

ON PARTIAL DIFFERENCE EQUATIONS IN MATHEMATICAL PHYSICS

ANDRÉ J. ROBERT

Central Analysis Office, Meteorological Service of Canada, Toronto, Ontario

FREDERICK G. SHUMAN and JOSEPH P. GERRITY, JR.

National Meteorological Center, Weather Bureau, ESSA, Washington, D.C.

ABSTRACT

A rather general theory of nonlinear computational stability is reported. Instability is caused by both spatial and temporal high frequencies that, if not present initially, will appear from nonlinear interactions. It appears that through simple remedies relative stability, if not perfect stability, can be achieved.

1. INTRODUCTION

Several ideas are gathered in this manuscript to form a basis for a rather general theory of computational stability of difference approximations to the nonlinear meteorological equations. Although we discuss here only applications to difference systems centered in time and space, the approach can be used to investigate stability properties of other classes of difference systems. The approach can also be extended to other areas of mathematical physics, which explains the generality of the title immodestly borrowed.

So far, the theory has explained the relative stability of space-averaged difference forms, the stability of certain integrations of the pure gravity wave, and the observed association of instability with high frequencies in space and time. Finally, we have used the theory to devise a new difference scheme for which computational stability was predicted successfully. We have now hardly begun to approach the full set of meteorological equations with our new ideas. Much remains to be done before they can be fully exploited in large operational atmospheric prediction models.

In outline, the paper:

1) develops the notion of aliasing, which allows us to restrict our attention to oscillations two increments and longer;

2) develops the notion of "folding," an idea related to aliasing, which allows us to regard high frequencies as low frequencies modulated by the two-increment oscillation;

3) discusses the origin of temporal high frequencies (so-called computational mode) as well as the temporal low frequencies (so-called physical mode) in numerical solu-

tions of the centered difference advection equation (the computational mode in the more general sets of hydrodynamic equations must feed back into the integration through undifferentiated factors, such as the advecting velocity; this feedback, along with the feedback of spatial high frequencies is, we claim, a root cause of nonlinear instability);

4) analyzes linearized equations for nonlinear computational stability criteria (the linearization consists of neglecting low-frequency variations in undifferentiated coefficients; in the case of high frequencies, only the modulating factor is therefore retained); and

5) demonstrates a simple technique for achievement of stability for a nonlinear set.

The theory is not complete, having been developed through linearization techniques; and, therefore, we are dealing with *relative* stability and *necessary*, not *sufficient*, conditions for stability. The one reported experiment, designed for stability according to the theory, however, did exhibit perfect stability.

The reader will recognize that many of the ideas are not original, but they are reported for completeness. The analysis of instability due to temporal high, spatial low, frequencies is due to Robert (1969) and to our knowledge is new. Indeed, his analysis motivated us to develop the theory at this time. Also to the best of our knowledge, this is the first time all of these ideas have been brought together into so general a theory of nonlinear computational stability.

Before closing the introduction, a word on notation is in order. For convenience in writing, we have adopted the following notation. Let a dimension, x , be divided by grid points into equal increments Δx . The grid points will be

serially numbered, ... 0, 1, 2, ..., $j-1, j, j+1, \dots$. The operator $(\)_x$ applied to an arbitrary variable f is defined by

$$f_x = \frac{1}{\Delta x} (f_{j+1} - f_{j-1}).$$

The operator $(\)^x$ is defined by

$$\bar{f}^x = \frac{1}{2} (f_{j+1} + f_{j-1}).$$

As a slight generalization, the prefix "2" to an operating variable extends the action of the operator to two increments, thus:

$$f_{2x} = \frac{1}{2\Delta x} (f_{j+1} - f_{j-1})$$

and

$$\bar{f}^{2x} = \frac{1}{2} (f_{j+1} + f_{j-1}).$$

Note that

$$f_{2x} = \bar{f}^x_x,$$

and

$$\bar{f}^{2x} = \bar{f}^{xx} + \left(\frac{\Delta x}{2}\right)^2 f_{xx}.$$

It will aid in following the derivations in sections 5 and 6 to understand that

$$\overline{(fg)}_x = \bar{f}^{2x-x} g_x + \bar{f}_x^{x-2x} g.$$

Further, note that at grid points (j an integer)

$$\overline{(e^{i\pi j})}_x = 0$$

and

$$\overline{(e^{i\pi j})}^{2x} = -e^{i\pi j}$$

where

$$i = \sqrt{-1}.$$

2. ALIASING

Consider a sinusoidal oscillation with k cycles in J equal increments, Δx , of any dimension x ,

$$F = \exp i \frac{2\pi k j}{J} \tag{1}$$

where $j = x/\Delta x$. We first show, as is well known, that if the wavelength, J/k increments, is less than two, the oscillation cannot be distinguished from one whose wavelength is longer than two increments. This phenomenon is called "aliasing."

To illustrate, in equation (1) let $J/k < 2$ ($k/J > 1/2$). For m any integer, $\exp 2\pi m i = 1$, and at grid points, therefore, we may write

$$F = \exp 2\pi i \left(\frac{k}{J} - m\right) j.$$

Thus an integer, m , may always be chosen so that

$$\left| \frac{k}{J} - m \right| < \frac{1}{2}, \text{ that is, } \left| \frac{J}{k - mJ} \right| > 2.$$

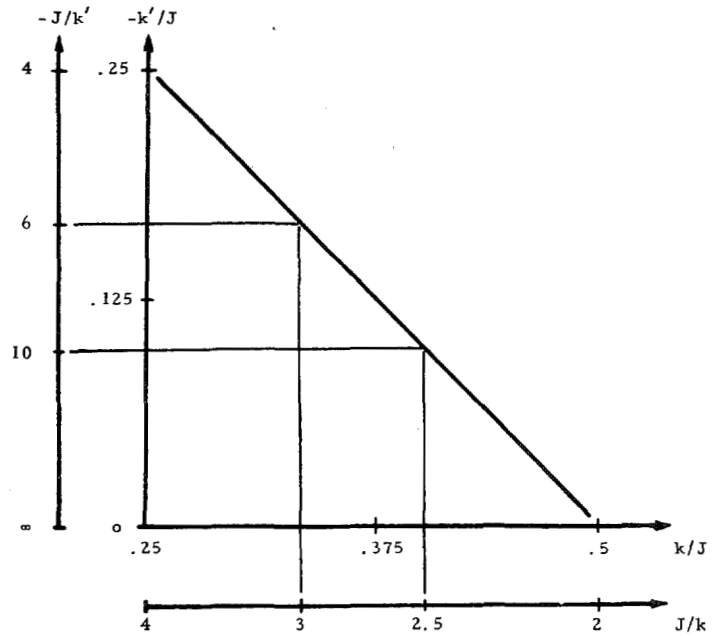


FIGURE 1.—Graph of $k'/J = k/J - 1/2$.

This is the basis for the custom of regarding the discrete spectral distribution as extending from the infinitely long, $k=0$, to only the two-increment-long, $k = 1/2 J$.

3. "FOLDING"

We next divide the spectrum into two equal parts, low frequency and high frequency. The low frequency will be defined by $J/k \geq 4$ and the high frequency by $2 \leq J/k \leq 4$. We have ambiguously included the four-increment oscillation in both groups, which here is no cause for concern since its categorization is irrelevant to the problem at hand.

We now show that any high-frequency oscillation may be expressed as a low-frequency oscillation modulated by the highest frequency oscillation, $J/k=2$. We may rewrite equation (1) as

$$F = F'' F' \tag{2}$$

where

$$F'' = \exp i\pi j \text{ and } F' = \exp i \frac{2\pi(k - \frac{1}{2}J)j}{J}.$$

F'' is the highest frequency oscillation, with length of two increments, for if we define k'' by $2\pi k'' j/J = \pi j$, then $J/k'' = 2$. Indeed, at grid points, $F'' = (-1)^j$. In the case of F' , if we define k' by $2\pi k' j/J = 2\pi(k - 1/2 J)j/J$, then $k'/J = (k/J) - 1/2$. Now if $2 < J/k < 4$, F is therefore high frequency, then $4 < \frac{J}{k'} < \infty$ and F' is therefore low frequency. It should further be noted that the higher is the frequency k/J of F , the lower is the frequency k'/J of F' . For example, as indicated in figure 1, a three-increment oscillation "folds" into a modulated six-increment oscillation; a two-and-one-half-increment oscillation folds into a modulated 10-increment oscillation.

4. THE COMPUTATIONAL MODE

Generally, all spatial frequencies from the shortest, two increments long, to the infinitely long are present in

integrations of the nonlinear equations of meteorological hydrodynamics and thermodynamics. If they are not there initially, they develop through nonlinear interactions. Thus, in space we must deal with both high and low frequencies.

It is important to establish that both high and low frequencies are also present in time. There will be nothing new in this stage of our argument, but for the sake of completeness, we establish it here through a simple example.

Consider a simple advective differential equation

$$\partial f/\partial t + U(\partial f/\partial x) = 0$$

where f is the dependent variable, t time, x distance, and U a constant advecting speed. Consider its centered difference form

$$\bar{f}_t' + U\bar{f}_x' = 0. \tag{3}$$

Solution of equation (3) may be expressed by sums of the components

$$f_{q,r} = A_{q,r} \exp 2\pi i \left(\frac{qn}{N} + \frac{rj}{J} \right)$$

where q and r are integers and $N\Delta t$ and $J\Delta x$ are the fundamental period and wavelength, respectively. Substitution into equation (3) yields the frequency equation

$$\sin \frac{2\pi q}{N} + \frac{U\Delta t}{\Delta x} \sin \frac{2\pi r}{J} = 0.$$

We first note, as a matter of course, that since we must account for $0 \leq r/J \leq 1/2$, that $-1 \leq \sin(2\pi r/J) \leq +1$ and, therefore, it is necessary and sufficient that $0 \leq (U\Delta t/\Delta x)^2 < 1$ to avoid the instability analyzed by Courant et al. (1928) (CFL). With the CFL criterion satisfied, we next note the presence of two solutions, one the so-called physical mode, q' , for which $0 \leq q'/N \leq 1/4$ and which is therefore low frequency by our definition. The other, the so-called computational mode, q'' , yields the same sine, being related to q' by $2\pi q''/N = \pi - (2\pi q'/N)$. Any multiple of 2π may be added to the right-hand side, but this would result in aliasing into either q' or q'' . The relationship between q' and q'' together with the limits on q' gives $1/4 \leq q''/N \leq 3/4$. The computational mode, q'' , is therefore high frequency according to our definition.

In a calculation with the linear difference equation (3), it is well known that the amplitude of the computational mode may be controlled, indeed eliminated entirely, through an appropriate choice of the two necessary sets of initial data at two levels of initial time. In practice, when we deal with the corresponding nonlinear sets of equations, it is customary to start the integration in time with a single distribution of data in space, and to derive a distribution at the next level in time by means of a difference equation centered in space but uncentered, forward, in time. Such a procedure does not eliminate the computational mode in the linear case, but analysis shows

that the procedure makes its amplitude very small. Experience, on the other hand, has almost universally been that the nonlinear centered difference equations eventually develop large-amplitude temporal high frequencies. We here interpret this phenomenon as development of the high-frequency, computational mode (a linear concept) through nonlinear interactions.

5. NONLINEAR INSTABILITY

In meteorology we deal with a whole set of equations, at least six in number in the more general cases, and the advecting components of velocities themselves are predicted by equations containing terms like those of equation (3) in f .

Therefore, we should expect that even though the integration is begun with only low frequencies in the advecting velocities, high frequencies will develop, in both space and time. In equation (3), the advecting speed, U , is constant. It is fair to interpret its analysis not only in terms of precisely constant U but also in terms of low frequencies in U , oscillating in both space and time. In the latter case the analysis should be regarded as holding for intervals in space and time that are short compared to the length of the wave in space and time, short enough so that variations of U are very small within the intervals.

With this idea in mind, we now turn to analysis of cases wherein the advecting speed is not confined to low frequencies but includes high frequencies as well. In including high frequencies we will think of them as folded into low frequencies modulated by the highest, two-increment-long frequency. We will neglect the variation of the modulated low frequency, for example, F' in equation (2), and include in the analysis only the modulation itself, for example, F'' in (2).

Consider the difference equation

$$\bar{f}_t' + (U_0 + U_1 e^{i\pi j} + U_2 e^{i\pi n} + U_3 e^{i\pi(j+n)}) \bar{f}_x' = 0 \tag{4}$$

where $U_0, U_1, U_2,$ and U_3 are constant. Application of the operator $(\bar{\quad})_x'$ to equation (4) yields

$$\bar{f}_{xt}'' + [(U_0 - U_3 e^{i\pi(j+n)}) - (U_1 e^{i\pi j} - U_2 e^{i\pi n})] \bar{f}_{xx}'' = 0.$$

Application of the operator $(\bar{\quad})_t'$ to equation (4) yields

$$\bar{f}_{tt}'' + [(U_0 - U_3 e^{i\pi(j+n)}) + (U_1 e^{i\pi j} - U_2 e^{i\pi n})] \bar{f}_{xt}'' = 0.$$

Elimination of \bar{f}_{xt}'' from the latter pair yields

$$\bar{f}_{tt}'' - [(U_0^2 - 2U_0 U_3 e^{i\pi(j+n)} + U_3^2) - (U_1^2 - 2U_1 U_2 e^{i\pi(j+n)} + U_2^2)] \bar{f}_{xx}'' = 0. \tag{5}$$

This is a second-order difference equation in which differences are taken over double increments in both space and time. There are therefore four interleaved sets of grid points in the x, t -net, on each of which the solution of the second-order equation (5) is independent of the other three. We note, on the other hand, that the first-

order difference equation (4) has only two sets of grid points, each carrying a solution independent of the other. The two sets of (4) are interleaved in checkerboard fashion: for one set $j+n$ is even, for the other set $j+n$ is odd. The four sets in the case of the second-order difference equation (5) can be divided into two pairs, each pair constituting one of the sets of the first-order equation (4).

We therefore lose no generality by considering two equations, one for even $j+n$,

$$\bar{f}_{ii}'' - [(U_0 - U_3)^2 - (U_1 - U_2)^2] \bar{f}_{zz}'' = 0,$$

and one for odd $j+n$

$$\bar{f}_{ii}'' - [(U_0 + U_3)^2 - (U_1 + U_2)^2] \bar{f}_{zz}'' = 0.$$

These are simple wave equations whose stability criteria are well known. For the former the stability criterion is

$$0 \leq \left(\frac{\Delta t}{\Delta x}\right)^2 [(U_0 - U_3)^2 - (U_1 - U_2)^2] < 1. \quad (6a)$$

For the latter the stability criterion is

$$0 \leq \left(\frac{\Delta t}{\Delta x}\right)^2 [(U_0 + U_3)^2 - (U_1 + U_2)^2] < 1. \quad (6b)$$

Since both sets of grid points are to be considered, both criteria must be satisfied for stability.

There is a simple historical sequence behind (6). Courant et al. (1928) showed the right-hand condition, which depends on the magnitude of Δt . Their analysis also implied the left-hand condition in a trivial way for $U_1 = U_2 = U_3 = 0$. Phillips (1959) captured the essence of the left-hand condition for $U_0 = U_2 = 0$, and later Richtmyer (1962) for only $U_2 = 0$. For example, consider the equation Richtmyer analyzed, which may be written $\bar{u}_i^t - \bar{u}^{2x} \bar{u}_x^x = 0$. From the result of his analysis, $\bar{u}^{2x} = U_0 + U_1 \cos \pi j + U_3 \cos \pi(j+n)$, where $|U_0|$ is his $|V|$, $|U_1|$ is his $\frac{1}{2}|A+B|$, and $|U_3|$ is his $\frac{1}{2}|A-B|$. His criterion for stability is identical to our criteria (6) without U_2 , but which he could have included by allowing his V to be time dependent. It is clear that, for a self-contained nonlinear equation such as his, our generalization applies to the interaction of packages of very short and very long waves with a package of middling, nearly four-increment-long waves. Robert (1969) showed the left-hand condition for nonvanishing U_2 , but with $U_0 = U_1 = U_3 = 0$. Finally, the paper in hand brings all combinations of high and low frequencies in space and time into consideration, which allows interesting, rather general interpretations of experience and, we trust, the invention of specific stabilizing devices.

The relative stability of difference systems, in which advecting velocity components have spatial high-frequency smoothing operators on them, is explained by the analysis. The smoothing operators effectively suppress the terms in (4) with coefficients U_1 and U_3 , so that the criteria (6) reduce to

$$0 \leq (\Delta t / \Delta x)^2 (U_0^2 - U_2^2) < 1.$$

At the same time, the uncentered, forward start customarily used makes the amplitude of the computational mode small initially. Thus U_2 is initially small, and our criterion therefore indicates stability initially. Generally instability eventually sets in, which we interpret as an eventual growth of U_2 to levels violating the left-hand inequality of the criterion, and perhaps later the right-hand side.

For even greater stability, if not perfect stability, not only must the spatial high frequencies be suppressed, as with smoothing operators on advecting coefficients in the equations, but also the temporal high frequencies must be similarly suppressed. The analysis in the next section on the gravity wave indicates that these remarks apply not only to coefficients of advecting velocity but to undifferentiated coefficients generally.

6. THE GRAVITATIONAL OSCILLATION

Long unexplained has been the perfect computational stability of certain integrations of the isolated gravity wave. Consider the set of equations for an incompressible homogeneous fluid under the hydrostatic approximation and with slab symmetry:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + g \frac{\partial h}{\partial x} = 0, \quad (7a)$$

$$\frac{\partial h}{\partial t} + u \frac{\partial h}{\partial x} + h \frac{\partial u}{\partial x} = 0, \quad (7b)$$

and

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} = 0. \quad (7c)$$

Here, x and t are the horizontal space and time coordinates, u and v the x and y components of velocity, y being the other horizontal space coordinate, h the height of the free surface, and g a constant gravitational acceleration. The set is a special case of the full set in two spatial dimensions, in which u , v , and h are not functions of y . It can easily be shown that, if such a condition prevails at any instant, it prevails for all time.

The so-called semimomentum form has always exhibited "perfect" stability—neither amplification nor damping—for u and h (Shuman and Stackpole 1968). Note that the first two equations (7a) and (7b), of the set are complete in themselves, being two equations in the two dependent variables, u and h . In the set (7), therefore, the gravity wave is isolated from other mechanisms.

We have recently experimented numerically with the third equation (7c) as well as the first two, (7a) and (7b), and v has generally exhibited instability. The experiments were with the so-called semimomentum forms, that is,

$$\bar{u}_i^t + \bar{u}^x u_x + g \bar{h}_x^x = 0, \quad (8a)$$

$$\bar{h}_i^t + \bar{u}^x h_x + \bar{h}^x u_x = 0, \quad (8b)$$

and

$$\bar{v}_i^t + \bar{u}^x v_x = 0. \quad (8c)$$

The instability in v is explained by Robert (1969) and the analysis in the preceding section. By reason of the $(\bar{\quad})^x$ operation on the advecting velocity in (8c), $U_1=U_3=0$, and the stability criteria (6) reduce to the single criterion,

$$0 \leq (\Delta t / \Delta x)^2 (U_0^2 - U_2^2) < 1.$$

Since in the calculations u varies about zero, it is more than plausible that U_0 is small and the left-hand inequality is somewhere sometime violated. Robert's (1969) analysis was for the case $U_0=0$ as well as $U_1=U_3=0$ and showed unconditional instability.

The perfect stability of the gravitational oscillation, however, is not explained by our analysis of the advective equation. For the explanation we will perform an analysis of the two gravity wave equations.

Similar to the advective equation (4) we consider

$$\bar{u}_t^i + U \bar{u}_x^x + g \bar{h}_x^x = 0 \tag{9a}$$

and

$$\bar{h}_t^i + U \bar{h}_x^x + H \bar{u}_x^x = 0 \tag{9b}$$

where

$$U = U_0 + U_1 e^{i\pi j} + U_2 e^{i\pi n} + U_3 e^{i\pi(j+n)}$$

and

$$H = H_0 + H_1 e^{i\pi j} + H_2 e^{i\pi n} + H_3 e^{i\pi(j+n)}.$$

U and H correspond to the undifferentiated u and h in equations (7). Since both u and h can be expected to contain high frequencies, these have been incorporated in U and H as above.

Following the derivation in section 5, we apply the operator $(\bar{\quad})_t^i$ to (9a) and (9b), then eliminate the resulting \bar{u}_{xt}^x and \bar{h}_{xt}^x from the resulting set by first applying the operator $(\bar{\quad})_x^x$ to (9a) and (9b) and then substituting. We thus obtain

$$\bar{u}_{tt}^i - A \bar{u}_{xx}^x - B \bar{h}_{xx}^x = 0 \tag{10a}$$

and

$$\bar{h}_{tt}^i - C \bar{u}_{xx}^x - D \bar{h}_{xx}^x = 0 \tag{10b}$$

where

$$A = \bar{U}^{2t} \bar{U}^{2x} + g \bar{H}^{2x},$$

$$B = g(\bar{U}^{2t} + \bar{U}^{2x}),$$

$$C = \bar{U}^{2t} \bar{H}^{2x} + \bar{U}^{2x} \bar{H}^{2t},$$

and

$$D = \bar{U}^{2t} \bar{U}^{2x} + g \bar{H}^{2t}.$$

Multiply (10b) by an arbitrary variable E and add to (10a), obtaining

$$\bar{u}_{tt}^i + E \bar{h}_{tt}^i - (A + CE) \bar{u}_{xx}^x - (B + DE) \bar{h}_{xx}^x = 0.$$

Let

$$B + DE = E(A + CE). \tag{12}$$

Then

$$\bar{u}_{tt}^i + E \bar{h}_{tt}^i - (A + CE) (\bar{u}_{xx}^x + E \bar{h}_{xx}^x) = 0.$$

Now let E be of the functional form

$$E = E_0 + E_1 e^{i\pi j} + E_2 e^{i\pi n} + E_3 e^{i\pi(j+n)}.$$

Then

$$\overline{(Eh)}_{tt}^i = E \bar{h}_{tt}^i$$

and

$$\overline{(Eh)}_{xx}^x = E \bar{h}_{xx}^x.$$

We may therefore write

$$\overline{(u + Eh)}_{tt}^i - (A + CE) \overline{(u + Eh)}_{xx}^x = 0.$$

This is a wave equation, and if $A + CE$ is constant, the stability criterion is

$$0 \leq (\Delta t / \Delta x)^2 (A + CE) < 1. \tag{13}$$

We now show that $A + CE$ may be regarded as constant for each of two sets of points, as in section 5, for the set where $j+n$ is even and for the set where $j+n$ is odd. After solving equation (12) for E , expanding the operators in (11), and substituting, we find for even $j+n$

$$A + CE = (U_0 - U_3)^2 - (U_1 - U_2)^2 + g(H_0 - H_3) \pm \sqrt{g^2(H_1 - H_2)^2 + 4g(U_0 - U_3)[(U_0 - U_3)(H_0 - H_3) - (U_1 - U_2)(H_1 - H_2)]}$$

and for odd $j+n$

$$A + CE = (U_0 + U_3)^2 - (U_1 + U_2)^2 + g(H_0 + H_3) \pm \sqrt{g^2(H_1 + H_2)^2 + 4g(U_0 + U_3)[(U_0 + U_3)(H_0 + H_3) - (U_1 + U_2)(H_1 + H_2)]}$$

As in section 5, we must deal with both sets of grid points, so both definitions of $A + CE$ must be considered for the stability criterion (13).

The explanation for the relative stability of the pure gravity wave equations (8a) and (8b), compared to pure advective equations, for example (8c), lies in the overwhelming role of the mean height, H_0 , of the free surface in the definition of $A + CE$.

7. A DEMONSTRATION

A theory that explains observations satisfies our curiosity, but its proof must be given by successful prediction, and only through prediction does it become useful. Having developed the theory to this stage, we ventured a prediction, that if the spatial and temporal high-frequency modes were suppressed in the undifferentiated factors in the equations, we would achieve relative, if not perfect, stability.

Such suppression could be accomplished either by smoothing in space and time the fields of dependent variables, or by inserting in the equations devices which suppress high frequencies in the equations but retain their presence in the fields. The former, we felt, would not be as convincing a test as the latter and in any case might be difficult because the smoothing would have to be adjusted to the growth of high frequencies through nonlinear interactions, something we know little about. We therefore invented a "star" operator $(\quad)^* \equiv \frac{1}{2}[(\quad)_{n-1} + (\quad)_n]$, which

is simply an average of the given function at the current and immediately previous time steps.

We predicted at least relative stability for the system

$$\overline{u}_t + \overline{u} \overline{u}_x + \overline{gh}_x = 0, \quad (14a)$$

$$\overline{h}_t + \overline{u} \overline{h}_x + \overline{h} \overline{u}_x = 0, \quad (14b)$$

and

$$\overline{v}_t + \overline{u^*} \overline{v}_x = 0. \quad (14c)$$

This set of three equations differs from the former set (8) only by the addition of the star operator on u in (14c). It is an important, though modest, test.

The results shown in figure 2 are from integrations of both (8) and (14). Following Shuman and Stackpole (1968), the initial data were

$$u = U \sum_{r=1}^{23} \sin(\pi r j / 24), \quad h = H, \quad \text{and}$$

$$v = V \sum_{r=1}^{23} \cos(\pi r j / 24),$$

where $U = V = 8.5 \text{ m sec}^{-1}$ and $H = 7620 \text{ m}$. The region of integration extended from $j = 0$ to $j = 24$. At each boundary, $u = \overline{u}^2_x = h_{2x} = v_{2x} = 0$, as boundary conditions throughout the integration. Data at the first time level after initial time were derived by a forward time step. The time step was 10 min, the space increment 381 km.

As before, u and h behaved with perfect stability, which we have explained but had not predicted. In the experiment with (14), v also exhibited perfect stability, as shown in figure 2. Since we had predicted stability for v , this is a substantiation of the theory.

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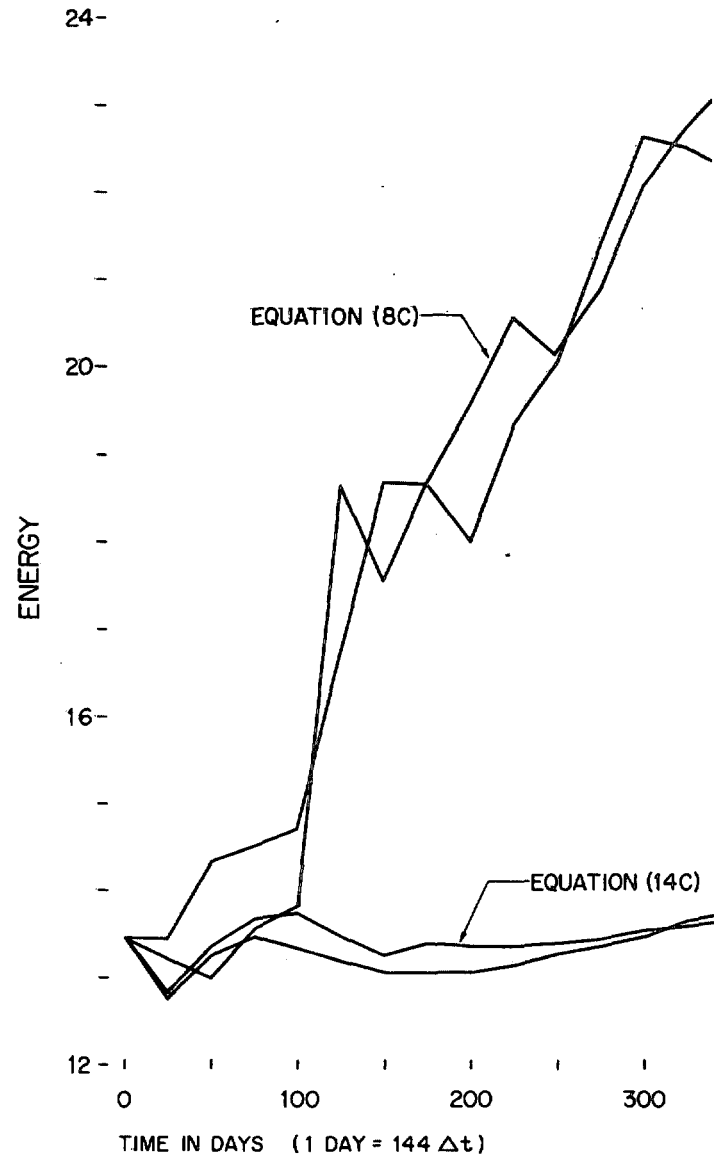


FIGURE 2.—The ordinate, labeled "energy," is $\log_{10} \frac{1}{2} \overline{hu^2}$ where the bar indicates a spatial average. In each pair of curves, one shows values at even time steps, the other odd.

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