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A Method for the Integration in Time of Certain Partial Differential Equations

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A method for the numerical solution of ordinary differential equations is analyzed that is explicit and yet can conserve the quadratic quantities conserved by the equations. The method can be a useful alternative to the usual leapfrog technique, in that it does not suffer from the occurrence of blowup phenomena. Numerical examples concerning the Korteweg–de Vries equation and the nonlinear Schrödinger equation are given.

1. INTRODUCTION

In [27] one of the present authors suggested a finite-difference scheme for the numerical study of the Korteweg–de Vries equation that is explicit and conserves exactly the "energy" of the computed solution. The main novelty of the scheme lay in the device employed for the integration in time, which was reminiscent of the usual leapfrog technique and yet did not suffer from the notorious blowup associated in some cases with leapfrog schemes [9, 10, 24]. Some indications regarding the extension of the suggested device to more general equations were also given in [27] and have been recently implemented by Mitchell and Morris [22] in the case of a nonlinear Schrödinger equation.

The present article develops the material in [27] in three different directions. First the suggested method for the integration in time of partial differential equations is presented in its full generality and analyzed. The method will then be applied to the Korteweg–de Vries equation as in [27] but with more thorough testing. Finally we shall consider the nonlinear Schrödinger equation studied in [22]. Our implementation is different from that used by Mitchell and Morris and a comparison will be drawn. The numerical experiments indicate that the schemes based on the suggested idea perform better than conventional leapfrog procedures.

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2. The Circularly Exact Leapfrog Method

In this section we shall be concerned with the numerical solution of the system of ordinary differential equations

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(\mathbf{y}), \tag{2.1}$$

where $\mathbf{y}$ is a vector with d components.

In the applications we have in mind, (2.1) will arise from the discretization in space of a system of partial differential equations, but at this stage no assumption on the properties or structure of $\mathbf{f}$ will be made.

The system (2.1) is discretized by means of the two-step method

$$\mathbf{y}^{n+1} - \mathbf{y}^{n-1} = 2\tau_n \mathbf{f}^n \tag{2.2a}$$

$$\tau_n = (\mathbf{y}^n - \mathbf{y}^{n-1})^T \mathbf{f}^n / (\mathbf{f}^{nT} \mathbf{f}^n) \tag{2.2b}$$

which can be derived [21] by fitting a circle to the past information: $\mathbf{y}^n$, $\mathbf{y}^{n-1}$, $\mathbf{f}^n$. Here $\mathbf{f}^n = \mathbf{f}(\mathbf{y}^n)$ and $\mathbf{y}^n$ is meant to approximate $\mathbf{y}(t_n)$, where the values t_n are computed recursively according to

$$t_{n+1} - t_{n-1} = 2\tau_n. \tag{2.2c}$$

Formulas (2.2a, b) were first suggested by Lambert and McLeod [18] for the case $d = 2$ and extended to the general case by Laurie [20]. These authors did not use formula (2.2c), as in the particular applications they considered thay were concerned with computing values of $\mathbf{y}$ and not with finding the correspondence of those values with t. The method enjoys the following property referred to as circular exactness: whenever the trajectory described in the d-dimensional space by the solution of (2.1) is a circle, all the computed points will lie on that circle provided that $\mathbf{y}_0, \mathbf{y}_1$ do [21]. Since (2.2a) is clearly reminiscent of the usual leapfrog or midpoint rule, we shall use the term circularly exact leapfrog method (CELF) to refer to formulas (2.2). Note that substitution of (2.2b) in (2.2a) shows that we are dealing with a rational method, i.e., a method which demands that products and quotients of the past information be formed. However, it is not related to the rational methods described in the literature [17, 19]. Rational methods are far more difficult to analyze than linear methods.

Throughout this paper, Euler's method

$$\mathbf{y}^1 = \mathbf{y}^0 + k\mathbf{f}^0, \tag{2.3a}$$

$$t_1 = t_0 + k, \tag{2.3b}$$

will be employed to initialize the CELF method. Of course alternative starting procedures may be considered.

It should be emphasized that the parameter k in (2.3) provides only the initial step-

length while subsequent step-lengths are obtained from (2.2b). Thus the CELF method is a *variable step method*, in which the initial step-size is the only control upon the sequence of step-sizes.

The main properties of the method will now be studied.

(i) *Order of Accuracy*

Taylor expansion of (2.2b) shows that *if* $\mathbf{y}^{n-1}$, $\mathbf{y}^n$ *are exact*, i.e., $\mathbf{y}^{n-1} = \mathbf{y}(t_{n-1})$, $\mathbf{y}^n = \mathbf{y}(t_n)$, the next time level is

$$t_{n+1} = t_n + (t_n - t_{n-1}) - (t_n - t_{n-1})^2 \frac{\mathbf{y}''(t_n)^{\mathrm{T}}\, \mathbf{y}'(t_n)}{\mathbf{y}'(t_n)^{\mathrm{T}}\, \mathbf{y}'(t_n)} + O((t_n - t_{n-1})^3) \tag{2.4}$$

and then expansion of $\mathbf{y}(t_{n+1})$ and (2.2a) lead to

$$\mathbf{y}^{n+1} - \mathbf{y}(t_{n+1}) = O((t_n - t_{n-1})^3), \tag{2.5}$$

so that we are dealing with a method of second order of *consistency* [16, p. 28]. Numerical evidence supports the claim the method possesses second order of *convergence*, i.e., $\|\mathbf{y}^n - \mathbf{y}(t_n)\| = O(k^2)$, but no theoretical proof of this fact is available.

(ii) *Equidistributing Property*

It is easily shown that $\|\mathbf{y}^{n+1} - \mathbf{y}^n\| = \|\mathbf{y}^n - \mathbf{y}^{n-1}\|$; i.e., the method equidistributes the dependent variable [35], as distinct from the equidistribution of the independent variable $t_{n+1} - t_n = t_n - t_{n-1}$, associated with standard ODE solvers (in fixed-step implementations), cf. [21].

In fact, for the scalar equation $dy/dt = f(y)$, formulas (2.2) can be rewritten as

$$\begin{aligned} y^{n+1} - y^n &= y^n - y^{n-1} = \text{const}, \\ t_{n+1} - t_{n-1} &= 2(y^n - y^{n-1})/f(y^n), \end{aligned} \tag{2.6}$$

which is precisely the result of applying the usual midpoint rule [16] to the equation $dt/dy = 1/f(y)$, in which the roles of the dependent and independent variables have been interchanged. This remark also proves the $O(k^2)$ convergence of the method in the *scalar* case.

It might be useful to point out that in [27] two schemes were suggested; one is the CELF method and the other (called in [27] fixed-step conservative) is given by (2.2a, b) and the formula $t_{n+1} = t_n + k$. It is easily seen that application of the fixed-step conservative scheme to the scalar equation leads to $y^{n+1} - y^n = \text{constant}$, $t_{n+1} - t_n = \text{constant}$ and therefore convergence cannot take place.

(iii) *Stability*

Recall that the stability of linear methods [16] is usually investigated by applying them to the model equation $y' = \lambda y$. This analysis is relevant because consideration of

normal modes extends it to any linear system. For the CELF method it is possible to solve the difference equations (2.2) in closed form when (2.1) takes the model form. However, for rational methods the conclusions cannot be extended to more general systems, due to the lack of a superposition principle for the solution. This consideration also precludes the use of a normal mode analysis in the applications of the method to PDEs.

(iv) *Rounding Errors*

Our attention is now directed to a discussion on rounding errors, as these will play an important role later in the paper.

We consider first the problem $dy/dt = 1$, $y(0) = 0$. In the absence of round-off error, formulas (2.2), (2.3) yield $y^n = nk$ with no error. Let us assume that an error is perpetrated leading to $\hat{y}^1 = y^1 + \varepsilon$. If no further round-off errors are present, the values of y are $\hat{y}^n = y^n + n\varepsilon$, so that for large n the difference $\hat{y}^n - y^n$ can be significant. However, the computed values of t are given by $\hat{t}_n = t_n + n\varepsilon$ if n is even, $\hat{t}_n = t_n + n\varepsilon - \varepsilon$ if n is odd, and therefore the propagated error $\hat{y}^n - \hat{t}_n$ is 0 or ε, respectively. Thus the presence of round-off has altered the sequence of step-sizes but not impaired greatly the accuracy of the method. Similar analyses can be conducted to study the effects of round-off errors in the computation of τ_n or t_n. The conclusion above is not altered.

In order to ascertain whether the same results hold for more general equations, the problem $y' = y$, $y(0) = 1$ was solved in a short word-length pocket calculator by the CELF method, with a random noise added to the right-hand side of each of the equations (2.2). The noise was uniformly distributed in the interval $[-\beta/2, \beta/2]$. Some of the results are displayed in Table I, where it is shown, in agreement with the previous discussion, that severe rounding errors result in an alteration of the step-length but propagate in a rather stable manner. Note also the $O(k^2)$ behaviour of the error in the last row.

(v) *Conservation of the L^2 Norm*

We now make the assumption that the identity

$$\mathbf{z}^T\mathbf{f}(\mathbf{z}) = 0 \tag{2.7}$$

TABLE I

	$k = 0.0250$		$k = 0.0125$	
β	t^{40}	Error $\times 10^6$	t^{80}	Error $\times 10^6$
10^{-3}	1.8844	2672	1.99165	7231
10^{-4}	1.9884	139	1.9930	703
10^{-5}	1.9988	−126	1.9993	35
0	2.0000	−156	2.0000	−39

for all d-dimensional vectors $\mathbf{z}$. Then the "energy" $\mathbf{y}^T\mathbf{y} = \sum y_i^2 = \|\mathbf{y}\|^2$ is a constant of motion for the solutions of (2.1). In a partial differential equation setting, this implies the conservation of the discrete counterpart of the integral of the square of the solution. The importance of the conservation of energy, both from the numerical and the physical point of view cannot be overemphasized (see the discussion in [24, 27]). It was shown in [27] that the CELF method is energy conserving whenever (2.7) holds. Therefore is not subject to the appearence of the blowup phenomena due to nonlinear interactions which is the main drawback in the application of leapfrog schemes to the study of waves. Newell and his co-workers [5, 26] have analyzed the mechanism leading to blowups.

It can be proved that there is no explicit, energy conserving Runge–Kutta or linear multistep method. There exist of course *implicit*, energy-conserving standard methods, but their conservation properties are lost if the implicit equations are not solved "exactly" (i.e., the iteration must be continued until the error is within the level of round-off). On the other hand, conservation laws of any kind can always be enforced in an a posteriori manner (see Navon [25, 39, 40]). For instance, the scheme

$$\begin{aligned} \hat{\mathbf{y}}^{n+1} &= \mathbf{y}^{n-1} + 2k\mathbf{f}^n, \\ \mathbf{y}^{n+1} &= (\|\mathbf{y}^0\|/\|\hat{\mathbf{y}}^{n+1}\|)\,\hat{\mathbf{y}}^{n+1}, \end{aligned} \tag{2.8}$$

which we call normalized leapfrog, has obviously the energy $\|\mathbf{y}\|$ as a conserved quantity. Note, however, that (2.8) can only approximate systems which satisfy (2.7), while the CELF method can be applied to any system of ordinary differential equations. A comparison between the normalized leapfrog and CELF methods will be given in Section 4. An alternative way of preventing the blowup phenomenon is the use of filters [41].

Before closing this paragraph, some comments on the implementation of the method should be made. When identity (2.7) holds, it is possible to rewrite formula (2.2b) in the form

$$\tau_n = -\mathbf{y}^{n-1^T}\mathbf{f}^n/(\mathbf{f}^{n^T}\mathbf{f}^n) \tag{2.9}$$

which is marginally more economical. An error of $\boldsymbol{\varepsilon}$ in the evaluation of $\mathbf{f}^n$ alters the numerator of (2.9) by an amount $(\mathbf{y}^{n-1})^T\boldsymbol{\varepsilon}$ and that of (2.2b) by an amount $(\mathbf{y}^n - \mathbf{y}^{n-1})^T\boldsymbol{\varepsilon}$. Since in a typical computation these quantities are $O(\|\boldsymbol{\varepsilon}\|)$ and $O(k\|\boldsymbol{\varepsilon}\|)$, respectively, it seems that formula (2.2b) should be preferred. Note that in a system arising from partial differential equations the evaluation of $\mathbf{f}$ can require a very large number of arithmetical operations.

(vi) *Other Conserved Quantities*

If the identity

$$\mathbf{z}^T M\mathbf{f}(\mathbf{z}) = 0, \tag{2.10}$$

rather than (2.7), holds, then the conserved quantity becomes $\mathbf{y}^T M\mathbf{y}$. Here we assume

that M is a constant, symmetric, positive-definite matrix. Accordingly, in this case (2.2b) would be replaced by

$$\tau_n = [(\mathbf{y}^n - \mathbf{y}^{n-1})^{\mathrm{T}} M \mathbf{f}^n]/(\mathbf{f}^{n\mathrm{T}} M \mathbf{f}^n), \tag{2.11}$$

in order to obtain the conservation of $(\mathbf{y}^n)^{\mathrm{T}} M \mathbf{y}^n$. In a finite-element setting [23], $\mathbf{f}$ would take the form $M^{-1}\mathbf{g}$, with M the mass matrix, and (2.11) would become

$$\tau_n = [(\mathbf{y}^n - \mathbf{y}^{n-1})^{\mathrm{T}} \mathbf{g}^n]/[\mathbf{g}^{n\mathrm{T}} (M^{-1}\mathbf{g}^n)] \tag{2.12}$$

and therefore the CELF method requires only the evaluation of two inner products per step in addition to the computational effort of the usual leapfrog scheme.

3. The Korteweg–De Vries Equation

There are many available methods for the numerical solution of the Korteweg–de Vries equation

$$u_t + uu_x + \varepsilon u_{xxx} = 0, \qquad \varepsilon > 0. \tag{3.1}$$

References include Zabusky and Kruskal [37], Vliegenthart [33], Greig and Morris [12], Gazdag [11], Canosa and Gazdag [6], Abe and Inoue [1], Alexander and Morris [3], Wahlbin [34], Sanz-Serna and Christie [29], Schoombie [30, 31], Kuo and Sanz-Serna [14], Christie *et al.* [7], Kuo and Wu [15], Winther [36], and Arnold and Winther [4].

We are concerned with the initial-value problem given by (3.1) together with the initial condition

$$u(x, 0) = F(x). \tag{3.2}$$

It is assumed that the interest is centered in solutions that, for the range of time under consideration are negligible outside an interval $0 < x < L$, although the situation is not greatly altered when periodic solutions are considered. The equation is discretized in space by introducing a grid $x_j = jh$, $j = 0, 1, \ldots, J$, $J = L/h$, and approximating $u(x_j, t)$ by $U_j(t)$, where the nodal values $U_j(t)$ satisfy

$$U_0(t) = U_1(t) = U_{J-1}(t) = U_J(t) = 0, \tag{3.3}$$

and

$$\begin{aligned}(d/dt)\, U_j(t) + (1/6h)(U_{j+1}(t) + U_j(t) + U_{j-1}(t))(U_{j+1}(t) - U_{j-1}(t)) \\ + (\varepsilon/2h^3)(U_{j+2}(t) - 2U_{j+1}(t) + 2U_{j-1}(t) - U_{j-2}(t)) = 0,\end{aligned} \tag{3.4}$$

$j = 2, 3, \ldots, J-2$. Thus a system of ordinary differential equations is obtained for the vector $\mathbf{y} = [U_2, \ldots, U_{J-2}]^{\mathrm{T}}$. It is easily verified that for this system (2.7) holds, leading to conservation of the L^2 norm.

When (3.4) is discretized in time by the usual leapfrog technique the resulting scheme is identical to that suggested by Zabusky and Kruskal [37]. This scheme is $O(k^2 + h^2)$, it accurately reproduces the wave profile (Abe and Inoue [1]), and, unlike higher-order methods (cf. [31]), does not introduce spurious oscillations. Unfortunately it is subject to blowup phenomena [1, 27].

In [27] the CELF method was employed as an alternative in the discretization of (3.4). The resulting scheme is not subject to the occurrence of blowup, due to the exact conservation of energy. Numerical results reported in [27] show that this "stabilization" is obtained without sacrificing accuracy and Figs. 1 and 2 indicate that the CELF method faithfully reproduces the wave profiles. In both figures $h = 0.01$, $k = 0.0008$, and $\varepsilon = 0.000484$; the method is run for 3000 steps. Figure 1 describes the evolution of a single soliton with amplitude 0.9, initially located at $x = 0.5$. In this experiment $L = 2$. The interaction of two solitons with amplitudes 2.1 and 0.3 and initial positions 0.5 and 1.5, respectively, is pictured in Fig. 2, which has $L = 4$.

The evolution of the time-step for the reported interaction of solitons is monitored in Table II. The step-size is found to remain nearly constant troughout the integration. Note that in the propagation of a wave, equidistribution of y would result in an approximate equidistribution of t (Section 2(ii)). In fact we found that the average time step t_n/n depends on the initial step k and on the grid spacing h, but *not* on the particular solution under consideration. For a fixed value of h the behaviour of t_n/n is as follows. There is a critical value $k_c(h)$ such that when $k \leqslant k_c(h)$ the steps are all nearly equal to the initial value k. If, however, $k \geqslant k_c(h)$ the step-size is reduced, so that the average t_n/n approaches $k_c(h)$ as n increases. An example of this

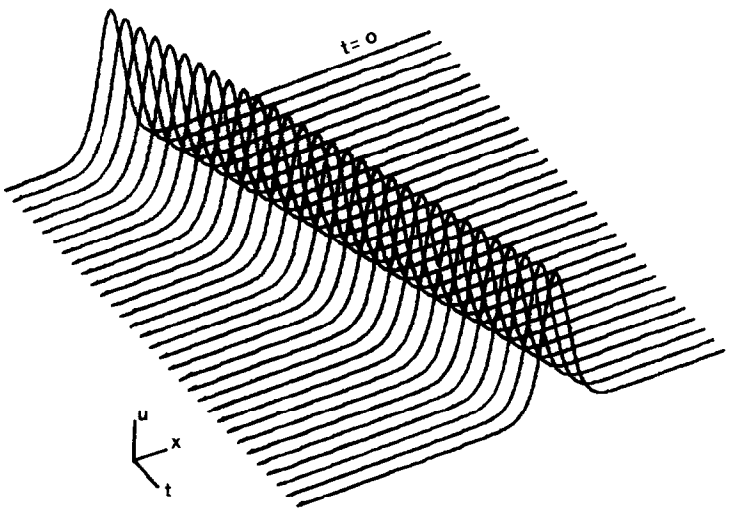

FIGURE 1

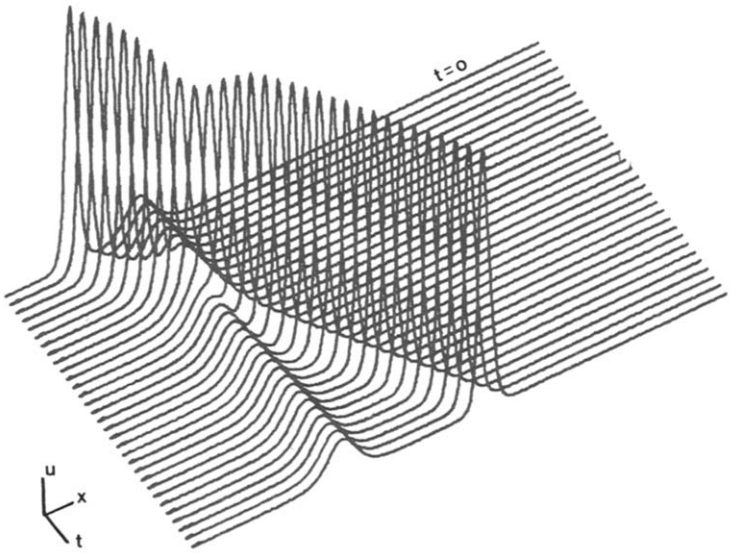

FIGURE 2

is provided in Table III, which gives the observed average step in $0 \leqslant t \leqslant 1$ when $h = 0.01$. Furthermore we have found that the critical value $k_c(h)$ is precisely the maximum time-step that can be allowed if the *usual* leapfrog scheme is to be linearly stable for that value of h. For the KdV equation the linearized stability condition reads [27]: $\sqrt[3]{3}\, k \leqslant 2h^3$. When $h = 0.01$, $\varepsilon = 0.000484$ the maximum k allowed by the condition above is 0.000795, which is in good agreement with the values reported in Tables II and III.

It should be emphasized that a choice of k above $k_c(h)$ in the CELF method does not result in an increase of the errors as the experiments in [27] showed. On the other hand, for the usual leapfrog scheme $k \geqslant k_c(h)$ leads to overflow at an early stage of the computation (linear instability) and even if $k \leqslant k_c(h)$ overflow may arise after some period of time (nonlinear blowup) [1, 26]. This will be illustrated in the next section.

TABLE II

Steps	Time	Average
500	0.398387	0.000797
1000	0.796091	0.000796
1500	1.193826	0.000796
2000	1.591293	0.000796
2500	1.988377	0.000795
3000	2.385329	0.000795

TABLE III

$k \times 10^4$	Average step $\times 10^4$
4.	4.002
5.	5.002
6.	6.003
7.	7.003
8.	7.963
9.	7.915
10.	7.930

4. A Nonlinear Schrödinger Equation

Our second test equation is the cubic Schrödinger equation

$$iu_t + u_{xx} + |u|^2 u = 0; \qquad i^2 = -1. \tag{4.1}$$

For numerical work it is convenient to decompose the complex field u into its real and imaginary parts v and w, respectively, leading to the system

$$\begin{aligned} v_t + w_{xx} + (v^2 + w^2)w &= 0, \\ w_t - v_{xx} - (v^2 + w^2)v &= 0. \end{aligned} \tag{4.2}$$

The nonlinear Schrödinger equation has been used to model a number of physical situations involving nonlinearity and dispersion; see [8, 13, 32, 38] and references therein. A survey of its mathematical theory is given by Strauss [2]. In 1970 Zakharov and Shabat [38] succeeded in applying the inverse scattering method to the pure initial value for (4.1). This problem possesses an infinite number of conservation laws including

$$\int u^2(x, t)\, dx \tag{4.3}$$

$$\int (2|u_x|^2 - |u|^4)\, dx \tag{4.4}$$

and also has solitons, which are given by

$$u(x, t) = \sqrt{2\alpha}\, \exp[i(\tfrac{1}{2}c[x - \gamma] - [\tfrac{1}{4}c^2 - \alpha]t)]\, \operatorname{sech}(\sqrt{\alpha}(x - \gamma - ct)). \tag{4.5}$$

Here γ merely determines the initial position of the solition, while α and c control the amplitude and speed, respectively.

Ablowitz and Ladik [2] developed a complicated discrete analog of (4.1) for which

an inverse scattering theory applies. The interest of this finite-difference scheme appears to be mainly theoretical. Delfour *et al.* [8] have proposed a useful finite-difference scheme which conserves the discrete analog of both (4.3) and (4.4). Although they do not provide indications regarding the computational cost of their method it would not be unfair to assume that the solution of the nonlinear equations up to the level of round-off required to achieve conservation is expensive. Griffiths *et al.* [13] use a predictor–corrector pair which requires the solution of two linear systems per step and does not conserve either (4.3) or (4.4). (Note that (4.4) is not positive definite and therefore form the numerical point of view its conservation may be less valuable than that of (4.3).) A proof of the convergence of the cited schemes is given in [28].

A scheme will now be constructed which is both explicit and energy conserving. Equation (4.1) is supplemented by the boundary conditions

$$u_x = 0, \qquad x = a, \quad x = b, \quad t > 0. \tag{4.6}$$

Periodic or homogeneous Dirichlet conditions can also be considered. A grid $x_j = a + jh$, $j = 0, 1, \ldots, J$, $h = (b-a)/J$ is introduced and $v(x_j, t)$, $w(x_j, t)$ are approximated by $V_j(t)$, $W_j(t)$, where

$$\begin{aligned} &(d/dt)\, V_j(t) + (1/h^2)(W_{j+1}(t) - 2W_j(t) + W_{j-1}(t)) + W_j(t)(V_j(t)^2 + W_j(t)^2) = 0, \\ &(d/dt)\, W_j(t) - (1/h^2)(V_{j+1}(t) - 2V_j(t) + V_{j-1}(t)) - V_j(t)(V_j(t)^2 + W_j(t)^2) = 0, \end{aligned} \tag{4.7}$$

$j = 0, 1, \ldots, J$. Here $V_{-1} \equiv V_1$, $W_{-1} \equiv W_1$, $V_{J+1} \equiv V_{J-1}$, $W_{J+1} \equiv W_{J-1}$. The set of equations (4.7) provides a system of ordinary differential equations for the vector $\mathbf{y} = [V_0, W_0, \ldots, V_J, W_J]^T$, which has

$$\tfrac{1}{2}V_0^2 + \tfrac{1}{2}W_0^2 + V_1^2 + W_1^2 + \cdots + V_{J-1}^2 + W_{J-1}^2 + \tfrac{1}{2}V_J^2 + \tfrac{1}{2}W_J^2, \tag{4.8}$$

as a conserved quantity, and therefore use of the CELF method for the discritization in time leads to the scheme required. Note that other spatial discretizations can be used. For example, the experience gained by Griffiths *et al.* [13] may suggest Galerkin's method based on piecewise-linear functions.

The CELF method for (4.7) was implemented and found to perform satisfactorily. An example is provided in Fig. 3, which depicts the modulus of the computed complex solution in the interaction of two solitons. In this computation $a = -20$, $b = 80$, $h = 0.25$, $k = 0.015$, and 3000 time-step were taken. The speeds, amplitudes, and initial positions of the solitons are 2.0 and 0.02, 1.0 and 1.0, 0 and 20, respectively. Other numerical experiments will be reported later in the section.

The behaviour of the time-step is found to be analogous to that of the *K dV* equation. For instance, the maximum allowable step when $h = 0.25$ and the usual leapfrog method is applied to the solution of system (4.7) *wihtout the nonlinear terms* (i.e., linearization around the zero solution) is $0.25h^2 = 0.0156$. This should be compared with Table IV which gives the average time-steps over $0 < t < 30$ in the study of a single solition with the CELF scheme.

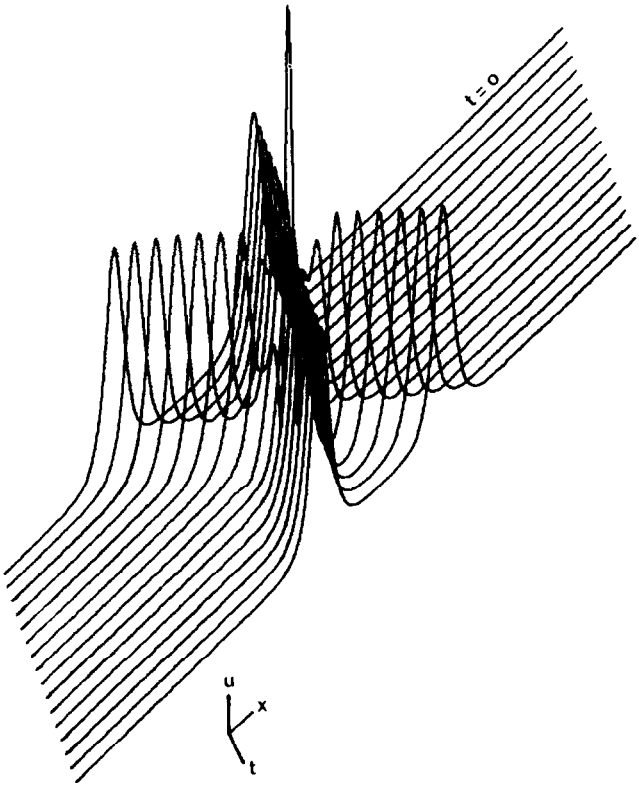

FIGURE 3

In order to draw a comparison between the usual leapfrog, the normalized leapfrog (2.8), and the CELF techniques as used to discretize (4.7) the following experiments are made. The three methods are applied with $h = 0.5$, $a = -30$, $b = 70$ to the study of a single soliton with $\alpha = 0$, $c = 1$ and initially placed at $x = 0$. The critical value of k is now $0.25h^2 = 0.0625$. We first set $k = 0.05$ (subcritical). The performance of the

TABLE IV

k	Average step
0.012	0.0118
0.013	0.0128
0.014	0.0137
0.015	0.0147
0.016	0.0156
0.017	0.0156
0.018	0.0156

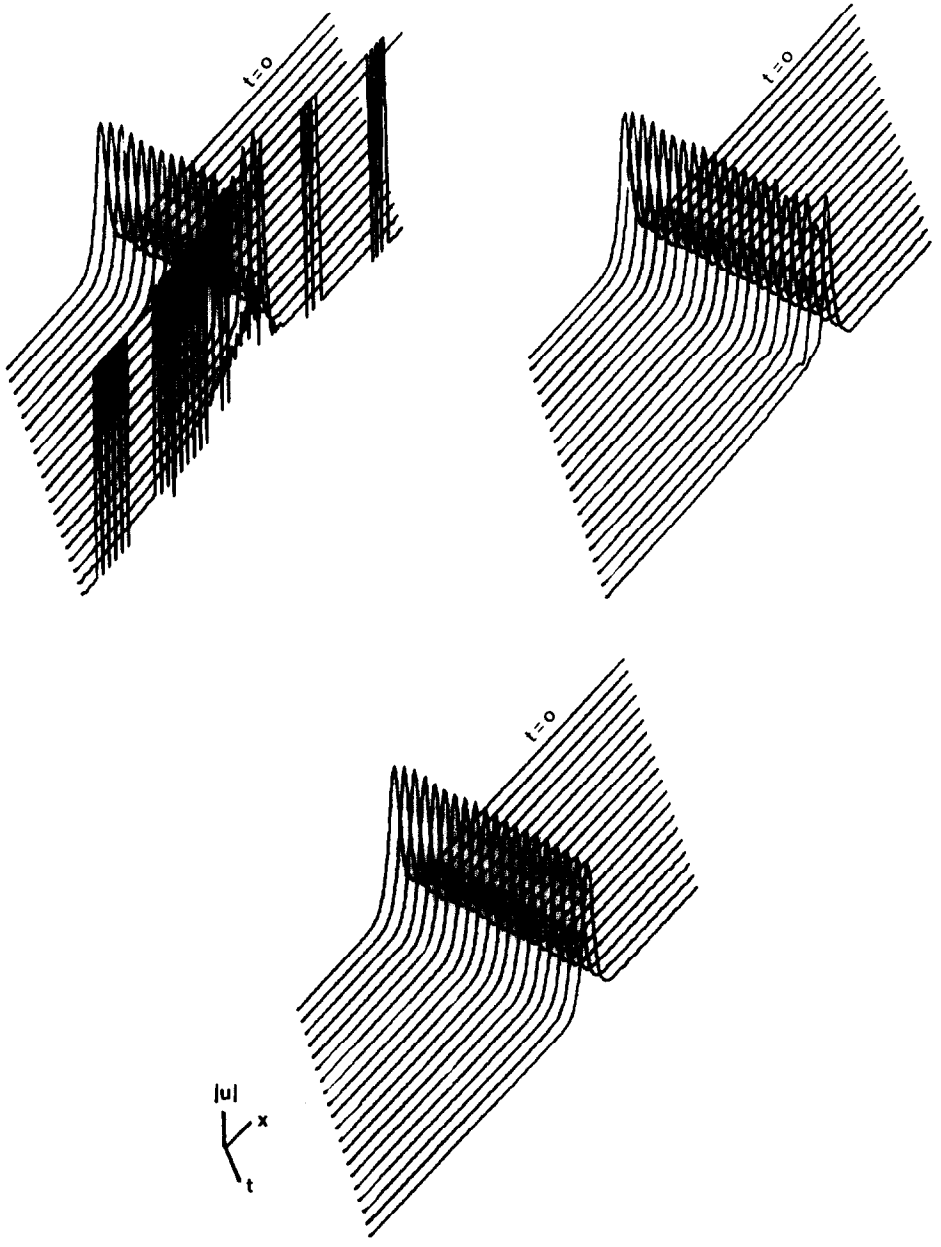

FIGURE 4

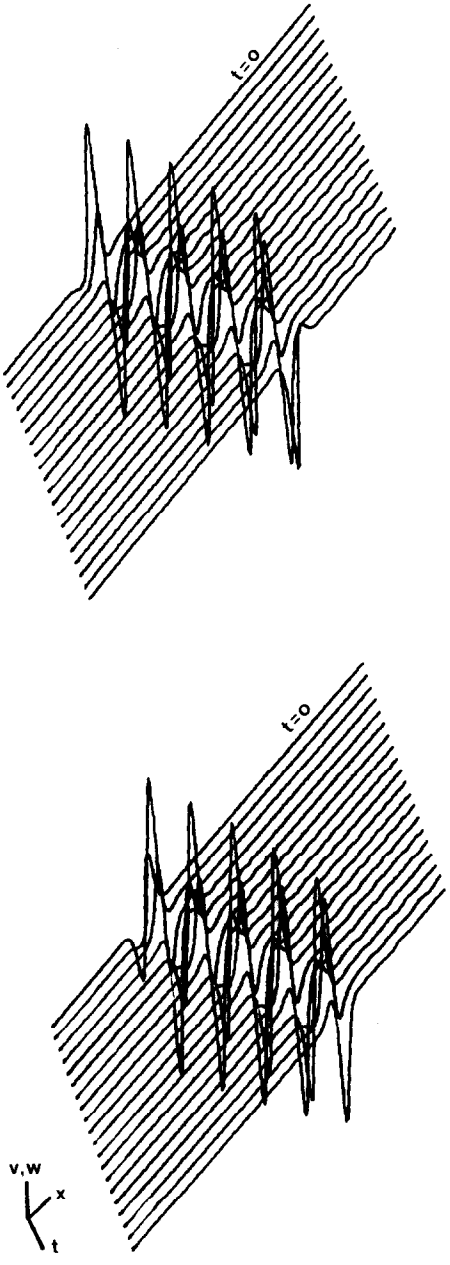

FIGURE 5

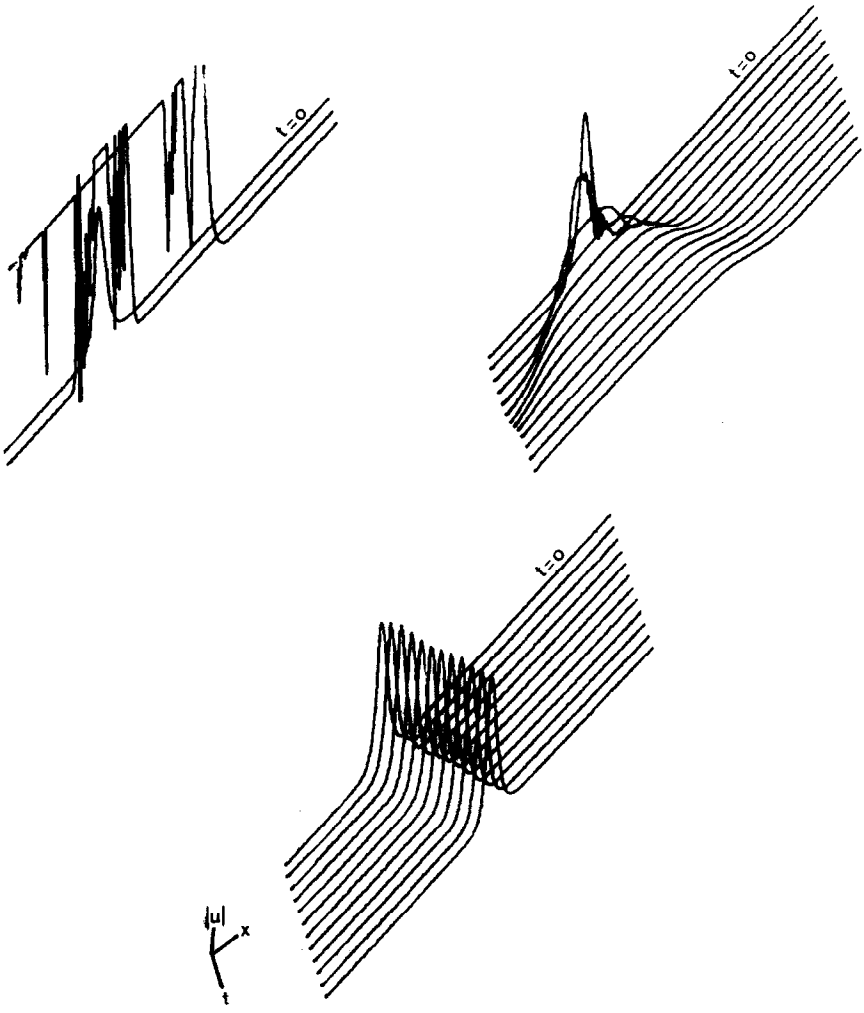

FIGURE 6

methods is displayed in Fig. 4. The usual leapfrog scheme (i) exhibits a blowup phenomenon at $t \simeq 32$. To avoid graphing meaningless large numbers U, V were truncated by the plotting routine. The normalized method (ii) remains "stable" although the profile of the soliton is altered. The displacement of the wave is faithfully described by the CELF method (iii). Figure 5 shows the behaviour of the real and imaginary parts of the solution of this problem, as integrated by the CELF procedure.

When k is increased to 0.08 (supercritical) (Fig. 6) the leapfrog scheme produces overflow at the first steps of the computation. The normalized leapfrog yields a wrong picture of the situation: the height of the wave is greatly reduced. Again the right

behaviour is given by the CELF procedure, which exhibits an average step of 0.0620, i.e., almost equal to the critical value. Note that both the CELF and the normalized leapflog methods conserve exactly (4.8).

Finally it should be pointed out that the present CELF scheme for the nonlinear Schrödinger equation (4.1) was also considered by Mitchell and Morris [22]. However, they computed τ_n according to formula (2.9), rather than (2.2b), and found that in some cases the step-length was steadily and greatly reduced. There is little doubt that this anomalous behaviour was due to rounding errors via the mechanism discussed in Section 2.

All the numerical computations in Sections 3 and 4 were carried out in single precission on the DEC 10 of the University of Dundee.

5. Conclusions

A method for the numerical solution of ordinary differential equations has been suggested that is explicit and second order. The method can conserve any quadratic quantity conserved by the continuous system and therefore may be useful for the integration in time of partial differential equations with quadratic constants of motion. Examples concerning the Korteweg–de Vries equation and the nonlinear Schrödinger equation show that the method improves on the leapfrog technique in two ways. It does not suffer from blowup phenomena and it can operate without difficulties at the maximum allowable time step associated with the linearized analysis of the usual leapflog method.

A comparison with the a posteriori enforcement of conservation laws has also breen drawn, to the advantage of the suggested method.

It is the authors' feeling that at the moment the understanding of the nonlinear stability phenomena involved is limited and that further research on the subject should be pursued.

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