A SYMPLECTIC SOLVER FOR LATTICE EQUATIONS

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Abstract

We describe an Ordinary Differential Equation solver for lattice dynamics equations in Hamiltonian form, which is more accurate, more efficient and easier to programme than the commonly used Runge-Kutta methods. An important feature of the solver is that it preserves the symplectic nature of the differential equations. We illustrate the application of scheme in a variety of examples of one and two space dimensional lattices, including the Toda lattice and a discrete version of the K.P. equation. We also show some comparisons with standard Runge-Kutta methods.

1 Introduction

We describe an Ordinary Differential Equation solver for lattice equations which can be written in the form

$$\frac{d^2}{dt^2}q_j = -\frac{\partial}{\partial q_j}G(\underline{q}) \tag{1}$$

for integers j, where q_j is the displacement of the jth lattice point from its equilibrium position and $\underline{q}$ is a vector containing the q_j's. For example, the choice

$$G(\underline{q}) = \sum_j V(q_j - q_{j-1}) \quad \Rightarrow \quad \frac{d^2}{dt^2}q_j = V'(q_{j+1} - q_j) - V'(q_j - q_{j-1}) \tag{2}$$

for integers j, where $V(\Delta q)$ is the potential. The well-known Toda lattice [9] is obtained with potential $V(s) = a\exp(-bs)/b + as$ where a, b are constants and $a, b > 0$. It is also common to see (2) written as

$$\frac{d^2}{dt^2}s_j = V'(s_{j+1}) - 2V'(s_j) + V'(s_{j-1}) \tag{3}$$

for integers j, where $s_j = q_j - q_{j-1}$ is the deviation of the bond length from its equilibrium. The extension to lattices in more than one space dimension is straightforward.

The rest of the paper is organised as follows. In section 2 we describe the symplectic Ordinary Differential Equation solver and compare its structure with the commonly used explicit classical Runge-Kutta method. In section 3 we describe the results of a series of experiments to evaluate the accuracy, Hamiltonian conservation and efficiency of the symplectic solvers applied to lattice equations in one and two space dimensions.

2 Symplectic ODE Solver

In recent years, much effort has been devoted to the development of solvers which preserve the symplectic properties of Hamiltonian systems of Ordinary Differential Equations. Surveys of this work can be found in [8] and [2]. Briefly, the main arguments in support of these methods are: the symplectic property determines much of the Hamiltonian dynamics and so should be preserved by the approximate solver; symplectic methods produce approximate solutions which stay close to the exact solution manifold over very long time periods; in general, although they do not exactly conserve the Hamiltonian and other quantities, they approximately conserve them to high precision with little change over long time periods (see [6] for example). The main reason that they are not in common use (apart from the fact that they are not yet widely known) is that the easily obtainable symplectic schemes are fully implicit Runge-Kutta methods, which are very computationally expensive since they involve the solution of systems of nonlinear algebraic equations at each time step. However, the special form of the lattice equations we are considering allows the use of a very cheap symplectic scheme which does not suffer this drawback.

We adapt a fourth order accurate, fixed time step, symplectic algorithm described in [1, 10] for lattice equations. We concentrate on one dimensional lattices, and the extension to two dimensional lattices is obvious. This scheme is designed for ODEs with a separable Hamiltonian form i.e.

$$\dot{p}_j = -\frac{\partial}{\partial q_j} H(\underline{p}, \underline{q}) \quad , \quad \dot{q}_j = \frac{\partial}{\partial p_j} H(\underline{p}, \underline{q}) \quad \text{with} \qquad H(\underline{p}, \underline{q}) = F(\underline{p}) + G(\underline{q}) \; . \tag{4}$$

The lattice equation (1) can be written in a particularly simple, separable form as

$$\dot{p}_j = -\frac{\partial}{\partial q_j} G(\underline{q}) \quad , \quad \dot{q}_j = p_j \quad \text{with} \qquad H(\underline{p}, \underline{q}) = G(\underline{q}) + \frac{1}{2} \sum_j (p_j)^2 \; . \tag{5}$$

The symplectic scheme to advance the solution from time $n\tau$ to $(n+1)\tau$ using a fixed time step size τ is written in pseudo-code as

(a) For all j do $q_j := q_j + b_1 p_j$.

(b) For $s = 2, \ldots, 4$ do

(b.1) For all j do $p_j := p_j + a_s A_j(\underline{q})$.

(b.2) For all j do $q_j := q_j + b_s p_j$.

where

$$A_j(\underline{q}) = -\frac{\partial}{\partial q_j} G(\underline{q})$$

and the constants b_s, a_s are given by

$$a_2 = a_4 = \tau(2 - 2^{1/3})^{-1}, \quad a_3 = \tau(1 - 2^{2/3})^{-1},$$

$$b_1 = b_4 = \tau(2 + 2^{1/3} + 2^{-1/3})/6, \quad b_2 = b_3 = \tau(1 - 2^{1/3} - 2^{-1/3})/6 \; .$$

At the start of step (a), the vectors $\underline{p}, \underline{q}$ contain the values of approximate solution at time $n\tau$ and at the end of step (b), they contain the approximate solution at time $(n+1)\tau$.

The symbol := indicates that we evaluate the right hand side and overwrite the storage locations on the left with the result. It is important to complete step (b.1) before starting step (b.2).

The computational cost of the algorithm is dominated by the three $\underline{A}(\underline{q})$ evaluations required for each time step and the main storage requirement is space for two vectors $\underline{p}, \underline{q}$. In comparison, the Classical 4th order Runge-Kutta method, which is often used in the solution of lattice equations, uses four evaluations of vector function $\underline{A}(\underline{q})$ and a large number of other vector operations each time step. If we use a simple coding of the Runge-Kutta method, then the storage required is 5 pairs of vectors the same size as $\underline{p}, \underline{q}$. With more complicated coding and at the expense of vectorisation, the storage can be cut to 1 pair of vectors. The symplectic scheme requires fewer auxiliary calculations also and the net result is that it is cheaper than the Runge-Kutta on all counts. This is confirmed in the experiments reported in the next section which showed it to take about 0.75 of the time required by the Runge-Kutta for each time step.

3 Numerical Results

In this section we describe the results of computations designed to investigate the stability of travelling wave solutions on one and two space dimensional lattices. In most cases we use initial data obtained by the approximation method described in [4, 5] which uses path following and spectral methods. We test the solver on finite lattices with periodic boundary conditions, so that the solitary wave is in effect travelling around a ring in the one space dimension case and over a torus in two.

We first consider lattice equations in one space dimension which can be written as (2) and then rewritten in first order Hamiltonian form as

$$\dot{p}_j = V'(q_{j+1} - q_j) - V'(q_j - q_{j-1}) \quad , \quad \dot{q}_j = p_j \ . \tag{6}$$

We consider various forms of potential energy function $V(\cdot)$, including the Toda and electrical potentials and the quartic polynomial potential

$$V_4(s) = \tfrac{1}{2}s^2 + \tfrac{1}{4}as^4 \ . \tag{7}$$

The change of variables,

$$s_j = q_{j+1} - q_j \ , \quad r_j = p_{j+1} - p_j \tag{8}$$

allows us to rewrite (6) again to obtain,

$$\dot{r}_j = V'(s_{j+1}) - 2V'(s_j) + V'(s_{j-1}) \quad , \quad \dot{s}_j = r_j \ . \tag{9}$$

The direct application of the symplectic scheme to lattice equations in the non-Hamiltonian form above is exactly equivalent to applying the scheme to the Hamiltonian form (6) and computing s_j from $s_j = q_j - q_{j-1}$, thus preserving the useful features of the scheme.

In all the examples tested, the Hamiltonian is conserved with considerable accuracy. The quartic potential results with $\tau = 0.01$ shown in figure 1 show an apparently constant upper bound on the error in the Hamiltonian up to (and beyond) 4 million time steps.

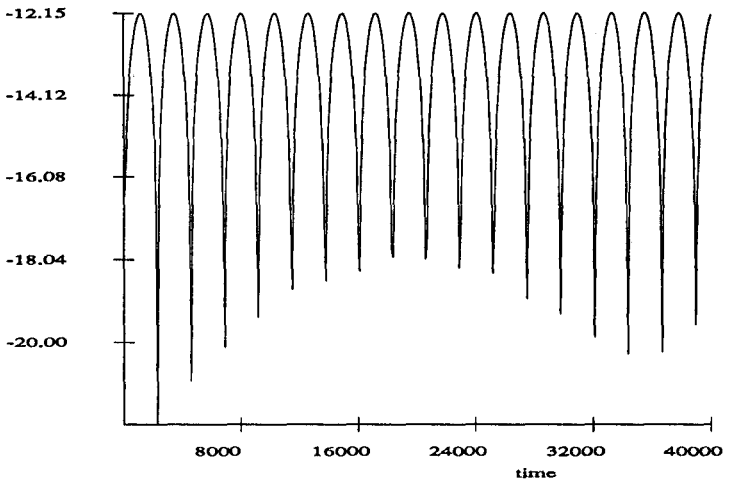

Figure 1: Graph of $\log_e(\frac{|H(t)-H(0)|}{H(0)})$ vs time for the symplectic solver on the quartic potential showing the large time control of $H(t)$. Parameters $\tau = 0.01$, 50 lattice points, $c \approx 3.8$.

For a given potential, the relative size of the error in the Hamiltonian is dependent on the time step size used and the height (and hence the speed) of the initial pulse. One would expect the relative error in the Hamiltonian to vary as $O(\tau^4)$ for small enough τ in this fourth order accurate scheme, and experiments on the quartic potential with different values of τ confirm this. For example, successively halving τ from $\tau = 0.04$ shows the maximum error decreasing by factors 15.5, 19.1, 17.6 etc. which is close to the predicted value 16.

We find apparent long time instabilities in the pulse solutions of the quartic potential problem when the initial data is perturbed slightly (actually by a mismatch between the number of lattice points used in the path following code and in the ODE solver). In this case, the pulse propagates as expected initially, but ripples develop after some time, at the expense of the pulse's height and speed. As the wave travels around the ring it interacts with these small linear waves, accelerating its decay. This behaviour is illustrated in figure 2, where the wave is travelling around a lattice of 50 nodes. We should remark that initially the wave has travelled around the ring slightly *more* than three times between each plot, and at later times slightly *less* than three times and has not reversed its direction (as it appears). These same examples have been calculated using the Classical fourth order Runge-Kutta scheme where ripples also develop and a similar picture is seen. However the Runge-Kutta scheme damps the solution causing a steady decrease in the Hamiltonian, at first more severely, but later less so, once the soliton has been mostly eroded. See figure 3 for a more quantitative description.

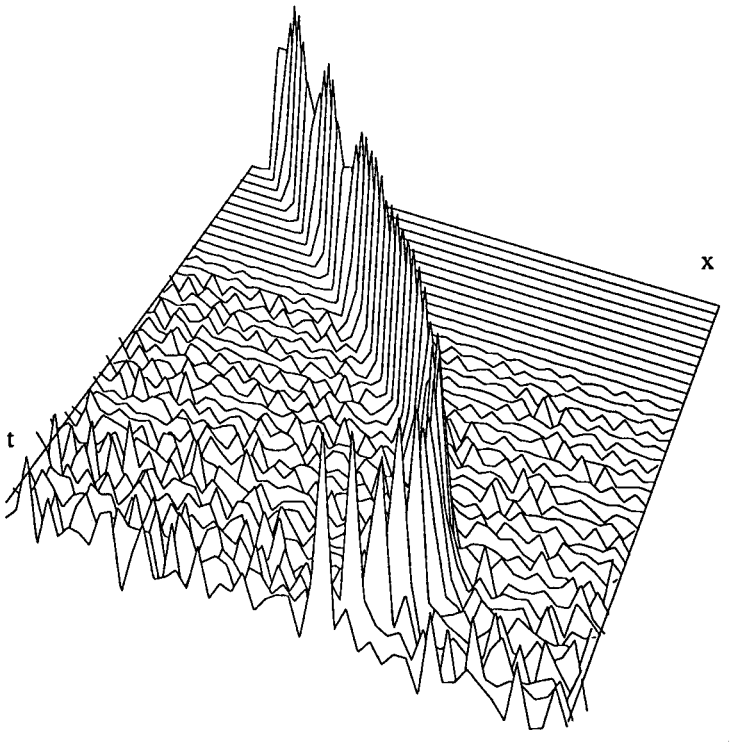

Figure 2: Solution profiles on quartic lattice at regular time intervals with about three revolutions between each plot. See text for details.

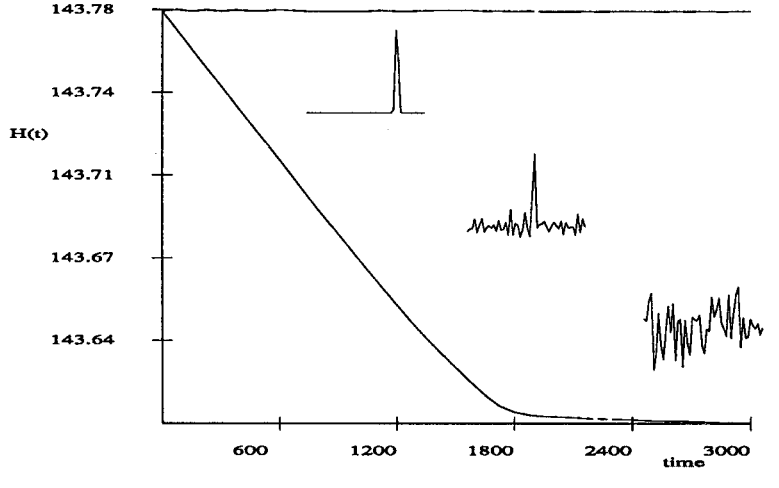

Figure 3: The main graph shows the behaviour of the Hamiltonian for the Symplectic scheme (upper line) and for the classical Runge-Kutta scheme (lower). The insets show the solution profile at times roughly corresponding to their position on the main graph.

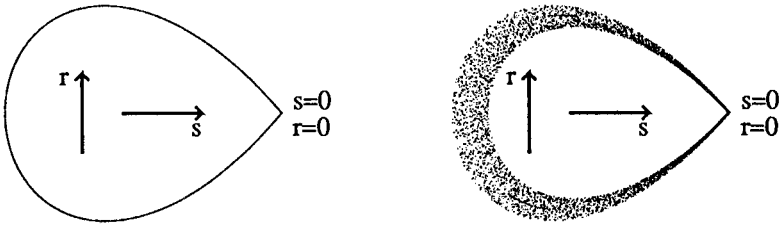

Figure 4: Phase plane portraits of a solitary wave in the lattice equation (9) with the Toda potential using the symplectic algorithm (left) and the Classical Runge-Kutta (right). 400000 time steps shown.

A slightly different example is given by the problem of electrical transmission lines [7, 5]. The simplest form of the equation of motion is

$$\frac{d^2}{dt^2}(w_n - aw_n^2) = w_{n+1} - 2w_n + w_{n-1}. \tag{10}$$

where $a > 0$. To put this into the form of equation 9, the substitution $u_n = w_n - aw_n^2$ is used. This is not a 1-1 transformation, so we have to take care in inverting it. Solving the quadratic and taking the negative branch, we obtain $V'(u) = (1 - \sqrt{1 - 4au})/2a$ giving,

$$V(u) = \frac{(1-4au)^{\frac{3}{2}}}{12a^2} + \frac{u}{2a} - \frac{1}{12a^2} \tag{11}$$

and we can solve this as before. The very sharp peak or cusp which appears at larger speeds (see [5]) makes determining the initial data harder, but once it is found the symplectic algorithm propagates this unusual solitary wave with little distortion and at the correct speed. The Hamiltonian was conserved to 9 significant figures in these tests.

Another clear indication of the advantages of the symplectic scheme can be seen in the phase plane portraits shown in figure 4. These show a solitary wave on the Toda lattice of 32 points, sampled at the same mesh point every 10 time steps for 400,000 steps and computed using the symplectic and Runge-Kutta methods with identical step sizes $\tau = 1/8$. The symplectic results are very sharp, but the Runge-Kutta results show the solution decaying in amplitude.

Finally we turn to a two dimensional example. We examine the KP lattice described in [3]

$$\begin{aligned} \frac{d^2}{dt^2}s_{i,j} &= (s_{i+1,j} - 2s_{i,j} + s_{i-1,j}) + \epsilon^2(s_{i,j+1} - 2s_{i,j} + s_{i,j-1}) \\ &+ \frac{1}{4}\epsilon^2(s_{i+1,j}^2 - 2s_{i,j}^2 + s_{i-1,j}^2). \end{aligned} \tag{12}$$

which can be solved using the symplectic method, modified to cover all the points in this two dimensional grid. We again show phase portraits of solitary waves in figure 5. We use a 150×200 mesh with appropriate periodic boundary conditions, time step size $\tau = 1/16$ and waves at angles 0 and $\tan^{-1}(3/4)$ to the i-axis at speeds close to 1. The phase portraits are again sharp over many timesteps, apart from the inner one (after magnification) which was given slightly perturbed initial data.

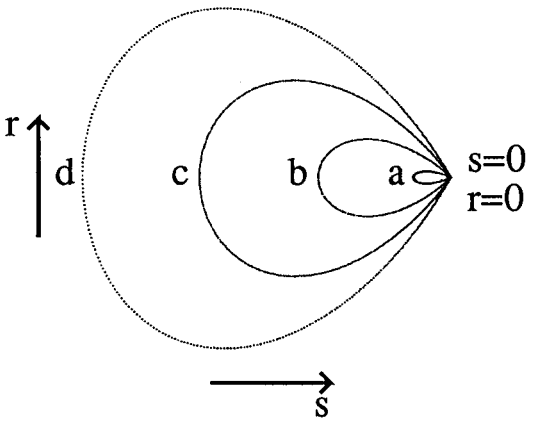

Figure 5: Phase plane diagram for the discrete KP equation on a two dimensional lattice showing (a) $\theta = 0, c = 1.053$ (b) $\theta = 0, c = 1.175$ (c) $\theta = \tan^{-1} 3/4, c = 1.054$ (d) $\theta = \tan^{-1} 3/4, c = 1.155$. (Note that $r = \dot{s}$)

4 Conclusion

The symplectic ordinary differential equation solver we describe is a useful tool for investigations of solitary waves on discrete lattices. It is simple, efficient and accurate.

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