NOTE

Accuracy Characteristics of Traditional Finite Volume Discretizations for Unsteady Computational Fluid Dynamics

INTRODUCTION

Recently Manson et al. [1] demonstrated the shortcoming of traditional finite volume approaches, typified by Patankar's SIMPLE algorithm [2], for discretizing the equations of fluid flow, heat transfer, and associated transport processes. They were able to show for one severe test case-low spatial resolution and zero diffusion-that traditional finite volume approaches are ineffective for unsteady state problems with significant convective effects. They are ineffective because there exists a time step limitation, even for implicit methods, which is imposed by accuracy constraints rather than stability constraints. The objective of the present paper is to show that the poor performance of these methods in that paper was not simply due to the severity of the test case. This paper will demonstrate the same inadequacy prevails for a range of spatial resolutions and non-zero diffusion cases. This knowledge is already documented but its significance still seems to elude the CFD community who persist with traditional discretizations for unsteady advection.

ADVECTION-DIFFUSION TRANSPORT AND TRADITIONAL FINITE VOLUME DISCRETIZATION

In one dimension advection-diffusion is represented in a conservative form by

$$\frac{\partial \phi}{\partial t} + \frac{\partial (u\phi)}{\partial x} = \frac{\partial}{\partial x} \left(K \frac{\partial \phi}{\partial x} \right), \tag{1}$$

where ϕ is the advected variable, *u* the advecting velocity, taken here to be uniform, steady, and positive, and *K* is a diffusion coefficient which will also be taken to be uniform, steady, and constant. Adopting the notation of Patankar, and referring to Fig. 1, the finite volume representation of (1) is given by integrating it over the control volume,

$$\int_{w}^{e} \left[\int_{t}^{t+\Delta t} \frac{\partial \phi}{\partial t} dt \right] dx = -\int_{t}^{t+\Delta t} \frac{\partial u \phi}{\partial x} dt dx + \int_{w}^{e} \left[\int_{t}^{t+\Delta t} \frac{\partial}{\partial x} \left(K \frac{\partial \phi}{\partial x} \right) dt dx \right] dx.$$
(2)

Employing Green's theorem for the diffusion term the discrete equation becomes

$$(\phi_P - \phi_P^0) \Delta x + (f(u\phi_e - u\phi_w) + (1 - f)(u\phi_e^0 - u\phi_w^0)) \Delta t$$
$$= \Delta t \left(f\left(K \frac{u\phi_E - u\phi_P}{\Delta x} - K \frac{u\phi_P - u\phi_W}{\Delta x} \right) + (1 - f) \left(K \frac{u\phi_E^0 - u\phi_P^0}{\Delta x} - K \frac{u\phi_P^0 - u\phi_W^0}{\Delta x} \right) \right),$$
(3)

where f is a Crank-Nicolson temporal weighting factor. A stability analysis indicates that as long as $f \ge 0.5$ this discretization is unconditionally stable [3], thus the choice of time step is not limited by stability considerations. In (3) the unknown values of ϕ at the future time have no superscript while known values at the present time are given the 0 superscript. We may rearrange (3) as below with all known quantities appearing on the right hand side of the equation,

$$\phi_P + \frac{u\Delta t}{\Delta x} f(\phi_e - \phi_w) - \frac{K\Delta t}{\Delta x^2} f(\phi_E - 2\phi_P + \phi_W)$$

$$= \phi_P^0 - \frac{u\Delta t}{\Delta x} (1 - f)(\phi_e^0 - \phi_w^0) \qquad (4)$$

$$+ \frac{K\Delta t}{\Delta x^2} (1 - f)(\phi_E^0 - 2\phi_P^0 + \phi_w^0).$$

In (4), $u\Delta t/\Delta x$ is the Courant number (Cr) and $K\Delta t/\Delta x^2$ will be termed the diffusion number (Di). Interpolation functions are required for the face values, ϕ_e and ϕ_w , in terms of the nodal values (ϕ_W , ϕ_P , ϕ_E , etc.). In this study quadratic upstream interpolation for convective kinematics (QUICK) [4] was used in keeping with current wisdom in CFD. In practice this gives rise to interpolating functions of the form

$$\phi_e = \frac{1}{2} (\phi_E + \phi_P) - CF(\phi_E - 2\phi_P + \phi_W).$$
(5)

CF is a curvature correction factor which is taken here to be constant with value 0.125.



FIG. 1. Control volume for discretization.

When these interpolation functions are incorporated into (4) the result is a formula for ϕ_P in terms of ϕ_{WW} , ϕ_W , and ϕ_E ,

$$a_P \phi_P = f \sum_{nb} a_{nb} \phi_{nb} + (1 - f) \sum_{nb} a_{nb}^0 \phi_{nb}^0 + a_P^0 \phi_P^0, \quad (6)$$

where *a* is some coefficient which is a function of the Courant number and/or the diffusion number. The nb subscript indicates a neighboring node to node P (i.e., E, W and WW). Equation (6) is written for each node and the resulting equations may be assembled into the solution matrix. Boundary conditions are required to solve the system. At the inlet, ϕ was specified and a zero gradient boundary condition was employed at the outlet.

 σ . This represents a Gaussian profile, with maximum value given by α , the standard deviation given by σ , and the location of the peak at μ . In the present study, μ takes the value 8000.0 mm and σ is varied to give different initial spatial resolutions. The severity of the test case will vary with σ because the numerical method must resolve the difference between maximum and zero over about (3σ) Δx) grid spacings. The initial spatial resolution will hence be defined here as $(3\sigma/\Delta x)$. The velocity is 0.45 mm/s, Δx is 200 mm, and the time step, Δt , is chosen to give Courant numbers $(u\Delta t/\Delta x)$ of 0.45 and 6.45. Two values of the time weighting factor, f, are investigated: 0.5 and 1.0. The simulation time of 20,000.0 s allows the profile to translate 9000.0 mm downwind. Figures 2 and 3 show the results with an initial spatial resolution of 5.82. Figure 2 shows results with a diffusion number of 0.025 while Fig. 3 shows results with a diffusion number ten times greater. Figures 4 and 5 show the results with an initial spatial resolution of 18.97. Figure 4 shows the case with the diffusion number equal to 0.025 and Fig. 5 shows the case with the diffusion number equal to 0.25. In all figures the exact solution is shown as a continuous line while the numerical solutions are shown as broken and dotted lines.

RESULTS

EXAMPLE RUNS

Several test cases will be used. The initial condition is always taken to be $\phi(x, 0) = \alpha e^{-X^2}$, where $X = (x - \mu)/2$

When all figures are considered a trend emerges. The trend suggests that the accuracy of the traditional finite volume approach is low for Courant numbers in excess of



FIG. 2. Initial spatial resolution = 5.82; diffusion number = 0.025.



FIG. 3. Initial spatial resolution = 5.82; diffusion number = 0.25.



FIG. 4. Initial spatial resolution = 18.97; diffusion number = 0.025.



FIG. 5. Initial spatial resolution = 18.97; diffusion number = 0.25.

unity regardless of the initial spatial resolution or the amount of stabilizing diffusion present. If the time weighting factor is set to be 0.5 the inaccuracy manifests itself by producing unphysical oscillations whereas for a time weighting factor of 1 the inaccuracy is due to an artificial smearing of the profile.

The method is most accurate if the Courant number is kept less than one and the time weighting factor is fixed at 0.5. In fact even for low initial spatial resolutions (shear layers resolved over about 6 grid spaces) the method performs well if these conditions are satisfied.

CONCLUSIONS AND RECOMMENDATIONS

This study suggests that the conclusions of Manson *et al.* [1] for a pure advection, low initial spatial resolution test case may be generalized to all one dimensional cases. As stated in that paper traditional implicit finite volume formulations for transport equations do not work for unsteady simulations to any greater Courant number than do explicit methods when the convective terms are significant. If practitioners to use QUICKended traditional finite volume codes for unsteady simulations then the recommendations of Manson *et al.* [1] should be considered.

These conclusions have far reaching consequences for commercial CFD code developers. It seems clear that future code development must address the implementation of alternative advection treatments. This may be a bitter pill for developers to swallow as this will inevitably require some re-thinking of the computer algorithm used. Recent work by Manson and Wallis [5] (DISCUS), Roache [6] (FBMMOC), and Leonard, Lock, and MacVean [7] (NIRVANA) may suggest ways to achieve unconditionally stable and accurate unsteady simulations.

On a positive note these simulations do suggest what an adequate resolution would be for unsteady simulations if a traditional finite volume approach is used.

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