ON THE FOLDED LEAPFROG EXAMPLE; ESTIMATES AT A POINT FOR SOLUTIONS OF FINITE DIFFERENCE SCHEMES

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On the Folded Leapfrog Example; Estimates at a Point for Solutions of Finite Difference Schemes

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Abstract. The folded leapfrog problem is a simple example in the theory of initial-boundary value problems for difference schemes that has, at first sight, a counter-intuitive result. In this paper we examine this problem and explain the source of the difficulty. The analysis leads to the consideration of L^2 norms in time of the finite difference solution at a point and estimates of these norms in terms of the initial data. Several theorems are presented giving optimal estimates.

1. Introduction

This paper presents several new estimates for solutions of finite difference schemes in one spatial dimension. These estimates are for the solution as a function of time at a point in space. We determine when the L^2 estimates over time of the solution at a point can be bounded by the L^2 norm of the initial data.

The motivation for this work came from an examination of a simple example in the theory of initial-boundary value problems, called the folded leapfrog problem. The folded leapfrog problem was discovered by L.N. Trefethen in about 1978 [4], and has, at first sight, a counter-intuitive result. In this paper we present the original folded-leapfrog example and discuss its consequences. We show that the example leads to the question of what conditions must hold in order to obtain L^2 estimates over time on the solution to a finite difference scheme at a fixed point. We then present several theorems related to the 'folded leapfrog' behavior.

For schemes in general, we obtain the best possible bounds on the growth of the L^2 norm in time of the solution at a point, and also an estimate for dissipative schemes. The analysis also leads to a conjecture, given at the end of section 5, as to when the L^2 norm in time of the solution at a point can be estimated by the L^2 norm of the initial data.

2. The Folded Leapfrog Problem

Consider the partial differential equation, the one-way wave equation,

$$u_t + au_x = 0 \tag{2.1}$$

for $x \in R$ and $t > 0$. The coefficient a is a real number. (The subscripts in (2.1) denote partial differentiation.) The initial value problem for (2.1) has the solution

$$u(t, x) = u_0(x - at)$$

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where u_0 is the initial data. The initial value problem for (2.1) is often used as a prototype for hyperbolic systems of partial differential equations, e.g., [2]. One estimate satisfied by the solution to (2.1) that concerns us in this paper is

$$\int_0^\infty |u(t,0)|^2 dt \leq |a|^{-1} \int_{-\infty}^\infty |u(0,x)|^2 dx\,. \tag{2.2}$$

Similar estimates hold for solution of more general hyperbolic systems. For example, for a general hyperbolic partial differential equation in n spatial dimensions, the L^2 norm of the solution over time on a $(n-1)$ dimensional sub-space is bounded by the L^2 norm of the initial data.

We now consider the 'folded' problem arising from (2.1), obtained by 'folding' the negative real portion of the spatial domain on top of the positive real portion. That is, define

$$v(t,x) = u(t,-x)$$

and by considering only positive values of x, we obtain the system

$$\begin{aligned} u_t + a u_x &= 0 \\ v_t - a v_x &= 0. \end{aligned} \tag{2.3}$$

To make the system (2.3) equivalent to (2.1) we have the one boundary condition

$$u(t,0) = v(t,0)\,. \tag{2.4}$$

There is no difficulty in showing that the 'folded' initial-boundary value problem (2.3) with (2.4) is equivalent to the original initial value problem (2.1).

However, a difficulty arises when considering finite difference approximations to the original initial-boundary value problem. We use the leapfrog scheme as an example. Consider a finite difference grid with space step h and time step k. We consider grid functions f_m^n defined at time level n and spatial point m. The time at time level n is nk, and the value of x at grid point m is mh for $m \in Z$. The leapfrog scheme for (2.1) is

$$\frac{u_m^{n+1} - u_m^{n-1}}{2k} + a\frac{u_{m+1}^n - u_{m-1}^n}{2h} = 0\,. \tag{2.5}$$

Thus if initial data is given at $n = 0$, and values are obtained at $n = 1$ by some means, for example,

$$u_m^1 = u_m^0 - a\frac{k}{2h}(u_{m+1}^0 - u_{m-1}^0)\,, \tag{2.6}$$

then the scheme (2.5) can be used to determine values of u_m^n for $n \geq 2$ and $m \in Z$. We set $\lambda = k/h$. The leapfrog scheme (2.5) is stable if and only if $|a|\lambda < 1$ is satisfied, e.g., [3]. (The use of (2.6) does not affect the stability of the leapfrog scheme.)

As was done with the partial differential equation, the finite difference scheme (2.5) can be converted to the folded problem

$$\begin{aligned} \frac{u_m^{n+1} - u_m^{n-1}}{2k} + a\frac{u_{m+1}^n - u_{m-1}^n}{2h} &= 0 \\ \frac{v_m^{n+1} - v_m^{n-1}}{2k} - a\frac{v_{m+1}^n - v_{m-1}^n}{2h} &= 0 \end{aligned} \tag{2.7}$$

for $n \geq 2$ and $m \geq 1$ with the two boundary conditions

$$u_0^n = v_0^n$$
$$\frac{u_0^{n+1} - u_0^{n-1}}{2k} + a\frac{u_1^n - v_1^n}{2h} = 0\,. \tag{2.8}$$

Values of u_m^1 and v_m^1 can be obtained similar to (2.6).

The initial-boundary value problem (2.7) and (2.8) is obviously equivalent to the initial value problem (2.5), yet the initial-boundary value problem (2.7) and (2.8) is unstable according to the theory developed by Gustafsson, Kreiss, and Sundström [1]. The analysis for this result is given in Section 7. We refer to this theory as the GKS theory.

The Folded Leapfrog Difficulty. *Why is the folded initial-boundary value problem* (2.7) - (2.8) *unstable when the original initial value problem is stable?*

In the next section we discuss the folded leapfrog difficulty and explain why it occurs. We also show that the difficulty occurs for schemes other than the leapfrog scheme, and determine, in Theorem 3.1, necessary and sufficient conditions for this to occur with conservative schemes.

Other theorems and results are given in section 5, along with some questions about possible estimates.

3. The Explanation of the Difficulty

We can explain the folded leapfrog difficulty by examining more closely the notions of stability for both the initial value problem and the initial-boundary value problem for finite difference schemes. Stability, in general, means that the solution as measured by some norm is bounded by the data in some norm. We now discuss the norms used in the definition of stability for the initial value problem and the initial-boundary value problem.

The von Neumann stability analysis for finite difference schemes applied to the initial value problem for (2.5) with initial data (2.6) requires that the L^2 estimate

$$||u^n||_h \leq C||u^0||_h \tag{3.1}$$

hold for some constant C. The norm is given by

$$||f||_h = \left(h \sum_{m=-\infty}^{\infty} |f_m|^2\right)^{1/2}. \tag{3.2}$$

For this particular problem the constant C can be taken independent of t, depending only on $|a|\lambda$. For general finite difference problems the constant C must be replaced by a function of t, see e.g., [3]

The initial-boundary value analysis of the GKS theory considers the estimate

$$|u_0|_{k,\eta} + ||u||_{k,h,\eta} + ||v||_{k,h,\eta} \leq C_\eta(||u^0||_h + ||v^0||_h) \tag{3.3}$$

for the problem (2.7) - (2.8) where the norms $|\cdot|_{k,\eta}$ and $||\cdot||_{k,h,\eta}$ are defined by

$$|f|_{k,\eta} = \left(k\sum_{n=0}^{\infty} |e^{-\eta nk} f^n|^2\right)^{1/2}$$
$$||f||_{k,h,\eta} = \left(kh\sum_{n=0}^{\infty}\sum_{m=-\infty}^{\infty} |e^{-\eta nk} f_m^n|^2\right)^{1/2},$$

and η is positive. The analysis required by the GKS theory, see Section 7, shows that the estimate (3.3) can not hold for (2.7) - (2.8).

Using (3.1) it is not difficult to obtain the estimate

$$\|u\|_{k,h,\eta} + \|v\|_{k,h,\eta} \leq C\eta^{-1/2}(\|u^0\|_h + \|v^0\|_h) \tag{3.4}$$

for the initial-boundary value problem. Comparison of (3.3) with (3.4) leads us to consider the term $|u_0|_{k,\eta}$ in the estimate (3.3). The term $|u_0|_{k,\eta}$ is a weighted L^2 norm, and by comparison with the estimate (2.2) we consider when the finite difference analog of (2.2) holds for finite difference schemes.

As we show, the basic difference between the folded differential equation problem and the folded finite difference problem is that the finite difference analog of (2.2) does not hold for the leapfrog scheme. We also show that there are many other schemes for which this estimate does not hold.

The characterization of those schemes for which this estimate does hold requires the study of the amplification factors of a finite difference scheme. For our purposes, the amplification factors $g_j(\theta)$ of a finite difference scheme are those functions such that

$$v_m^n = g_j(\theta)^n e^{im\theta}$$

is a solution of the finite difference scheme. The stability of the schemes is determined by the magnitude of the amplification factors. For the simple cases treated here we may use the restricted von Neumann condition, requiring

$$|g_j(\theta)| \leq 1 \quad \text{for all } j \text{ and } \theta.$$

Also required for stability is the condition that two amplification factors, g_j and g_k, can not be equal if their modulus is 1. See a text on finite difference schemes for a more general analysis, e.g., [3]. If there is only one amplification factor we write it as $g(\theta)$.

Since we frequently refer to the leapfrog scheme, we now determine its amplification factors, and the condition for stability. Substituting $u_m^n = g^n e^{im\theta}$ into the scheme (2.5), we obtain the equation

$$g^2 - 1 + 2ia\lambda g \sin\theta = 0$$

as the equation that g must satisfy to be a solution. We have set $\lambda = k/h$, as we do throughout this paper. The two solutions of this equation are

$$\begin{aligned} g_0(\theta) &= -ia\lambda\sin\theta + \sqrt{1 - a^2\lambda^2\sin^2\theta} \\ g_1(\theta) &= -ia\lambda\sin\theta - \sqrt{1 - a^2\lambda^2\sin^2\theta}. \end{aligned} \tag{3.5}$$

The condition that the magnitude of g_j not exceed 1 is that $|a\lambda|$ be at most 1. In this case we have $|g_j(\theta)| = 1$. The condition that g_0 not be equal to g_1 is that $|a\lambda|$ be strictly less than 1. The leapfrog scheme is stable if and only if $|a\lambda|$ is less than 1.

Schemes for which the amplification factors are all equal to 1 in modulus are called conservative schemes. These schemes are also called strictly non-dissipative schemes. The leapfrog scheme is an example of a conservative scheme.

The Crank-Nicolson scheme for (2.1) is

$$\frac{v_m^{n+1} - v_m^n}{2k} + a\frac{v_{m+1}^{n+1} - v_{m-1}^{n+1}}{4h} + a\frac{v_{m+1}^n - v_{m-1}^n}{4h} = 0$$

and is also an example of a conservative scheme. Its amplification factor is

$$g = \frac{1 - \frac{1}{2}ia\lambda\sin\theta}{1 + \frac{1}{2}ia\lambda\sin\theta}. \tag{3.6}$$

The Crank-Nicolson scheme is stable for all values of λ.

The next theorem characterizes those conservative schemes for which the the folded initial-boundary value problem is unstable. It reduces to showing when the finite difference analog of estimate (2.2) holds for conservative schemes.

Theorem 3.1. *For a conservative stable finite difference scheme with amplification factors* $g_0(\theta), \ldots, g_\nu(\theta)$ *there exists a constant* C *such that the inequality*

$$k\sum_{n=0}^{\infty} |v_0^n|^2 \le Ch \sum_{m=-\infty}^{\infty} |v_m^0|^2 \tag{3.7}$$

holds for all solutions to the finite difference scheme if and only if the functions

$$\frac{\partial g_j(\theta)}{\partial\theta}, \quad j = 0, \ldots, \nu \tag{3.8}$$

do not vanish for $\theta \in [-\pi, \pi]$.

Defining the norms

$$\|f\|_k = \left(k\sum_{n=0}^{\infty} |f^n|^2\right)^{1/2} \tag{3.9}$$

and

$$\|f\|_{k,N} = \left(k\sum_{n=0}^{N} |f^n|^2\right)^{1/2} \tag{3.10}$$

analogous to (3.2) we may restate (3.7) as

$$\|v_0\|_k \le C\|v^0\|_h.$$

For conservative schemes, the vanishing of the derivative of an amplification factor, i.e., (3.8), is equivalent to the vanishing of a group velocity of the scheme. This can be seen by writing $g(\theta) = e^{-i\psi(\theta)}$ and noting that the group velocity is given by the derivative of ψ with respect to θ, see e.g., [3]. The basic idea of Theorem 3.1 is that if the group velocity vanishes, then the modes associated with the vanishing group velocity do not propagate away, but remain, with only a small dispersive effect to slowly weaken them.

To prove the necessity of the derivatives (3.8) not vanishing for the estimate (3.7) to hold, we will construct a family of solutions to finite difference schemes for which the derivatives (3.8) vanish and for which the L^2 norm in time at a point grows without bound. As the construction is of some interest, we state the following theorems which show the growth rates that may be obtained if the derivatives (3.8) vanish.

Theorem 3.2. *If the group velocity vanishes at a point θ_0, i.e., $\psi_j'(\theta_0) = 0$, and $\psi_j''(\theta_0) \neq 0$ for some j, then there exists a family of solutions to the finite difference initial value problem v_m^n, and constants, C_0 and C_1, with C_0 positive, such that*

$$\|v_0\|_{k,N} \geq C_0 \|v^0\| \left((\ln N)^{1/2} - C_1 \right) . \tag{3.11}$$

Theorem 3.3. *If the group velocity vanishes at a point θ_0, i.e., for some j, $\psi_j'(\theta_0) = 0$, and $\psi_j^{(k)}(\theta_0) = 0$ for $1 \leq k < \ell$, with $\psi^{(\ell)}(\theta_0) \neq 0$, then there exists a family of solutions to the finite difference initial value problem v_m^n, and constants, C_0 and C_1, with C_0 positive, such that*

$$\|v_0\|_{k,N} \geq C_0 \|v^0\| N^{1/2 - 1/\ell} \left(1 - C_1 N^{-1/\ell} \right) . \tag{3.12}$$

In section 6, we give the results of computations demonstrating the growth rates (3.11) and (3.12) in particular cases.

4. The Proof of the Main Estimate

To prove Theorem 3.1, which is the chief result of this paper, we begin by considering the case of only one amplification factor. We have then the representation of the solution

$$v_m^n = \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} g(h\xi)^n e^{imh\xi} \hat{v}^0(\xi) d\xi \,, \tag{4.1}$$

see [3]. For a conservative scheme we may write

$$g(\theta) = e^{-i\psi(\theta)} \tag{4.2}$$

where $\psi(\theta)$ is a well-defined smooth function of θ in $[-\pi, \pi]$. Note that $\partial g / \partial \theta \neq 0$ implies that $\psi'(\theta) \neq 0$. Restricting (4.1) to m equal to 0, we then have

$$v_0^n = \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} e^{-in\psi(h\xi)} \hat{v}^0(\xi) d\xi \,. \tag{4.2}$$

From (4.2) we obtain

$$k \sum_{n=0}^{\infty} |v_0^n|^2 = \int_{-\pi/h}^{\pi/h} \overline{z(\xi)} \hat{v}^0(\xi) d\xi \tag{4.3}$$

where

$$z(\xi) = \frac{k}{\sqrt{2\pi}} \sum_{n=0}^{\infty} e^{in\psi(h\xi)} v_0^n \,.$$

If we consider the discrete function w^n which is v_0^n for nonnegative n and is 0 for negative n, we see that its Fourier transform in time can be written as

$$\hat{w}(\omega) = \frac{k}{\sqrt{2\pi}} \sum_{n=0}^{\infty} e^{-ink\omega} v_0^n \,.$$

This shows that

$$z(\xi) = \hat{w}(-k^{-1}\psi(h\xi)) \,. \tag{4.4}$$

From the relation (4.3) we have

$$\int_{-\pi/h}^{\pi/h} \overline{z(\xi)}\hat{v}^0(\xi)d\xi \le \|z\|_h \|v^0\|_h \,, \tag{4.5}$$

where

$$\|z\|_h^2 = \int_{-\pi/h}^{\pi/h} |z(\xi)|^2 d\xi \,.$$

Note that by Parseval's relation we have

$$\int_{-\pi/h}^{\pi/h} |\hat{v}^0(\xi)|^2 \, d\xi = h \sum_{m=-\infty}^{\infty} |v_m^0|^2 = \|v^0\|_h^2.$$

By (4.4) we have

$$\begin{aligned} \|z\|_h^2 &= \int_{-\pi/h}^{\pi/h} |\hat{w}(-k^{-1}\psi(h\xi))|^2 d\xi \\ &= h^{-1}\int_{-\pi}^{\pi} |\hat{w}(-k^{-1}\psi(\theta))|^2 d\theta \\ &= \left(\frac{k}{h}\right) \int_{-A\pi/k}^{A\pi/k} |\hat{w}(\omega)|^2 \frac{d\omega}{|\psi'(\theta)|} \end{aligned} \tag{4.6}$$

where $\pi A = \max|\psi(\theta)|$, and $\psi(\theta) = \omega$. (Recall that since $|\psi'| > 0$, ψ is monotone, and so $A = |\psi(\pi)|/\pi$.)

From (4.6) we obtain the upper bound

$$\begin{aligned} \|z\|_h^2 &\le \frac{\lceil A \rceil \lambda}{\min|\psi'(\theta)|} \int_{-\pi/k}^{\pi/k} |\hat{w}(\omega)|^2 d\omega \\ &= \frac{\lceil A \rceil \lambda}{\min|\psi'(\theta)|} \|v_0\|_k^2 \end{aligned}$$

by Parseval's relation. From this relation, (4.3), and (4.5) we obtain

$$\|v_0\|_k \le \left(\frac{\lceil A \rceil \lambda}{\min|\psi'(\theta)|}\right)^{1/2} \|v^0\|_h \,. \tag{4.7}$$

This proves that the condition (3.7) holds if the group velocity does not vanish for one-step schemes.

For the case when there are several amplification factors, we have in place of (4.1)

$$v_0^n = \sum_{j=0}^{\nu} \int_{-\pi/h}^{\pi/h} g_j(h\xi)^n \hat{v}^{0,j}(\xi) d\xi \tag{4.8}$$

for some functions $v^{0,j}(\xi)$. Each integral in the sum in (4.8) can be estimated as in the previous case. Moreover, since the $g_j(\theta)$ are bounded away from each other and an initialization is used to compute the solution at levels $j = 1, \dots, \nu$, e.g., (2.6), we have, see [3],

$$\sum_{j=0}^{\nu} \|v^{0,j}\|_h \le C\|v^0\|_h \,.$$

Next we show that if the group velocity vanishes, then the estimate (3.7) can not hold. This will follow from Theorems 3.2 and 3.3.

We first prove Theorem 3.2; the proof of Theorem 3.3 will be sketched later. Let θ_0 be a value where the group velocity vanishes, i.e., $\psi'(\theta_0) = 0$. Let $z(\theta)$ be a smooth 2π-periodic function normalized such that $z(\theta_0) = 1$ and z vanishes in a neighborhood of all other points where $\psi'(\theta)$ vanishes. We consider then the grid functions $\hat{v}^0(\xi)$, depending on h, defined by

$$\hat{v}^0(\xi) = h\hat{z}(h\xi)\,. \tag{4.9}$$

Define the constant c_0 by

$$c_0 = \int_{-\pi}^{\pi} |z(\theta)|^2 d\theta\,.$$

We assume also that $\psi''(\theta_0)$ does not vanish.

We now show that for v_m^n with v^0 defined by (4.9) that

$$k\sum_{n=0}^{N} |v_0^n|^2 \geq \frac{\lambda\|v^0\|^2}{c_0|\psi''(\theta_0)|}(\ln N - C) \tag{4.10}$$

for some constant C. Here and throughout this paper we will use C to denote an arbitrary constant, its use should be clear from the context.

By (4.2) and the definition of $\hat{v}^0$, see (4.9),

$$v_0^n = \frac{1}{\sqrt{2\pi}}\int_{-\pi}^{\pi} e^{-in\psi(\theta)}z(\theta)d\theta\,. \tag{4.11}$$

By our choice of $\hat{v}$, we see from (4.11) that the value of v_0^n is independent of k and h, depending only on n.

We next obtain an estimate for the magnitude of v_0^n as a function of n. We need several lemmas first.

Lemma 4.1. *If $[a,b]$ is an interval on which $|\psi'(\theta)| > c_1 > 0$, then there exists a constant C, depending on $[a,b]$, z, and ψ, such that*

$$\left|\int_a^b e^{-in\psi(\theta)}z(\theta)d\theta\right| \leq \frac{C}{n}$$

for all $n \geq 1$.

Lemma 4.2. *If $\psi'(\theta_0) = 0$ with $\psi''(\theta_0) \neq 0$ then for each $\varepsilon > 0$ there is a constant C, depending on ε, z, and ψ, such that*

$$\left|\int_{\theta_0-\varepsilon}^{\theta_0+\varepsilon} e^{-in\psi(\theta)}z(\theta)d\theta \;-\; e^{-in\psi(\theta_0)}z(\theta_0)\frac{\sqrt{2\pi}}{\sqrt{i\psi''(\theta_0)n}}\right| \leq \frac{C}{n}$$

for all $n \geq 1$. The square root in the denominator is the root with positive real part.

To prove Lemma 4.2 we need to estimate integrals of the form

$$\int_a^{\infty} e^{i\beta\eta^2}\, d\eta \tag{4.12}$$

where β is a parameter taking real values. The integral (4.12) is not Lebesgue integrable, but is given the value

$$\lim_{\varepsilon\to 0+}\int_a^{\infty} e^{-\varepsilon\eta^2}e^{-i\beta\eta^2}\, d\eta\,.$$

In particular,

$$\int_{-\infty}^{\infty} e^{-i\beta\eta^2}\, d\eta = \frac{1}{\sqrt{i\beta}}\int_{-\infty}^{\infty} e^{-s^2} ds$$

$$= \begin{cases} \sqrt{\dfrac{\pi}{\beta}}\,(1-i) & \text{for } \beta > 0, \\ \sqrt{\dfrac{\pi}{|\beta|}}\,(1+i) & \text{for } \beta < 0. \end{cases} \tag{4.13}$$

For $a > 0$, we have using integration by parts,

$$\int_a^{\infty} e^{-i\beta\eta^2}\, d\eta = \frac{1}{2i\beta a} e^{-i\beta a^2} - \frac{1}{2i\beta}\int_a^{\infty} \frac{e^{-i\beta\eta^2}}{\eta^2}\, d\eta\,.$$

So

$$\left|\int_a^{\infty} e^{-i\beta\eta^2}\, d\eta\right| \le \frac{C}{|a\beta|}\,. \tag{4.14}$$

Finally, if $f(\eta)$ is a smooth function and $a < 0 < b$, then

$$\left|\int_a^{b} e^{-i\beta\eta^2}\eta f(\eta)\, d\eta\right| \le C/|\beta|\,. \tag{4.15}$$

This result is easily proved by integration by parts.

We now prove Lemmas 4.1 and 4.2.

Proof of Lemma 4.1.

Using integration by parts we have

$$\int_a^b e^{-in\psi(\theta)} z(\theta) d\theta$$

$$= i\frac{z(b)}{n\psi'(b)} e^{-in\psi(b)} - i\frac{z(a)}{n\psi'(a)}$$

$$+ \frac{1}{n}\int_a^b e^{-in\psi(\theta)} \frac{d}{d\theta}\Big(\frac{z(\theta)}{\psi'(\theta)}\Big) d\theta\,.$$

Thus

$$\left|\int_a^b e^{-in\psi(\theta)} z(\theta)\, d\theta\right| \le \frac{C}{n}$$

where

$$C = \left|\frac{z(b)}{\psi'(b)}\right| + \left|\frac{z(a)}{\psi'(a)}\right| + \int_a^b \left|\frac{d}{d\theta}\left(\frac{z(\theta)}{\psi'(\theta)}\right)\right| d\theta.$$

Proof of Lemma 4.2.

Define a new variable of integration on the interval $[\theta_0 - \varepsilon, \theta_0 + \varepsilon]$ by

$$\psi(\theta) = \psi(\theta_0) + \frac{1}{2}\sigma\eta^2$$

where $\eta_- \le \eta \le \eta_+$ and $\sigma = \psi''(\theta_0)$. It then follows that

$$\int_{\theta_0-\varepsilon}^{\theta_0+\varepsilon} e^{-in\psi(\theta)} z(\theta) d\theta = e^{-in\psi(\theta_0)} \int_{\eta_-}^{\eta_+} e^{-in\sigma\eta^2/2} z(\theta(\eta)) \frac{d\theta}{d\eta}\, d\eta\,.$$

We need to evaluate $d\theta/d\eta$ at $\eta = 0$. We have

$$\psi'(\theta)\frac{d\theta}{d\eta} = \sigma\eta.$$

Using l'Hôpital's rule at $\eta = 0$, we have

$$\frac{d\theta}{d\eta}_{|\eta=0} = \lim_{\eta\to 0}\frac{\sigma\eta}{\psi'(\theta)} = \lim_{\eta\to 0}\frac{\sigma}{\psi''(\theta)d\theta/d\eta}\,.$$

Since we may determine the sign of $d\theta/d\eta$,

$$\frac{d\theta}{d\eta}(0) = 1.$$

Proceeding with the estimate of the integral, we have

$$\begin{aligned}\int_{\eta_-}^{\eta_+} e^{-in\sigma\eta^2/2} z(\theta(\eta))\frac{d\theta}{d\eta}\,d\eta =& z(\theta_0)\int_{\eta_-}^{\eta_+} e^{-in\sigma\eta^2/2}\,d\eta \\ &+ \int_{\eta_-}^{\eta_+} e^{-in\sigma\eta^2/2}[z(\theta(\eta))\frac{d\theta}{d\eta}(\eta) - z(\theta_0)]\,d\eta\,.\end{aligned} \tag{4.16}$$

Now

$$\begin{aligned}\int_{\eta_-}^{\eta_+} e^{-in\sigma\eta^2/2}\,d\eta =& \int_{-\infty}^{\infty} e^{-in\sigma\eta^2/2}\,d\eta \\ &- \int_{\eta_+}^{\infty} e^{in\sigma\eta^2/2}\,d\eta - \int_{-\infty}^{\eta_-} e^{in\sigma\eta^2/2}\,d\eta\,.\end{aligned}$$

By formulas (4.13) and (4.14) we have

$$\left|\int_{\eta_-}^{\eta_+} e^{-in\sigma\eta^2/2}\,d\eta - e^{-in\psi(\theta_0)}\frac{\sqrt{2\pi}}{\sqrt{in\sigma}}\right| \le \frac{C}{n}\,.$$

This estimates the first term on the right-hand side of (4.16). For the second term on the right-hand side in (4.16) we have

$$z(\theta(\eta))\frac{d\theta}{d\eta}(\eta) - z(\theta_0) = \eta f(\eta)$$

where $f(\eta)$ is a smooth function on $[\eta_-, \eta_+]$. By (4.15) we have that this term is on the order of n^{-1}. This proves Lemma 4.2.

To complete the proof of Theorem 3.2, we have from (4.11)

$$v_0^n = \frac{1}{\sqrt{2\pi}}\int_{\theta_0-\varepsilon}^{\theta_0+\varepsilon} e^{-in\psi(\theta)}z(\theta)d\theta + \frac{1}{\sqrt{2\pi}}\int_{|\theta-\theta_0|>\varepsilon} e^{-in\psi(\theta)}z(\theta)d\theta\,.$$

Using estimates on these integrals from Lemmas 4.1 and 4.2, we obtain

$$\left|v_0^n - e^{-in\psi(\theta_0)}z(\theta_0)\frac{1}{\sqrt{i\sigma n}}\right| \le \frac{C}{n}$$

for $n \ge 1$. (Recall that we have chosen $z(\theta)$ to be zero at all zeros of ψ' other than θ_0.)

We then easily obtain that

$$\begin{aligned}k\sum_{n=0}^{N}|v_0^n|^2 &\ge \frac{1}{|\sigma|}k\sum_{n=1}^{N}\frac{1}{n} - Ck\sum_{n=1}^{N}\frac{1}{n^{3/2}} \\ &= \frac{1}{|\sigma|}k\ln N - CkO(1)\,.\end{aligned}$$

Recall that $z(\theta_0) = 1$. Now

$$\|v^0\|^2 = \int_{-\pi/h}^{\pi/h} |\hat{v}(\xi)|^2 \, d\xi = h \int_{-\pi}^{\pi} |z(\theta)|^2 \, d\theta$$
$$= hc_0 \,.$$

Letting $\lambda = k/h$, we obtain

$$\|v_0\|^2_{k,N} \geq \frac{1}{|\sigma|} \lambda c_0^{-1} (\ln N - C) \|v^0\|^2.$$

This proves Theorem 3.2.

We now sketch the proof of Theorem 3.3. If $\psi''(\theta_0)$ does vanish, and ℓ is the order of the first non-zero derivative of ψ at θ_0, then Lemma 4.2 is replaced by the following lemma.

Lemma 4.3. *If $\psi^{(k)}(\theta_0) = 0$ for $1 \leq k < \ell$ with $\psi^{(\ell)}(\theta_0) \neq 0$, then for each $\varepsilon > 0$ there is a constant C, depending on ε, ψ, and z, such that*

$$\left| \int_{\theta_0-\varepsilon}^{\theta_0+\varepsilon} e^{-in\psi(\theta)} z(\theta) d\theta - e^{-in\psi(\theta_0)} z(\theta_0) \frac{\gamma_0}{n^{1/\ell}} \right| \leq \begin{cases} \dfrac{C}{n^{2/\ell}} & \text{if } \ell \text{ is odd,} \\ \dfrac{C}{n^{3/\ell}} & \text{if } \ell \text{ is even,} \end{cases}$$

for all $n > 0$. The constant γ_0 is given by

$$\gamma_0 = \int_{-\infty}^{\infty} e^{-i\alpha^\ell/\ell!} \, d\alpha.$$

Lemma 4.3 is proved by changing to the new variable η defined by

$$\psi(\theta) = \psi(\theta_0) + \sigma\eta^\ell/\ell!$$

where $\sigma = \psi^{(\ell)}(\theta_0)$. The integral

$$\int_{\eta_-}^{\eta_+} e^{-in\sigma\eta^\ell/\ell!} z(\theta(\eta)) \frac{d\theta}{d\eta} \, d\eta$$

is evaluated by expressing z as a Taylor polynomial in η about 0 plus terms of order $\eta^{\ell-1}$. The estimation of each term gives the result.

5. Estimates for the General Case

Theorem 3.1 naturally raises the question of what estimates analogous to (2.2) hold for schemes in general. In this section we give a partial answer to that question by considering different estimates of v_0^n in terms of $\|v^0\|$.

We begin by considering a one-step stable scheme for simplicity. By the definition of the amplification factor, see (4.1), we have

$$v_0^n = \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} g(h\xi)^n \hat{v}^0(\xi) d\xi \,.$$

Using the Fourier inversion formula, we obtain

$$v_0^n = \sum_{m=-\infty}^{\infty} p(n,m) v_m^0 \tag{5.1}$$

where

$$p(n,m) = \frac{h}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} g(h\xi)^n e^{-imh\xi} d\xi$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} g(\theta)^n e^{-im\theta} d\theta .$$

Thus $p(n,m)$ is the mth Fourier coefficient of $g(\theta)^n$, considered as a function on $[-\pi, \pi]$. By Parseval's relation, and the stability of the scheme,

$$\sum_{m=-\infty}^{\infty} |p(n,m)|^2 = \int_{-\pi}^{\pi} |g(\theta)^n|^2 d\theta \leq 2\pi . \tag{5.2}$$

From this we obtain our first estimate.

Theorem 5.1. *For a stable one-step finite difference scheme, the estimate*

$$\|v^n\|_{k,N} \leq (2\pi\lambda(N+1))^{1/2} \|v^0\|_h \tag{5.3}$$

holds for all $N \geq 0$. For a stable multistep finite difference scheme, there is a constant C depending on the scheme and the initialization such that the estimate

$$\|v^n\|_{k,N} \leq C(N+1)^{1/2} \|v^0\|_h$$

holds for all $N \geq 0$.

Proof.

We have by (5.1) and (5.2)

$$k \sum_{n=0}^{N} |v_0^n|^2 = k \sum_{n=0}^{N} \sum_{m=-\infty}^{\infty} \overline{v_0^n} p(n,m) v_m^0$$
$$\leq \left(k \sum_{n=0}^{N} \sum_{m=-\infty}^{\infty} |v_0^n|^2 |p(n,m)|^2 \right)^{1/2} \left(k \sum_{n=0}^{N} \sum_{m=-\infty}^{\infty} |v_m^0|^2 \right)^{1/2}$$
$$\leq \sqrt{2\pi} \left(k \sum_{n=0}^{N} |v_0^n|^2 \right)^{1/2} (N+1)^{1/2} \lambda^{1/2} \left(h \sum_{m=-\infty}^{\infty} |v_m^0|^2 \right)^{1/2} .$$

This easily gives (5.3).

For multistep schemes we have the representation

$$v_m^n = \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} G(h\xi, n) e^{imh\xi} \hat{v}^0(\xi) d\xi ,$$

where $G(\theta, n)$ is a linear combination of powers of the amplification factors. For example, if all amplification factors are distinct

$$G(\theta, n) = \sum_{j=0}^{\nu} A_j(\theta) g_j(\theta)^n$$

for some coefficients $A_j(\theta)$ depending on the initialization. Stability of the scheme implies that $|G(\theta, n)|$ is bounded independently of θ and n. Defining $p(n,m)$ by

$$p(n,m) = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} G(\theta, n) e^{-im\theta} d\theta$$

easily gives the result.

Comparison of Theorem 5.1 with (3.12) shows that both results are sharp. That is, the growth of $O(N)^{1/2}$ is the best bound that can be obtained for general stable schemes. We next investigate how dissipation can affect the estimate.

Theorem 5.2. *For a dissipative one-step finite difference scheme, dissipative of order $2r$, there is a constant C_0 such that all solutions satisfy*

$$\|v_0\|_{k,N} \le C_0 N^{1/2-1/4r}\, \|v^0\|_h \tag{5.4}$$

for $N \ge 1$.

Proof.

For a scheme to be dissipative of order $2r$ means that there is a constant c such that

$$|g(\theta)| \le e^{-c\theta^{2r}} \quad \text{for} \quad |\theta| \le \pi\,.$$

Using this estimate, we replace (5.2) with

$$\begin{aligned}\sum_{m=-\infty}^{\infty} |p(n,m)|^2 &= \int_{-\pi}^{\pi} |g(\theta)^n|^2 d\theta \le \int_{-\pi}^{\pi} e^{-2cn\theta^{2r}} d\theta \\ &\le \varepsilon_n = \begin{cases} Cn^{-1/(2r)} & n \ge 1, \\ 2\pi & n = 0. \end{cases}\end{aligned}$$

We use this to modify the proof of Theorem 5.1, as follows,

$$\begin{aligned} k\sum_{n=0}^{N} |v_0^n|^2 &\le \Big(k\sum_{n=0}^{N}\sum_{m=-\infty}^{\infty} |v_0^n|^2 \varepsilon_n^{-1} |p(n,m)|^2\Big)^{1/2} \Big(k\sum_{n=0}^{N}\sum_{m=-\infty}^{\infty} \varepsilon_n |v_m^0|^2\Big)^{1/2} \\ &\le C\Big(k\sum_{n=0}^{N} |v_0^n|^2\Big)^{1/2} \lambda^{1/2}\Big(h\sum_{m=-\infty}^{\infty} |v_m^0|^2\Big)^{1/2}\Big(\sum_{n=0}^{N}\varepsilon_n\Big)^{1/2}. \end{aligned}$$

Now

$$\sum_{n=1}^{N} n^{-1/(2r)} \le 1 + \int_1^N x^{-1/(2r)}\, dx = 1 + \left(1 - \frac{1}{2r}\right)^{-1} (N^{(1-1/(2r))} - 1).$$

This easily proves the theorem.

An examination of the analysis used thus far leads us to the following conjecture.

Conjecture. *For a stable finite difference scheme there is a constant C such that*

$$\|v_0\|_k \le C\|v^0\|_h$$

if and only if each of the amplification factor of the scheme, g_j, satisfies

$$\frac{\partial g_j}{\partial \theta}(\theta) \ne 0 \quad \text{when} \quad |g_j(\theta)| = 1\,.$$

In the next section we give computational evidence in support of this conjecture.

6. Examples

In this section we present several examples which illustrate the theory. We present several schemes which do or do not satisfy the different hypotheses of the theorems and give some numerical evidence showing the growth rates predicted by the preceding analysis.

As an example of a conservative scheme for which the estimate (3.7) holds we consider the Wendroff box scheme for $u_t + au_x = 0$. The scheme is

$$\frac{1}{2k}\left\{\left(v_m^{n+1} + v_{m+1}^{n+1}\right) - \left(v_m^n + v_{m+1}^n\right)\right\}$$
$$+\frac{a}{2h}\left\{\left(v_{m+1}^{n+1} + v_{m+1}^n\right) - \left(v_m^{n+1} + v_m^n\right)\right\} = 0 .$$

The amplification factor is

$$g(\theta) = \frac{\cos\frac{1}{2}\theta - ia\lambda\sin\frac{1}{2}\theta}{\cos\frac{1}{2}\theta + ia\lambda\sin\frac{1}{2}\theta},$$

and so the function ψ is given by

$$\tan\frac{1}{2}\psi(\theta) = a\lambda\tan\frac{1}{2}\theta .$$

From $\sec^2\frac{1}{2}\psi\,\psi' = a\lambda\sec^2\frac{1}{2}\theta$, we obtain

$$\psi'(\theta) = a\lambda\frac{\sec^2\frac{1}{2}\theta}{\sec^2\frac{1}{2}\psi} = a\lambda\frac{(1+\tan^2\frac{1}{2}\theta)}{(1+a^2\lambda^2\tan^2\theta)} .$$

We see that $\psi'(\theta)$ does not vanish, that $\min|\psi'|$ is $\min(|a|\lambda, |a\lambda|^{-1})$, and that $\psi(\pi) = \pi$. Thus we obtain by (4.7)

$$||v_0||_k \le \frac{1}{|a|^{1/2}}||v^0||_h$$

for $|a|\lambda \le 1$ and

$$||v_0||_k \le |a|^{1/2}\lambda||v^0||_h$$

for $|a|\lambda > 1$, for the Wendroff box scheme.

To illustrate the different growth rates shown by equation (4.10) we present some computational results. The first case uses the leapfrog scheme

$$\frac{v_m^{n+1} - v_m^{n-1}}{2k} + \frac{v_{m+1}^n - v_{m-1}^n}{2k} = 0 \tag{6.1}$$

and the second case uses the Crank-Nicolson scheme

$$\frac{v_m^{n+1} - v_m^n}{2k} + \frac{v_{m+1}^{n+1} - v_{m-1}^{n+1}}{4h} + \frac{v_{m+1}^n - v_{m-1}^n}{4h} = 0 \tag{6.2}$$

for $u_t + u_x = 0$. The amplification factors for the leapfrog scheme are given by (3.5) and for the Crank-Nicolson scheme by (3.6) Notice that the derivative with respect to θ of each amplification factor vanishes at θ equal to $\pm\pi/2$. Since the second derivative does not vanish these schemes can give the $O(\ln(N)^{1/2})$ growth.

We take as initial data the function

$$v_m^0 = \begin{cases} -.1 & \text{if } m = -3, \\ -.9 & \text{if } m = -1, \\ .9 & \text{if } m = \ \ 1, \\ .1 & \text{if } m = \ \ 3, \\ 0 & \text{otherwise} . \end{cases} \tag{6.3}$$

Note that $z(\theta) = (9\sin\theta + \sin 3\theta)/10$.

Thee calculations were was on the domain $-40 \leq x \leq 40$. The first case was for $0 \leq t \leq 55$, the grid spacing was .01 with $\lambda = 0.9$. This means that the maximum value of N was 6112. The first time step was computed with the forward-time central-space scheme.

The Crank-Nicolson calculation in the second case used the same initial data with a grid spacing of .02 and $\lambda = 1$. Computing to time 40 results in 2000 time steps.

Because of the expected growth rate of $O(\ln N)^{1/2}$ is quite slow, it is difficult to determine the exact growth rate from the computed results. What we have done is to consider the two quantities

$$r_1 = \frac{\|v_0\|_{k,N}}{\|v^0\|_h (\ln N)^{\frac{1}{2}}} \quad \text{and} \quad r_2 = \frac{\ln(\|v_0\|_{k,N}/\|v^0\|_h)}{\ln\ln N}. \tag{6.4}$$

The quantity r_1 should tend to a constant if $\|v_0\|_{k,N}/\|v^0\|_h$ grows like $O(\ln N)^{1/2}$, and r_2 should determine the exponent α such that $\|v_0\|_{k,N}/\|v^0\|_h$ is $O(\ln N)^\alpha$.

The values of r_2 that were obtained are displayed in Table 1. The discussion of the results is given after all the four cases are presented.

As an example of a conservative scheme having a growth rate of $O(N^{1/4})$ we have the modified leapfrog scheme

$$\frac{v_m^{n+1} - v_m^{n-1}}{2k} + \delta_0 v_m^n - \frac{h^2}{3}\delta_0^3 v_m^n = 0$$

where δ_0 is the usual central difference operator. For this scheme we have the two amplification factors

$$g_\pm = -iS \pm \sqrt{1 - S^2}$$

where

$$S = S(\theta) = \lambda(\sin\theta - \frac{1}{3}\sin^3\theta).$$

The grid spacing and other parameters for this third case are the same as for the first case. This scheme is stable if $|S| < 1$, i.e., for $|\lambda| < 3/2$. Since $S'(\pi/2) = S''(\pi/2) = S'''(\pi/2) = 0$, with $S^{(4)}(\pi/2) \neq 0$, we should get a growth of $O(N^{1/4})$ for $\|v_0\|_{k,N}$ for some initial data, according to Theorem 3.3.

For this scheme we define r_1 and r_2 by

$$r_1 = \frac{\|v_0\|_{k,N}}{\|v^0\|_h N^{1/4}}$$

and

$$r_2 = \frac{\ln(\|v_0\|_{k,N}/\|v^0\|_h)}{\ln N}$$

As our fourth case we present a scheme which is not a conservative scheme, but should have unbounded growth if the conjecture at the end of section 5 is true. This is the modified, first-order accurate, Crank-Nicolson scheme,

$$\begin{aligned} \frac{v_m^{n+1} - v_m^n}{k} + \beta\frac{v_{m+1}^{n+1} - v_{m-1}^{n+1}}{2h} + (1-\beta)\frac{v_{m+1}^n - v_{m-1}^n}{2h} \\ - \gamma\frac{v_{m+2}^n - 2v_m^n + v_{m-2}^n}{4h} = 0. \end{aligned}$$

The amplification factor is

$$g = \frac{1 - i(1-\beta)\lambda\sin\theta - \gamma\lambda\sin^2\theta}{1 + i\beta\lambda\sin\theta}$$

and so,

$$|g|^2 = \frac{(1-\gamma\lambda\sin^2\theta)^2 + (1-\beta)^2\lambda^2\sin^2\theta}{1+\beta^2\lambda^2\sin^2\theta}.$$

If

$$(1-\gamma\lambda)^2 + (1-2\beta)\lambda^2 = 1,$$

then the scheme is stable, and $|g| = 1$ only if $\sin^2\theta$ is 0 or 1. Moreover, at $\theta_0 = \pm\pi/2$ we have $|g(\theta_0)| = 1$ and $g'(\theta_0) = 0$. Thus, if $||v_0||_{k,N}$ appears to be unbounded, as the computationœ shows, this supports the conjecture given at the end of section 5. Based on the proofs given in section 5, we can expect that this scheme could have $O(\ln N)^{1/2}$ growth as does the usual Crank-Nicolson scheme.

The computation for this fourth case used the same parameters as the Crank-Nicolson calculation in the second case. The value of β was 0.30. The values of r_1 and r_2 were computed as in (6.4).

For all of these cases the values of r_1 and r_2 appeared to be converging to limits, but the trends were exceedingly slow. This is not unexpected and can be appreciated by noticing that the expected deviation in r_1 from the theoretical limit in cases 1, 2, and 4 is on the order of $O(\ln N)^{-1/2}$. This requires very large values of N before an accurate value can be obtained. Similarly, r_2 converges to its limiting value as $O(\ln(\ln N))^{-1}$, again a very slow rate of convergence.

The values of r_2 and their behavior near the end of the computation are given in Table 1. The values of r_1 are not given, but in each case they were changing at a very slow rate at the end of the computations. In spite of the less than perfect agreement between the theoretical limit and the observed values, it must be emphasized that for all examples it is quite evident that $||v_0||_{k,N}$ is unbounded.

Figure 1 displays the graphs of r_1 and r_2 for case 3. As can be seen r_1 appears to be slowly tending to a constant value, and r_2 is greater than 0.25 and is slowly decreasing, but the limit is difficult to judge.

Case	r_2(theoretical)	r_2(computation)	r_2 behavior
1	0.50	0.448	slowly decreasing
2	0.50	0.412	slowly increasing
3	0.25	0.260	slowly decreasing
4	0.50	0.480	slowly increasing

Table 1

7. The GKS Theory Applied.

In this appendix we present the analysis of the folded leapfrog and folded Crank-Nicolson problems by the GKS theory.

We begin by checking for non-zero solutions of the finite difference equations (2.7) of the form

$$\begin{aligned} u_m^n &= Az^n\kappa_1^m \\ v_m^n &= Bz^n\kappa_2^m \end{aligned} \tag{7.1}$$

with $|z| \geq 1$, $|\kappa_1| \leq 1$, and $|\kappa_2| \leq 1$. We find that κ_1 and κ_2 must satisfy the equations

$$z - \frac{1}{z} + a\lambda(\kappa_1 - \frac{1}{\kappa_1}) = 0\,, \tag{7.2}$$

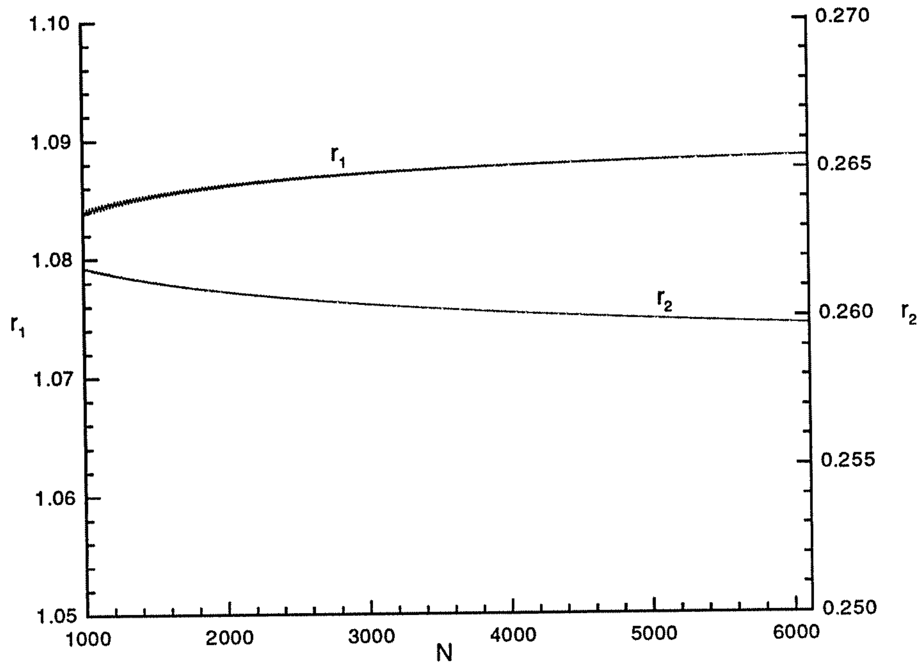

Figure 1

$$z - \frac{1}{z} - a\lambda(\kappa_2 - \frac{1}{\kappa_2}) = 0\,. \tag{7.3}$$

It is easy to see that for each value of z with $|z| > 1$, there is one value of κ_1 with $|\kappa_1| < 1$ and one value of κ_2 with $|\kappa_2| < 1$. Note that (7.2) and (7.3) also have solutions with $\kappa_1| > 1$ and $\kappa_2 > 1$, respectively. For z with $|z| = 1$, we take $\kappa_1(z)$ to be the value defined by

$$\kappa_1(z) = \lim_{\varepsilon \to 0+} \kappa_1(z(1+\varepsilon)) \tag{7.4}$$

where $|\kappa_1(z(1+\varepsilon))| < 1$, and similarly for $\kappa_2(z)$. By stability of the scheme $|\kappa_i| \neq 1$ if $|z| > 1$.

We next check the boundary conditions with the solutions (7.1). From $u_0^n = v_0^n$ we deduce that $A = B$, and without loss of generality we may set $A = B = 1$.

Checking the second boundary condition in (2.8) we obtain

$$z - \frac{1}{z} + a\lambda(\kappa_1 - \kappa_2) = 0\,. \tag{7.5}$$

From (7.2) and (7.5) we see that these equations can only be satisfied if

$$\kappa_2 = \kappa_1^{-1}\,, \tag{7.6}$$

and this implies that $|\kappa_1| = |\kappa_2| = |z| = 1$.

Set $\kappa_1 = e^{i\theta}$, $\kappa_2 = e^{-i\theta}$, and $z = e^{i\phi}$, then by (7.2) and (7.3) we have

$$\sin\phi = -a\lambda \sin\theta\,. \tag{7.7}$$

This does not assure us of a nontrivial solution of the type sought for, since we have not checked condition (7.4). To check condition (7.4) set

$$\begin{aligned} z &= (1+\varepsilon)e^{i\phi} \\ \kappa_1 &= (1-\delta_1)e^{i\theta} \\ \kappa_2 &= (1-\delta_2)e^{-i\theta}\,. \end{aligned} \tag{7.8}$$

If there are solutions of the form (7.8) with both Re $\delta_1 > 0$ and Re $\delta_2 > 0$ for $\varepsilon > 0$, then the initial-boundary value problem (2.7) and (2.8) is unstable in the GKS sense.

From (7.2) and (7.8) we obtain

$$\begin{aligned} &2i\sin\phi + 2\varepsilon\cos\phi + O(\varepsilon^2) \\ &\quad = -\,a\lambda(2i\sin\theta - 2\delta_1\cos\theta + O(\delta_1^2))\,, \end{aligned}$$

which, by (7.7), implies

$$\varepsilon\cos\phi = +2a\lambda\delta_1\cos\theta + O(\delta_1^2)$$

and similarly from (7.3)

$$\varepsilon\cos\phi = -2a\lambda\delta_2\cos\theta + O(\delta_2^2).$$

These two relations show that δ_1 and δ_2 must have opposite signs, for small ε, unless $\cos\theta$ vanishes. (If $\cos\theta$ does not vanish then the solutions to (7.2), and (7.3), satisfying (7.7) satisfy either $|\kappa_1| > 1$ or $|\kappa_2| > 1$ for $|z| > 1$.)

If $\cos\theta = 0$, then $\cos\phi_0 = \pm\sqrt{1-a^2\lambda^2} \neq 0$ and we obtain

$$2\varepsilon\cos\phi_0 = -ia\lambda\delta_1^2 + O(\delta_1^3)$$

and

$$2\varepsilon\cos\phi_0 = +ia\lambda\delta_2^2 + O(\delta_2^3)\,.$$

Therefore, if $a\lambda\cos\phi_0$ is positive, then

$$\begin{aligned} \delta_1 &= (1+i)\sqrt{\varepsilon\left|\frac{\cos\phi_0}{a\lambda}\right|} + O(\varepsilon) \\ \delta_2 &= (1-i)\sqrt{\varepsilon\left|\frac{\cos\phi_0}{a\lambda}\right|} + O(\varepsilon) \end{aligned}$$

are the solutions with positive real parts, and δ_1 and δ_2 are equal to the conjugates of these values if $a\lambda\cos\phi_0$ is negative. Thus the the folded leapfrog initial-boundary value problem is unstable in the GKS sense.

For the folded Crank-Nicolson problem we start with the solution (7.1) and obtain the two equations

$$\begin{aligned} \frac{z-1}{z+1} &= -\frac{a\lambda}{4}(\kappa_1 - \frac{1}{\kappa_1}) \\ \frac{z-1}{z+1} &= +\frac{a\lambda}{4}(\kappa_2 - \frac{1}{\kappa_2}) \end{aligned}$$

from the schemes and from the first boundary condition we obtain that $A = B$. From the second boundary condition we have

$$\frac{z-1}{z+1} = -\frac{a\lambda}{2}(\kappa_1 - \kappa_2)$$

corresponding to the boundary condition (7.5). Again we see that κ_2 must equal κ_1^{-1}.

Checking condition (7.8), we set $z = e^{i\phi}(1+\varepsilon)/(1-\varepsilon)$ and $\kappa_1 = (1-\delta_1)e^{i\theta}$, $\kappa_1 = (1-\delta_2)e^{-i\theta}$, where

$$\tan\frac{1}{2}\phi = -\frac{a\lambda}{2}\sin\theta\,.$$

We obtain

$$i\tan\frac{1}{2}\phi\Big(\frac{1-i\varepsilon\cot\frac{1}{2}\phi}{1+i\varepsilon\tan\frac{1}{2}\phi}\Big) = -\frac{a\lambda}{4}(2i\sin\theta - 2\delta_1\cos\theta) + O(\delta_1^2)$$

or

$$\varepsilon(1+\tan^2\frac{1}{2}\phi) = +\frac{a\lambda}{2}\delta_1\cos\theta + O(\delta_1^2)$$

and

$$\varepsilon(1+\tan^2\frac{1}{2}\phi) = -\frac{a\lambda}{2}\delta_2\cos\theta + O(\delta_2^2)\,.$$

Again, we must have $\cos\theta = 0$ to allow δ_1 and δ_2 to both have positive real parts. In this case

$$\delta_1 = (1-i)\sqrt{\frac{2\varepsilon}{|a\lambda|}}\left|\sec\frac{1}{2}\phi\right| + O(\varepsilon)$$

$$\delta_2 = (1+i)\sqrt{\frac{2\varepsilon}{|a\lambda|}}\left|\sec\frac{1}{2}\phi\right| + O(\varepsilon)$$

if $a\lambda\sin\theta_0$ is positive, and the δ_1 and δ_2 are the conjugates of these values if $a\lambda\sin\theta_0$ is negative. Thus, the folded Crank-Nicolson problem is also unstable in the GKS sense.

A check of these two examples shows that the difficulties occur for precisely those values of θ at which the derivative of the amplification factors vanish, in agreement with Theorem 5.1.

8. Conclusions

Although we have explained the apparent contradiction arising with the folded leapfrog example, there are several other issues that should raised. One is to note that the folded problems, being stable as initial value problems, are stable as initial-boundary value problems, but with a set of norms other than those used in the GKS theory. Thus the GKS theory should be modified to include this case. There is also the possibility that there are other initial-boundary value problems that are unstable in the GKS sense, but are not unstable in a slightly weaker sense. It would be nice to have a theory that incorporated these considerations.

One interesting question is whether there can be reasonable norms for which the norm in time of the solution at a point is bounded by the initial data. If there were, these might be good choices to use in a theory of initial-boundary value problems for finite difference schemes. However, judging from the nature of the the growth, it is quite unlikely that these norms would be very useful.

It should also be pointed out that the growth rates of $\|v_0\|_{k,N}$ are so slow that it is quite likely not to be seen in most calculations. It is only the modes associated with very high frequencies that are subject to this growth and they would usually be dominated by lower frequencies. Indeed, unless one is measuring the L^2 norm in time of the solution at a point, and this would rarely be done, there is no concern about the growth of this norm in practical computations.

Finally, the generalization of these results to more than one spatial dimension should be of interest.

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