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The Influence of Differencing and CFL Number on Implicit Time-Dependent Non-linear Calculations

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This paper is concerned with the stability and precision of transient implicit finite difference algorithms. The test problem is the Burgers equation. The influence of space discretisation and initial values is studied. Linear analysis provides incomplete stability conditions for both continuous and weak solutions and we derive a simple criterion of "augmented" stability taking into account the non-linearity of the problem. The real stability limits appear to be a combination of the linear stability analysis criterion and of this "augmented" stability criterion.

1. INTRODUCTION

Recent progress in the numerical solution of the Euler equations has been accomplished by the development of noniterative implicit methods. These methods are attractive because they are more stable and generally more efficient than explicit schemes (see Refs. [1–7] for some recent contributions to this field).

Many aspects of these methods are still the subject of intensive research. One important problem is that of the spatial differencing scheme. Recent activity has concentrated on the development of schemes which avoid spurious oscillations and allow a rapid rate of convergence to the steady state. An interesting class of such schemes is known as the total variation diminishing (TVD) algorithms (see, for example, Yee, Warming, and Harten [1]).

Another point of concern is that of the accuracy of the transient solution. Indeed most of the implicit methods, although based on time-dependent formulations, are only used to determine the steady state solution of the dynamic equations. In these circumstances the time steps are merely used as relaxation steps in an iterative search of the steady state solution. However, in many problems transient accuracy is also of importance. For example, in problems of turbulent reactive flows, quantities like the turbulent kinetic energy, the dissipation, and the species mass fractions must remain positive at all times. Now if in the course of the calculation

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spurious ripples are allowed to develop then in many cases the computation rapidly diverges.

In the present paper we wish to contribute to the analysis of these two aspects. For simplicity we consider as a test problem the Burgers equation under various initial conditions and we center the analysis on the linearized block implicit (LBI) method of McDonald and Briley [5, 6]. We also restrict the study to cases where the boundary conditions have no influence. This is achieved by considering the semi-infinite half-space $0 \leqslant t < \infty$, $-\infty < x < +\infty$ and stopping the calculation when the solution reaches the boundaries of the computational domain.

Our scope is to examine the conditions under which schemes of the LBI type provide stable, ripple-free, and accurate solutions. We shall demonstrate that an examination of the solution after the first time step provides interesting clues to the possible non-linear growth of spurious oscillations. In the present case this method may be used to enhance the stability and precision of the time-dependent calculation.

Section 2 describes the test problem and the LBI type difference schemes under examination. The results of linear stability analysis are presented in Section 3. A non-linear analysis of the growth of spurious oscillations is carried out in Section 4 by first considering shock-free solutions of the Burgers equation. Section 5 concerns solutions with shocks. A non-linear criterion for transient accuracy is put forward for such cases.

2. Formulation of the Test Problem and Finite Difference Schemes

We use as a test problem the Burgers equation

$$\frac{\partial u}{\partial t} + L(u) = 0, \tag{1}$$

where

$$L(u) = \frac{\partial}{\partial x}\left(\frac{u^2}{2}\right) - \nu \frac{\partial^2 u}{\partial x^2}$$

in the infinite domain $-\infty < x < +\infty$, $t \geqslant 0$.

The Burgers equation constitutes a good model for the evolution of non-linear waves in a dissipative medium and it has many features in common with the Navier–Stokes equations. (See Karpman [11] for a complete analysis of Burgers equation properties.) The term $\nu \partial^2 u/\partial x^2$ is associated with the viscous dissipation effect and will be neglected here because we are essentially interested in the non-linear phenomena associated with $u \partial u/\partial x$.

As initial conditions we consider the following cases (Fig. 1):

(a) $u(x, 0) = 0$ for $x < 0$; $u(x, 0) = u_0$ for $x \geqslant 0$;

(b) $u(x, 0) = u_0$ for $x < 0$; $u(x, 0) = 0$ for $x \geqslant 0$.

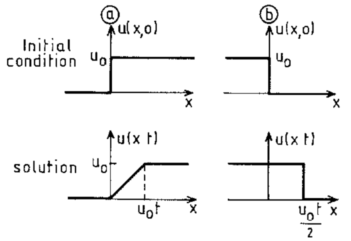

FIG. 1. Initial conditions and analytical solutions for the Burgers equation: (a) Expansion fan, (b) shock.

The solutions corresponding to these initial conditions are shown in Fig. 1. Condition (a) generates an expansion fan: $u(x, t) = 0$ for $x < 0$, $u(x, t) = x/t$ for $0 \leqslant x \leqslant u_0 t$, $u(x, t) = u_0$ for $x > u_0 t$.

Condition (b) produces a shock propagating at speed $u_0/2$: $u(x, t) = u_0$ for $x < u_0 t/2$, $u(x, t) = 0$ for $x \geqslant u_0 t/2$.

In the previous set of initial conditions, u_0 is a characteristic value of the field u. It is then convenient to define the dimensionless field $U = u/u_0$ and work with the modified equation

$$\frac{\partial U}{\partial t} + u_0 \cdot L(U) = 0, \qquad \text{where } L(U) = U \cdot \frac{\partial U}{\partial x}. \tag{2}$$

Finite Difference Methods

We restrict the present study to the linearized block implicit scheme of Briley and McDonald [5, 6].

In accord with these references, Eq. (2) is first replaced by a discrete form with respect to time

$$\frac{U^{n+1} - U^n}{\Delta t} = -\beta u_0 L(U^{n+1}) - (1-\beta)\, u_0 L(U^n), \tag{3}$$

where β is a constant parameter $(0 \leqslant \beta \leqslant 1)$. Then the nonlinear term $L(U^{n+1})$ is expanded in Taylor series around U^n. For this we let

$$L(U) = UU_x = M(U, U_x).$$

Then

$$L(U^{n+1}) \simeq L(U^n) + \left(\frac{\partial M}{\partial U}\right)^n \cdot (U^{n+1} - U^n) + \left(\frac{\partial M}{\partial U_x}\right)^n \cdot (U_x^{n+1} - U_x^n).$$

Here $\partial M/\partial U = U_x$ and $\partial M/\partial U_x = U$ and the previous expansion becomes

$$L(U^{n+1}) \simeq L(U^n) + (U_x)^n (U^{n+1} - U^n) + U^n (U_x^{n+1} - U_x^n). \tag{4}$$

We now introduce the difference between the solutions at time steps $n+1$ and n, $\psi^{n+1} = U^{n+1} - U^n$. With this definition expression (4) becomes

$$L(U^{n+1}) \simeq L(U^n) + \frac{\partial}{\partial x}(U^n \psi^{n+1}).$$

Substituting this approximation in Eq. (3) yields the "delta" form

$$[1 + \beta u_0 \Delta t\, G(U^n)]\, \psi^{n+1} = -u_0 \Delta t\, L(U^n), \tag{5}$$

where

$$G(U^n) = U^n \frac{\partial}{\partial x} + \frac{\partial U^n}{\partial x}$$

and

$$\psi^{n+1} = U^{n+1} - U^n. \tag{6}$$

To discretize the spatial operator $\partial/\partial x$ appearing in L and G we use a linear combination of the classical forward and backward operators. Thus

$$\left(\frac{\partial F}{\partial x}\right)_i = \frac{1}{\Delta x}\,[\alpha D_+ + (1-\alpha)\, D_-]\, F_i + \left(\alpha - \frac{1}{2}\right) O(\Delta x) + O(\Delta x^2), \tag{7}$$

where $D_+ F_i = F_{i+1} - F_i$ and $D_- F_i = F_i - F_{i-1}$.

The values $\alpha = 0$, $1/2$, and 1 correspond respectively to backward, centered, and forward differencing.

Substitution of Eq. (7) in the delta form (5) yields a tridiagonal system of equations

$$-a_i \psi_{i-1}^{n+1} + b_i \psi_i^{n+1} - c_i \psi_{i+1}^{n+1} = d_i, \tag{8}$$

where

$$a_i = \beta\lambda(1-\alpha)\, U_{i-1}^n$$

$$b_i = 1 + \beta\lambda(1-2\alpha)\, U_i^n$$

$$c_i = -\beta\lambda\alpha U_{i+1}^n$$

$$d_i = -\frac{\lambda}{2}\,\{\alpha[(U_{i+1}^n)^2 - (U_i^n)^2] + (1-\alpha)[(U_i^n)^2 - (U_{i-1}^n)^2]\}$$

and

$$\lambda = u_0 \Delta t / \Delta x.$$

3. Linear Stability Analysis

To obtain the linear stability conditions we apply the Von Neumann method to the difference scheme defined by expression (8). In this method the non-linear operators are linearized and the solution is assumed to be spatially periodic and of the form

$$U_i^n = V^n \exp(j(ik\Delta x)) \qquad \text{for } i = 0, ..., N+1, \tag{9}$$

where $j^2 = -1$.

The amplification factor defined by $\xi^n = V^{n+1}/V^n$ is determined by inserting expression (9) in the linearized difference scheme (8).

Linear stability is assured if $\|\xi^n\| \leqslant 1$. Straightforward calculations yield

$$\|\xi^n\|^2 = \frac{[1 + (\beta - 1)\,\lambda(1 - \cos\theta)(1 - 2\alpha)]^2 + [\lambda(\beta - 1)\sin\theta]^2}{[1 + \beta\lambda(1 - \cos\theta)(1 - 2\alpha)]^2 + [\lambda\beta\sin\theta]^2}, \tag{10}$$

where $\theta = k\Delta x$. It is then possible to show that stability is obtained if the parameters α, β, and λ satisfy the sets of inequalities

$$\beta < \tfrac{1}{2}, \qquad \alpha < \tfrac{1}{2}, \qquad \lambda \leqslant (1 - 2\alpha)/(1 - 2\beta) \tag{11}$$

or

$$\beta \geqslant \tfrac{1}{2} \qquad \text{and} \qquad \alpha \leqslant \tfrac{1}{2}.$$

4. Augmented Stability of Shock-Free Solutions

It is well known that the standard linear stability analysis only provides necessary conditions for the stability of a finite difference approximation of a non-linear equation. Linear analysis alone does not yield clues to the possible growth and development of oscillations in the numerical solution. Such oscillations may give rise to important difficulties in many circumstances. It is therefore interesting to augment the stability criterion with additional conditions ensuring that oscillations do not arise. These conditions may be obtained in various ways. A simple method consists of examining the numerical solution after a single time step. Clearly, this strategy of suppressing oscillations after a single step does not provide a sufficient condition for stability or accuracy. A necessary condition is obtained which may only be used in combination with the classical linear stability results to improve the stability and precision of the calculation. The main difference between the classical linear analysis and the present approach is that the former isolates a single Fourier mode and considers its growth or decay while the latter is concerned with the complete solution, as it evolves after one time step. It is then possible to determine the conditions under which this solution remains free of ripples or

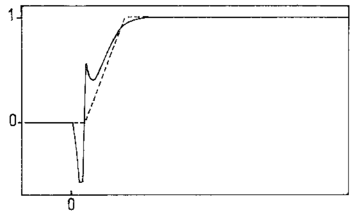

FIG. 2. Expansion fan. Numerical solution after six time steps. $\alpha = 0.5$, $\beta = 0.5$, CFL = 2, $\Delta t = 0.04$ s, $t = 0.24$ s.

overshoot (and undershoot) values, and in this sense the criterion obtained is non-linear. Now, if the initial conditions have a simple form it is most convenient to determine the solution after the first time step. To illustrate this approach let us consider the initial condition (a) corresponding to an expanding fan. At $t = 0$, the discrete values of U^0 are $U_i^0 = 0$ for $i = 0,..., M - 1$ and $U_i^0 = 1$ for $i = M,..., N + 1$.

It is then a simple matter (see Appendix A) to directly calculate the solution U_i^1 after the first time step. This solution remains bounded by 0 and 1 and thus does not undershoot or overshoot only if the following two conditions are satisfied:

$$\alpha = 0$$
$$\lambda \leqslant 2/(1 - 2\beta) \qquad \text{for } 0 \leqslant \beta \leqslant \tfrac{1}{2}. \tag{12}$$

A smooth solution is obtained if the spatial differencing is upwind and if the CFL number λ is less than $2/(1 - 2\beta)$ for $0 \leqslant \beta \leqslant \frac{1}{2}$. This basic result is illustrated in Figs. 2, 4, and 5. The numerical solution obtained after 6 time steps with $\alpha = 0.5$ (central differencing in space) is displayed in Fig. 2. A strong oscillation develops around the origin of the expansion fan leading to divergence of the calculations after 10 time steps. No choice of β or CFL number λ is able to stabilize the calculations if α differs from zero (i.e., if the spatial differencing is not fully upwind). For $\alpha \neq 0$ the negative value generated at the left of the expansion fan goes to $-\infty$ after a few time steps. As we shall see later this situation does not prevail when the initial conditions produce a moving shock. In that case a stable undershoot may be obtained.

Now let us set $\alpha = 0$ (upwind differencing) and analyse the behavior of the

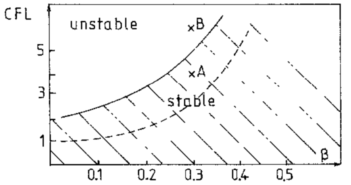

FIG. 3. Stability regions in the case of an expansion fan. $\alpha = 0$. Shaded area, observed stability region; solid line, result of non-linear analysis (Eq. (12)); dotted line, result of linear theory (Eq. (11)).

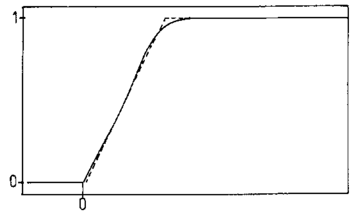

FIG. 4. Expansion fan. Numerical solution at $t = 0.48$ s, $\alpha = 0$, $\beta = 0.3$, CFL = 4, $\Delta t = 0.08$ s. Condition (12) is satisfied.

numerical scheme as a function of the CFL number λ and parameter β. The stability limit obtained from the linear analysis of Section 3 and the criterion (11) are plotted in Fig. 3. The numerical scheme is unconditionaly stable for $\beta \geq \frac{1}{2}$. It is linearly stable for $\beta = 0$ (explicit scheme) if the CFL number λ does not exceed 1. Now if $0 < \beta < \frac{1}{2}$, the calculations remain stable for CFL numbers λ bounded by $2/(1-2\beta)$ as predicted by criterion (12). This limit exceeds that obtained from the linear stability analysis. This interesting aspect is illustrated in Figs. 4 and 5, which respectively correspond to couples of parameters ($\beta = 0.3$, $\lambda = 4$) and ($\beta = 0.3$, $\lambda = 6$), points A and B of Fig. 3. As expected the calculation is stable for the first set of parameters and unstable for the second.

When stability is assured it is still possible to obtain further limitations of the CFL number by considering the precision of the numerical scheme. At time $t = n\Delta t$, a measure of the numerical error is provided by

$$E^n = \|U^n - U\| = \frac{1}{N} \sum_{I=1}^{N} \left| U_I^n - U\left(\left(I - M + \frac{1}{2}\right) \Delta x, n\Delta t\right) \right|, \tag{13}$$

where U^n is the calculated solution and U the exact solution. This error is plotted in Fig. 6 with respect to β for a given time t and different values of the CFL number λ. It is interesting to note that schemes using $\beta = 0.3$ are the most precise. However, this choice of β implies a CFL limitation of 5. Clearly the large CFL numbers used in many time-marching calculations of steady state flows do not assure transient accuracy. McDonald and Briley [5] indicate that CFL numbers of the order of 10^3

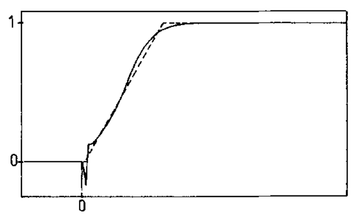

FIG. 5. Expansion fan. Numerical solution at $t = 0.48$ s, $\alpha = 0$, $\beta = 0.3$, CFL = 6, $\Delta t = 0.12$ s. Condition (12) is not satisfied.

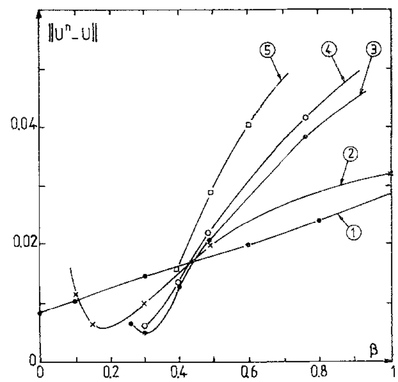

FIG. 6. Expansion fan. Effect of the CFL number on transient accuracy. $\alpha=0$, $t=0.48$ s, U^n = numerical solution, U = exact solution. 1: CFL = 1; 2: CFL = 2; 3: CFL = 4; 4: CFL = 5; 5: CFL = 10.

may be used to obtain the steady state solution of the gas dynamic equations but they note that transient accuracy is not achieved when λ exceeds 2.2 for $\beta=1$, $\alpha=\frac{1}{2}$.

In the case of Burgers equation $\alpha=0$, $\beta=0.3$, $\lambda=4$ appears to be a good choice for the determination of shock-free solutions.

5. Augmented Stability of Solutions Containing Shocks

The results of the linear stability analysis of Section 3 may be used in the present case. However, it is well known that non-linear instabilities may develop even if the linear stability criteria are satisfied (see, for example, Yee *et al.* [1]). As a consequence it is important to obtain additional information on the possible growth of oscillations. This may be achieved by examining the discrete solution obtained after the first time step. This calculation, performed in Appendix B, indicates that the solution remains bounded by 0 and 1 if

$$\alpha=0 \qquad \text{and} \qquad \lambda \leqslant 2. \tag{14}$$

The condition $\lambda \leqslant 2$ is equivalent to the Von Neumann–Richtmeyer condition $u_s \Delta t/\Delta x \leqslant 1$, where u_s is the shock propagation speed which here is $u_s = u_0/2$ [8].

The linear stability limit and the non-linear condition (14) are plotted in Fig. 7. Clearly, condition (14) sets a strong limitation on the CFL number λ.

The previous discussion is well illustrated by the following numerical calculations. We first consider a case where $\alpha=0.5$. In this circumstance the solution is expected to oscillate and this is indeed observed (see Figs. 8 and 9). The oscillations remains bounded if the CFL number is below the linear stability limit (Eqs. (10) and (11)). This behavior is illustrated in Fig. 8 with a typical result of

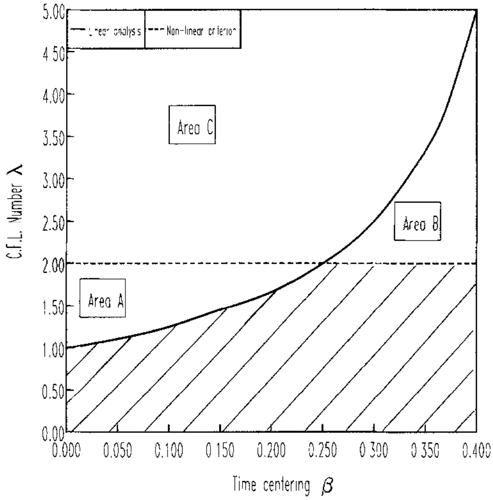

FIG. 7. Stability regions for shock calculations. Shaded area, observed stability region; solid line, result of linear theory (Eq. (11)); dotted line, result of non-linear analysis (Eq. (14)).

calculation corresponding to centered difference ($\alpha = 0.5$), a CFL number $\lambda = 2$, and a parameter $\beta = 0.8$. Otherwise the oscillation grows without bound as exemplified in Fig. 9 ($\alpha = 0.5$, CFL $= 2$, $\beta = 0.3$) with a result obtained a few time steps before complete divergence of the calculation.

These results provide some insight on the coupling between linear and non-linear instability modes. For a CFL number satisfying the linear stability limit an oscillation is generated by a non-zero value of the spatial differencing parameter α. The amplitude of this oscillation first grows and then reaches a bounded value typical of certain non-linear oscillations. Now, if the linear stability condition is not satisfied, the oscillation is constantly amplified and cannot reach a bounded amplitude. This may explain why schemes using centered space differencing ($\alpha = 0.5$) can be stabilized with small artificial viscosity terms. For such schemes and sufficiently small CFL numbers only finite amplitude non-linear oscillations are generated and these may be diminished or dissipated with artificial viscosity.

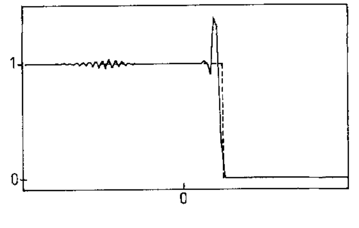

FIG. 8. Evolution of oscillations in shock calculations. Stable overshooting. (Condition (11) is satisfied.) $\alpha = 0.5$, $\beta = 0.8$, CFL $= 2$, $\Delta t = 0.04$ s, $t = 0.48$ s.

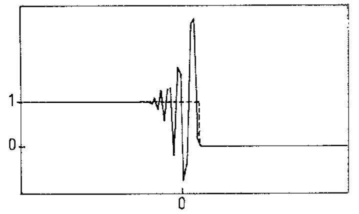

FIG. 9. Evolution of oscillations in shock calculations. Unstable overshooting. (Condition (11) is not satisfied.) $\alpha = 0.5$, $\beta = 0.3$, CFL = 2, $\Delta t = 0.04$ s, $t = 0.2$ s.

When $\alpha = 0$, corresponding to upwind differencing, linear stability is assured for values of the CFL number satisfying (11) with $\alpha = 0$;

$$\lambda \leqslant 1/(1-2\beta), \tag{15}$$

and the solution remains bounded by 0 and 1 if in addition $\lambda \leqslant 2$. For values of β and λ taken in the shaded area of Fig. 7, the solution is stable and smooth. This area corresponds to the inequalities (15) and (14), respectively. The linear stability region is restricted here by the non-linear criterion. If conditions (14) and (15) are both satisfied, i.e., if β and λ belong to the shaded area, the stability of the finite difference scheme is assured for weak solutions. In region A, where condition (15) is not satisfied, and in region B, where condition (14) is not satisfied, the finite difference schemes are unstable. This result differs from that obtained in the case of the expansion fan (Section 4). There we found that implicit schemes enhance the linear and non-linear stability of the calculation. For a shock however the non-linear criterion (14) sets a limit to the gain, which may be obtained by increasing the value of β. For β larger than 0.25 the CFL number must be kept less than or equal to 2 (Fig. 7).

Figures 10 and 11 illustrate the previous discussion. The values of β and λ belong to the shaded area displayed in Fig. 7. The shock width is a function of β and λ. High values of β produce wide transitions layers. Sharp shocks are obtained for a CFL number of 2. The width of the shock increases as the CFL number λ is decreased below 2.

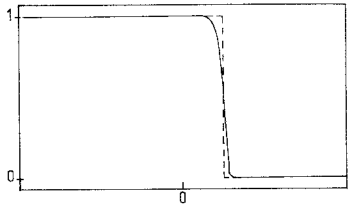

FIG. 10. Influence of CFL number on shock width. $\alpha = 0$, $\beta = 1$, $t = 0.52$ s, $\Delta t = 0.03$ s, CFL = 1.5.

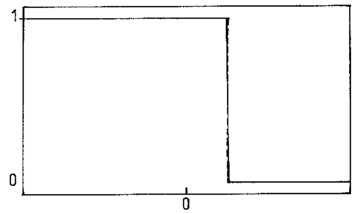

FIG. 11. Influence of CFL number on shock width. $\alpha = 0$, $\beta = 1$, $t = 0.52$ s, $\Delta t = 0.04$ s, CFL = 2.

Starting from Eq. (B10) of Appendix B it is easy to verify that the case $\lambda = 2$ corresponds to a translation of the shock discontinuity without modification. The shock is followed in a "quasi-Langrangian" way from one node to the next for each time step. The shock speed is in this case $u_s = u_0/2$ and the transition layer is then reduced to a single cell. This situation is exceptional and cannot be expected to occur in more complicated calculations. A significant result of this analysis is that the growth of ripples in calculations involving shocks is strongly dependent on the spatial differencing and CFL number. Similar conclusions are obtained from numerical simulations of inviscid nozzle flows.

CONCLUSION

The present analysis has been concerned with the Burgers equation and its solution with linearized block implicit-type schemes. The following results have been obtained:

(1) If no artificial viscosity is introduced in the finite difference scheme then any spatial differencing except upwind differencing ($\alpha = 0$) induces spurious oscillations in the neighborhood of discontinuities. Whether these oscillations grow in time depends on the existence of shocks and on the CFL number. A stable ripple may arise in shock calculations if the CFL number is less than a certain limit function of the time centering parameter β (Eqs. (10) and (11)) and always less than 2. In the case of shock-free solutions the oscillations always grow without bound if the differencing scheme is not upwind (i.e., if $\alpha \neq 0$). Therefore schemes corresponding to $\alpha \neq 0$ (for example, the centered scheme $\alpha = 0.5$ of McDonald and Briley) must be stabilized by explicit artificial viscosity [8, 9].

(2) Upwind differencing schemes do not require explicit artificial viscosity. The maximum CFL number is 2 for shock calculations and a function of β for continuous solutions (Eq. (12)). Unconditional stability and the absence of spurious ripples are obtained for $\beta \geqslant \frac{1}{2}$. However, the best transient accuracy is found for $\beta = 0.3$ and CFL = 4.

(3) It is well known that upwind differencing schemes have a good behavior in computations involving discontinuities [2, 7, 10]. This study shows that they have

the *best* behavior among first-order or centered (second-order) differencing schemes. Furthermore they provide the greatest precision and allow the use of the highest CFL numbers if they are used in an implicit code with an adequate time centering.

It must be noticed that results concerning the Burgers equation are not directly applicable to more complicated systems like the Navier–Stokes equations. However, these equations have some common features and the Burgers equation constitutes a pertinent model problem. The calculations performed in this paper indicate that the simple non-linear criterion obtained by examining the solution after a single time step may be used to augment the stability of the scheme. In fact the solution obtained after one time step contains indications of the behavior of the solution for later times. No rigorous demonstration of this property may be given at present. However, as suggested by a reviewer it might be possible to study the non-linear interaction of elementary perturbations and actually link the analysis performed in this paper to the usual linear Fourier analysis which assumes that no interactions take place. This approach may rely, for example, on the recent contributions of Briggs *et al.* [13] and Hunter and Keller [14].

Appendix A

We consider as initial conditions those corresponding to an expansion fan and write system (8) after the first time step

$$\psi_i^1 = 0 \qquad \text{for } 0 \leqslant i \leqslant M-2 \tag{A2}$$

$$\psi_{M-1}^1 + \beta\lambda\alpha\psi_M^1 = -\lambda\alpha/2 \tag{A2}$$

$$[1 + \beta\lambda(1-2\alpha)]\,\psi_M^1 + \beta\lambda\alpha\psi_{M+1}^1 = -\lambda(1-\alpha)/2 \tag{A3}$$

$$-\beta\lambda(1-\alpha)\,\psi_{i-1}^1 + [1 + \beta\lambda(1-2\alpha)]\,\psi_i^1 + \beta\lambda\alpha\psi_{i+1}^1 = 0 \qquad \text{for } M+1 \leqslant i \leqslant N \tag{A4}$$

$$\psi_{N+1}^1 = 0. \tag{A5}$$

In these equations ψ_i^1 represents the increment in the difference solution after the first time step: $\psi_i^1 = U_i^1 - U_i^0$. To solve the previous set of equations we use the associated sequence ϕ_i defined by

$$-a\,\phi_{i-1} + b\,\phi_i + c\,\phi_{i+1} = 0 \tag{A6}$$

for $i = M-1$ to N

$$\phi_{N+1} = 0, \tag{A7}$$

where $a = \beta\lambda(1-\alpha)$, $b = 1 + \beta\lambda(1-2\alpha)$, and $c = \beta\lambda\alpha$. Equations (A6), (A7) are formally equivalent to (A4), (A5). Now, the sequence ϕ_i is completely determined by

Eq. (A6) and two additional conditions. One condition is given by (A7) while the second may consist of

$$\phi_M = \psi^1_M. \tag{A8}$$

As a consequence

$$\phi_i = \psi^1_i \qquad \text{for } i = M \text{ to } N+1.$$

Then, ϕ_{M-1} may be determined from Eq. (A6) written for $i = M$.

$$\begin{aligned}\phi_{M-1} &= (b\,\phi_M + c\,\phi_{M+1})/a \\ &= (b\,\psi^1_M + c\,\psi^1_{M+1})/a\end{aligned}$$

and Eq. (A3) then yields

$$\phi_{M-1} = \frac{-\lambda(1-\alpha)/2}{\beta\lambda(1-\alpha)} = -\frac{1}{2\beta}. \tag{A9}$$

Now each term of the sequence may be written in the form

$$\phi_i = k_1 r^i_1 + k_2 r^i_2, \tag{A10}$$

where r_1, r_2 are the roots of the characteristic equation

$$c\,r^2 + b \;\; - a = 0.$$

The product of the two roots

$$r_1 r_2 = -a/c = -(1-\alpha)/\alpha$$

is negative while the sum of the two roots

$$r_1 + r_2 = -(1 + \beta\lambda(1-2\alpha))/\beta\lambda\alpha$$

is also negative. In fact, $r_1 + r_2$ might be positive for large values of the CFL number λ ($\lambda > 1/(\beta(2\alpha - 1))$) when $\alpha > 1/2$: as we expect stability to be achieved for all CFL numbers between $\lambda = 0$ and a certain limit, we keep the sign of $r_1 + r_2$ corresponding to the lower CFL number, i.e., $r_1 + r_2 < 0$. As a consequence, if r_1 designates the negative root of the characteristic equation then $r_1 < 0 < r_2$ and $|r_1| > |r_2|$.

The constants k_1 and k_2 may now be determined by imposing the conditions (A7) and (A9) on the general solution (A10). This yields

$$\phi_i = -\frac{1}{2\beta}\,\frac{r_2^{N+1}\,r_1^i - r_1^{N+1}\,r_2^i}{r_2^{N+1}\,r_1^{M-1} - r_1^{N+1}\,r_2^{M-1}} \qquad \text{for } M-1 \leqslant i \leqslant N+1. \tag{A11}$$

It is now possible to determine ψ^1_{M-1} and ψ^1_M by making use of Eqs. (A2), (A8), and (A11):

$$\psi^1_{M-1} = -\frac{\lambda\alpha}{2}\left[1 - r_1 \cdot \frac{1-(r_1/r_2)^{N+1-M}}{1-(r_1/r_2)^{N+2-M}}\right] \tag{A12}$$

$$\psi^1_M = -\frac{1}{2\beta} \cdot r_1 \cdot \frac{1-(r_1/r_2)^{N+1-M}}{1-(r_1/r_2)^{N+2-M}}. \tag{A13}$$

It is then a simple matter to verify that ψ^1_M is negative and that ψ^1_{M-1} and α have opposite signs. The only way to avoid such negative values (corresponding to a negative solution U^1) consists of choosing $\alpha = 0$.

In that particular case $\psi^1_{M-1} = 0$ and $\psi^1_M = -\lambda/2(1+\beta\lambda)$. Since $U^1_M = \psi^1_M + U^0_M = \psi^1_M + 1$ must be positive, the maximum CFL number is given by

$$\lambda \leqslant 2/(1-2\beta).$$

Appendix B

We now consider as initial conditions those corresponding to a propagating shock and write system (8) after the first time step:

$$\psi^1_0 = 0 \tag{B1}$$

$$-\beta\lambda(1-\alpha)\,\psi^1_{i-1} + (1+\beta\lambda(1-2\alpha)))\,\psi^1_i + \beta\lambda\alpha\psi^1_{i+1} = 0 \qquad \text{for} \quad 1 \leqslant i \leqslant M-2 \tag{B2}$$

$$-\beta\lambda(1-\alpha)\,\psi^1_{M-2} + (1+\beta\lambda(1-2\alpha))\,\psi^1_{M-1} = \lambda\alpha/2 \tag{B3}$$

$$-\beta\lambda(1-\alpha)\,\psi^1_{M-1} + \psi^1_M = \lambda(1-\alpha)/2 \tag{B4}$$

$$\psi^1_i = 0 \qquad \text{for } M+1 < i < N+1. \tag{B5}$$

We again consider an associated sequence ϕ_i defined by

$$-a\,\phi_{i-1} + b\,\phi_i + c\,\phi_{i+1} = 0 \qquad \text{for } 1 \leqslant i \leqslant M-1 \tag{B6}$$

$$\phi_0 = 0 \tag{B7}$$

$$\phi_{M-1} = \psi^1_{M-1} \tag{B8}$$

Clearly the two sequences ψ^1_i and ϕ_i coincide for $0 \leqslant i \leqslant M-1$. Now ϕ_M may be determined by writing Eq. (B6) for $i = M-1$ and making use of Eq. (B3). This leads to

$$\phi_M = -1/2\beta. \tag{B9}$$

The general solution of Eq. (B6) satisfying the conditions (B7) and (B9) is then easily cast in the form

$$\phi_i = -\frac{1}{2\beta} \frac{r_1^i - r_2^i}{r_1^M - r_2^M},$$

where r_1, r_2 are the roots of the characateristic equation $c\,r^2 + b\,r - a = 0$. These two roots have opposite signs and if r_1 designates the negative root $r_1 < 0$ then $|r_1| > |r_2|$. In these circumstances ϕ_i is an alternating sequence and this is also the case for ψ_i^1, $1 \leqslant i \leqslant M-2$. An oscillation is generated behind the shock. This oscillation only vanishes when $\alpha = 0$. In this case, corresponding to upwind differencing, Eqs. (B2) and (B3) give

$$\psi_i^1 = 0 \qquad \text{for } 1 \leqslant i \leqslant M-1$$

while ψ_M^1 obtained from (B4) becomes

$$\psi_M^1 = \lambda/2. \tag{B10}$$

To avoid an overshoot at the shock, $\psi_M^1 \leqslant 1$ and as a consequence the CFL number λ should be bounded by 2.

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