JOURNAL OF COMPUTATIONAL PHYSICS 22, 377–388 (1976)

A Stable Difference Scheme for the Solution of Hyperbolic Equations Using the Method of Lines

J. C. HEYDWEILLER

Department of Chemical Engineering, Kansas State University, Manhattan, Kansas, 66506

AND

R. F. SINCOVEC

Department of Computer Science, Kansas State University, Manhattan, Kansas 66506

Received February 23, 1976

A new differencing scheme is proposed for the solution of hyperbolic partial differential equations by the method of lines. The accuracy of the scheme is shown to be between first and second order while the instability associated with the use of centered second-order differences is avoided. The method is successfully demonstrated on problems which have smooth solutions.

INTRODUCTION

A system of partial differential equations may be transformed into a coupled system of ordinary differential equations by discretizing all the equations in all but one independent variable. This procedure is known as the method of lines [11, 12]. In this paper, hyperbolic partial differential equations depending on time and one spatial variable will be considered. Finite differencing in the spatial variable leads to a set of time dependent ordinary differential equations. The number of ordinary differential equations is equal to the number of partial differential equations times the number of grid points used.

The advantage of using the method of lines is that sophisticated packages [1, 4, 7, 15] exist for the numerical solution of ordinary differential equations. These packages contain iterative methods for handling nonlinearities and feature automatic step-size adjustment and integration-order selection to maintain a user-specified error and to solve the problem with near optimal efficiency. Previous applications of the method of lines to solve partial differential equations [12, 16] have been geared to parabolic equations and have generally used centered, second-order differences. Using these differences on hyperbolic equations can lead to unstable solutions. To add stability, upstream (backward or forward) first-order differences could be used for the spatial discretization but these differences require the use of more grid points than centered differences for a given spatial accuracy. An artificial dissipation (or viscosity) term [14] is often added to a centered-differencing scheme to add stability but it is difficult to determine the magnitude of this term required for the stability and the effect of this term on the solution. Other stabilizing techniques [3, 8, 9, 14] which have been employed in explicit finite difference procedures are generally not applicable to the method of lines approach because they involve manipulation of terms in both the time and space discretizations.

The method presented in this paper uses a three-point difference which is a biased average of forward and backward differences. The direction and amount of the bias are adjusted to give stable difference schemes with an accuracy between the usual first- and second-order schemes. Use of these biased differences allows the efficient solution of hyperbolic partial differential equations by the method of lines. This method of solution is especially attractive for coupled sets of hyperbolic and parabolic equations.

Accuracy

The difference scheme to be studied is given by

$$\frac{df_i}{dx} = \frac{Af_{i+1} + Cf_i - Bf_{i-1}}{(A+B)\,\Delta x} + E_T, \tag{1a}$$

$$C = B - A = \pm 1, \tag{1b}$$

where A and B are integers greater than or equal to zero, $A + B$ is an odd integer, and E_T is the truncation error. This equation may be rearranged to give

$$\frac{df_i}{dx} = \frac{1}{A+B}\left[A\left(\frac{f_{i+1} - f_i}{\Delta x}\right) + B\left(\frac{f_i - f_{i-1}}{\Delta x}\right)\right] + E_T. \tag{2}$$

This arrangement shows that the proposed scheme is a weighted average of A forward differences and B backward differences. By replacing the two differences with their Taylor series expansions, one obtains

$$\begin{aligned}\frac{df_i}{dx} = {} & \frac{A}{A+B}\left[\frac{df_i}{dx} + \frac{\Delta x}{2}\frac{d^2f_i}{dx^2} + \frac{(\Delta x)^2}{6}\frac{d^3f_i}{dx^3} + \cdots\right] \\ & + \frac{B}{A+B}\left[\frac{df_i}{dx} - \frac{\Delta x}{2}\frac{d^2f_i}{dx^2} + \frac{(\Delta x)^2}{6}\frac{d^3f_i}{dx^3} + \cdots\right] + E_T.\end{aligned} \tag{3}$$

Since $B - A = \pm 1$, this equation reduces to

$$E_T = \pm \frac{1}{A+B} \frac{\Delta x}{2} \frac{d^2 f_i}{dx^2} - \frac{(\Delta x)^2}{6} \frac{d^3 f_i}{dx^3} \pm \cdots \tag{4}$$

For $A + B$ equal to 1, the difference scheme reduces to either the usual forward or backward difference with its associated first-order truncation error. When $A + B$ is greater than 1, the first-order term of the truncation error is reduced by a factor of $A + B$. In the limit as $A + B$ approaches infinity, this difference scheme approaches the second-order accuracy of a centered difference.

Stability

As the stability of a three-point differencing scheme is difficult to analyze, the theoretical study of stability will be limited to the equation

$$\partial U/\partial t = C_0 \, \partial U/\partial x. \tag{5}$$

An implicit in time difference scheme for this equation is given by

$$\frac{U_i^{n+1} - U_i^{\,n}}{\Delta t} = C_0 \left[\frac{A U_{i+1}^{n+1} + C U_i^{n+1} - B U_{i-1}^{n+1}}{(A+B)\,\Delta x} \right], \tag{6}$$

where $U_i^{\,n}$ is the solution to the difference equation at x_i and t_n. To show unconditional stability with the Fourier method of analysis [14], one assumes that the solution of the difference equation is of the form

$$U_i^{\,n} = \gamma^n e^{jpi\Delta x}, \tag{7}$$

where $j = (-1)^{1/2}$ and then shows that the magnitude of the complex constant γ is less than 1 (the von Neumann condition). Substituting this expression for $U_i^{\,n}$ into Eq. (6) and simplifying leads to

$$\gamma = (1 - rC - rAe^{jp\Delta x} + rBe^{-jp\Delta x})^{-1}, \tag{8}$$

where

$$r = C_0 \Delta t/(A + B)\,\Delta x. \tag{9}$$

This equation may be rewritten as

$$\gamma = (1 - rC(1 - \cos p\,\Delta x) - rj(A + B) \sin p\,\Delta x)^{-1}. \tag{10}$$

For this procedure (Eq. (6)) to be unconditionally stable, the magnitude of γ must be less than 1. The requirement is satisfied if

$$1 - rC(1 - \cos p\,\Delta x) > 1. \tag{11}$$

This condition may also be written as

$$C(C_0\,\Delta t/(A + B)\,\Delta x)(1 - \cos p\,\Delta x) < 0. \tag{12}$$

Since $\cos p\,\Delta x \leqslant 1$, C must be positive if C_0 is negative and C must be negative if C_0 is positive. This implies that $A < B$ for $C_0 < 0$ and $A > B$ for $C_0 > 0$. To maintain stability, the averaging of the forward and backward differences is biased upstream relative to the motion of the wave. As $A + B$ increases in value, the magnitude of γ approaches 1, which is the condition of marginal stability.

For an explicit in time procedure, the finite difference scheme for Eq. (5) is given by

$$(U_i^{n+1} - U_i^{\,n})/\Delta t = C_0[(AU_{i+1}^n + CU_i^{\,n} - BU_{i-1}^n)/(A + B)\,\Delta x]. \tag{13}$$

The Fourier method of analysis is applied again. Using Eq. (7) and simplifying, one obtains

$$\gamma = 1 + rC + rAe^{jp\Delta x} - rBe^{-jp\Delta x}, \tag{14}$$

where r is given by Eq. (9). The expression for the magnitude of this complex number may be written as

$$|\,\gamma\,| = \{1 + r[2C(1 - \cos p\,\Delta x)] + r^2[C^2(1 - \cos p\,\Delta x)^2 + (A + B)^2 \sin^2 p\,\Delta x]\}^{1/2}. \tag{15}$$

By setting $|\,\gamma\,|$ equal to 1, solving for r, and performing some algebra, one can obtain the equation

$$r = -C/(A^2 + B^2 + 2AB\cos p\,\Delta x). \tag{16}$$

The smallest value of r will occur when $\cos p\,\Delta x$ equals one. This condition leads to the restriction

$$\Delta t \leqslant -C\,\Delta x/C_0(A + B) \tag{17}$$

on the size of the time step. Since Δt and Δx are both positive, this equation gives the same relationship between the signs of C and C_0 as that found for the implicit case.

For $A + B$ equal to 1, Eq. (17) gives the time step restriction for an explicit procedure based on forward ($C_0 > 0$) or backward ($C_0 < 0$) differencing. As $A + B$ increases, the time step restriction appears to become more severe. However, since the spatial truncation error is reduced by a factor of $A + B$, a value of Δx that is $A + B$ times as large can be used with the biased difference scheme for the same spatial truncation error. Therefore, for a given error, the maximum time step allowed for stability of the biased difference scheme is independent of the value of $A + B$ as long as the first-order term dominates the truncation error. Since a larger value of Δx is used with the biased difference scheme, fewer difference equations must be solved per time step.

The method of lines procedure gives the ordinary differential equation

$$dU_i/dt = C_0[(AU_{i+1} + CU_i - BU_{i-1})/(A + B)\,\Delta x]. \tag{18}$$

The stability of this procedure is dependent on the integrator (type and order) used. In the previously mentioned packages for the solution of ordinary differential equations, the lowest-order method uses an explicit Euler's method for a predictor and an implicit Euler's method for a corrector. Since the explicit and implicit Euler's methods correspond to the explicit and implicit finite difference schemes given in Eqs. (13) and (6), respectively, the method of lines procedure is conditionally stable for the simplest integration method. The procedure should be conditionally stable for the higher-order integration methods in these packages because all of these methods are stable for the same class of equations [2].

Results and Discussion

To use the method of lines to solve partial differential equations, a suitable integrator must be chosen to solve the ordinary differential equations resulting from the spatial discretization. The integrator used was developed by Hindmarsh [4] and is of the type first proposed by Gear [1]. For all the problems solved, the nonstiff option was used. With this option, the Adams methods are used with functional iteration so there is no associated matrix problem.

The first problem solved was

$$\partial U/\partial t = -\partial U/\partial x, \tag{19a}$$

with

$$U(0, t) = 0 \tag{19b}$$

and

$$U(x, 0) = U_0(x); \qquad 0 \leqslant x \leqslant 1. \tag{19c}$$

The exact solution, $U(x, t) = U_0(x - t)$, is shown as the triangular wave in Fig. 1 at time 0.4. The numerical results for this problem are presented to show the effect of the size of $A + B$ on the accuracy and stability of the procedure. The numerical solutions are plotted in Fig. 1 for $A + B$ equal to 1 (backward difference), 11, 101, and infinity (centered difference) at times of 0.1, 0.2, 0.3, and 0.4. Although the value of 0.01 used for Δx is not small enough to give much accuracy, it is sufficient for a visual comparison of the numerical solutions for the different values of $A + B$ with the exact solution. As is expected, increasing $A + B$ improves the accuracy but is detrimental to stability. By a time of 0.4, the shape of the wave is severely distorted for $A + B$ equal to one while the oscillations are continuing to increase in magnitude for $A + B$ equal to infinity. For problems of this type, the choice of $A + B$ is dependent on the desired accuracy, the value of Δx and the length of the time integration interval which determines the number of time steps.

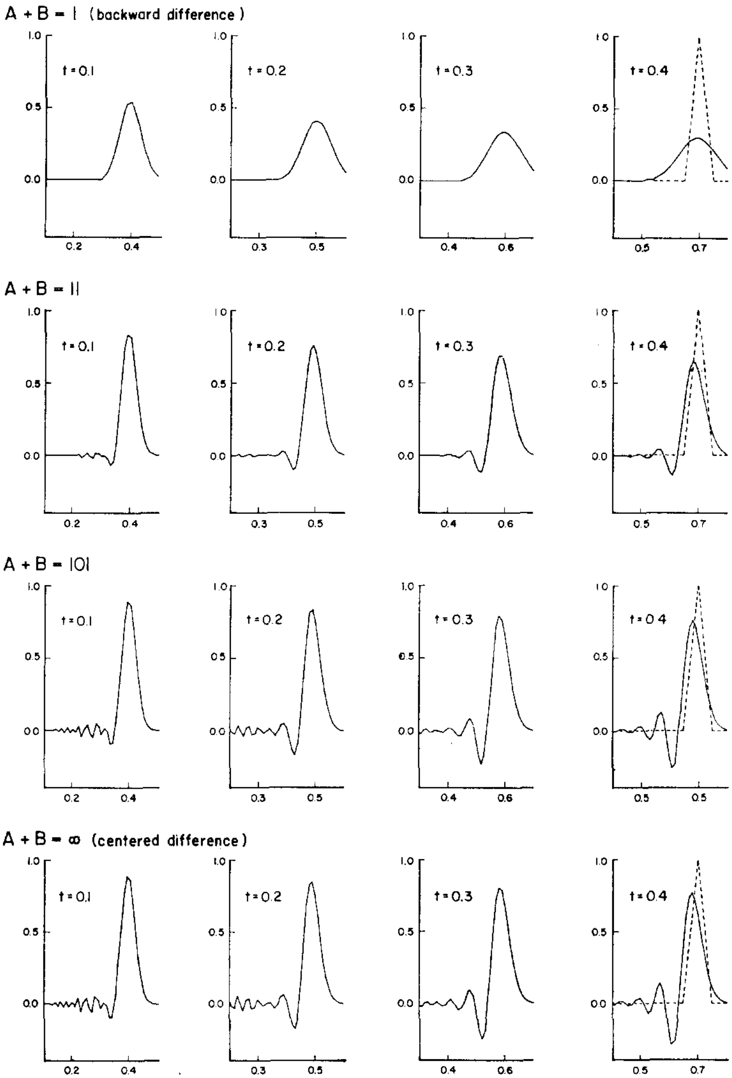

FIG. 1. Effect of $A + B$ on solution of Eq. (19) (– – – exact solution).

The second problem solved was

$$\partial U/\partial t = -(\partial/\partial x)(\tfrac{1}{2}U^2), \tag{20a}$$

with

$$U(0, t) = 0 \tag{20b}$$

and

$$U(x, 0) = x; \qquad 0 \leqslant x \leqslant 1. \tag{20c}$$

This example is due to Richtmyer [13] and is discussed in [14]. The proper direction of bias was determined from the linearized form of the equation. A value of 0.01 was chosen for Δx. To test the effect of $A + B$ on accuracy, values of 1, 11, 101, and infinity were used while the maximum time integration error was fixed at 10^{-6}. To maintain accuracy at the right boundary, the following one-sided, second-order difference scheme was used.

$$(\partial/\partial x)(\tfrac{1}{2}U_I^2) = \tfrac{1}{2}[(3U_I^2 - 4U_{I-1}^2 + U_{I-2}^2)/2(\Delta x)], \tag{21}$$

where U_I is evaluated at x equal to 1.

The analytical solution to this problem is given by

$$U(x, t) = x/(1 + t). \tag{22}$$

For each of the values of $A + B$ used, the maximum error of the numerical solution in the interval is given for times of 0.5, 1, 5, and 10 in Table I. Increasing $A + B$ from 1 to 11 reduces the error by an order of magnitude while almost another order of magnitude decrease is gained by increasing $A + B$ from 11 to 101. For the centered difference case ($A + B$ equal to infinity), the maximum error always occurred at or near the right boundary. This is due to the fact that the truncation error of the difference equation used at the right boundary, Eq. (21), is twice as large as the truncation error for the centered differences used for the interior points.

TABLE I
Effect of $A + B$ on Truncation Error[a]

	Maximum error			
	Time			
$A + B$	0.5	1.0	5.0	10.0
1	$0.135 * 10^{-2}$	$0.173 * 10^{-2}$	$0.149 * 10^{-2}$	$0.109 * 10^{-2}$
11	$0.123 * 10^{-3}$	$0.158 * 10^{-3}$	$0.136 * 10^{-3}$	$0.994 * 10^{-4}$
101	$0.135 * 10^{-4}$	$0.181 * 10^{-4}$	$0.150 * 10^{-4}$	$0.201 * 10^{-4}$
∞	$0.477 * 10^{-6}$	$0.140 * 10^{-5}$	$0.123 * 10^{-4}$	$0.115 * 10^{-4}$

[a] Solution of Eq. (20).

The third problem solved was

$$\partial\Psi/\partial\tau = -(\partial\Psi/\partial\zeta) - \kappa\Psi^N, \tag{23a}$$

with

$$\Psi(0, \tau) = 1 \tag{23b}$$

and

$$\Psi(\zeta, 0) = 0; \qquad 0 < \zeta \leqslant 1. \tag{23c}$$

This equation describes the disappearance of a chemical species by an Nth-order reaction in a plug flow reactor [10] in terms of dimensionless reactant concentration (Ψ), time (τ), and axial position (ζ). The solution was obtained for κ equal to 1, 5, and 10 and N equal to 1, 2, and 3. A value of 0.01 was used for $\Delta\zeta$ and since the convective term is the same as that of the first test problem, Eq. (19), $A + B$ was chosen to be 11. No difficulties were encountered solving this problem with any combination of the parameters. A typical solution is shown in Fig. 2. The small disturbance behind the front remains bounded and actually decreases with time. At a time of 1.5, the front has passed through the reactor and the solution is close to steady state.

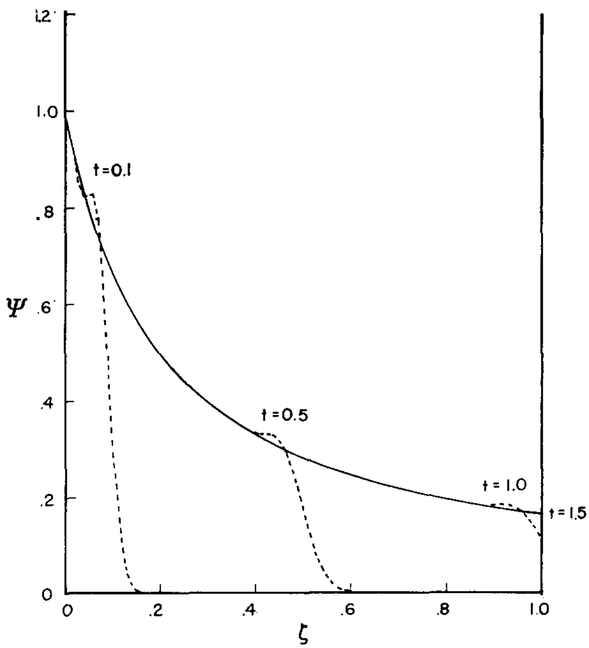

FIG. 2. Solution of Eq. (23) for $\kappa = 5$ and $N = 2$.

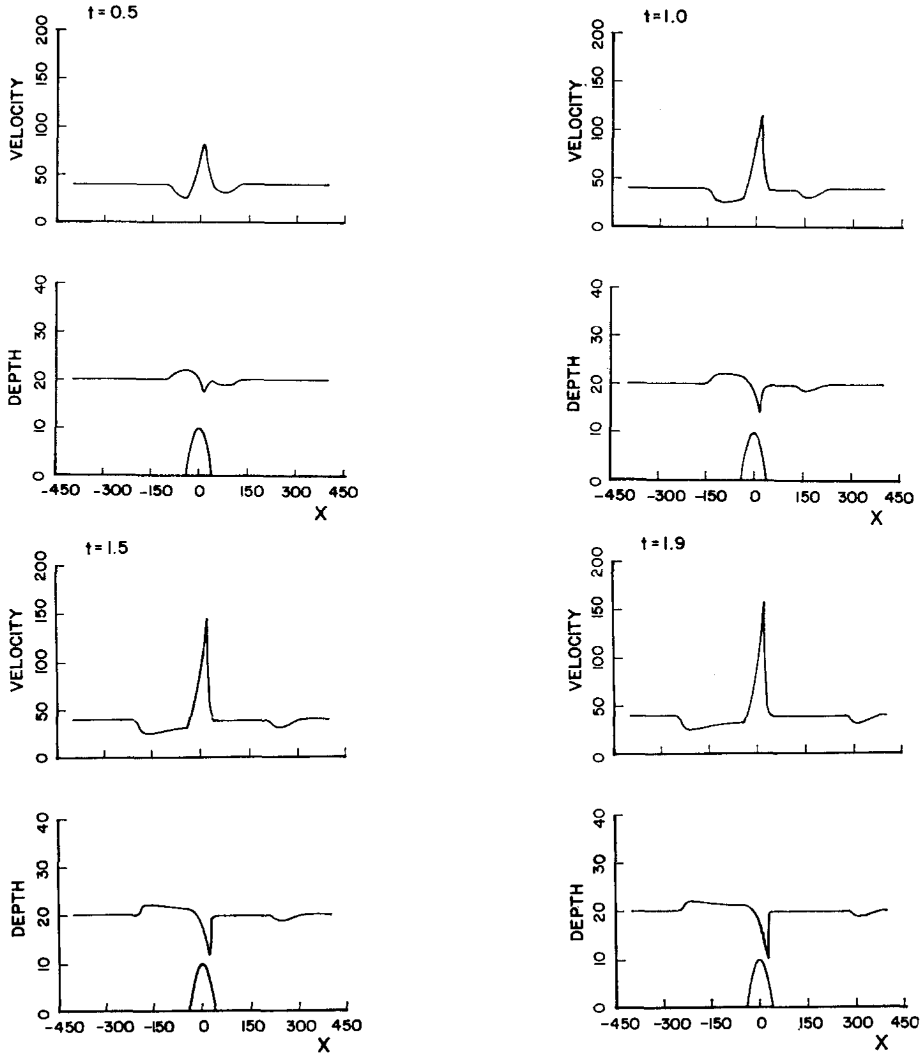

FIG. 3. Solution of Eq. (24) with dissipation added.

The last problem attempted was

$$\partial U/\partial t = -(\partial/\partial x)(\tfrac{1}{2}U^2) - 980((\partial\Phi/\partial x) + (dH/dx)), \tag{24a}$$

$$\partial\Phi/\partial t = -(\partial/\partial x)(U\Phi), \tag{24b}$$

with

$$U(0, x) = 40, \tag{24c}$$

$$\Phi(0, x) = 20 - H(x), \tag{24d}$$

$$U(t, -400) = U(t, 400) = 40, \tag{24e}$$

$$\Phi(t, -400) = \Phi(t, 400) = 20, \tag{24f}$$

$$H(x) = \max[0, 10 - 10(x/40)^2]. \tag{24g}$$

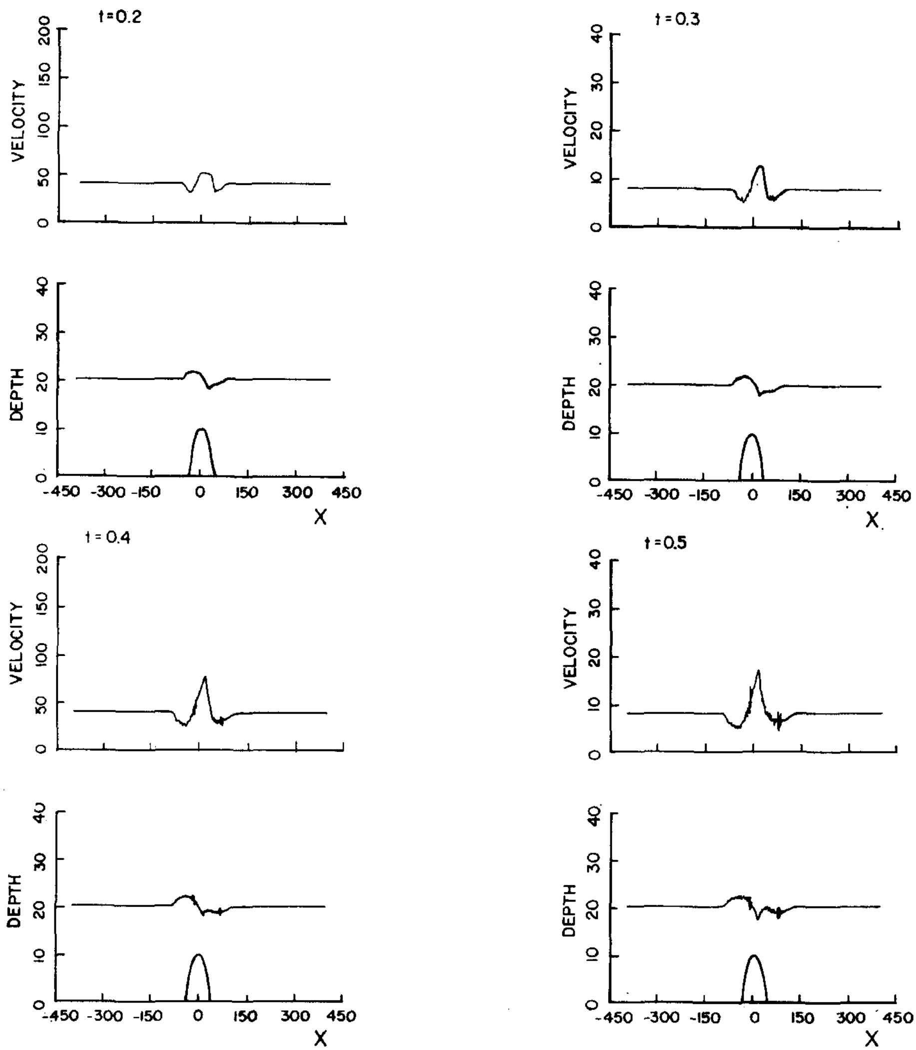

FIG. 4. Unstable solution of Eq. (24) with $A + B = 11$.

These equations have been studied by Houghton and Kasahara [5, 6]. The equations represent the flow of a fluid over a barrier, $H(x)$. The fluid velocity in the x-direction is denoted by U while Φ denotes the fluid depth. The solution is presented in Fig. 3. Besides a major stationary shock developing on the downstream side of the barrier, the solution contains smaller fronts moving in both the positive and negative x directions.

A value of 2 was used for Δx and the direction of bias was determined from the linearized form of the equation. Values of 1, 11, 101, 1001, and infinity were tried for $A + B$. It was found that increasing $A + B$ had a stabilizing effect. This is probably because a centered difference can best account for the movement of fronts in opposite directions. The biased difference scheme did not yield a stable solution for any value of $A + B$. Fig. 4 shows the growth of numerical instabilities for the case of $A + B$ equal to 11. The solution presented in Fig. 3 was obtained by adding dissipative terms to a centered difference scheme.

Conclusions

The biased differencing scheme given in Eq. (1) can be used with a suitable ordinary differential equation integrator to solve many hyperbolic partial differential equations by the method of lines. It has been successfully used on both linear and nonlinear equations which have sufficiently smooth solutions. This procedure has failed to solve a set of equations whose solution develops a shock discontinuity without the addition of dissipative terms.

From the example problems, it appears that the biased differences will give stable solutions to any problem which can be solved using upstream, first-order differences. Because of the greater accuracy of the biased differences, more efficient solutions can be obtained by using them in place of the upstream differences.

Acknowledgment

Gratitude is expressed to Dr. L. T. Fan for his support during the preparation of this manuscript.

References

1. C. W. Gear, *Comm. ACM* 3 (1971), 176.
2. C. W. Gear, "Numerical Initial Value Problems in Ordinary Differential Equations," Prentice-Hall, Englewood Cliffs, N.J., 1971.
3. S. K. Godnov, *Mat. Sb.* 47 (1959), 271.
4. A. C. Hindmarsh, "Gear: Ordinary Differential Equation System Solver," Lawrence Livermore Laboratory, Report UCID-30001, Rev. 3 (1974).

5. D. D. HOUGHTON AND A. KASAHARA, *Comm. Pure Appl. Math.* **21** (1972), 603.
6. A. KASAHARA AND D. D. HOUGHTON, *J. Computational Phys.* **4** (1969), 377–388.
7. F. T. KROGH, "An Integrator Design," Jet Propulsion Lab. Tech. Memo. 278, California Institute of Technology, Pasadena, Calif., 1971.
8. P. D. LAX, *Com. Pure Appl. Math.* **1** (1954), 159.
9. P. D. LAX AND B. WENDROFF, *Comm. Pure Appl. Math.* **13** (1960), 217.
10. O. LEVENSPIEL, "Chemical Reaction Engineering," 2nd ed., Wiley, New York, 1972.
11. O. A. LISKOVETS, *Difference Equations* **1** (1965), 1308.
12. N. K. MADSEN AND R. F. SINCOVEC, The Numerical Method of Lines for the Solution of Nonlinear Partial Differential Equations, in "Computational Methods in Nonlinear Mechanics" (J. T. Oden *et al.*, Eds.), Texas Institute for Computational Mechanics, Austin, Tex., 1974.
13. R. D. RICHTMYER, "The Stability Criterion of Godunov and Ryabenkii for Difference Schemes," Rept. No. NYO-1480-4, Courant Institute of Mathematical Sciences, New York University, New York, 1964.
14. R. D. RICHTMYER AND K. W. MORTON, "Difference Methods for Initial Value Problems," 2nd ed., Interscience, New York, 1967.
15. L. F. SHAMPINE AND M. K. GORDON, "Computer Solution of Ordinary Differential Equations: Initial Value Problems," Freeman, San Francisco, 1975.
16. R. F. SINCOVEC AND N. K. MADSEN, *ACM Trans. Math. Software* **1** (1975), 232.