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Note

The Role of Diagonal Dominance and Cell Reynolds Number in Implicit Difference Methods for Fluid Mechanics Problems

The success of implicit methods for certain classes of problems, notably boundary layer flows where marching steps hundreds of times the explicit stability step size limit are used [1], leads to the question of their use for more general flows, i.e., Navier-Stokes solutions. The purpose of this paper is to identify some of the difficulties associated with implicit solution methods for the Navier-Stokes equations.

Analysis of Burgers' Equation

A simple equation which has both hyperbolic and parabolic properties is Burgers' equation

$$u_\xi + a u_\eta = \nu u_{\eta\eta}, \tag{1}$$

where a can be a function of u, ξ, η. The two-dimensional boundary layer equations integrated into the inviscid region is another example. Equation (1) can be differenced implicitly using forward time, central space differences

$$\frac{u_j^{n+1} - u_j^{n}}{\Delta\xi} + a\left(\frac{u_{j+1}^{n+1} - u_{j-1}^{n+1}}{2\Delta\eta}\right) = \nu\left(\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{\Delta\eta^2}\right). \tag{2}$$

Performing the usual linear von Neumann stability analysis on Eq. (2), with

$$u_j^{n} = U_0(n)\, e^{i\kappa j \Delta\eta},$$

gives, for the amplification factor, G,

$$|G|^2 = \left|\frac{U_0(n+1)}{U_0(n)}\right|^2 = \frac{1}{(1+\omega)^2 + \beta^2}, \tag{3}$$

where

$$\omega = \frac{2\nu\,\Delta\xi}{\Delta\eta^2}(1 - \cos\phi), \qquad \beta = \frac{a\,\Delta\xi}{\Delta\eta}\sin\phi, \qquad \phi = \kappa\,\Delta\eta.$$

Now, examining the condition for diagonal dominance of the matrix which arises from the differencing (2), i.e.,

$$(-C/2 - D)\, u_{j-1}^{n+1} + (1 + 2D)\, u_j^{n+1} + (C/2 - D)\, u_{j+1}^{n+1} = u_j^{\,n} \tag{4}$$

gives

$$| 1 + 2D | \geqslant | C/2 + D | + | C/2 - D |$$

where

$$C = \frac{a\, \Delta\xi}{\Delta\eta}, \qquad D = \frac{\nu\, \Delta\xi}{\Delta\eta^2}.$$

Solving this gives

$$1 + 2D \geqslant | C |, \tag{5a}$$

when

$$| C |/2D > 1. \tag{5b}$$

When $| C |/2D \leqslant 1$, the matrix is always diagonally dominant. This quantity which governs the diagonal dominance condition is

$$\frac{| C |}{2D} = \frac{1}{2} \frac{| a |\, \Delta\eta}{\nu} = \frac{1}{2} R_c, \tag{6}$$

where R_c is the cell Reynolds number. Rewriting operations (5a) and (5b) gives

$$| C | \leqslant \frac{1}{1 - 2/R_c}, \qquad R_c > 2, \tag{7}$$

to maintain diagonal dominance.

Hence, if one is concerned with diagonal dominance, keeping $R_c \leqslant 2$ assures the condition independent of the size of the marching step. For values of $R_c > 2$, Eq. (7) gives the marching step size, $\Delta\xi$, which must be used to assure diagonal dominance. As R_c increases, Eq. (7) indicates that the inviscid limit, $C \leqslant 1$, is approached, and thus the usefulness of implicit methods is progressively weakened.

When confronted with a Navier–Stokes solution in which large inviscid regions appear, one might be tempted to think of this extreme Reynolds number case, i.e., $C \leqslant 1$, as imposing a stability limitation on the marching step. This argument has two flaws. First, when an equation of the type (1) is differenced, even in an inviscid region, the terms involving ν are still present. In inviscid regions ν does not go to zero, but rather the cumulative effect of the entire diffusive term; the second derivative itself becomes negligible. Equation (2) is still the result of differencing a "viscous" equation in an inviscid region. Thus, Eq. (7) governs the diagonal dominance of the matrix, not the $C \leqslant 1$ limit obtained when $\nu = 0$.

Even in cases when $\nu = 0$ could be considered the correct physical description of the process being studied, condition (7) does not imply the differencing (2) is unstable, since it was not derived from any stability analysis. The stability of Eq. (2) is implied in the result of Eq. (3). If ν, hence ω, is zero, the amplification factor is still less than or equal to one; thus the difference equation (2) is always stable. Relation (7) simply indicates that the sufficient condition for convergence of the matrix inversion is guaranteed by $|C| \leqslant 1$. Violation of this sufficient condition implies the possibility of round-off error destroying the inversion. However, being only a sufficient condition, violation does not mean the Thomas algorithm will not work, only that it might not. If assurance of inversion is sought, possibly a partial pivoting technique could be employed. The main point that should be noted is that condition (7) does not arise from a stability analysis, and is not a restriction on the implicit differencing method. Only a different matrix inversion might be necessary when Eq. (7) is violated.

In addition to the possibility of round-off error accumulation if the cell Reynolds number is greater than two, the use of central differences for the convection term affects the resolution of the results. This is manifested by the "wiggles" in the solution as described by Roache [2]. These wiggles are not round-off error but are the exact algebraic solution of the equations.

Numerical Experiments with Burgers' Equation

The step size behavior (effects of the Courant number, C), cell Reynolds number behavior, and their effects on the diagonal dominance of the solution matrix were tested on the numerical solution of Burgers' equation. For the numerical calculations, Burgers' equation was solved using a wave oriented coordinate system. The nonconservative form of the equation is

$$\frac{\partial u}{\partial \xi} + (u - U)\frac{\partial u}{\partial \eta} = \nu \frac{\partial^2 u}{\partial \eta^2}, \tag{8}$$

where U is the steady state wave speed. The boundary conditions were taken to be

$$u(\eta, t) = 1.0, \qquad \eta \to -\infty,$$
$$u(\eta, t) = 0, \qquad \eta \to \infty.$$

Using forward time, central space differences Eq. (8) becomes

$$\frac{u_j^{n+1} - u_j^n}{\Delta\xi} + (u_j^{n+1} - U)\left(\frac{u_{j+1}^{n+1} - u_{j-1}^{n+1}}{2\Delta\eta}\right) = \nu\left(\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{\Delta\eta^2}\right). \tag{9}$$

To effect a solution the nonlinear coefficient was iterated at each time step. The wave speed U was set equal to 1/2.

Different values of ν and $\Delta\xi$ were used for a fixed value of $\Delta\eta = 0.2$. Fifty-one grid points were used. A linear velocity distribution was used to start the solution. The Thomas algorithm was employed to solve the resultant set of simultaneous algebraic equations at each time step. The solution was assumed to have reached steady-state when the maximum change in u between time steps was less than 10^{-5}.

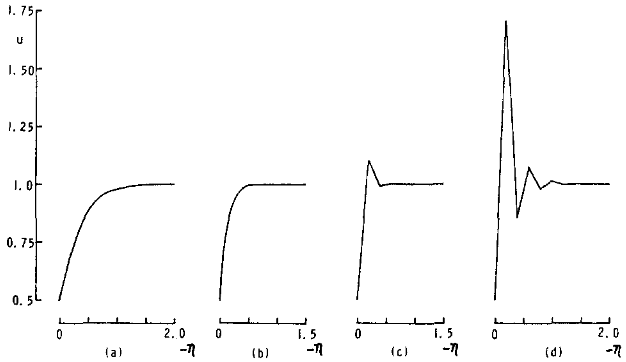

FIG. 1. Effect of cell Reynolds number on computed solutions to Burgers' equation. (a) $\nu = 1/8$, $R_c = 0.8$, (b) $\nu = 1/16$, $R_c = 1.6$, (c) $\nu = 1/24$, $R_c = 2.4$, (d) $\nu = 1/48$, $R_c = 4.8$.

For the cases where $\nu = 1/8$ and $\nu = 1/16$ (cell Reynolds numbers of 0.8 and 1.6, respectively), the solutions converged rapidly to steady state values for u (see Fig. 1) which compared well with the analytic solution [3]. Various values of C ($0.25 \leqslant C \leqslant 10^6$) were used with no deletrious effects on the solution; however, beyond $C = 500$ the number of steps needed to reach steady state was constant, e.g., for $\nu = 1/16$

Courant no.	Steps to steady state
0.25	206
0.5	113
1	65
5	25
10	20
50	16
100	16
500	15
⋮	⋮
10^6	15

For cases of lower viscosity, values of $\nu = 1/24$ and $\nu = 1/48$ were used, the maximum cell Reynolds number exceeded 2 ($R_{c_{\max}} = 2.4$ and 4.8, respectively) and diagonal dominance was lost. When solutions could be obtained they exhibited oscillations as shown in Fig. 1, which qualitatively reproduce the behavior shown by Roache [2]. It was possible to compare point by point the $\nu = 1/24$ solution to one obtained by simple forward time, centered space explicit differencing [2]. The results were identical to seven decimal places. Thus, the "wiggles" appear, independent of the method, due solely to the central differencing of convection. The converged solutions obtained all had values of $C \gg 1$.

An attempt was made to determine why no degradation of the solution occurred when the diagonal dominance condition was not satisfied. The implementation of the Thomas algorithm requires a back substitution for the unknown U_m from the formula [4] $U_m = \omega_m U_{m+1} + g_m$ where for no round-off error $|\omega_m| \leqslant 1$. Following Mitchell, a typical ω_m can be written as

$$\omega_m = \frac{\gamma_m}{\beta_m - \alpha_m \omega_{m-1}},$$

where the α, β, γ terms are the coefficients of the matrix equations

$$-\alpha_m U_{m-1} + \beta_m U_m - \gamma_m U_{m+1} = \delta_n .$$

Assuming all $\omega_m < 1$ until the present point m, we can examine

$$|\omega_m| = \left| \frac{\gamma_m}{\beta_m - \alpha_m} \right| \leqslant 1. \tag{10}$$

From the difference equation (4), substituting for the coefficients yields

$$\omega_m = \frac{(C/2 - D)}{[1 - (C/2 - D)]}. \tag{11}$$

The most severe case occurs when the denominator vanishes, i.e.

$$C/2 - D = C(1/2 - 1/R_c) = 1.$$

Thus when

$$C = 2R_c/(R_c - 2), \tag{12}$$

the error growth might be expected to be near maximum. Test cases were examined using the value of C from Eq. (12) for $\nu = 1/24$ and $\nu = 1/48$. For $\nu = 1/24$ convergence was obtained for $1.0 < C < 10^6$. For $\nu = 1/48$, the solution would not converge for a C given by Eq. (12), but as C was increased beyond 25, the solution again converged. This $\nu = 1/48$ behavior may be interpreted from Eq. (11).

As C grows, Eq. (11) can be expanded for large C as

$$\omega_m \simeq -1 - 2/C + \mathcal{O}(1/C^2).$$

When C is large, although $|\omega_m|$ is still greater than one, the error growth is so small that no accumulation occurs in the number of steps used for this particular matrix inversion.

The convergence of the $\nu = 1/24$ case can be explained by reexamining the matrix inversion technique. To get Eq. (10), all previous values of ω_m were assumed to have their maximum allowable value, i.e., $|\omega_m| = 1$. If, as occurs in the $\nu = 1/24$ calculation, the values are quite small, i.e., $|\omega_m| = \epsilon \ll 1$, then Eq. (10) becomes

$$|\omega_m| = \left| \frac{\gamma_m}{\beta_m - \alpha_m \epsilon} \right| \leqslant 1.$$

The analog of Eq. (11) is then

$$\omega_m = \frac{(C/2 - D)}{(1 + 2D)}$$

neglecting the ϵ term. This value of ω_m is always less than one for $\nu = 1/24$, and so no error growth occurs.

Another test was to artifically induce a small error on one of the boundaries to see if this induced error affected the solution. A boundary condition change from $u = 1.0$ to $u = 1.0 + 10^{-5}$ was investigated. For the cell Reynolds number less than 2, the solution converged rapidly to a steady state. When $\nu = 1/24$ ($R_c = 2.4$) was used, for a time step which previously gave the converged result of figure 1, no converged solution was obtained. Changing the values of C in this case did not alter the resulting nonconvergence.

Conclusions

The findings of this investigation show that the accuracy of the inversion of a tridiagonal matrix obtained from implicit differencing is governed by the cell Reynolds number. For $R_c \leqslant 2$, the matrix inversion is assured. For $R_c > 2$, diagonal dominance, which assures the matrix inversion, is lost and round-off error can degrade the solution.

As R_c increases, the diagonal dominance condition reduces the size of the effective marching step until, in the limit $R_c \gg 1$, the explicit stability limit, $C \leqslant 1$, is obtained as the condition for maintaining diagonal dominance of the implicit method. Solutions which are obtained for $R_c > 2$ may be inaccurate, although there is no a priori way to determine if this is so.

It should be noted that central differences were used throughout this discussion. Other techniques might produce different cell Reynolds number behavior, e.g., upwind differencing produces a matrix which is always diagonally dominant.

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