ANALYSIS OF EXPLICIT FINITE DIFFERENCE METHODS USED IN COMPUTATIONAL FLUID MECHANICS

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1. INTRODUCTION

It is now commonplace to simulate fluid motion by numerically solving the governing partial differential equations on high speed digital computers.

Finite difference techniques, because of their relative simplicity and their long history of successful application, are the most commonly used. They have, for example, been used in depth-averaged and three-dimensional time dependent tidal modelling by many oceanographers and coastal engineers : see, for example, Noye and Tronson (1978), Noye et.al. (1982) and Noye (1984a).

However, like finite element techniques and boundary integral methods, finite difference methods of solving the Eulerian equations of hydrodynamics seldom model the advective terms accurately. Errors in the phase and amplitude of waves are usual, particularly the former.

The accuracy of various explicit finite difference methods applied to solving the advection equation, namely

$$\frac{\partial\bar{\tau}}{\partial t} + u\frac{\partial\bar{\tau}}{\partial x} = 0, \; 0 \le x \le 1, \; t > 0, \; u \text{ a positive constant,} \tag{1.1}$$

is investigated in this work. The boundary condition to be used in practice is that $\bar{\tau}(0,t)$ is defined for $t > 0$, with no values prescribed at $x = 1$.

The von Neumann amplication factor is not only used to find the stability criteria of the methods investigated, but also to determine the wave deformation properties of the technique. These properties are then linked to the "modified" equation; that is, the partial differential equation which is equivalent to the finite difference equation, after the former has been modified so it contains only the one temporal derivative, $\partial\bar{\tau}/\partial t$, all other derivatives being spatial.

It will be seen that successively more accurate methods can be developed by systematic elimination of the higher order terms in the truncation error, which is the difference between the modified equation and the given equation (1.1).

The approach used by Molenkamp (1968) and Crowley (1968) to assess the accuracy of the numerical method to the advection equation is also used to illustrate the conclusions reached from the mathematical analysis; that is, the numerical method is applied to a simple problem whose exact solution is known, and the numerical solution is compared with the exact solution. The problem chosen is that of an infinite train of Gaussian pulses, used as initial condition to (1.1), for which the exact solution at time t on the infinite domain $-\infty < x < \infty$ is the same train displaced a distance ut to the right along the x-axis. The corresponding numerical solution of this process is obtained using cyclic boundary conditions at $x = 0$ and $x = 1$.

Higher order techniques, such as the third order upwind biassed method and Rusanov's methods, are clearly more accurate than the more widely used methods such as first order upwind and the Lax-Wendroff methods. The increased accuracy justifies the increased computational time and complications near the boundary due to extension of the computational molecule for certain higher order methods.

2. THE FIRST-ORDER UPWIND METHOD

At the gridpoint $(j\Delta x, n\Delta t)$, $j = 1, 2, .., J$, $n = 1, 2, 3, ...,$ $\Delta x = 1/J$, the advection equation

$$(2.1) \qquad \left.\frac{\partial\bar{\tau}}{\partial t}\right|_j^n + u\left.\frac{\partial\bar{\tau}}{\partial x}\right|_j^n = 0,$$

becomes, on using the two-point forward time approximation and the two-point backward space approximation,

$$(2.2) \qquad \frac{\tau_j^{n+1} - \tau_j^n}{\Delta t} + u\left\{\frac{\tau_j^n - \tau_{j-1}^n}{\Delta x}\right\} = 0.$$

On rearrangement, this gives the two point upwind equation, see Godunov (1959),

$$(2.3) \qquad \tau_j^{n+1} = c\tau_{j-1}^n + (1-c)\tau_j^n,$$

where τ_j^n is an approximation to $\bar{\tau}(j\Delta x, n\Delta t)$ and $c = u\Delta t/\Delta x > 0$ is the Courant number.

The amplification factor, $G(c,N_\lambda)$, of the von Neumann method of stability analysis is obtained by substituting $\tau_j^n = (G)^n \exp\{i(2\pi j/N_\lambda)\}$, $i = \sqrt{-1}$, into (2.3), where the parameter N_λ is the number of grid-spacings per wavelength of a particular Fourier mode contained in the initial conditions. For this method we obtain

(2.4) $$G(c,N_\lambda) = \{1 - 2c \sin^2(\pi/N_\lambda)\} - i\{c \sin(2\pi/N_\lambda)\}.$$

The stability requirement is that $|G| \leq 1$ for all $N_\lambda \geq 2$, which is true so long as $0 < c \leq 1$.

The amplification factor also yields information about the difference between the numerical and exact solutions for an initial condition consisting of an infinite sine wave of wavelength $N_\lambda \Delta x$. While the advection equation (1.1) propagates this wave at speed u and unchanged amplitude, a finite difference equation may transmit the wave at another speed u_N and a different amplitude. These effects of the finite difference method may be described by two parameters, the relative wave speed and the amplitude attenuation which occurs in one wave period. The relative wave speed is denoted and defined by

(2.5) $$\mu = u_N/u = -N_\lambda \, \mathrm{Arg}\{G(c,N_\lambda)\}/2\pi c,$$

and the amplitude attenuation per wave period is given by

(2.6) $$\gamma = |G(c,N_\lambda)|^{N_\lambda/c},$$

(see Noye, 1984b, p.193).

The wave deformation parameters, μ and γ, of the first order upwind equation (2.3) are graphed against N_λ for various c, in Figure 1.

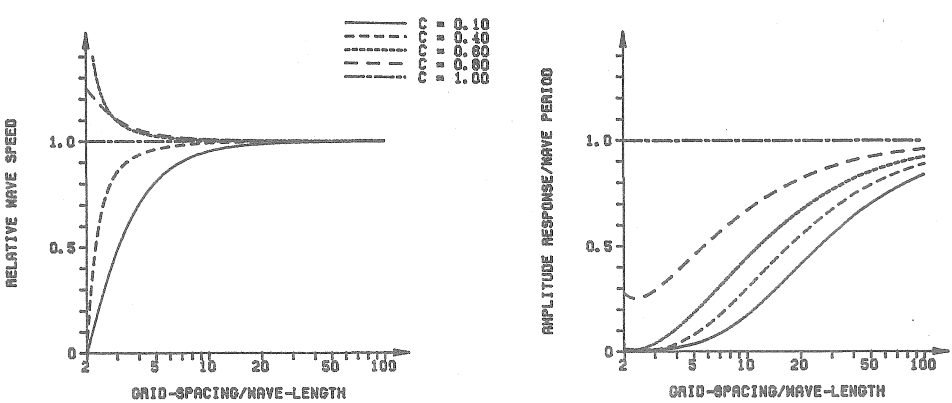

Fig. 1 : Wave propagation parameters for first order upwind method.

The loss of amplitude of component waves is very large; for instance, with $N_\lambda = 40$ and $c = 0.4$, the amplitude after one wave period falls to 0.7 of its original value, so that after two wave periods the amplitude is less than half its original value.

The effect of this is seen in Figure 2, in which is shown the numerical solution after 10 periods for the following test case. The initial conditions consist of an infinite set of Gaussian peaks (see dashed curve), symmetrical about $x = (P + \frac{1}{2})$, $P = 0, \pm 1, \pm 2, \ldots$, so it is periodic in space with period 1; that is, $\bar{\tau}(x+1,t) = \bar{\tau}(x,t)$. With $\Delta x = 0.025$ and $c = 0.4$, the numerical solution is obtained using cyclic boundary conditions; that is with $\tau_j^n = \tau_{j+J}^n$, $j = 0,1,\ldots,J-1$. The excessive wave damping is clear. In spite of this, "first-order upwinding is the industry standard in chemical, civil and mechanical engineering" (Leonard, 1981). First-order upwinding is the basic differencing scheme in many books including Gosman et.al. (1969) and Patankar (1980).

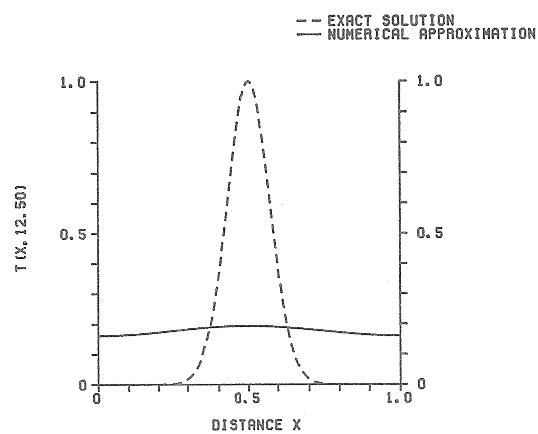

Fig. 2 : Gauss pulse problem solved using the first order upwind method.

The consistency analysis of (2.3) involves Taylor series expansions of each term of the finite difference equation about the gridpoint $(j\Delta x, n\Delta t)$. This yields at this gridpoint the equivalent partial differential equation

$$\frac{\partial \tau}{\partial t} + u\frac{\partial \tau}{\partial x} = -\frac{\Delta t}{2}\frac{\partial^2 \tau}{\partial t^2} + \frac{u\Delta x}{2}\frac{\partial^2 \tau}{\partial x^2} - \frac{(\Delta t)^2}{6}\frac{\partial^3 \tau}{\partial t^3} - \frac{u(\Delta x)^2}{6}\frac{\partial^3 \tau}{\partial x^3} + \ldots \tag{2.7}$$

from which may be derived the "modified" equation

$$(2.8) \qquad \frac{\partial\tau}{\partial t} + u\frac{\partial\tau}{\partial x} = \frac{u\Delta x}{2}(1-c)\frac{\partial^2\tau}{\partial x^2} - \frac{u(\Delta x)^2}{6}(1-c)(1-2c)\frac{\partial^3\tau}{\partial x^3} + \ldots$$

on successive substitution of (2.7) in itself to replace the temporal derivatives on the right side, by spatial derivatives (see Warming and Hyett, 1974). Clearly the finite difference equation (2.3) is consistent with the partial differential equations (1.1), because the right sides of (2.7) and (2.8) tend to zero as the grid-spacings Δt, Δx both tend to zero.

Equation (2.8), which has the general form

$$(2.9) \qquad \frac{\partial\tau}{\partial t} + u\frac{\partial\tau}{\partial x} = c_2\frac{\partial^2\tau}{\partial x^2} + c_3\frac{\partial^3\tau}{\partial x^3} + c_4\frac{\partial^4\tau}{\partial x^4} + c_5\frac{\partial^5\tau}{\partial x^5} + \ldots$$

is related to the amplitude response per wave period γ by the relation

$$(2.10) \qquad \gamma = \exp\{-\frac{4\pi^2}{N_\lambda}[\frac{c_2}{u\Delta x} - (\frac{2\pi}{N_\lambda})^2\frac{c_4}{u(\Delta x)^3} + \ldots]\},$$

and to the relative wave speed μ by

$$(2.11) \qquad \mu = 1 + (\frac{2\pi}{N_\lambda})^2\frac{c_3}{u(\Delta x)^2} - (\frac{2\pi}{N_\lambda})^4\frac{c_5}{u(\Delta x)^4} + \ldots .$$

(see Noye, 1984b, p.242). Clearly, the coefficients of the even derivatives of x, namely c_2, c_4, c_6, ..., contribute to the amplitude error, whereas the odd coefficients c_3, c_5, c_7, ..., contribute to the wave speed error. Thus, if c_2 is negative, γ is larger than 1, and the amplitude of any perturbation will grow exponentially as N_λ becomes very large. In such a case, the finite difference equation is unstable.

For the first order upwind equation (2.3) the amplitude response per wave period is

$$(2.12) \qquad \gamma = \exp\{\frac{-2\pi^2(1-c)}{N_\lambda}[1 - (\frac{2\pi}{N_\lambda})^2\frac{(1-6c+6c^2)}{12} + \ldots]$$

$$\to 1(-) \text{ as } N_\lambda \to \infty \text{ for fixed } c \text{ in } 0 < c < 1.$$

The relative wave speed is

$$(2.13) \qquad \mu = 1 - (\frac{2\pi}{N_\lambda})^2\frac{(1-c)(1-2c)}{6}[1 - (\frac{2\pi}{N_\lambda})^2\frac{(1-12c+12c^2)}{20} + \ldots]$$

$$\to \left\{\begin{array}{l} 1(-) \text{ for fixed } c \text{ in } 0 < c < \frac{1}{2} \\ 1(+) \text{ for fixed } c \text{ in } \frac{1}{2} < c < 1 \end{array}\right\} \text{ as } N_\lambda \to \infty.$$

These asymptotic properties of γ and μ for large N_λ are seen in Figure 1.

3. TWO OTHER FINITE DIFFERENCE METHODS

If the two-point forward time and two-point centred space approximations are substituted into Equation (2.1), the following centred space finite difference equation is obtained:

$$\tau_j^{n+1} = \tfrac{1}{2}c\tau_{j-1}^n + \tau_j^n - \tfrac{1}{2}c\tau_{j+1}^n. \tag{3.1}$$

The corresponding modified equation is

$$\frac{\partial\tau}{\partial t} + u\frac{\partial\tau}{\partial x} = -\frac{u\Delta x}{2}c\frac{\partial^2\tau}{\partial x^2} - \frac{u(\Delta x)^2}{6}(1+2c^2)\frac{\partial^3\tau}{\partial x^3} - \ldots \tag{3.2}$$

Equation (3.2) is consistent with (1.1), but the negative coefficient of $\partial^2\tau/\partial x^2$ indicates that perturbations will magnify exponentially so the equation is unstable.

If the three-point backward space approximation is used with the two-point forward time approximation, the following three-point upwind finite difference equation is obtained:

$$\tau_j^{n+1} = -\tfrac{1}{2}c\tau_{j-2}^n + 2c\tau_{j-1}^n + \tfrac{1}{2}(2-3c)\tau_j^n. \tag{3.3}$$

The corresponding modified equation is

$$\frac{\partial\tau}{\partial t} + u\frac{\partial\tau}{\partial x} = -\frac{u\Delta x}{2}c\frac{\partial^2\tau}{\partial x^2} + \frac{u(\Delta x)^3}{3}(1-c^2)\frac{\partial^3\tau}{\partial x^3} + \ldots \tag{3.4}$$

which indicates that (3.3) is unstable because, like (3.2), the coefficient of $\partial^2\tau/\partial x^2$ is always negative.

In spite of their instability, it is seen in the next Section that Equations (3.1) and (3.3) may be used with (2.3) to give more accurate finite difference methods than (2.3).

4. SOME HIGHER ORDER METHODS

If the modified equations (2.8) and (3.2) are multiplied by c and (1-c) respectively, then added, the term containing $\partial^2\tau/\partial x^2$ in the truncation error of Equation (2.9) is eliminated. Applying the same procedure to the finite difference equations (2.3) and (3.1) yields the Lax-Wendroff equation

$$\tau_j^{n+1} = \tfrac{1}{2}c(1+c)\tau_{j-1}^n + (1-c)(1+c)\tau_j^n - \tfrac{1}{2}c(1-c)\tau_{j+1}^n, \tag{4.1}$$

with corresponding modified equation

$$\frac{\partial \tau}{\partial t} + u\frac{\partial \tau}{\partial x} = -\frac{u(\Delta x)^2}{6}(1-c^2)\frac{\partial^3 \tau}{\partial x^3} - \frac{u(\Delta x)^3}{8}c(1-c^2)\frac{\partial^4 \tau}{\partial x^4} + \ldots \quad (4.2)$$

Equation (4.1) is stable for $0 < c \leq 1$.

Graphs of the wave propagation parameters of (4.1) are shown in Figure 3. These properties are discernable in the results of the Gauss pulse test, Figure 4, which shows the main peak in the numerical solution ($N_\lambda = 40$) lagging behind the true solution. The small peak which appears ahead of the true solution ($N_\lambda \simeq 14$) is actually trailing behind the peak at x = 1.5 in the exact solution.

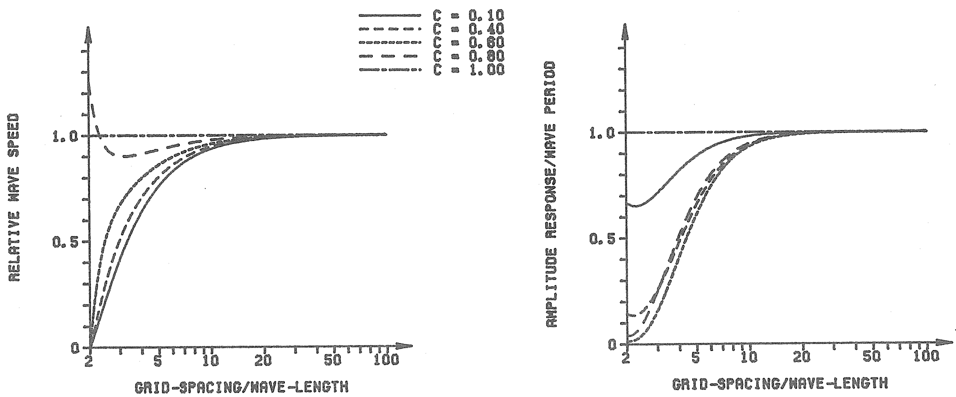

Fig. 3 : Wave propagation parameters for the Lax-Wendroff method.

Alternatively, the coefficient c in the modified equation may be made zero by adding equations (2.8) and (3.4) multiplied by the same weights as before, c and (1-c) respectively. When the finite difference equations (2.3) and (3.3) are treated similarly, the optimal three-point upwind equation is obtained:

$$\tau_j^{n+1} = -\tfrac{1}{2}c(1-c)\tau_{j-2}^n + c(2-c)\tau_{j-1}^n + \tfrac{1}{2}(1-c)(2-c)\tau_j^n, \quad (4.3)$$

which is stable for $0 < c \leq 2$ and has the corresponding modified equation

$$\frac{\partial \tau}{\partial t} + u\frac{\partial \tau}{\partial x} = \frac{u(\Delta x)^2}{6}(1-c)(2-c)\frac{\partial^3 \tau}{\partial x^3} - \frac{u(\Delta x)^3}{8}(1-c)^2(2-c)\frac{\partial^4 \tau}{\partial x^4} + \ldots \quad (4.4)$$

The results of applying (4.3) to solve the Gauss pulse problem are shown in Figure 5. Component waves travel too fast in the numerical solution if $0 < c < 1$, which is in accord with the fact that the coefficient of $\partial^3\tau/\partial x^3$ (c_3 of Equation (2.9)) is positive.

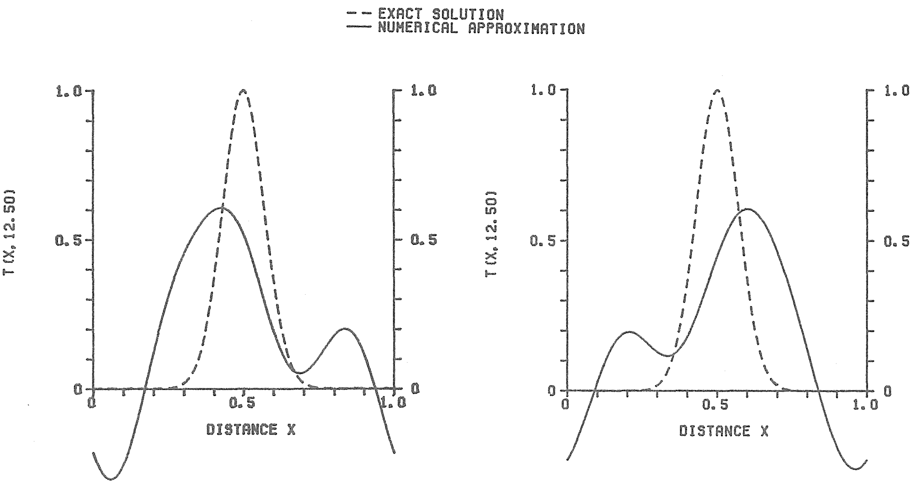

Fig. 4 : Gauss pulse test with Lax-Wendroff method.

Fig. 5 : Gauss pulse test with optimal 3-pt. upwind method.

We have seen that, for $0 < c < 1$, the finite difference equation (4.1) propagates component waves too slowly whereas (4.3) propagates them too quickly. Taking the arithmetic mean of these two equations would give a wave speed which is nearer the exact value. This yields Fromm's (1968) "zero-average" phase error method, stable for $0 < c \leq 1$,

$$(4.5)\qquad \tau_j^{n+1} = -\tfrac{1}{4}c(1-c)\tau_{j-2}^n + \tfrac{1}{4}c(5-c)\tau_{j-1}^n + \tfrac{1}{4}(1-c)(4+c)\tau_j^n - \tfrac{1}{4}c(1-c)\tau_{j+1}^n$$

in which the coefficient c_3 of the derivative $\partial^3\tau/\partial x^3$ of the truncation error in (2.9) is smaller than those in (4.2) and (4.4). However, the coefficient of $\partial^3\tau/\partial x^3$ in the modified equation (2.9) can be made zero by multiplying (4.1) by $(2-c)/3$ and adding (4.3) multiplied by $(1+c)/3$. The result is a third-order upwind biassed equation, stable for $0 < c \leq 1$,

$$(4.6)\qquad \tau_j^{n+1} = -\frac{1}{6}c(1-c)(1+c)\tau_{j-2}^n + \tfrac{1}{2}c(2-c)(1+c)\tau_{j-1}^n + \tfrac{1}{2}(1-c)(2-c)\tau_j^n - \frac{1}{6}c(1-c)(2-c)\tau_{j+1}^n,$$

with the modified equation

$$(4.7)\qquad \frac{\partial\tau}{\partial t} + u\frac{\partial\tau}{\partial x} = -\frac{u(\Delta x)^3}{24}(1-c)(2-c)(1+c)\frac{\partial^4\tau}{\partial x^4} + \frac{u(\Delta x)^4}{60}(1-c)(2-c)(1+c)(1-2c)\frac{\partial^5\tau}{\partial x^5} + \ldots$$

Use of Fromm's equation (4.5) and the upwind biassed equation (4.6) to solve the Gauss pulse problem (see Figures 6, 7) indicates the superiority of both over the Lax-Wendroff and the optimal three-point upwind equations. The peaks in the numerical solutions are now more nearly aligned with those of the exact solution, particularly for the third-order upwind biassed equation. Leonard (1984) states that, in his opinion, "third-order upwinding is the rational basis for the development of clean and robust algorithms for computational fluid mechanics". However, more accurate higher order methods can be derived from (4.6).

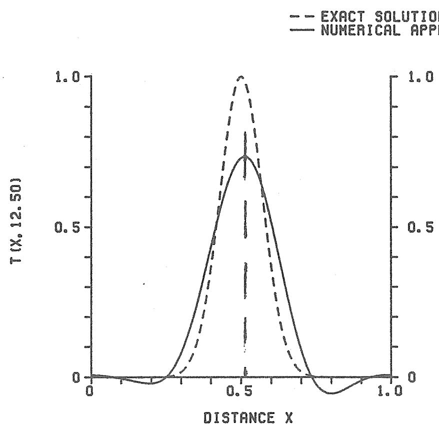

Fig. 6 : Gauss pulse test with Fromm's method.

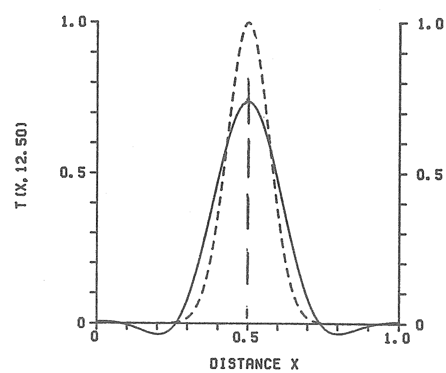

Fig. 7 : Gauss pulse test with 3rd-order upwind biassed method.

Replacing Δx by $-\Delta x$ in (4.6) and (4.7) yields the finite difference equations

$$(4.8) \qquad \tau_j^{n+1} = \frac{1}{6}c(1+c)(2+c)\tau_{j-1}^n + \tfrac{1}{2}(1+c)(2+c)(1-c)\tau_j^n - \tfrac{1}{2}c(2+c)(1-c)\tau_{j+1}^n + \frac{1}{6}c(1+c)(1-c)\tau_{j+2}^n$$

with corresponding modified partial differential equation

$$(4.9) \qquad \frac{\partial\tau}{\partial t} + u\frac{\partial\tau}{\partial x} = \frac{u(\Delta x)^3}{24}(1+c)(2+c)(1-c)\frac{\partial^4\tau}{\partial x^4} + \frac{u(\Delta x)^4}{60}(1+c)(2+c)(1-c)(1+2c)\frac{\partial^5\tau}{\partial x^5} + \ldots$$

Since addition of (4.7) multiplied by $(2+c)/4$ and (4.9) multiplied by $(2-c)/4$ eliminates the coefficient of $\partial^4\tau/\partial x^4$ in the modified equations, then similar operations applied to the finite difference equations (4.6) and (4.8) yield the fourth-order accurate equation, see Rusanov (1970) and Burstein and Mirin (1970):

$$(4.10)\quad \tau_j^{n+1} = -\frac{1}{24}c(1-c)(1+c)(2+c)\tau_{j-2}^n + \frac{1}{6}c(2-c)(1+c)(2+c)\tau_{j-1}^n + \tfrac{1}{4}(1-c)(2-c)(1+c)(2+c)\tau_j^n - \frac{1}{6}c(1-c)(2-c)(2+c)\tau_{j+1}^n + \frac{1}{24}c(1-c)(1+c)(2+c)\tau_{j+2}^n.$$

This is generally referred to as Rusanov's "Minimum amplitude error" method and is stable for $0 < c \leq 1$.

Rusanov's "minimum phase error" method may be obtained in a similar way, by eliminating the coefficients of $\partial^5\tau/\partial x^5$ from (4.7) and (4.9) by multiplying by $(1+2c)(2+c)/10c$ and $(1-2c)(2-c)/10c$ respectively, and subtracting. Applying this procedure to the finite difference equations (4.6) and (4.8) yields the equation, stable for $0 < c \leq 1$:

$$(4.11)\quad \tau_j^{n+1} = -\frac{1}{60}c(1-c)(1+c)(1+2c)(2+c)\tau_{j-2}^n + \frac{1}{30}(2-c)(1+c)(2+c)(1+4c)\tau_{j-1}^n + \frac{1}{5}(1-c)(2-c)(1+c)(2+c)\tau_j^n + \frac{1}{30}(1-c)(2-c)(2+c)(1-4c)\tau_{j+1}^n - \frac{1}{60}(1-c)(1-2c)(2-c)(1+c)\tau_{j+2}^n.$$

Results from the use of (4.10) and (4.11) to solve the Gauss pulse problem are seen in Figures 8 and 9. The improvement in amplitude response of the "minimum amplitude error" method over the third order upwinding equation (4.6) is evident, as is the improvement in wave speed of the "minimum phase error" method. Although the Rusanov equations appear to involve an additional spatial gridpoint compared to the third-order upwind-biassed equation, the fact that the velocity u may be either positive or negative in a realistic situation means that, in practice, they all require two spatial gridpoints each side of the central gridpoint. The problems which then remain, are that, firstly, values of the dependent variable τ at the gridpoint next to the boundary $x = 0$ (i.e. $j = 1$) must be interpolated with an accuracy at least that of the method being used and, secondly, in order to reach a given gridpoint $(j\Delta x, n\Delta t)$ in x-t space, the initial set of values may need to extend well beyond values at $j\Delta x$ because of the triangular shape of the computational domain. However, these complications are more than compensated for, by the much greater accuracy of the higher order methods.

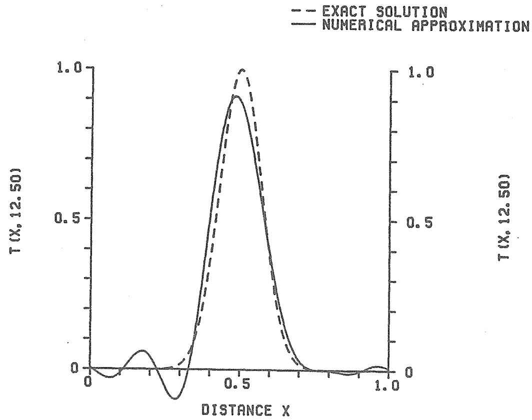

Fig. 8 : Gauss pulse test with Rusanov's min. amplitude error method.

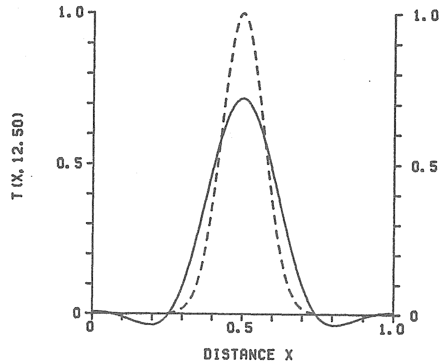

Fig. 9 : Gauss pulse test with Rusanov's min. phase error method.

5. SUMMARY

This article reviews in a systematic fashion some of the explicit finite difference methods of solving the advection equation. Use of the modified partial differential equation which is equivalent to a finite difference equation used to solve the advection equation, contains in the truncation error terms of the form $c_p\ \partial^p T/\partial x^p$, p=2,3,4,.. The even indexed terms contribute to the error in amplitude response, γ, and the odd indexed terms contribute to the error in relative wave speed, μ. By successively eliminating these terms, it has been shown that methods of increasing order of accuracy are obtained. This procedure can be continued, in order to produce even more accurate schemes in which the spurious oscillations are almost eliminated. This is the subject of a further article on this work.

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