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A Reynolds Number Dependent Scheme for the
Solution of "Diabolic" Equations*

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ABSTRACT

A numerical procedure for solving "Diabolic Equations" (conservative equations containing positive source terms) is presented. The solution scheme is forward differenced in time and centrally differenced in space. Every term except the time derivative is expressed as a convex combination of the present and the advanced time step. The selection of the convex combination is determined by analyzing the magnitude of the coefficients of a linear one-dimensional model equation

$$\frac{\partial \phi}{\partial t} + U \frac{\partial \phi}{\partial x} = A \phi + D \frac{\partial^2 \phi}{\partial x^2}$$

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together with the spatial and temporal step sizes. Typical examples of numerical solutions to this equation are compared for different convex combinations. These results indicate that the judicious choice of the combination may avoid some of the difficulties encountered when using purely implicit or purely explicit schemes.

In the course of this study, a computer automated method of analysis is developed with particular application to reacting flows, mixed phase flows and some aspects of turbulence modeling.

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INTRODUCTION

This study was motivated by various attempts to the authors to solve numerically systems of equations which are coupled by source or sink terms or which contain source or sink terms occurring naturally. Examples of physical equations including source terms are the conservation equations governing multiphase flow in Nuclear Reactor pressure suppression systems. The source terms appear as coupling terms in the condensation and vaporization of the working fluid (steam/water) (for example, see Rivard and Torrey¹ or Hirt and Romero²).

A particular set of the turbulence model equations help to describe the motion of turbulent fluid flow in a time-dependent system and contain all of the elements of the general conservation equations: a time derivative, a convective derivative, a diffusive derivative, and often, a source term. The form of these equations is parabolic in the strict mathematical sense, however, there are natural flow regimes in which the convective derivative becomes large and the systems behave as if they were hyperbolic. In general, implicit solution schemes devised for parabolic equations do not work very well or are costly for hyperbolic equations. As a result, flow regimes where this problem occurs can cause a great deal of difficulty to the person trying to obtain a solution. The presence of a positive source term in the equations can further complicate matters and cause the solution to grow exponentially. When this is combined with numerical dispersion as described by Chin³, the solution scheme appears to be unstable.

Physical governing equations containing all of the terms described above are often solved explicitly and the magnitude of the time-step associated the criteria for stability is prohibitively small. Many of the flow conditions are such that a more rapid solution procedure (larger problem time-step) could be used. This occurs particularly in the boundary layer region close to the

wall where in this limit the Navier-Stokes equations commonly take on a parabolic form. This also occurs in other regions for solutions involving time decay of inertial derivatives so that the magnitude of diffusive effects becomes more influential than that of convective effects. Counter examples in which the equations become elliptic near a wall occur in separating flows or on boundaries with massive wall blowing or suction.

This paper is a discussion of the development of a solution scheme for flows in which the numerical stability is weakly dependent on the cell Reynolds number of the flow and strongly dependent on the magnitude of the source term. This development attempts to incorporate advantages of the reduced dependence on the time step associated with doing implicit or mixed implicit/explicit calculations. The mixed scheme in this sense refers to a combination of terms involving both the present and the advanced time step. A model equation is solved numerically as a test. The method is then applied to the turbulence model equations of Saffman⁴, as modified by Wilcox and Alber⁵ and Saffman and Wilcox⁶.

The Model Equations

The one-dimensional model equation is considered

$$\frac{\partial \phi}{\partial t} + \frac{\partial (U_1 \phi)}{\partial x_1} = S(\phi) + \frac{\partial}{\partial x_1} \left(\frac{D \partial \phi}{\partial x_1} \right) \quad (1)$$

where the source term $S(\phi)$ may be linear as in the case for turbulent production and dissipation

$$S(\phi) = A\phi \quad (2)$$

or exponential as in the energy equation for reacting flow

$$S(\phi) = \lambda e^{1/\phi} \quad (3)$$

In equation (1), the symbol D represents a diffusion coefficient while ϕ represents the particular dependent variable of interest.

Solution Procedure

For purposes of analysis, the one dimensional form of the model equation, Eq. (), is linearized by assuming U and D to be constant. The finite difference form of this equation is written as a convex combination of the explicit and implicit schemes as

$$\begin{aligned} \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + (1-F) U \delta \phi_i^{n+1} + F U \delta \phi_i^n &= (1-F) A \phi_i^{n+1} + D(1-F) \delta^2 \phi_i^{n+1} \\ &+ DF \delta^2 \phi_i^n + FA \phi_i^n, \end{aligned}$$

$$0 \leq F \leq 1, \quad (4)$$

where the difference operators δ and δ^2 are central difference operators, are defined in terms of ϕ as

$$\delta \phi = (\phi_{i+1} - \phi_{i-1}) / 2\Delta x \quad (5)$$

$$\delta^2 \phi = (\phi_{i+1} - 2\phi_i + \phi_{i-1}) / \Delta x^2 \quad (6)$$

In Eqn. (4), the superscript n refers to the time-step and the subscript, i refers to the spatial location with Δt and Δx defined as the time and spatial step sizes.

A functional form for the quantity F is sought so that a natural selection of an all implicit $F = 0$, all explicit $F = 1$, or a mixed scheme is made automatically. The determination of F is based on a numerical stability argument. It is clear that when an all explicit scheme is selected, stability restrictions on Δt make it prohibitively expensive to solve many problems. It is, therefore, desirable to use an implicit scheme wherever possible. However, for certain combinations of the cell Reynolds number, Δt and the source term coefficient A , the coefficient matrix of an all implicit solution scheme is nearly singular and gives rise to a numerical instability (and possibly problems of convergence). With this in mind, F must be selected as close to zero as possible and still avoid the region of numerical instability. Traditionally, solution schemes have been used with F as a fixed value that is set to 0 or 1 or to some intermediate value. In some calculations, different values of F have been selected within some problem for different spatial regimes. However, to our knowledge, no smooth automatic transition method exists for changing F from 0 to 1 during a calculation. This present work emphasizes a formalization and extension of these earlier ideas on mixed schemes with a goal of developing an automated procedure for the transition.

To determine the function F , it is convenient to define,

$$G = 1 - F \quad (7)$$

then expand (4) using (5) and (6) and rewrite (4) as

$$\begin{aligned}
 & G \left[\frac{U \Delta x}{2D} - 1 \right] \phi_{i+1}^{n+1} + \left[\frac{\Delta x^2}{D \Delta t} + G \left(2 - \frac{A \Delta x^2}{D} \right) \right] \phi_i^{n+1} \\
 & + G \left[-\frac{U \Delta x}{2D} - 1 \right] \phi_{i-1}^n = F \left[-\frac{U \Delta x}{D} + 1 \right] \phi_{i+1}^n \\
 & + \left[\frac{\Delta x^2}{D \Delta t} + F \left(\frac{A \Delta x^2}{D} - 2 \right) \right] \phi_i^n + F \left[\frac{U \Delta x}{D} + 1 \right] \phi_{i-1}^n
 \end{aligned} \tag{8}$$

The quantity $\frac{U \Delta x}{D}$ is the cell Reynolds number,

$$Re_{Cell} = \frac{U \Delta x}{D} \tag{9}$$

which Chin¹ suggests must be less than 2 to prevent numerical dispersion for the linear case and less than $\sqrt{3}$ for the non-linear case.

Eqn. (8) results in a matrix equation

$$B_{ij} \phi_j = d_i \quad i = 1, I; j = i-1, i, i+1 \tag{10}$$

except for the first and last rows. The coefficient matrix B_{ij} is banded and of the form

$$B_{ij} = \begin{bmatrix} b & a & 0 & \dots & 0 & \dots \\ c & b & a & \dots & 0 & \dots \\ 0 & c & b & a & \dots & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & b & a \end{bmatrix} \tag{11}$$

The eigenvalues of B_{ij} are given by

$$\lambda_i = b + 2\sqrt{ac} \cos \frac{i\pi}{I+1} ; i = 1, I \quad (12)$$

which for our particular coefficients are

$$\lambda_i = \frac{\Delta x^2}{\Delta t} + G \left[2 - \frac{A \Delta x^2}{D} + 2\sqrt{1 - \alpha^2} \cos \frac{i\pi}{I+1} \right], \quad i = 1, I \quad (13)$$

where $\alpha = \frac{Re}{2} \text{Cell}$.

Without loss of generality, we may multiply (13) by $\frac{D \Delta t}{\Delta x^2}$ and rewrite it as

$$\lambda_i = 1 + G \Delta t \left[\frac{2D}{\Delta x^2} \left(1 + \sqrt{1 - \alpha^2} \cos \frac{i\pi}{I+1} \right) - A \right] \quad (14)$$

The function G is defined to avoid the numerical instability by examining the eigenvalues λ_i . The system is unstable when any of the λ_i is close to zero. To insure a well conditioned matrix, the λ_i may be moved away from zero by adjusting the value of G . Note by inspection of Eq. (14) when G approaches zero, all λ_i collapse to 1.

For real λ_i we must consider the three cases:

- all of the λ_i are positive
- some λ_i are negative and some are positive
- all of the λ_i are negative

For Case a. If the smallest λ_i is far from zero, then G may just be set to 1.

If λ_i is close to zero, reducing G will move all of the λ_i to the right so that the smallest eigenvalue λ_1 is sufficiently greater than some small value of δ .

For Case b. May be treated exactly as the second part of Case a. By reducing G until all λ_i are positive and $\lambda_1 > \delta$.

For Case c. If all λ_i are far to the left, then setting $G = 1$ will insure that all λ_i remain removed from D . When the largest λ_i is close to zero, reducing G will again move the λ_i to the right until $\lambda_1 > \delta$

For all situations except that where $\lambda_1 \ll 0$, the procedure is to choose G such that the smallest eigenvalue λ_1 remains positive. To keep λ_1 away from zero, some small value δ is chosen such that

$$\lambda_1 > \delta \quad (15)$$

We may replace $\cos \frac{i\pi}{1+i}$ with -1 and write (15) as

$$G \left[\frac{A\Delta x^2}{D} + 2\sqrt{1 - \alpha^2} - 2 \right] \leq \frac{\Delta x^2}{\Delta t} - \delta \quad (16)$$

The upper and lower bounds on G are such that it lies in the interval

$$0 \leq G \leq 1$$

So that as long as $\frac{\Delta x^2}{D\Delta t} > \delta$ we set $G = 1$ if

$$\frac{A\Delta x^2}{D} + 2\sqrt{1-\alpha^2} - 2 \leq \frac{\Delta x^2}{D\Delta t} - \delta \quad (17)$$

and $G = 0$ when $G \leq \delta$. For the case where $\lambda_1 \ll 0$, $G = 1$.

The magnitude of δ was arbitrarily set to be

$$\delta = 0.1 \frac{\Delta x^2}{D\Delta t} \quad (18)$$

When neither of the above cases are true, then G is calculated from

$$G = \frac{\frac{\Delta x^2}{D\Delta t} - \delta}{\frac{A\Delta x^2}{D} + 2\sqrt{1-\alpha^2} - 2} \quad (19)$$

Another point that needs to be discussed here is the case when we purposely violate Chin's³ dispersion criterion so that

$$\alpha > 1 \quad (20)$$

For this case, the eigenvalues of B_{ij} are complex and of the form

$$\lambda_i = \lambda + j\gamma_i \quad (21)$$

where $j = \sqrt{-1}$.

Here the λ_i are displaced on a vertical line with the value or the real intercept λ , hence if λ is sufficiently far from zero, then the absolute value $|\lambda_i| > 0$ and the coefficient matrix is well conditioned. For this case, the selection of G is based on the inequality

$$G\Delta t \left[A - \frac{2D}{\Delta x^2} \right] \ll 1. \quad (22)$$

or

$$G\Delta t \left[A - \frac{2D}{\Delta x^2} \right] \gg 1. \quad (23)$$

In cases represented here, the largest possible value of G is sought for which the solution scheme remains stable. Care must be taken when the system approaches the all explicit case $G = 0$. Here the time step selected for computation must be adjusted so that it does not exceed the explicit stability criterion (usually a more restrictive time step). This is given by

$$\frac{\Delta t}{\Delta x^2} \leq 1/2 \quad (24)$$

The procedure for the explicit limit depends on an automatic adjustment of the time step and will be discussed in a later publication.

Turbulence Model Equations

The flow equations considered as an example in our study are written in terms of the mean flow variables and the local properties of the turbulence (using the notation of Saffman and Wilcox⁶),

$$\frac{\partial}{\partial t} (\rho e) + \frac{\partial}{\partial x_j} (\rho U_j e) = [\alpha^* (2 S_{ij} S_{ij})^{1/2} - \beta^* \rho \Omega - \epsilon \frac{\partial U_k}{\partial x_k}] \rho e \quad (25)$$

$$+ \frac{\partial}{\partial x_j} [(\nu + \sigma^* \rho \epsilon) \frac{\partial e}{\partial x_j}]$$

and

$$\frac{\partial}{\partial t} (\rho \Omega^2) + \frac{\partial}{\partial x_j} (\rho U_j \Omega^2) = [\alpha (\frac{\partial U_i}{\partial x_j} \frac{\partial U_j}{\partial x_i})^{1/2} - \beta \rho \Omega] \rho \Omega^2 \quad (26)$$

$$+ \frac{\partial}{\partial x_j} [(\nu + \sigma \rho \epsilon) \frac{\partial \Omega^2}{\partial x_j}]$$

where

$$\epsilon = \frac{e}{\rho \Omega} \quad (27)$$

and ρ , U_j , x_j , t are the mean density, velocity, spatial coordinate and time, e is the local turbulent kinetic energy, and Ω is a "psuedo vorticity" (actually an effective dissipation time scale). α^* , α , β^* , β , ρ , σ , σ^* are universal constants and ν and ϵ are the kinematic and turbulent viscosities.

Input to these equations is supplied by the numerical solution of the mass averaged flow equations for conservation of mass, momentum, and energy.

Both equations (25) and (26) contain the ingredients alluded to in the foregoing problem statement; namely, the competing convective and diffusive derivatives and the source term.

Results

Results for the one-dimensional model equation are shown for a variety of cases. The results given here are not all-inclusive, but serve to exemplify the ideas developed in the preceding section.

The first three figures are included to show the effect of violating Chin's³ numerical dispersion criterion. Numerical dispersion is present in all three cases and appears as a bounded oscillation in the solution. As indicated, dispersion is independent of the solution scheme used. Figure 1a is a single time frame from an explicit calculation which is stable, however the cell Reynolds number exceeds the minimum required to prevent numerical dispersion. Figure 1b is the same calculation run in an all implicit mode and Figure 1c is again the same calculation using the method described in the previous section. Figure 1d is the mixed mode calculation with a reduced spatial step size so that the cell Reynolds number is less than 2 which eliminates the numerical dispersion. The values of the coefficients used in Eq. (14) and the spatial and time step sizes are indicated on the figures.

To demonstrate the strong effect of the source term in determining the value of G in Eq. (14), a set of variables was chosen for the source term coefficient, $A = 100$, the time step, $\Delta t = 0.05$, which would be unstable

if used in an all implicit calculation. These two values were determined by setting Eq. (14) equal to zero, $G = 1$, and adjusting the product $A\Delta t$ for a representative set of the variables $\Delta x = 0.05$, $D = 0.05$, and $U = 5$. The results of the all implicit calculation are shown in Figure 2a for the first time cycle and are clearly unstable. The calculation repeated, using an all explicit scheme was also unstable and is shown for the first time cycle in Figure 2b and at a later time step in Figure 2c. The results of implementing a mixed mode calculation are given in Figure 2d. The computation automatically selects a value of $G = 0.33$ which is stable, but displays some numerical dispersion because of the relatively large cell Reynolds number of 5. The inaccuracy of the calculation is a result of the large time step value $\Delta t = 0.05$.

Another example is shown in Figure 3a and 3b for a smaller source term coefficient, $A = 58$, at a smaller time step, $\Delta t = 0.02$. This example was selected to have a fairly large cell Reynolds number of 25 and, similar to the second example, the values of A and Δt were selected by setting Eq. (14) equal to zero, $G = 1$, and the variables $\Delta x = 0.05$, $D = 0.01$, and $U = 5$. In these two cases, numerical dispersion is obvious, however, the pronounced numerical instability of the all-implicit calculation with $G = 1$ shown in Figure 3a is eliminated and the effect of the dispersion is considerably reduced by selecting $G = 0.99$, as shown by Figure 3b.

To get better resolution of the solution behavior, another series of calculations similar to those shown in Figure 1a through 1d were carried

with a smaller time step $\Delta t = 0.01$. The explicit calculation in Figure 4a was unstable, however, could be made stable by reducing the time step Δt to 5×10^{-4} . Both the implicit and the mixed mode calculations were identical and are shown in Figures 4b and 4c. In the automatic selection mode case, G was chosen to be 1. A comparison of an all explicit and an all implicit calculation were carried out for the same time step and are shown in Figure 5a and 5b. The curve in Figure 5b does not reveal a smearing of the wave front which is apparent when the actual numbers used to generate the plot are closely inspected. This smearing is typical of the obal nature of the implicit method. Examples where this smearing has an adverse effect occur since implicit solutions violate shock and discontinuity propagation in supersonic flow.

Calculations on the Saffman Wilcox model equations, Eqs. (25) through (27), are being carried out and will be discussed at the conference, however, they were not complete at the time of this printing.

Conclusions

It has been demonstrated that the presence of a positive source term in a linear one-dimensional equation, incorporating the features of most conservation equations, may prevent a stable solution using an all *implicit technique*. It has also been shown that a stable explicit solution to this same equation may require a time step so small that the cost of the calculation becomes uneconomical. The proper convex combination of implicit and explicit terms in the solution scheme may relieve both of these difficulties. If large time steps are required and this convex combination of implicit/explicit terms meets stability requirements, then it may be possible to automatically adjust the mixed mode method to achieve an acceptable and economic level of accuracy. However, this work represents only the initial phase of a much more extensive effort to investigate all aspects of convex combination solution schemes.

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Fig. 1 Examples showing numerical dispersion independent of solution scheme: a) explicit b) implicit c) automatic selection made $G=1$ d) implicit with dispersion removed.

Fig. 2 Effect of a large source term and large time step on solution stability: a) unstable all implicit, b) unstable all explicit, c) unstable all explicit at a later time step, d) stable but inaccurate automatic mode $G=0.99$.

Fig. 3 Effect of a large source term on stability at a lower time step: a) implicit, b) automatic $G=0.99$.

Fig. 4 Comparison of time step requirements for stable explicit and implicit solution: a) unstable explicit b) stable implicit, c) stable automatic $G=1$.

Fig. 5 Stable calculations with small source term, small dispersion: a) explicit, b) implicit or $G=1$.

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