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STUDIES IN NUMERICAL NONLINEAR INSTABILITY I. WHY DO LEAPFROG SCHEMES GO UNSTABLE?*

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Abstract. It is well known that leapfrog (explicit mid-point) discretizations of partial differential equations may have unbounded solutions for any choice of mesh-sizes, (even for choices satisfying conditions for linear stability). We provide a means for forecasting the qualitative behaviour of the computed leapfrog points, thus explaining the dynamics of the nonlinear instability phenomenon.

Key words. nonlinear instability, leapfrog schemes, dynamical systems

1. Introduction. Leapfrog (explicit mid-point) schemes are often used in those meteorological or oceanographic computations where the interest lies in monitoring the global evolution of physical magnitudes over long periods of time. In these circumstances, nondissipative leapfrog schemes may be more advisable than some dissipative alternative methods [14]. However, the lack of dissipativity, while preventing gross global losses of energy, vorticity, etc., ..., entails some disadvantages from the stability point of view. Here the word stability must be understood to refer to the behaviour of the numerical solution for *fixed* values of the mesh-sizes, as the number of computed time-levels grows. (As distinct from the notions of Lax–Richtmyer stability or Dahlquist stability [16], which provide conditions related to the concept of convergence as the mesh-sizes tend to zero.)

In linear, constant coefficient problems with suitable boundary conditions, the stability of leapfrog schemes is easily investigated, for in such cases the discrete equations are solvable in closed form, via Fourier analysis. Often a relationship between the various mesh-sizes (the so-called linear stability condition) can be derived which ensures boundedness of the numerical solution as the number of computed levels grows.

In linear, variable coefficient or nonlinear problems describing wave phenomena, it may happen that the leapfrog solution is unbounded for *any choice of meshsizes* (even for choices which satisfy the linear stability conditions associated with all the problems obtainable from the given one by linearizing and freezing the coefficients.) This fact was first noted by Phillips [17] in the nonlinear case and Miyakoda [13] in the variable coefficient case. Phillips attributed this offending behaviour (the so-called *nonlinear instability*) to the presence of *aliasing*. However Arakawa [1] constructed a continuous-time difference scheme for the inviscid vorticity transport equation which suffers from aliasing and yet exactly conserves vorticity, its square and kinetic energy, thus ensuring boundedness of the computed solution. (See Morton [14] for an excellent survey of the role played by *quadratic conserved quantities* and its relation with Galerkin's method.) When Arakawa's scheme is discretized in time by means of the leapfrog technique, the quadratic invariants are only *approximately* conserved and nonlinear stability can arise, (cf. [19]). In practice, leap-frog schemes must be supplemented by filtering or artificial viscosity [12] in order to prevent the onset of nonlinear instability. A modification of the leapfrog technique which is free from the occurrence of blowups has been introduced and analyzed in [19], [21], [22].

In this paper we present a technique, whereby *the qualitative behaviour of leapfrog approximations can be forecast* a priori (or explained a posteriori). In particular we provide an explanation of the nonlinear instability phenomenon.

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Our research was inspired by a paper by Ushiki [26].

Little is known concerning the qualitative behaviour, for fixed values of the mesh-sizes, of discretizations of nonlinear evolutionary problems. In the ordinary differential equation field, interest has been centered around the issue of *contractivity* (see Dekker and Verwer [4] for a thorough summary). The experience gained by Ushiki [26] and the contents of the present paper, appear to suggest that the investigation of stability properties may benefit from an interaction with the field of *dynamical systems*. However our study does not rely heavily on concepts of that field and the reader only needs to be familiar with the basic elementary techniques in the qualitative study of ordinary differential systems (see among others [7]).

Another useful connection is that between nonlinear instability in numerical analysis and nonlinear stability in fluid mechanics, explored by Newell [15].

An outline of the paper is as follows. Section 2 contains the main idea. The linear and nonlinear ordinary differential equation cases are described in §§ 3 and 5, respectively. Partial differential equations are investigated in § 6. The fourth section is devoted to some technical results and the seventh contains several concluding remarks.

2. The augmented system. We consider initial value problems for the system

$$\mathbf{y}' = \mathbf{f}(\mathbf{y}), \tag{2.1}$$

where a prime denotes differentiation with respect to t and $\mathbf{f}:\mathbb{R}^d \to \mathbb{R}^d$ is a smooth (C^∞ say) function. The system (2.1) is discretized by means of the mid-point rule

$$\mathbf{y}_{n+2} = \mathbf{y}_n + 2h\mathbf{f}(\mathbf{y}_{n+1}), \tag{2.2}$$

where the step-length h is positive. If we fix a solution $\mathbf{y}(t)$ of (2.1) and choose $\mathbf{y}_0, \mathbf{y}_1$, close to $\mathbf{y}(0), \mathbf{y}(h)$ respectively, then each point $\mathbf{y}_n$, $n = 2, 3, \cdots$ generated by (2.2) will be "close" to the point $\mathbf{y}(nh)$, $n = 2, 3, \cdots$. In more (but not too) precise terms, if we consider a *family* $\mathbf{y}_0^h, \mathbf{y}_1^h$ of starting points, with h ranging in an interval $(0, h_0)$, $h_0 > 0$, then [10, p. 22]

$$\lim_{\substack{h\to 0\\ nh = a}} \mathbf{y}_n^h = \mathbf{y}(a) = \mathbf{y}(nh), \tag{2.3}$$

provided that

$$\lim_{h\to 0} \mathbf{y}_0^h = \lim_{h\to 0} \mathbf{y}_1^h = \mathbf{y}(0). \tag{2.4}$$

However, this *convergence* property does not imply that for a given, *fixed* value of h, and given $\mathbf{y}_0, \mathbf{y}_1$ (close to $\mathbf{y}(0), \mathbf{y}(h)$, respectively), the sequences in $\mathbb{R}^d$

$$\mathbf{y}_0, \mathbf{y}_1, \mathbf{y}_2, \cdots, \mathbf{y}_n, \cdots, \tag{2.5}$$

$$\mathbf{y}(0), \mathbf{y}(h), \mathbf{y}(2h), \cdots, \mathbf{y}(nh), \cdots, \tag{2.6}$$

exhibit the same *qualitative behaviour*. In fact, it is well known [6, p. 241] that if (2.1) is linear

$$\mathbf{y}' = A\mathbf{y} \tag{2.7}$$

and the spectrum of A is contained in $\{z: \operatorname{Re} z < 0\}$, so that $\lim_n \mathbf{y}(nh) = \mathbf{0}$, the leapfrog points $\mathbf{y}_n$ will, in general, be unbounded no matter how close $\mathbf{y}_0, \mathbf{y}_1$ are to $\mathbf{y}(0), \mathbf{y}(h)$.

In this paper a method is given for describing the qualitative behaviour of (2.5) for fixed h. We start by introducing the sequence in $\mathbb{R}^{2d}$

$$[\mathbf{y}_0, \mathbf{y}_1], [\mathbf{y}_2, \mathbf{y}_3], \cdots, [\mathbf{y}_{2n}, \mathbf{y}_{2n+1}], \cdots. \tag{2.8}$$

It is obvious that the knowledge of (2.8) implies that of (2.5) and vice versa. Nevertheless (2.8) is more advantageous in that each "augmented" vector $[\mathbf{y}_{2n}, \mathbf{y}_{2n+1}]$ is obtained from the previous vector $[\mathbf{y}_{2n-2}, \mathbf{y}_{2n-1}]$ by means of the *one-step* recursion

$$[\mathbf{y}_{2n}, \mathbf{y}_{2n+1}] = \mathcal{T}[\mathbf{y}_{2n-2}, \mathbf{y}_{2n-1}], \tag{2.9}$$

where $T: \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is the mapping

$$\mathcal{T}[\mathbf{p}, \mathbf{q}] = [\mathbf{p} + 2h\mathbf{f}(\mathbf{q}), \mathbf{q} + 2h\mathbf{f}(\mathbf{p} + 2h\mathbf{f}(\mathbf{q}))]. \tag{2.10}$$

One iteration of (2.9) is equivalent to *two* iterations of (2.2). The main point of this paper consists of the observation that (2.10) provides a *stable*, first-order *consistent*, one-step method for the numerical study of the system in $\mathbb{R}^{2d}$,

$$\mathbf{p}' = \mathbf{f}(\mathbf{q}), \qquad \mathbf{q}' = \mathbf{f}(\mathbf{p}), \tag{2.11}$$

which we call *augmented system* associated with the *original system* (2.1). More precisely, if we fix a solution $\mathbf{p}(t)$, $\mathbf{q}(t)$ of (2.11), then

$$\lim_{\substack{h \to \infty \\ 2nh = a}} T^n[\mathbf{p}_0^h, \mathbf{q}_0^h] = [\mathbf{p}(a), \mathbf{q}(a)] \tag{2.12}$$

provided that $\mathbf{p}_0^h$, $\mathbf{q}_0^h$ tend to $\mathbf{p}(0)$, $\mathbf{q}(0)$.

(The proof of this convergence result is trivial and will not be given here.) *We claim that the qualitative behaviour of* (2.8) *is governed by the qualitative behaviour of sequences*

$$[\mathbf{p}(0), \mathbf{q}(0)], [\mathbf{p}(h), \mathbf{q}(h)], \cdots, [\mathbf{p}(nh), \mathbf{q}(nh)], \cdots, \tag{2.10}$$

where $\mathbf{p}(t)$, $\mathbf{q}(t)$, *is a solution of the augmented* system (2.11).

Before we justify our claim, which concerns the fixed h, $n \to \infty$ behaviour of the computed solutions, let us examine the $h \to 0$, nh-fixed behaviour. We consider again a family of step-lengths h, $0 < h < h_0$; fix a solution $\mathbf{y}(t)$ of the original system and choose $\mathbf{y}_0^h$, $\mathbf{y}_1^h$ satisfying (2.4). This implies, after (2.3), convergence of $\mathbf{y}_n^h$ towards $\mathbf{y}(nh)$ (nh constant).

On the other hand, consideration of the augmented recursion (2.9), implies after (2.12) that

$$\lim_{\substack{h \to \infty \\ 2nh = a}} \mathbf{y}_{2n}^h = \mathbf{p}(a), \qquad \lim_{\substack{h \to \infty \\ 2nh = a}} \mathbf{y}_{2n+1}^h = \mathbf{q}(a) \tag{2.13}$$

where $\mathbf{p}(t)$, $\boldsymbol{q}(t)$ is the solution of the augmented system satisfying $\mathbf{p}(0) = \mathbf{q}(0) = \mathbf{y}(0)$. Now it is obvious that this solution is given by $\mathbf{p}(t) = \mathbf{q}(t) = y(t)$, so that (2.13) is just a restatement of (2.3). Thus, in the study of the $h \to 0$, nh-fixed case the introduction of the augmented system does not bring any new information. It can be proved that this conclusion is not altered if orders of convergence are taken into account. Incidentally, we note that only *diagonal solutions* of the augmented system (i.e. solutions with $\mathbf{p}(t) \equiv \mathbf{q}(t)$) have appeared in our argument: clearly there is a one-to-one correspondence between diagonal solutions of the augmented system and solutions of the original problem (2.1). It will turn out that in the study of the fixed h behaviour *nondiagonal solutions* of the augmented system will play an important role.

We now fix a solution $\mathbf{y}(t)$ of (2.1), fix a "small" value of h and choose fixed starting vectors $\mathbf{y}_0, \mathbf{y}_1$ "close" to $\mathbf{y}(0)$, $\mathbf{y}(h)$ respectively. Our aim is to describe the qualitative behaviour of (2.5). We rely on the concept of *local error*, as employed in the text by Shampine and Gordon [23, p. 22]. In these authors' words, when $\mathbf{y}_n$, and $\mathbf{y}_{n+1}$ have been computed, the best that the method (2.2) can do is to yield a point

$\mathbf{y}_{n+2}$ close to $\mathbf{u}(2h)$, where $\mathbf{u}(t)$ is the *local solution* defined by

$$\mathbf{u}' = \mathbf{f}(\mathbf{u}), \qquad \mathbf{u}(0) = \mathbf{y}_n.$$

Now, upon Taylor expanding we find that

$$\mathbf{y}_{n+2} - \mathbf{u}(2h) = 2h\mathbf{f}(\mathbf{y}_{n+1}) - 2h\mathbf{f}(\mathbf{u}(h)) + \mathbf{E},$$

where $\mathbf{E}$ can be bounded in the form $\|\mathbf{E}\| \leqq Ch^3$, with C independent of h. If we were in the $h \to 0$ study, we would argue that $\mathbf{y}_{n+1}$ is close to $u(h)$ and therefore the next computed point is close to $\mathbf{u}(2h)$, *i.e.* the computed points tend to follow approximately the *local solutions.* (More precisely if $\mathbf{y}_0 = \mathbf{y}(0)$ and $\mathbf{y}_1$ is obtained by means of a one-step, first order method, then $\mathbf{y}_{n+1} - \mathbf{u}(h) = O(h^2)$ and $\mathbf{y}_{n+2} - \mathbf{u}(2h) = O(h^2)$.) However for fixed h, n large, $\mathbf{y}_{n+1}$ and $\mathbf{u}(h)$ can be significantly different and thus $\mathbf{y}_{n+2}$ may not follow the local solution.

Let us consider what happens if we describe the computed points in terms of the augmented iteration (2.9). When $\mathbf{y}_{2n-1}, \mathbf{y}_{2n}$ have been computed, the method will attempt to approximate the local solution $\mathbf{v}, \mathbf{w}$ defined by

$$\mathbf{v}' = \mathbf{f}(\mathbf{w}), \qquad \mathbf{w}' = \mathbf{f}(\mathbf{v}),$$
$$\mathbf{v}(0) = \mathbf{y}_{2n-2}, \qquad \mathbf{w}(0) = \mathbf{y}_{2n-1},$$

and now Taylor expansion yields

$$\mathbf{y}_{2n} - \mathbf{v}(2h) = \mathbf{E}_1, \qquad \mathbf{y}_{2n-1} - \mathbf{w}(2h) = \mathbf{E}_2$$

with $\|\mathbf{E}_1\| + \|\mathbf{E}_2\| \leqq Ch^2$, C constant independent of h. In other words, the computed points will lie near the local solution of the augmented recursion. Note that these local solutions are in general nondiagonal.

Admittedly the previous discussion has been merely *heuristic* and it is difficult to see how a rigorous proof could be given when the term "qualitative" behaviour has not been mathematically defined. We recall that it is possible to define precisely what is meant by the statement "two differential systems have the same qualitative behaviour" [3, p. 92]. This line of thought is not pursued in this paper. However the linear case is *rigorously* treated in the next section.

3. The linear case. In this paragraph we consider the linear system (2.7) and assume for simplicity that A is real and can be diagonalized by a (possibly complex) linear change of variables. Within this section vectors will be allowed to belong to the complex space $\mathbb{C}^d$. We define qualitative behaviour as follows.

DEFINITION 1. Let (a_n), (b_n) be sequences of complex numbers. We say that they are linear with the same qualitative behaviour if they are both identically zero or if they are of the form $a_n = r \exp(nc)$, $b_n = s \exp(nd)$, with r, c, s, d complex numbers $r, s \neq 0$, sign Re c = sign Re d, sign Im c = sign Im d.

Note that if (a_n), (b_n) are linear with the same qualitative behaviour then either $|a_n| \uparrow \infty$, $|b_n| \uparrow \infty$, or $|a_n| =$ constant, $|b_n| =$ constant or $|a_n| \downarrow 0$, $|b_n| \downarrow 0$. Also as $n \uparrow \infty$, the arguments of a_n, b_n are either both increasing or both constant or both decreasing. There are *nine* possible qualitative behaviours for sequences other than the identically zero sequence.

For sequences of vectors we resort to uncoupling changes of variables as follows. ($\mathbf{e}_i$ denotes the ith column of the identity matrix.)

DEFINITION 2. If $(\mathbf{a}_n)$, $(\mathbf{b}_n)$ are sequences in $\mathbb{C}^d$, we say that they are linear with the same qualitative behaviour, if regular matrices M, N can be found such that, for each i, $1 \leqq i \leqq d$ the sequences of components $\mathbf{e}_i^T M \mathbf{a}_n$, $\mathbf{e}_i^T N \mathbf{b}_n$ are linear with the same qualitative behaviour in the sense of the previous definition.

THEOREM 1. *Let* $\mathbf{y}_0, \mathbf{y}_1$ *be given vectors in* $\mathbb{C}^d$ *and fix h such that* $|h \operatorname{Im} \lambda_i| < 1$ *for each* λ_i *in* Spec (A), *with A as above. Then there is a solution* $\mathbf{p}(t)$, $\mathbf{q}(t)$ *of the augmented system associated with* $\mathbf{y}' = A\mathbf{y}$, *such that the sequence* (2.10) *and the leapfrog sequence* (2.8) *are linear with the same qualitative behaviour in* $\mathbb{R}^{2d}$, *and furthermore* $\mathbf{p}(0) = \mathbf{y}_0$.

Remark. Note that here $\mathbf{y}_0, \mathbf{y}_1$ can be arbitrary. In practice $\mathbf{y}_0, \mathbf{y}_1$ approximate $\mathbf{y}(0)$, $\mathbf{y}(h)$, with $\mathbf{y}(t)$ a solution of the original system, and therefore the starting augmented vector $[\mathbf{y}_0, \mathbf{y}_1]$ will be close to the diagonal of $\mathbb{R}^d \times \mathbb{R}^d$, (i.e. $\mathbf{y}_0, \mathbf{y}_1$ will not be widely different).

Proof. As usual, it is enough to consider the scalar equation

$$y' = \lambda y, \quad \lambda \in \mathbb{C}, \quad |h \operatorname{Im} \lambda| < 1$$

with augmented system

$$p' = \lambda q, \qquad q' = \lambda p.$$

After the change of variables in R^2 given by

$$p + q = P, \qquad p - q = Q,$$

the solutions of the augmented systems are of the form $P = a \exp(\lambda t)$, $Q = b \exp(-\lambda t)$, with $a = p(0) + q(0)$, $b = p(0) - q(0)$. Therefore, in the P, Q variables, the sequence in (2.10) becomes

$$[a(\exp(\lambda h))^n, b(\exp(-\lambda h))^n]. \tag{3.1}$$

Now the theory of linear, constant coefficient difference equations shows that the sequence of computed leapfrog points (2.5) is given by

$$y_n = cr^n + d(-r^{-1})^n$$

where c, d depend on r, y_0, y_1 and r is related to h and λ through a function $r = g(H)$, $H = \lambda h$ given by

$$g(H) = H + \sqrt{1 + H^2}.$$

Here $\sqrt{z}$ denotes the square root of z with argument in the interval $(-\pi/2, \pi/2]$. Double roots of the characteristic equation are ruled out by the condition $|h \operatorname{Im} \lambda| < 1$. For the nth term in the augmented sequence (2.8), we have

$$\begin{bmatrix} y_{2n} \\ y_{2n+1} \end{bmatrix} = \begin{bmatrix} cr^{2n} + d(r^{-1})^{2n} \\ crr^{2n} - dr^{-1}(r^{-1})^{2n} \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ r & -r^{-1} \end{bmatrix} \begin{bmatrix} c(r^2)^n \\ d(r^{-2})^n \end{bmatrix}. \tag{3.2}$$

The matrix in (3.2) is regular. (The values $r = \pm i$ which render it singular are excluded by the requirement $|\operatorname{Im} H| < 1$.) Then a change of variables brings (3.2) to the "uncoupled" form $[c(r^2)^n, d(r^{-2})^n]$, which is compared with (3.1), after choosing $p(0)$, $q(0)$ such that $p(0) + q(0) = 2c$, $p(0) - q(0) = 2d$. For this choice $p(0) = c + d = y_0$.

We introduce the following subsets of $\mathbb{C}$, in correspondence with the possible nontrivial qualitative behaviours:

$$A_1 = \{0\},$$

$$A_2 = \{bi: 0 < b < 1\},$$

$$A_3 = \{bi: -1 < b < 0\},$$

$$A_4 = \{a: 0 < a < \infty\},$$

$$A_5 = \{a\colon -\infty < a < 0\},$$
$$A_6 = \{a+bi\colon 0 < a < \infty, 0 < b < 1\},$$
$$A_7 = \{a+bi\colon 0 < a < \infty, -1 < b < 0\},$$
$$A_8 = \{a+bi\colon -\infty < a < 0, 0 < b < 1\},$$
$$A_9 = \{a+bi\colon -\infty < a < 0, -1 < b < 0\}.$$

The proof is concluded if we show that

$$g(A_1) = \{1\},$$
$$g(A_2) = \{e^{i\theta}\colon 0 < \theta < \pi/2\},$$
$$g(A_3) = \{e^{i\theta}\colon -\pi/2 < \theta < 0\},$$
$$g(A_4) = \{a\colon 1 < a < \infty\},$$
$$g(A_5) = \{a\colon 0 < a < 1\},$$
$$g(A_6) \subset \{\rho\, e^{i\theta}\colon \rho > 1, 0 < \theta < \pi/2\},$$
$$g(A_7) \subset \{\rho\, e^{i\theta}\colon \rho < 1, -\pi/2 < \theta < 0\},$$
$$g(A_8) \subset \{\rho\, e^{i\theta}\colon \rho < 1, 0 < \theta < \pi/2\},$$
$$g(A_9) \subset \{\rho\, e^{i\theta}\colon \rho < 1, -\pi/2 < \theta < 0\}.$$

The conditions relative to A_i, $i = 1-5$ are verified straightforwardly. For A_6 note that g is univalued and analytic in the closure $\bar{A}_6$, except for the branch point at $H = i$. It is therefore sufficient to investigate the behaviour of the boundary of A_6 under the mapping $g(H)$. That boundary consists of A_1, A_2, A_4, already considered, and of the half line $L = \{a + i, 0 < a < \infty\}$. A simple computation shows that if z is in L then $\operatorname{Im} z > 1$, $\operatorname{Re} z > 0$. This accounts for A_6. For A_7 use the reflection principle. The remaining subsets (i.e., A_5, A_8, A_9) are easily dealt with via the symmetry $g(H) = (g(-H))^{-1}$.

Remark. It is very important to emphasize that the solution $[\mathbf{p}(t), \mathbf{q}(t)]$ given by the theorem does not in general satisfy $[\mathbf{p}(0), \mathbf{q}(0)] = [\mathbf{y}_0, \mathbf{y}_1]$. It is easily shown that these two 2-dimensional vectors differ by $O(h)$ terms for fixed, arbitrary $\mathbf{y}_0, \mathbf{y}_1$.

Before we close this paragraph, we describe some of the properties of *linear* augmented systems.

THEOREM 2. *Let A be as above.* (i) *If $\lambda \neq 0$ is an eigenvalue of A with multiplicity m, then $\lambda, -\lambda$ are eigenvalues of the matrix of the augmented system with multiplicity m each. If $\mathbf{a}$ is an eigenvector of A associated to $\lambda \neq 0$, then $[\mathbf{a}, \pm\mathbf{a}]$ are eigenvectors of the augmented matrix associated to $\pm\lambda$.*

(ii) *If 0 is an eigenvalue of A with multiplicity m then 0 is an eigenvalue of the augmented matrix with multiplicity $2m$. If $\mathbf{a} \neq \mathbf{0}$ is in the null space of A then $[\mathbf{a}, \mathbf{0}]$, $[\mathbf{0}, \mathbf{a}]$ are linearly independent and lie in the null space of the augmented matrix.*

Proof. It is easy and will not be given.

It follows from this theorem that the origin is a stable equilibrium of the augmented system if and only if the spectrum of A is purely imaginary. Theorem 1 implies then that the mid-point rule is absolutely stable for small h and linear constant-coefficient problems, if and only if these have purely imaginary spectra—a well-known result.

4. Some auxiliary results. We now turn our attention to general *nonlinear* augmented systems (2.11). If $\mathbf{p}_0, \mathbf{q}_0 \in \mathbb{R}^d$ we denote by $\mathbf{p}(t; \mathbf{p}_0, \mathbf{q}_0)$, $\mathbf{q}(t; \mathbf{p}_0, \mathbf{q}_0)$, the solution of (2.11) such that $\mathbf{p}(0; \mathbf{p}_0, \mathbf{q}_0) = \mathbf{p}_0$; $\mathbf{q}(0; \mathbf{p}_0, \mathbf{q}_0) = \mathbf{q}_0$. Then for fixed $t > 0$ the mapping $F_t = [\mathbf{p}_0, \mathbf{q}_0] \to [\mathbf{p}(t; \mathbf{p}_0, \mathbf{q}_0), \mathbf{q}(t; \mathbf{p}_0, \mathbf{q}_0)]$ is the t-time *flow* of the system (2.11). It is defined only at those vectors $[\mathbf{p}_0, \mathbf{q}_0]$ such that the corresponding solution $[\mathbf{p}(t; \mathbf{p}_0, \mathbf{q}_0), \mathbf{q}(t; \mathbf{p}_0, \mathbf{q}_0)]$ is defined at time t (i.e. has not reached infinity before that time).

THEOREM 3. (i) *For each fixed time t, the t-time flow F_t of any augmented system preserves the volume in* $\mathbb{R}^{2d}$.

(ii) *The equilibria of the augmented system* (2.11) *are precisely the points* $[\mathbf{a}, \mathbf{b}]$, *with* $\mathbf{a}, \mathbf{b}$ *equilibria of the original system. At a diagonal equilibrium* $[\mathbf{a}, \mathbf{a}]$ *the eigenvalues of the Jacobian matrix of the augmented system are given by* $\pm\lambda$, *with* λ *an eigenvalue of the Jacobian matrix at* $\mathbf{a}$ *of the original system* (2.1).

(iii) *If the original system is a gradient system i.e.* $\mathbf{f} = \mathbf{grad}\ V$, *for a scalar function V, then the augmented system takes the Hamiltonian form*

$$\mathbf{p}' = -\frac{\partial H}{\partial \mathbf{q}}, \qquad \mathbf{q}' = \frac{\partial H}{\partial \mathbf{p}}$$

for the Hamiltonian function $H(p, q) = V(p) - V(q)$. *In this case H is a first integral of the augmented system, i.e.* $H(\mathbf{p}(t), \mathbf{q}(t)) =$ *constant for solutions of* (2.11).

(iv) *If the original system has a quadratic first integral* $\mathbf{y}(t)^T M \mathbf{y}(t) =$ *constant, with M a constant, symmetric matrix, then the augmented system has the first integral* $\mathbf{p}(t) TM \mathbf{q}(t) =$ *constant.*

Proof. (ii)-(iv) are easy. For (i) note that $[\mathbf{f}(\mathbf{q}), \mathbf{f}(\mathbf{p})]$ is a divergence-free field in the $[\mathbf{p}, \mathbf{q}]$ space [2, p. 69].

For the augmented recursion we have, similarly, the next theorem.

THEOREM 4. (i) *The mapping T in* (2.10) *preserves the orientation and the volume.*

(ii) *The fixed points of T are of the form* $[\mathbf{a}, \mathbf{b}]$ *with* $\mathbf{a}, \mathbf{b}$ *equilibria of* $\mathbf{f}$.

(iii) *T is one-to-one and onto.*

(iv) *If the original system has a quadratic first integral* $\mathbf{y}(t)^T M \mathbf{y}(t) =$ *constant, with M a constant symmetric matrix, then the leapfrog points verify* $\mathbf{y}_n^T M \mathbf{y}_{n+1} =$ *constant,* $n = 0, 1, \cdots$.

Proof. Introduce the map

$$S\begin{bmatrix}\mathbf{p}\\ \mathbf{q}\end{bmatrix} = \begin{bmatrix}\mathbf{q}\\ \mathbf{p} + 2h\mathbf{f}(\mathbf{q})\end{bmatrix},$$

so that T is the composition $S \circ S$. It is clear that S is one-to-one and onto and this implies (iii). Furthermore the Jacobian matrix of S takes the form

$$J = \begin{bmatrix}0 & I\\ I & 2hD\mathbf{f}\end{bmatrix}$$

with $D\mathbf{f}$ the Jacobian of $\mathbf{f}(\mathbf{q})$ w.r.t. $\mathbf{q}$. Then $\det(J) = -1$ and the determinant of the Jacobian matrix of T equals 1. This proves i), ii) and iv) are trivial.

5. Nonlinear problems. In this section we prove, by means of examples, that the qualitative behaviour of the augmented sequence (2.8) is governed by the behaviour of the neighbouring solutions of the augmented system, in the sense that when $[\mathbf{y}_{2n}, \mathbf{y}_{2n+1}]$ has been computed $[\mathbf{y}_{2n+2}, \mathbf{y}_{2n+3}]$ lies near the corresponding local solution.

A. Our first example concerns the escalar equation $y' = y^2$, whose nonequilibrium solutions are monotonically *increasing* functions of t. The origin is the only equilibrium. If $y(0) < 0$, then $y(t)$ tends to 0 as t tends to ∞. If $y(0) > 0$, then $y(t)$ reaches in finite time.

The problem $y'=y^2$, $y(0)=-1$, is solved by the mid-point method with $h=0.1$, $y_0=-1$, and y_1 obtained by means of Euler's rule. The computed values y_n do not exhibit the monotonic behaviour of the points $y(nh)$. Some values of y_n are shown in Table 1.

TABLE 1

n	y_n
40	−0.308
41	−0.062
42	−0.307
43	−0.043
…	…
80	−0.220
81	0.267
82	−0.206
83	0.276
…	…
120	0.141
121	0.319
…	…
150	0.771
151	0.850
…	…
~180	overflow

The augmented system is, according to Theorem 3, Hamiltonian with $H(p,q)=\frac{1}{3}(p^3-q^3)$. In the (p,q) plane, solutions of the augmented system are contained in the level sets $p^3-q^3=\text{constant}$ (see Fig. 1). When the computed points are plotted in the

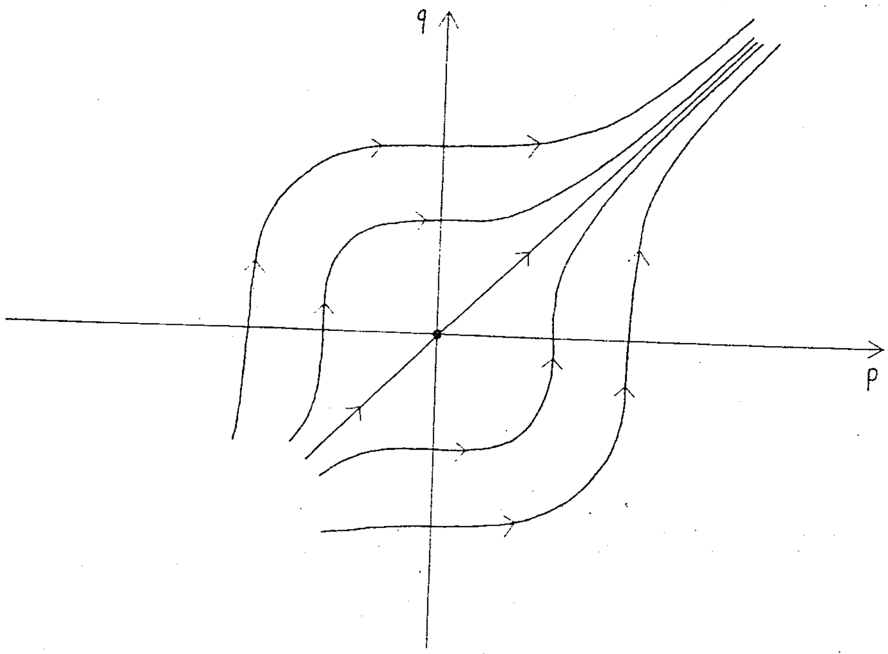

FIG. 1

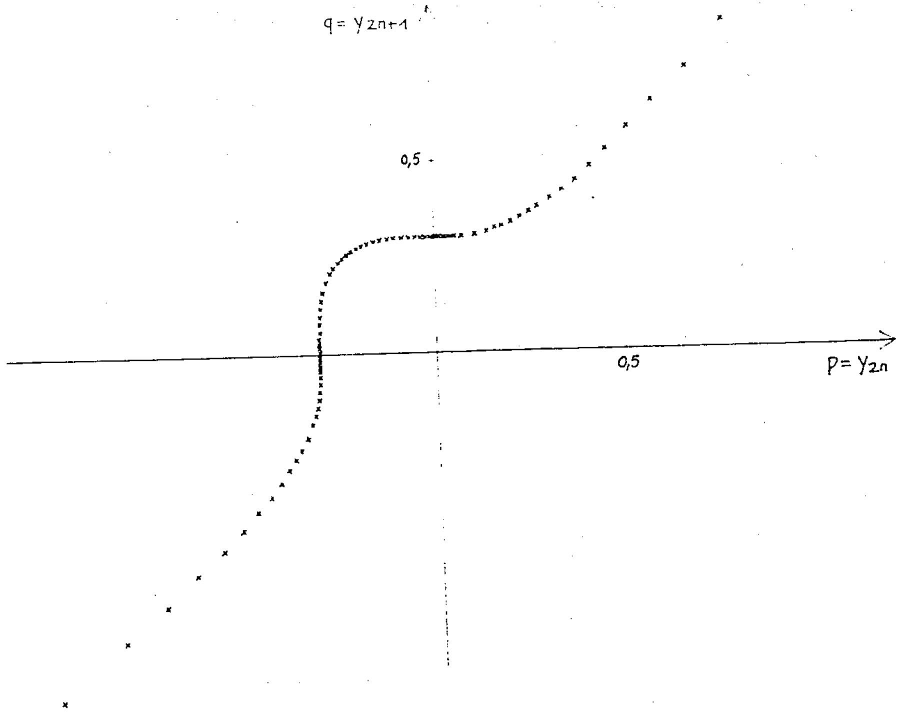

FIG. 2

(p, q) space $(p = y_{2n}, q = y_{2n+1})$ it is clear (Fig. 2) that their behaviour mimics that of solutions of the augmented system.

Note that while the points (y_{2n}, y_{2n+1}) remain near the diagonal, they roughly move towards the origin. In this range of values of n, the behaviour is that of the original equation $y' = y^2$ (more precisely that of the diagonal solutions of the augmented system). However the computed points move quickly away from the diagonal and then, as discussed in § 2, the dynamics of the augmented system takes over, leading to a rapid increase of the magnitude of the values y_n.

The fact that the blowup of leapfrog schemes is preceded by large discrepancies between consecutive values y_n, y_{n+1} (i.e. nondiagonal behaviour) has been known for a long time [11].

The following remark will be used later: *Any choice of* y_0, y_1 *leads to a leapfrog sequence with* $\lim y_n = \infty$. Strictly speaking there is a curve in the (p, q)-plane so that if (y_0, y_1) lies on C^- then (y_{2n}, y_{2n+1}) lie also on C and $\lim y_n = 0$, provided that no round-off is perpetrated.

The curve C^- plays, in the difference case, the role played by the bisectrix of the third quadrant in the augmented system (Fig. 1). Of course, in practice round-off is always present and so computationally $\lim y_n = \infty$ for every y_0, y_1.

The equation $q = \phi(p)$ for C^- near the origin is readily obtained by assuming an expansion

$$q = \phi(p) = a_1 p + a_2 p^2 + a_3 p^3 + \cdots$$

and imposing the requirement that the coordinates $T_{(1)}$, $T_{(2)}$ of the transformed point $T(p, \phi(p))$ satisfy $T_{(2)} = \phi(T_{(1)})$. Thus, we find

$$q = \phi(p) = p + hp^2 + h^2p^3 + O(p^5), \qquad p \to 0^-. \tag{5.1}$$

In order to numerically investigate the role of C^- the following experiment was carried out.

For $h=\frac{1}{2}$, we took $y_0=-0.1$ and successively set y_1 equal to -0.1, -0.095, -0.09525. This corresponds to choosing (y_0, y_1) on C^- except for terms $O(p^2)$, $O(p^3)$, $O(p^5)$ respectively. The smallest value of n for which y_n is larger than zero is given in Table 2.

TABLE 2

y_0	y_1	N
−0.1	−0.1	49
−0.1	−0.095	164
−0.1	−0.09525	1,045

It is useful to observe that -0.095, -0.09525 are precisely the values of y_1 furnished by Euler's rule and the second order Taylor expansion method, respectively.

Returning now to the flow in Fig. 1, it should be pointed out that, due to the divergence-free/area conserving property the behaviour of the contours $p^3-q^3=$ constant is similar to that of the streamlines in an incompressible flow. Thus these contours are sparsely distributed in the neighbourhood of the equilibrium (stagnation point) and converge near the diagonal of the first quadrant where the magnitude of the velocity of the flow is large. Hence the diagonal $p=q>0$ is an attractor of the flow of the augmented system. Analogously for the mapping T, there exists a curve C^+ in the region $p, q>0$ such that if (y_0, y_1) lies on C^+ then for all integers n, $T^n(y_0, y_1)$ lies on C^+ with

$$\lim_{n\to\infty} T^n(y_0, y_1)=(\infty, \infty), \qquad \lim_{n\to\infty} T^{-n}(y_0, y_1)=(0,0),$$

and C^+ attracts the flow of the discrete recursion defined by T.

The expression $q=\psi(p)$ near $p=0$ is again given by (5.1). Near $p=\infty$, $q=\psi(p)$ has an expansion in powers of $p^{1/2}$

$$q=2hp^2+(2h)^{-1/2}p^{1/2}+O(p^{-1/2}), \qquad p\to\infty.$$

Hence, we expect that for any choice of y_0, y_1, h and large n

$$y_{2n+1}\simeq 2hy_{2n}^2+(2h)^{-1/2}y_{2n}^{1/2}.$$

In fact, when $h=0.1$, $y_0=y_1=-1$, we find that for $n=36$, $y_{2n}=157.43$, $y_{2n+1}=4984.52$ and the discrepancy between the right- and left-hand sides in the expression above equals -0.937.

B. We now follow [26], [28] and consider the equation $y'=y-y^2$. This has the equilibria $y=0$ (unstable) and $y=1$ stable. Solutions with $y(0)>1$ decrease monotonically towards 1 and solutions with $0<y(0)<1$ increase monotonically towards 1. When $y(0)<0$ the solution reaches $-\infty$ in finite time. (Solutions in closed form are readily available, but quantitative features are disregarded here.)

The problem $y'=y-y^2$, $y(0)=0.5$ was integrated by the mid-point method with $h=0.1$, $y_0=0.5$ and y_1 obtained by means of Euler's rule. Some computed points are shown in Table 3.

Initially the values y_n grow and approach the equilibrium $y=1$. Then they oscillate with increasing amplitude around that equilibrium. When the oscillations become large enough, the computed points are "attracted" towards the *unstable* equilibrium $y=0$, a surprising behaviour. Later, the y_n recover the monotonic behaviour and eventually ($n=500$, 501) a situation very similar to the initial ($n=0, 1$) is attained.

TABLE 3

n	y_n
80	.99966
81	.99969
160	.99988
161	1.00013
240	.62801
241	1.31896
320	−.00320
321	.00262
360	−.00005
361	+.00005
440	.00286
441	.00316
500	.53534
501	.56013

The strange dynamics of the numerical solution is again readily explained by that of the augmented system. Now, we have $p'=q-q^2$, $q'=p-p^2$, with four equilibria $O=(0,0)$, $P=(1,1)$, $C_1=(0,1)$, $C_2=(1,0)$. According to Theorem 2, both O and P are saddles, while a simple computation shows that C_1 and C_2 are centers.

The augmented system is Hamiltonian with $H(p,q)=(1/2)(p^2-q^2)-(1/3)(p^3-q^3)$. The contour $H(p,q)=0$ consists of the diagonal $p=q$ and of the ellipse $3(p+q)=2(p^2+q^2+pq)$. The latter comprises the unstable manifold of P and the stable manifold of O. The phase portrait of the augmented system given in Fig. 3 can now be compared with the plot of the points $p=y_{2n}$, $q=y_{2n+1}$ given in Fig. 3 ($n=0$, $5, 10, \cdots, 450$).

We shall return to this example in § 7.

C. *First integrals.* Our next example concerns the system $y'_{(1)}=-y_{(1)}y_{(2)}$; $y'_{(2)}=y^2_{(1)}$. (Bracketed subindices denote components.) The system has the first integral $y^2_{(1)}+y^2_{(2)}=$ constant, implying that the origin is a stable equilibrium and that the solutions remain bounded as t increases. The points $y_{(1)}=0$, $y_{(2)}=r$ are equilibria, (stable for $r\geqq 0$, unstable for $r<0$). In the $(y_{(1)}, y_{(2)})$-phase plane a nonequilibrium solution, is represented by a circular arc connecting the initial point $(y_{(1)}(0), y_{(2)}(0))$ to the equilibrium:

$$y_{(1)}=0, \qquad y_{(2)}=(y^2_{(1)}(0)+y^2_{(2)}(0))^{1/2}.$$

The augmented system

$$\begin{aligned} p'_{(1)}&=-q_{(1)}q_{(2)},\\ p'_{(2)}&=q^2_{(1)},\\ q'_{(1)}&=-p_{(1)}p_{(2)},\\ q'_{(2)}&=p^2_{(1)}, \end{aligned} \tag{5.2}$$

inherits, according to Theorem 3, the first integral

$$p_{(1)}q_{(1)}+p_{(2)}q_{(2)}=\text{constant}. \tag{5.3}$$

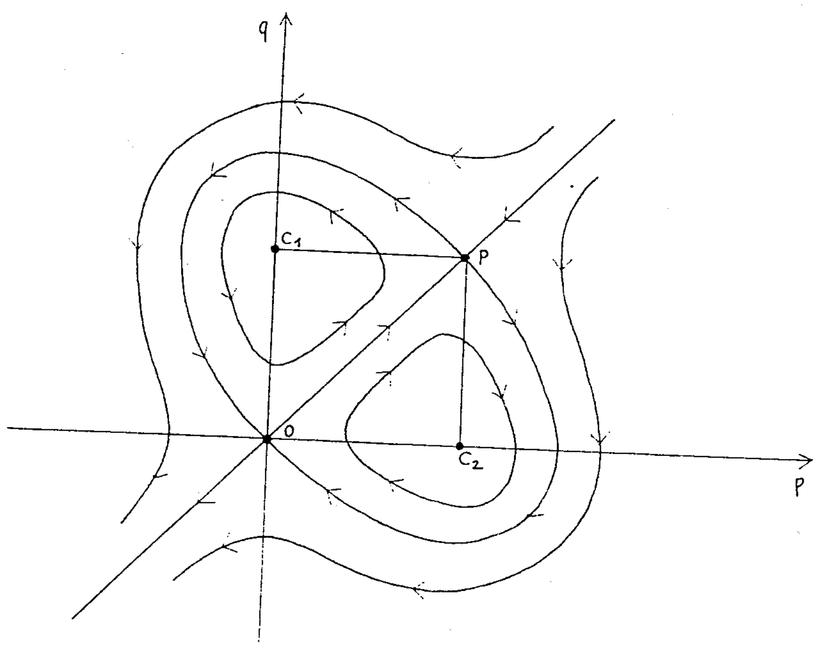

FIG. 3

However the surfaces in the $(p_{(1)}, p_{(2)}, q_{(1)}, q_{(2)})$-space whose equation is (5.3) are not bounded: now the first integral does not guarantee boundedness of the solutions. In fact, consider a diagonal point $\mathbf{p}^0$ with coordinates $p^0_{(1)} = q^0_{(1)} \neq 0$, $p^0_{(2)} = q^0_{(2)}$. From the theorem of continuous dependence on initial values, we conclude that solutions to the augmented system with initial data near $\mathbf{p}^0$ will reach the neighbourhood of the diagonal equilibrium $\mathbf{p}^e$, $p^e_{(1)} = q^e_{(1)} = 0$, $p^e_{(2)} = q^e_{(2)} = ((p^0_{(1)})^2 + (p^0_{(2)})^2)^{1/2}$. Study of the linearization of this equilibrium shows that, generically, solutions in the neighbourhood of $\mathbf{p}^e$ leave the regions

$$\{p_{(1)} > 0, p_{(2)} > 0, q_{(1)} > 0, q_{(2)} > 0\},$$
$$\{p_{(1)} > 0, p_{(2)} > 0, q_{(1)} < 0, q_{(2)} < 0\},$$

and enter the regions

$$R_1 = \{p_{(1)} > 0, p_{(2)} > 0, q_{(1)} < 0, q_{(2)} > 0\}$$

and

$$R_2 = \{p_{(1)} < 0, p_{(2)} > 0, q_{(1)} > 0, q_{(2)} > 0\}.$$

Now, it is easily seen that R_1, R_2 are positively invariant for the flow of (5.1), i.e. solutions of (5.1) cannot leave R_1 or R_2. We conclude that solutions of (5.1) which start near the diagonal, generically enter R_1 or R_2 and remain there. However, it is clear from the signs of the right-hand sides in (5.1) that solutions in R_1 or R_2 have components whose magnitude grow unboundedly. (In fact they reach ∞ in finite time, due to the quadratic interactions.) To sum up, solutions of (5.2) with initial data arbitrarily close to the diagonal will generically reach infinity in finite time.

Once more we found that the augmented system provides a reliable indication as to the dynamics of the mid-point rule solution to the original system. Some computed values ($h = 0.1$, $y_{(1)}(0) = 0.2$, $y_{(2)}(0) = 1.$) are shown in Table 4.

TABLE 4

n	$y_{(1)2n}$	$y_{(2)2n}$	$y_{(1)2n+1}$	$y_{(2)2n+1}$
4	0.090	1.015	0.079	1.017
5	0.075	1.017	0.064	1.018
...	...	...	...	...
15	0.019	1.019	−0.002	1.020
16	0.019	1.019	−0.006	1.021
...	...	...	...	...
40	3.23	3.38	−4.63	4.74
41	7.64	7.68	−16.3	16.4

The dynamics is, for small n, that of the original system: $y_{(1)n}$ decreases towards 0 and $y_{(2)n}$ increases. In the neighbourhood of the equilibrium $\mathbf{p}^e$ the points enter the region R_1 and once there the behaviour is monotonic towards $(\infty, \infty, -\infty, \infty)$.

As noted before, Theorem 4 (iv) ensures the conservation property (5.3). Therefore an unbounded growth of the solution y_n can only take place if one of the products $y_{(1)n}y_{(1)n+1}$ or $y_{(2)n}y_{(2)n+1}$ is negative.

6. Application to partial differential equations. We now turn our attention to the study of schemes for the numerical solution of evolutionary partial differential equations based on the leapfrog time stepping. It is supposed that the space variables are discretized first [20] (by means of finite differences, finite elements etc...) so as to approximate the original equation or system by a system of ordinary differential equations having the time as independent variable. The resulting system is in turn discretized in time by means of the leapfrog technique to obtain the fully discrete set of approximating equations.

For simplicity we restrict ourselves to the model equation [5]:

$$u_t + uu_x = 0, \qquad u(0, t) = u(1, t),$$

although our study can be readily extended among others to problems associated with the vorticity/stream-function formulation of the equations of inviscid, incompressible flow.

Let r be a real parameter. The interval $[0, 1]$ is divided into J intervals of equal length $\Delta x = 1/J$, by means of a grid $x_j = j\,\Delta x, j = 0, 1, \cdots, J$ and $u(x_j, t)$ is approximated by the solutions $U_j = U_j(t)$ of the system [5]:

$$U_j' + (r/2\Delta x)U_j(U_{j+1} - U_{j-1}) + ((1-r)/4\Delta x)(U_{j+1}^2 - U_{j-1}^2) = 0, \tag{6.1}$$
$$j = 1, \cdots, J-1, \quad U_J = U_0.$$

Error estimates for $U_j(t)$ are given in [9]. The dynamics of the solutions of (6.1) and of their leapfrog approximations is complicated indeed. A means of achieving some insight is to restrict the attention to J-dimensional vectors $[U_0, \cdots, U_{J-1}]$ representable as a superposition of a *small* number of *discrete Fourier modes*. The relevant set of modes must be chosen in such a way that it is closed under the quadratic interactions in (6.1), i.e. the product of two modes in the set must belong to the set. This simplifying approach was first taken by N. A. Phillips [17] for the vorticity transport equation. Later references include Richtmyer (reproduced in [18]) and Fornberg [5].

Here two sets of modes are considered:

(i) *One mode solution.* Assume that J is a multiple of 3.

Then [5] the system (6.1) has solutions

$$U_j(t) = a(t) \sin(2\pi j/3), \tag{6.2}$$

where the amplitude $a(t)$ satisfies

$$a'(t) = ca^2(t), \qquad c = \left(\frac{\sqrt{3}}{8\Delta x}\right)(1-3r). \tag{6.3}$$

Note that leapfrog discretization of the amplitude equation (6.3) yields, via (6.2), a solution to the fully discrete leapfrog partial difference equations, i.e. Fourier analysis and leapfrog differencing commute.

Fornberg [5] observed that if $r \neq 1/3$ and $a(0)$ and c are of the same sign, then $a(t)$ reaches infinity at a finite $O(1/\Delta x)$ time. Hence he concluded that the corresponding leapfrog approximations would grow unboundedly for increasing n. The condition on the sign of $a(0)$ means that, for a fixed value of r, only one among the sign patterns

$$0, +, -, 0, +, -, 0, +, -, \cdots, 0, +, -,$$

$$0, -, +, 0, -, +, 0, -, +, \cdots, 0, -, +$$

in $U_0(0), U_1(0), \cdots, U_{J-1}(0)$ will lead to the blow up predicted by Fornberg. Upon introducing the new variable $y = ca$, the equation (6.3) reads $y' = y^2$, so that from our analysis in the previous section we conclude that the blowup in the leapfrog solution will take place (if $r \neq 1/3$) either if the signs of $a(0)$ and c agree or not. In other words *both* sign patterns in $U_j(0)$, $j = 0, 1, \cdots, J-1$ lead to blowup.

(ii) *Two modes solution.* In the case $r \neq 1/3$ the instability described above is attributable to the space discretization.

Any method employed for the integration in time inherits that offending behaviour and this is particularly so with the mid-point rule, which, as we have seen, enlarges the class of initial conditions leading to blowup.

The value $r = 1/3$ is special in that it ensures the conservation law $\sum U_j^2(t) =$ constant, and therefore forces the boundedness of $U_j(t), j = 1, \cdots, J, t > 0$. (See Morton [14] or Kreiss and Oliger [8] for a discussion.) Hereafter we set $r = 1/3$, assume that J is multiple of four and look for solutions

$$U_j(t) = a(t)(\sin(\pi j/2) + \cos(\pi j/2)) + b(t) \cos \pi j.$$

The amplitudes a, b must satisfy

$$a' = \left(\frac{1}{3\Delta x}\right) ab, \qquad b' = -\left(\frac{1}{3\Delta x}\right) a^2,$$

a system whose leapfrog discretization entails blowup as shown in the previous section.

The material in this section is covered in detail and expanded in [27].

7. Integrability. Concluding remarks. We now return to Example B in § 5. It is important to point out that the similarity between Figs. 3 and 4 is deceptive. In fact the augmented system is an *integrable* Hamiltonian system [2], [25]. This simply means that due to the first integral $H(p(t), q(t)) =$ constant, the integration of the system is achievable by quadratures. (In systems with d degrees of freedom, d involutive first integrals are required.) For the time h flow F_h, integrability implies that all the iterates $F_h^n(p_0, q_0)$ of a point lie on a curve $H(p, q) =$ constant. These curves are closed in the region $H(p, q) < 0$. It may be conjectured from Fig. 4, that the mapping T, (which approximates F_h) also defines an integrable system, i.e. a nonconstant function $S(p, q)$ defined in all R^2 exists so that the iterates $T^n(p_0, q_0)$ are confined to lie on a level

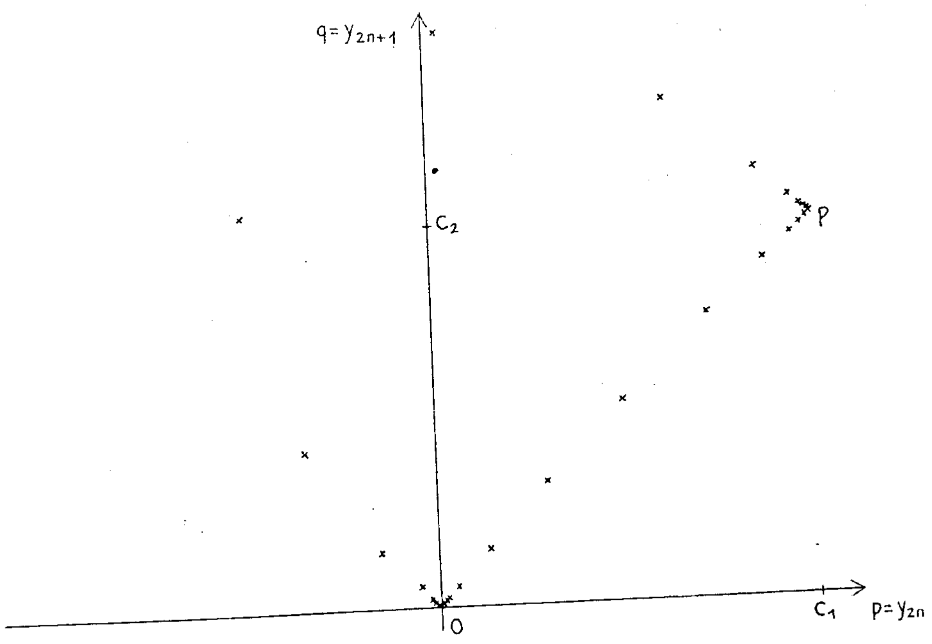

FIG. 4

curve $S(p, q) = \text{constant}$. However Ushiki [26] has proved that this is not the case. In fact he shows that the dynamics of T is *chaotic* in a sense made precise in his paper. This remark does not invalidate our claim that (y_{2n+2}, y_{2n+3}) lies near the local solution through (y_{2n}, y_{2n+1}); it only implies that the behaviour of the sequence (y_{2n}, y_{2n+1}), $n = 0, 1, \cdots$ may be far more complicated than that of sequences $(p(nh), q(nh))$, $n = 0, 1, \cdots$. In this regard linear systems are exceptional as shown by Theorem 1.

We would like to recall that there are many available results concerning the behaviour of area preserving mappings [24]. Some of them could be used in order to ascertain the properties of the dynamics of T. It is expected that such a dynamics will be highly involved. Some of the finer details will be numerically missed due to round-off. Of particular significance is the study of T near center equilibria, since, as noted before, these are the only nondegenerate equilibria in whose neighbourhood the leapfrog technique is useful. This point will be the subject of a forthcoming paper.

Finally, we observe that theories similar to the one presented in this paper can be constructed for any multistep method having $r^k - r^{k-2}$ as first characteristic polynomial. (Nystrom and generalized Milne–Simpson methods, in the terminology of [10].) For instance the dynamics associated with Milne's method

$$y_{n+2} - y_n = \frac{h}{3}(f_{n+2} + 4f_{n+1} + f_n),$$

would be governed by the enlarged system

$$p' = \tfrac{1}{3}(p + 2q), \qquad q' = \tfrac{1}{3}(2p + q).$$

Note. Prof. M. N. Spijker has recently let us know that the idea of augmented system had been considered by H. J. Stetter, *Symmetric two-step algorithms for ordinary differential equations*, Computing, 5 (1970), pp. 267–280. However the subject of Stetter's paper is completely different from ours.

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