We introduce and analyze a collection of difference schemes for the numerical solution of a model multi-dimensional equation of Schrödinger type with applications to the three dimensional parabolic wave equation arising from the sound propagation in the ocean. This collection of methods includes explicit and implicit schemes, 2-level and 3-level schemes and real and complex schemes. Many of these are analogous to classical schemes for the heat equation and the wave equation but some schemes are unique to the Schrödinger equation. Von Neumann type stability results are given for all the schemes. Numerical results arising from the application to an ocean acoustic problem are presented.

Difference Schemes for The Parabolic Wave Equation in Ocean Acoustics

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Research Report YALEU/DCS/RR-329
December 1984

The authors were supported in part by the Department of Energy under contract DE-AC02-81ER10996, by the Army Research Office under contract DAAG-83-0177, by the ONR Grant N00014-82-K-0184 and by Naval Underwater Systems Center Independent Research Project A65020.

Keywords: *Schrödinger's equation, parabolic wave equation, finite difference methods, stability, multi-dimensional problems.*

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1. Introduction

The parabolic wave equation (PWE) [18] is an equation that has been used frequently in the modelling of acoustic wave propagation in the ocean. This paper is concerned with numerical methods for solving it.

Many methods have been proposed for the solution of the PWE. Among these are the Fourier split-step [7], implicit finite difference (Crank Nicolson) [10], and method of lines based on the Adam-Bashforth formula [11]. In this paper, we present a collection of finite difference schemes for the solution of the PWE. Compared to Fourier type schemes, finite difference schemes are more generally applicable to variable coefficient problems, such as those that arise in the wide angle case [16, 17] and the variable density case [8]. Moreover, the treatment of solid bottom boundary conditions is considerably easier for finite difference schemes.

Traditionally, only *implicit* finite difference schemes have been used. As we shall show later, this is not too surprising because some of the more natural *explicit* schemes are unstable. In this paper, we shall show how to construct new and stable explicit schemes. We are particularily interested in explicit schemes because they are simple to implement, require less storage and are easier to vectorize on many pipeline computers. These advantages are especially pronounced for multi-dimensional problems.

For each of the proposed schemes, we present its stability and accuracy properties. All the stability results are given for the general multi-dimensional case. Only an outline is given here - the derivations and more general results can be found in [2, 3, 4].

In Section 2 we derive the parabolic equation and its model Schrödinger type equation. In Section 3 we discuss the definition of stability that we use for analyzing the schemes. The various schemes and their properties are presented in Sections 4 - 9. Some of the schemes are applied to an ocean acoustic problem, and the numerical results are presented in Section 10.

2. The Paraoblic Wave Equation and Its Model Equation

The propagation of acoustic waves in a stratified three-dimensional ocean can be described by the following wave equation in cylindrical coordinates:

$$\phi_{rr} + \frac{1}{r}\phi_r + \frac{1}{r^2}\phi_{\theta\theta} + \phi_{zz} + k_0^2 n^2(r,\theta,z)\phi = 0,$$

where $\phi(r,\theta,z)$ denotes the acoustic pressure field, z the depth variable, r the range variable, θ the azimuthal angular variable, k_0 the reference wave number, $n(r,\theta,z) = \frac{C_0}{C(r,\theta,z)}$ the index of refraction with $C(r,\theta,z)$ being the sound speed and C_0 a reference sound speed.

Following Tappert[18], we let $\phi(r,\theta,z) = u(r,\theta,z)v(r)$, where $u(r,\theta,z)$ depends only weakly on r. Then in the far-field with $k_0 r >> 1$, one can derive that u and v satisfy the equations:

$$v(r) = \sqrt{\frac{2}{\pi k_0 r}} e^{ik_0(r-\frac{\pi}{4})},$$

and

$$u_{rr} + 2ik_0 u_r + \frac{1}{r^2}u_{\theta\theta} + u_{zz} + k_0^2(n^2-1)u = 0.$$

Since u is assumed to be a slowly varying function of r, if we drop the u_{rr} term in the above equation, we arrive at the so called three-dimensional parabolic wave equation:

$$u_r = \frac{i}{2k_0}u_{zz} + \frac{i}{2k_0 r^2}u_{\theta\theta} + \frac{i}{2}k_0\left(n^2-1\right)u.$$

To facilitate the analysis of difference schemes for the parabolic wave equation, we consider the following constant coefficient model Schrödinger equation in m dimensions:

$$u_t = \sum_{l=1}^{m} ib_l u_{x_l x_l} + iau,$$

where a and $b_l > 0$ are real. Consider the one dimensional case ($m = 1$):

$$u_t = ibu_{xx} + iau.$$

A Fourier mode $e^{i2\pi\omega}$ will be propagated by this equation according to:

$$u(x,t) = e^{i2\pi\omega(x-2\pi\omega bt)}e^{iat}. \tag{2.1}$$

Thus, although the equation "appears" parabolic, it exhibits a dispersive wave behaviour.

3. Stability

The usual definition of stability is the so-called Von Neumann stability condition:

$$|R| \leq 1 + O(k) \quad as\ k,\ h \to 0,$$

where R is any root of the characteristic polynomial of the numerical scheme and k and h are the temporal and spatial mesh sizes. While this definition is sufficient to guarantee convergence of the numerical solution as k and h tend to 0 for any consistent scheme [14], for *fixed k and h*, it does allow numerical solutions that can ***grow*** with each time step. On the other hand, it follows from (2.1) that the exact solution of the PWE has the property that $||u(x,t)||_{L_2}$ is conserved at all time. It thus seems natural to require that the numerical solution also satisfy a similar property. Since it is more difficult to construct schemes that have exact conservation properties, we shall require only that the numerical solution does not grow with the time step. This is equivalent to the condition that

$$|R| \leq 1 \quad for\ any\ k\,, h.$$

This is sometimes known as the ***practical stability condition*** [1, 14] and is the one that we shall adopt in this paper.

For simplicity, we shall present only schemes for the simplified model equation:

$$u_t = \sum_{l=1}^{m} ib_l u_{x_l x_l}. \tag{3.1}$$

Under the Von Neumann stability definition, the addition of lower order terms, like the iau term in the PWE, does not affect the stability of a numerical scheme for (3.1). This is not so for the practical stability definition. In practice, the lower order term iau is multiplied by some positive powers of h in a numerical scheme and if h is small enough, its effect is usually negligible on the stabililty. In any case, since the practical stability condition obviously implies the Von Neumann condition, the stability conditions given here are sufficient to guarantee the convergence of the numerical solution as k and h tend to zero, even in the presence of lower order terms.

4. Simple Explicit Schemes in One Dimension

The instability of some standard explicit schemes can be illustrated in one dimension. Consider the Taylor series expansion:

$$u(x,t+k) = u(x,t) + ku_t + \frac{k^2}{2}u_{tt} + \cdots\cdots$$
$$= u(x,t) + k(iu_{xx}) + \frac{k^2}{2}(i^2 u_{xxxx}) + \cdots$$

A family of explicit difference schemes can be derived by replacing the spatial derivatives by their difference approximations:

$$\frac{u_j^{n+1} - u_j^n}{k} = \sum_{l=1}^{p} \frac{k^{l-1}}{l!}\left(iD_j^n\right)^l u,$$

where

$$D_j^n u = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}.$$

The truncation error is $O(k^p, h^2)$. The amplification factor is given by :

$$R = 1 - i\gamma - \frac{\gamma^2}{2} + \frac{i\gamma^3}{6} + \cdots,$$

where

$$\gamma = 4r\sin^2\frac{\theta}{2}, \quad \text{with } 0 \le \theta \le 2\pi, \; r = \frac{k}{h^2}.$$

Stability requires

$$|R| \le 1 \quad \text{for} \quad 0 \le \theta \le 2\pi.$$

For $p = 1$ (the Euler Scheme), $|R|^2 = 1 + \gamma^2 > 1$, and thus this scheme is unstable.

For $p = 2$ (a Lax Wendroff type scheme), $|R|^2 = 1 + \frac{\gamma^4}{4} > 1$, and thus this is also unstable. The next two members of this family are stable, however, with the stability conditions:

$$p = 3: \; r \le \frac{\sqrt{3}}{4},$$
$$p = 4: \; r \le \frac{\sqrt{3}}{2\sqrt{2}}.$$

5. Stable Explicit Schemes with Artificial Dissipation

The Euler scheme can be made stable by adding the appropriate amount of artificial dissipation. Consider the multi-dimension equation:

$$u_t = \sum_{l=1}^{m} ib_l u_{x_l x_l},$$

and the Euler scheme with artificial dissipation :

$$\frac{u_j^{n+1} - u_j^n}{k} = \sum_{l=1}^{m} b_l\left(iD_{j,l}^n u + (\alpha + i\beta)h_l^2\left(D_{j,l}^n\right)^2 u\right),$$

where α, β are arbitrary real constants, h_l denotes the spatial mesh size in the x_l direction and $D^n_{j,l}$ denotes the D^n_j operator in the x_l direction. The dissipative term corresponds to adding terms of the form $(\alpha + i\beta)h^2 u_{xxxx}$ to the model equation. It is proven in [4] that the stability condition is :

$$\alpha < 0 \quad \text{and} \quad k \leq \min\left(-\frac{2\alpha}{\sum_{l=1}^{m} \frac{b_l}{h_l^2}}, -\frac{\alpha}{\left[\alpha^2 + (\beta - \frac{1}{4})^2\right] \sum_{l=1}^{m} \frac{b_l}{h_l^2}} \right).$$

The scheme with the least restrictive stability condition is :

$$\alpha = -\frac{1}{4},\ \beta = \frac{1}{4},$$

with the stability condition:

$$k \leq \frac{1}{2 \sum_{l=1}^{m} \frac{b_l}{h_l^2}}.$$

6. General Two-Level Scheme

Consider the general two level scheme :

$$\frac{u_j^{n+1} - u_j^n}{k} = \mu \sum_{l=1}^{m} i b_l D_{j,l}^{n+1} u + (1 - \mu) \sum_{l=1}^{m} i b_l D_{j,l}^{n} u,$$

with $0 \leq \mu \leq 1$. With $\mu = 0$, we have the Euler scheme, while $\mu = \frac{1}{2}$ corresponds to the Crank-Nicolson scheme and $\mu = 1$, the backward Euler scheme.

The truncation error is :

$$\begin{cases} O(k, h^2) & \text{if} \quad \mu \neq \frac{1}{2} \\ O(k^2, h^2) & \text{if} \quad \mu = \frac{1}{2}. \end{cases}$$

The scheme is stable if $\frac{1}{2} \leq \mu \leq 1$, and unstable otherwise.

7. Leap-Frog

Consider the Leap-Frog scheme:

$$\frac{u_j^{n+2} - u_j^n}{2k} = \sum_{l=1}^{m} i b_l\, D_{j,l}^{n+1} u.$$

The truncation error is $O(k^2, h^2)$. The stability condition is :

$$k \leq \frac{1}{4 \sum_{l=1}^{m} \frac{b_l}{h_l^2}}.$$

Thus this scheme is explicit and conditionally stable. However, three time levels must be used.

8. Du-Fort Frankel

The Du-Fort Frankel scheme is a well-known explicit, unconditionally stable scheme for the heat equation. For our model equation, it is given by :

$$\frac{u_j^{n+2} - u_j^n}{2k} = \sum_{l=1}^{m} i b_l \, DF_{j,l}^{n+1} u,$$

where

$$D\,F_j^{n+1} u = \frac{1}{h^2}\left(u_{j+1}^n - u_j^{n-1} - u_j^{n+1} + u_{j-1}^n\right).$$

This scheme is also unconditionally stable. The truncation error is $O\left(k^2, h^2, \left(\frac{k}{h}\right)^2\right)$ and thus unless $\frac{k}{h} \to 0$, this scheme is inconsistent.

9. Real System

The previous schemes are all derived directly from the original complex model equation (3.1). If we let $u \equiv v + iw$, where v, w are the real and imaginary parts of u, then v and w satisfy the following equations :

$$v_t = -\sum_{l=1}^{m} b_l w_{x_l x_l},$$

$$w_t = \sum_{l=1}^{m} b_l v_{x_l x_l}.$$

Unlike the previous schemes, these two equations can be treated differently. For example, consider the following two-level *explicit* scheme :

$$\frac{v_j^{n+1} - v_j^n}{k} = -\sum_{l=1}^{m} b_l D_{j,l}^n w$$

$$\frac{w_j^{n+1} - w_j^n}{k} = \sum_{l=1}^{m} b_l D_{j,l}^{n+1} v.$$

The truncation error is $O(k, h^2)$. Note that it has the same stencil as the Euler scheme. However, it is conditionally stable, with the stability condition :

$$k \le \frac{1}{2\left(\sum_{l=1}^{m} \frac{b_l}{h_l^2}\right)}.$$

Other time differencing can be applied to the real system. For example, a scheme similar to the above one but based on the Leap Frog differencing has been recently proposed by Peggion and O'Brien [13]. The stability property is similar to that of the Leap Frog scheme presented in Section 7.

10. Numerical Examples

This section is divided into two parts. Part 1 presents the computations performed on two-dimensional problems and Part 2 presents the computations performed on a three-dimensional problem. All numerical results were required to satisfy an acceptable accuracy with a relative error less than 1 percent. These results were compared with known reference solutions for accuracy and speed. All computations were made on the VAX 11/780 computer with complex, single-precision arithmetic.

10.1. Two-Dimensional Problems

Two sets of numerical results are presented in this section. The first set shows the application of an explicit scheme to a real ocean acoustic problem; the accuracy of the results were then determined by comparing with results from other known reference solutions. The second set uses an exact reference solution to examine a set of explicit schemes; the accuracy of these results and the speed of the computation were then compared with those from the Crank-Nicolson solution. Both sets are shown in graphical and tabular form in this section.

10.1.1. An Application

Solutions to a real ocean acoustic problem such as arises in the Mediterranean Sea, were produced by a number of methods [2, 9, 10]. The real ocean scenario consists of a point source at a depth of 50 m and a frequency of 500Hz. The region of propagation is regular with an ocean depth of 100 m and a water column density of $1.0g/cm^2$. The receiver is also placed at 50 m. The sound travels at a constant speed of 1500 m/s. Starting at the origin, propagation is to be predicted up to 40 km. Below the bottom, a slight density change is anticipated ($1.2g/cm^2$) with an attenuation of 1db/wavelength. The existing Crank-Nicolson [10] solution partitions the depth direction interval into 200 points (i.e., the depth increment of 0.5 m). The Crank-Nicolson method marches with a range increment of 0.5 m. We selected Scheme 5 for the same application. Results for both solutions agree surprisingly well, as shown in Figure 1.

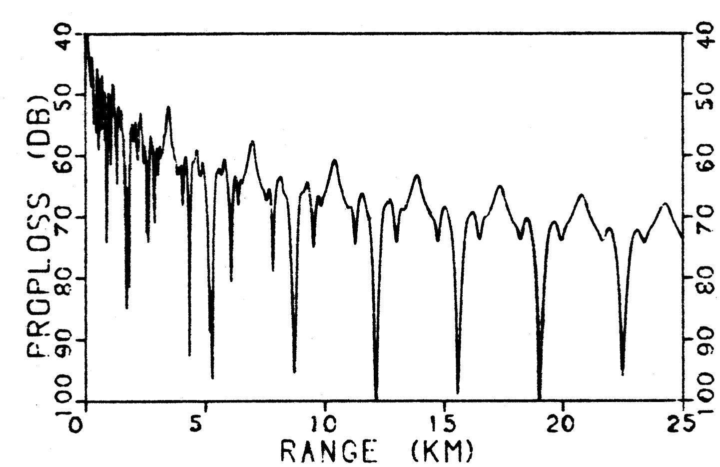

Figure 1: Propagation loss versus range

10.1.2. An Examination of Computational Speed

It was expected that for the same range step size, the explicit schemes would perform at a faster speed and with the same accuracy as did Crank- Nicolson scheme. The three explicit schemes selected (Schemes 5, 8, and 9) were used to solve a simple model equation with a known solution. This test required the same accuracy as did the test in the previous section (within 1 percent). The simple model equation is

$$u_r = \frac{i}{2k_0} u_{zz} \tag{10.1}$$

whose exact solution is

$$u(r,z) = \frac{1}{\sqrt{r}} e^{\frac{ik_0(z-50)^2}{2r}} \tag{10.2}$$

Most of the input parameters were chosen arbitrarily for the test. Specially chosen parameters included the depth increment (1 m) and the maximum range (200 m). Table 1 shows the accuracy requirement for the computations; it also shows the CPU time, using the same time step of 0.001 m.

METHOD	RANGE STEP SIZE (m)	ERROR Real	ERROR Imaginary	CPU Hr–min–sec
Crank–Nicolson	0.001	$-0.77E-02$	$-0.024E-02$	02–07–38.11
5–point	0.001	$-0.83E-02$	$-0.025E-02$	00–48–39.78
DuFord–Frankel	0.001	$-0.74E-02$	$-0.025E-02$	01–21–30.81
Real–Imaginary	0.001	$-0.76E-02$	$-0.024E-02$	00–53–14.00

Table 1: Two–Dimensional Results

Remarks: For two-dimensional problems, the Crank-Nicolson scheme is only required to solve a special tridiagonal system of equations and can thus take advantage of an efficient tridiagonal solver. For the same step size, the explicit schemes are faster than the Crank-Nicolson scheme. However, the Crank-Nicolson scheme can use a larger range step size than the other explicit scheme because of its unconditional stability. The real advantage of the explicit schemes in computational speed can only be appreciated in the next section where they are used to solve a three-dimensional problem.

10.2. Three-Dimensional Problem

In studying the three-dimensional ocean environmental effects, Lee and Siegmann [12] developed a three-dimensional wide angle wave equation in which the narrow angle wave equation is a special case, which is a parabolic equation of the Schrodinger type. To test the validity of this development, Lee and Siegmann constructed an exact solution of the form

$$u(r,\theta,z) = sin(\Omega z) e^{im\theta} e^{i\frac{m^2}{2k_0 r}} \tag{10.3}$$

This solution was designed to satisfy the three-dimensional narrow angle wave equation, a parabolic equation of the Schrodinger type, i.e.,

$$u_r = \frac{i}{2} k_0 (n^2(r,\theta,z) - 1) u + \frac{i}{2k_0} u_{zz} + \frac{i}{2k_0 r^2} u_{\theta\theta} \tag{10.4}$$

Schultz-Lee-Jackson [15] applied the Crank-Nicolson scheme and the Yale Sparse Matrix Package [5, 6] to solve Eq. (10.4). The main advantage of the explicit schemes is the saving in speed and memory storages - there is no need to solve a large sparse system. Because Scheme 5 produced satisfactory results for two-dimensional computations, we extended the scheme to solve Eq. (10.4) using the exact solution in Eq. (10.3) as a comparison; the Crank-Nicolson solution [15] was also compared. Most input parameters were the same as those for the two-dimensional problem. However, some additional information was needed for the three dimensional problem,including the azimuthal angular increment $\Delta\theta = 0.2$; the modal index m = 3; the angular sector $0 \leq \theta \leq 360^o$;

METHOD	ERROR Real	ERROR Imaginary	CPU Hr–min–sec
Crank–Nicolson	$0.18E-01$	$-0.12E-01$	03–47–09.63
5–point	$0.10E-01$	$-0.11E-01$	00–21–35.48

Table 2: Three-Dimensional Results

and $\Omega = \pi/100$. To ensure the same accuracy, the range increment was determined to be 0.001 m for both the Crank-Nicolson method and Scheme 5. Computations were made up to 500 range steps so that visible CPU time could be recorded for comparison. Table 2 displays the results at a receiver depth of $100m$.

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