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A General Corrective Procedure for the Numerical Solution of Initial-Value Problems[1]

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ABSTRACT

In many circumstances the finite difference equations used in the solution of an initial-value problem must be solved by an iteration process at each time step. This paper proposes a technique that permits crude iteration to be used without leading to a disastrous accumulation of error after many cycles of time advancement. The technique, which is quite general, is discussed for two examples. The second of these applications accounts for the success of the Marker-and-Cell computing method for the solution of incompressible fluid flow problems.

In the finite difference solution of an initial-value problem, the dependent variable configuration is advanced in time through a sequence of small steps of duration δt. In many circumstances the finite difference equations used for advancing the solution through one time step must be solved by an iteration or relaxation process. This occurs, for example, when the difference equations are nonlinear, or are sets of coupled linear equations. The use of an iterative procedure always introduces some error. To avoid a significant accumulation of this error, when a solution is carried through many time cycles, it is generally thought necessary to use a very fine convergence criterion for the iteration process. Usually, the required computing time increases rapidly with an increase in the fineness of the convergence criterion, and this often means prohibitive computing time to obtain a desired level of accuracy.

In this paper we propose a technique that permits the use of a coarse convergence criterion by prohibiting the usual accumulation of error. This technique, which is quite general, is adapted from a procedure proposed by Harlow and Welch [1] for a special case. The main purpose of this corrective technique is to save computing time. The technique significantly reduces the number of iterative subcycles that are required to preserve accuracy through a large number of time-advancement cycles.

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We first illustrate the basic idea by a simple example. The initial value problem

$$(d/dt)(Z + Z^5) + 2t(1 + 5Z^4) = 0, \tag{1}$$

with $Z = 1$ at $t = 0$ has the exact solution

$$Z = 1 - t^2. \tag{2}$$

To obtain a finite difference solution of (1) the following approximation could be used.

$$\begin{gathered}[Z^{n+1} + (Z^{n+1})^5] - [Z^n + (Z^n)^5] + 2\delta t(n\delta t)[1 + 5(Z^n)^4] = 0 \\ Z^0 = 1,\end{gathered} \tag{3}$$

where Z^n means the value of Z at time step n. For each cycle a non-linear equation must be solved for Z^{n+1}. This could be accomplished, for example, by iterating with a Newton-Raphson method [2].

If Eq. (3) is not iterated finely enough at each time step, it is possible for a significant error to develop after many cycles of calculation. To eliminate such an accumulation of error we propose that Eq. (1) be replaced by the equivalent set of equations,

$$\begin{aligned}\frac{dD}{dt} &= \frac{d}{dt}(Z + Z^5) + 2t(1 + 5Z^4), \\ D &= 0,\end{aligned} \tag{4}$$

which has the finite difference approximation

$$D^{n+1} = D^n + [Z^{n+1} + (Z^{n+1})^5] - [Z^n + (Z^n)^5] + 2\delta t(n\delta t)[1 + 5(Z^n)^4], \tag{5}$$

and

$$D^{n+1} = 0. \tag{6}$$

According to Eq. (6) we should solve Eq. (5) for a value of Z^{n+1} that makes the right-hand side of that equation equal to zero. A solution of this nonlinear equation for Z^{n+1} can be obtained by an iteration process. An iteration process, however, is usually terminated with some error, so that D^{n+1}, as defined by Eq. (5), can differ from zero by an amount that depends on the convergence criterion for Z^{n+1}. In the next cycle of calculation, step $n + 2$, this residual D^{n+1} is used for the value of D^n on the right-hand side of Eq. (5). In this way a correction is introduced at step $n + 2$ for the error made in Z^{n+1}. It is this corrective term that allows Eq. (5) to be solved for each Z^n with a relatively coarse convergence criterion without the usual accumulation of error as n increases.

To demonstrate the effect of the correction term we have calculated with Eqs. (3) and (5) for 100 cycles, with $\delta t = 0.01$. The equations were solved by

a Newton-Raphson iteration technique using the convergence criterion: the magnitude of the change in Z^{n+1} after an iteration had to be less than a specified constant ϵ. Three sets of calculations were performed, $\epsilon = 1.0$, $\epsilon = 0.1$, and $\epsilon = 0.01$. Figure 1 shows the results for $\epsilon = 1.0$ and $\epsilon = 0.1$. In the $\epsilon = 0.01$ case the corrected and uncorrected solutions agreed with the exact solution to within 0.1. The corrective procedure improved the approximate solutions in every case.

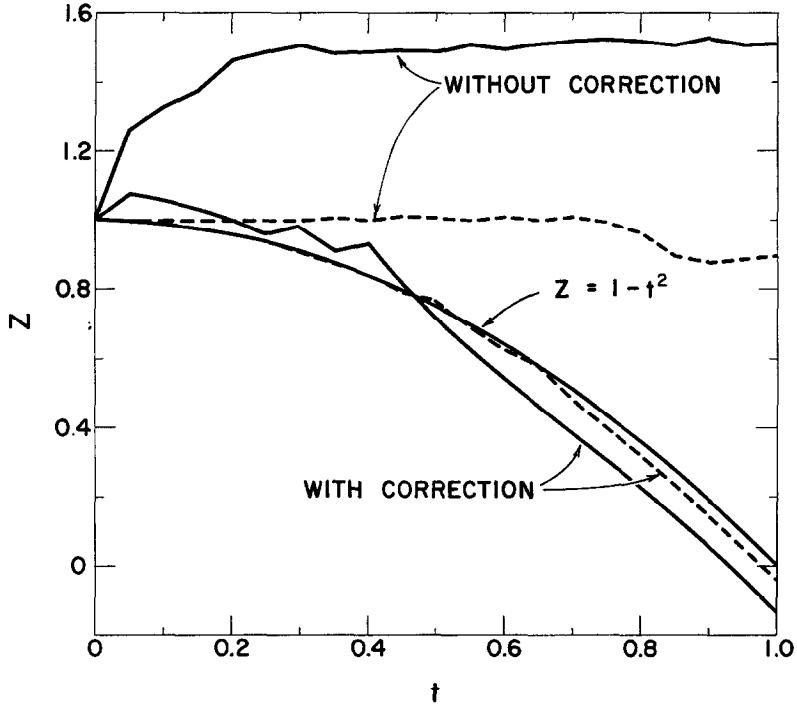

FIG. 1. The results for 100 cycles as obtained from Eq. (3), without correction, and Eq. (5), with correction, are compared with exact solution. Solid lines had a convergence criterion of 1.0, and dashed lines had a convergence criterion of 0.1.

Specifically, the corrected results obtained with convergence criterion 1.0 (0.1) are at least as accurate as the uncorrected results obtained with convergence criterion 0.1 (0.01).

Another example that illustrates this corrective procedure occurs in the Marker-and-Cell method [1]. This is a computing technique for solving the Navier-Stokes equations that describe the transient dynamics of an incompressible fluid. The

condition of incompressibility is that the divergence of the fluid velocity, $\mathbf{u}$, must vanish,

$$\nabla \cdot \mathbf{u} = 0. \tag{7}$$

The fluid pressure, p, must satisfy an equation that is derived by taking the divergence of the momentum equation (Navier-Stokes equation). Retaining all of the terms, we obtain

$$\frac{\partial}{\partial t}(\nabla \cdot \mathbf{u}) = -\nabla^2(p/\rho) + \nu\nabla^2(\nabla \cdot \mathbf{u}) - Q \tag{8}$$

where

$$Q = \nabla \cdot [\nabla \cdot (\mathbf{uu})], \tag{9}$$

ρ is the fluid density (a constant), and ν is the kinematic viscosity.

The incompressibility condition, Eq. (7), implies that Eq. (8) is a Poisson equation for the pressure. This equation must be solved at each step in the time advancement of a problem. A Poisson equation in finite difference form is most efficiently solved by an iteration process. Since an iteration process must be terminated after a finite number of iterations, some error is always introduced. Although the error introduced in one time cycle may be small, it can accumulate over many time cycles. This error corresponds to an error in the total volume of fluid, so it must remain small for the numerical solutions of the Navier-Stokes equations to be accurate. There are two ways to limit the *accumulation* of iteration errors. The iteration process can be carried to a high level of accuracy at each time cycle, or the self-correcting procedure that we are proposing can be used for a cycle-to-cycle adjustment. The latter method is preferred because it shortens computing time. In fact, it was in the Marker-and-Cell method that this corrective procedure was first described. If we define for each cell of the computing mesh the quantity

$$D = \nabla \cdot \mathbf{u}, \tag{10}$$

then Eqs. (7) and (8), for each cell, have a form similar to Eq. (4); the quantity that should be zero is instead set equal to $\partial D/\partial t$, and the auxiliary equation $D = 0$ is imposed.

The advantage gained in using this procedure in the Marker-and-Cell method is described in Ref. [3], p. 22. The corrective term cuts down the accumulation of incompressibility errors, even with a coarse pressure iteration. Thus, with relatively little computing time, an accuracy is achieved that would otherwise be possible only at the expense of many more iterative subcycles of the pressure equation, requiring as much as three or four times more computer time.

The corrective procedure described by the preceding two examples can be considerably generalized. Consider the matrix of equations

$$\frac{\partial \Phi(Z)}{\partial t} + \Gamma = 0, \tag{11}$$

in which Z is a set of unknown quantities, and Φ is a matrix of specified functions of Z. The term Γ represents a matrix of functions of the Z quantities, of various independent variables (for example, spatial variables), and of derivatives of Z with respect to these independent variables.

A finite difference approximation to Eq. (11) is

$$\Phi(Z^{n+1}) - \Phi(Z^n) + \delta t\, \Gamma^n = 0, \tag{12}$$

in which the derivatives of Z occurring in Γ are also approximated by finite differences. The index n counts time cycles, i.e., $t = n\delta t$. Some or all of the Z in Γ^n may also carry the index $n + 1$. In any case Eq. (12) is a (coupled) set of algebraic equations for the unknown quantities Z^{n+1}. If this set can be solved exactly, by efficient techniques, then the considerations of this paper do not apply. If an approximate solution is to be acquired through iteration, then our proposal eases the convergence criteria without introducing a loss of accuracy that could accumulate through many cycles of time advancement. We replace Eq. (11) by the equivalent pair of equations

$$\begin{aligned} \frac{\partial D}{\partial t} &= \frac{\partial \Phi(Z)}{\partial t} + \Gamma \\ D &= 0, \end{aligned} \tag{13}$$

which, become, in finite difference form,

$$\begin{aligned} D^{n+1} &= D^n + \Phi(Z^{n+1}) - \Phi(Z^n) + \delta t \Gamma^n \\ D^{n+1} &= 0. \end{aligned} \tag{14}$$

Thus, in each cycle one solves, with relatively coarse convergence criteria, the matrix of equations

$$D^n + \Phi(Z^{n+1}) - \Phi(Z^n) + \delta t\, \Gamma^n = 0, \tag{15}$$

in which

$$D^n = D^{n-1} + \Phi(Z^n) - \Phi(Z^{n-1}) + \delta t\, \Gamma^{n-1}. \tag{16}$$

The result is an efficient calculation with significantly less than the usual accumulation of error.

References

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