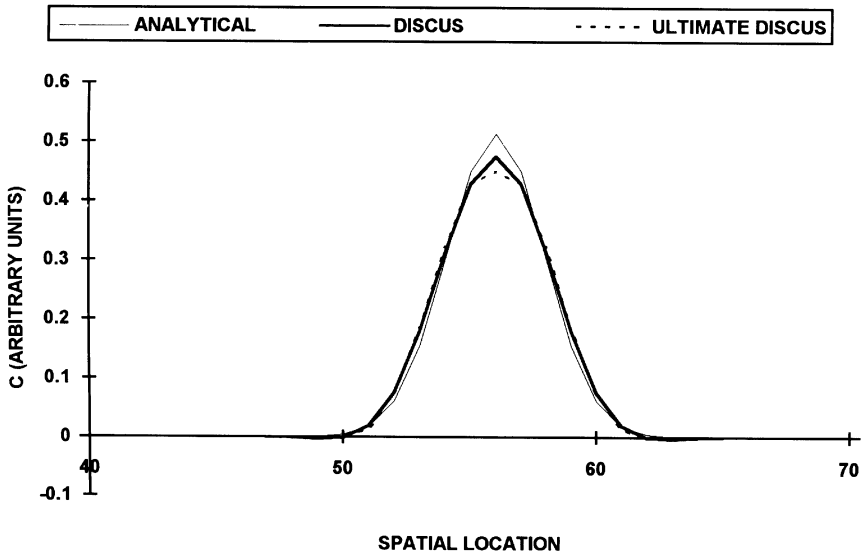

Figure 6(c). Analytical and numerical solutions; Courant number $N1 = 7{\cdot}5$, spatial resolution $N3 = 7{\cdot}76$

even higher spatial resolutions. Other simple accuracy norms such as a coefficient of determination[1] yielded similar trends to those illustrated in Figures 4 and 5.

Figures 6(a)–6(d) shows spatial profiles of C from both schemes at the end of the simulation for Courant numbers of 0·5, 2·5, 7·5 and 22·5 respectively. The analytical solution is also shown. The figures illustrate important aspects of the simulations and show the nature of the errors in them, the main features being: the computed profiles are symmetrical; the calculated peak value is too low in

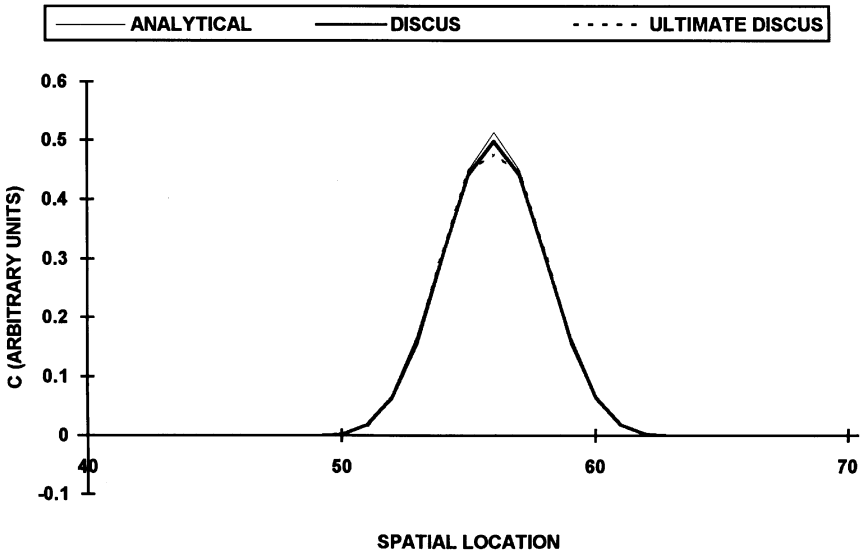

Figure 6(d). Analytical and numerical solutions; Courant number $N1 = 22{\cdot}5$, spatial resolution $N3 = 7{\cdot}76$

both schemes, with the error being greater with ULTIMATE DISCUS as indicated earlier; DISCUS creates oscillatory errors on the front and leading edges while ULTIMATE DISCUS produces monotonic profiles; and both schemes artificially widen the profile to a similar extent. The generally increasing accuracy of both schemes is demonstrated by comparing the visual size of these discrepancies across the four Courant numbers shown. It is noticeable that a significant error in the peak value remains in both schemes even when they appear to fit the rest of the profile. It is this so-called clipping error which the adaptive higher-order form of DISCUS or ULTIMATE DISCUS would remove.

The profile widening and accompanying peak error are caused by numerical diffusion in the QUICKEST algorithm. Clearly, the major side-effect of ULTIMATE DISCUS is the introduction of additional suppression of the peak with only a marginal effect on the profile width. This is the price of eliminating the wiggles and constraining the calculations to remove obviously non-physical modes while retaining mass conservation. The profile widening can be quantified by evaluating the spatial resolution of the profiles at the end of the simulations, *N*3 (final). Such data from the ULTIMATE DISCUS simulations are shown in Figure 7, which is a similar type of plot to Figure 4. This figure shows similar trends to those of the peak error norm discussed earlier. Similar data from the DISCUS simulations are not shown, because all *N*3-values are close to that of the initial profile. This does not imply that profile widening does not occur (see Figure 6); however, the negative parts of the profiles reduce the calculated variance in such a way that the total variance from all runs is always within about 1% of the initial value. Clearly, any error norm based on a simple calculation of variance is not a good discriminator of profile widening if wiggles are present.

Finally, we would stress that both schemes offer significant advantages in practical modelling exercises over existing schemes because they allow the use of larger time steps and hence offer the prospect of reduced computing time. Since the accuracy per time step is only dependent on the fractional Courant number and spatial resolution, the use of large time steps actually increases the basic accuracy of the scheme by reducing the number of spatial interpolation operations required to advect a profile over a fixed distance. Readers should be aware that recourse to traditional means of utilizing large time steps, i.e. the use of Eulerian implicit finite difference or finite element schemes,

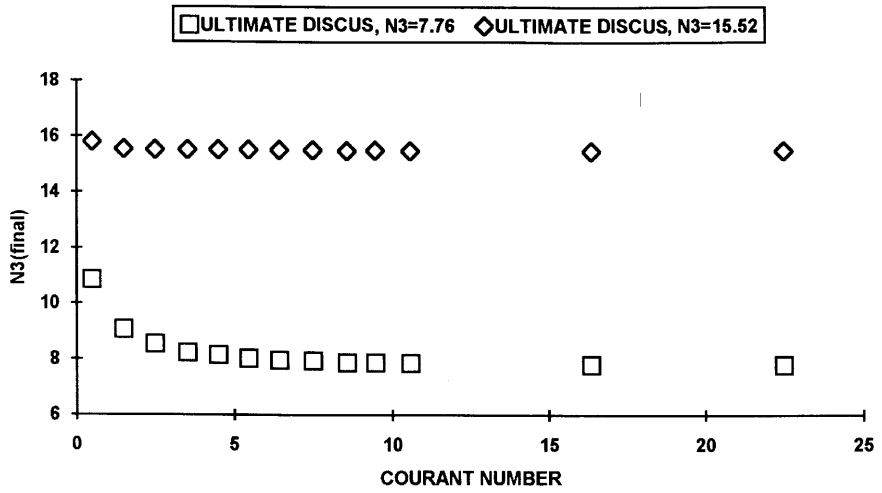

Figure 7. Spatial resolution of simulated profile at end of simulation, *N*3 (final), as a function of Courant number

is counter-productive and should be avoided[1] because their accuracy decreases with increasing Courant number greater than one.

CONCLUSIONS

This paper has described the ULTIMATE DISCUS algorithm for simulating advection. The philosophy of the algorithm is similar to Roache's FBMMOC method,[2] except that it uses the ULTIMATE QUICKEST scheme of Leonard[4] in place of the MUSCL scheme of van Leer.[6] The scheme offers the promise of stability, mass conservation, monotonic profiles and high accuracy at large time steps. The semi-Lagrangian nature of this scheme, which acknowledges the physical nature of advection, is the key to its success, because, for a fixed advection distance, larger time steps imply fewer spatial interpolations and hence the accuracy improves. In terms of simple error norms the original DISCUS scheme (which uses the QUICKEST algorithm) is generally more accurate than the new ULTIMATE DISCUS scheme (which uses the ULTIMATE QUICKEST algorithm). However, the monotonic profiles ensured by ULTIMATE DISCUS are more comforting physically, albeit at the cost of a few per cent loss in overall accuracy. Both schemes give more accurate solutions as the spatial resolution increases, as would be expected. If the computational cost of increasing spatial resolution in order to increase accuracy is too high, the use of the adaptive higher-order form of the ULTIMATE QUICKEST algorithm[4] within the DISCUS framework appears attractive, since the more costly calculations would only be required at relatively few grid points. A simpler remedy, however, would be to increase the time step! Indeed, this latter course is the first step current users of QUICKEST or ULTIMATE QUICKEST should follow in order to immediately increase the accuracy of their simulations. The second step is to locate the core cell using the (new) Courant number, i.e. to use equation (15) in place of the conventional control volume discretization.

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