EXACT SOLUTIONS FOR HAMILTONIAN SYSTEMS USING INTEGER ARITHMETIC

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1. Introduction

Numerical simulations usually aim to study the qualitative features of dynamical systems. For example, when we simulate disk galaxy dynamics we are concerned with the overall evolution of the galaxy rather than the fine details of individual stellar orbits.

In seeking practical numerical methods that correctly reproduce the qualitative behaviour of dynamical systems, it is always worthwhile to try to ensure that the basic mathematical structure of the system under study is not altered by the integration method. We present here a method for modifying a traditional integration scheme so that if the original system is Hamiltonian then the computed system is also exactly Hamiltonian. The effect of this method is to provide the exact solution for a Hamiltonian system that is slightly different from the system one really wishes to integrate. The method as stated here is applicable to an important class of problems in Hamiltonian dynamics. In particular, it can be used to perform exact integrations of Hamiltonian systems that closely approximate the gravitational N-body problem.

2. Hamiltonian Systems and Leapfrog

To a very good approximation, many of the dynamical systems that we study in astronomy are Hamiltonian systems. This means that a state of the system is described by a point in phase space and the time evolution is given by Hamilton's equations,

$$\dot{\mathbf{x}} = \frac{\partial H}{\partial \mathbf{v}}, \qquad \dot{\mathbf{v}} = -\frac{\partial H}{\partial \mathbf{x}}. \tag{1}$$

Here H is the Hamiltonian, the total energy expressed as a function of $\mathbf{x}$, $\mathbf{v}$, and t. A solution of these equations (1) gives a trajectory in phase space.

There are several important properties shared by all Hamiltonian systems. The most basic is that *phase trajectories do not intersect.* Hamiltonian systems have several other special properties, which can be expressed as integral invariants. The most fundamental of these is that *volume in phase space is preserved.* An ideal numerical integration scheme ought to preserve all these properties.

B. Sundelius (ed.) Dynamics of Disc Galaxies (1991) Göteborg, Sweden, pp. 137–141.

There are two major classes of dynamical systems: Hamiltonian systems and dissipative systems. While trajectories of Hamiltonian systems remain distinct, trajectories of dissipative systems tend to converge onto an "attractor". Standard numerical methods turn Hamiltonian systems into dissipative ones, destroying the Hamiltonian properties (although for good methods, the dissipation is weak and only leads to noticeable effects after integrating for a long time).

Numerical integration schemes give the state of the system at time $t + \Delta t$ given the state at time t. To do this exactly requires the evaluation of an infinite series. Since the series must be truncated after a finite number of terms, the computed new state is not exactly correct. In symplectic integration algorithms (*e.g.*, Channell and Scovel 1990) the bad effects of this *truncation error* are evaded by replacing the original system with a slightly different (but still Hamiltonian) system for which the series are always finite. Thus, despite the finite time step, all the Hamiltonian properties are preserved; the only error is that the Hamiltonian is slightly incorrect.

Unfortunately, this goal of preserving the Hamiltonian properties is not really achieved in practice. *Roundoff errors* make it impossible to perform the required finite computations exactly, so phase trajectories still intersect and phase volumes contract with time. The main point of this presentation is that *numerical integrations can be made exactly Hamiltonian despite roundoff error.*

The simplest symplectic integration algorithm is the standard "leapfrog" scheme,

$$\begin{aligned} \mathbf{x}(t+\Delta t) &= \mathbf{x}(t) + \Delta t\, \mathbf{v}(t+\Delta t)\,, \\ \mathbf{v}(t+\Delta t) &= \mathbf{v}(t) - \Delta t \frac{\partial U}{\partial \mathbf{x}}(\mathbf{x}(t))\,. \end{aligned} \tag{2}$$

This first-order method can be used to integrate trajectories described by any Hamiltonian that can be expressed in the form $H = \frac{1}{2}\mathbf{v}^2 + U(\mathbf{x})$ (an important special case is the gravitational N-body problem in cartesian coordinates). Equations (2) follow directly from Hamilton's equations (1) with the Hamiltonian $H = \frac{1}{2}\mathbf{v}^2 + U(\mathbf{x}) \sum_n \delta(t - n\Delta t)$. Thus truncation error is "cured" by multiplying the potential by a periodic time-dependent factor whose average value is unity.

We may now avoid roundoff error by adding a small, time-independent perturbation to the original potential $U(\mathbf{x})$, so that when the perturbed potential $\tilde{U}(\mathbf{x})$ is inserted in the leapfrog scheme (2) the required computations can always be done exactly. The idea is to ensure that the scheme (2) maps a lattice of points to itself. After a change of scale, lattice points will have integer coordinates so computers can do the required iteration of the "lattice map" without errors. If we choose a lattice with m points per unit, then we must choose the time-step Δt such that $m\Delta t$ is an integer. Then the "integerized leapfrog" scheme is

$$\begin{aligned} m\mathbf{x}(t+\Delta t) &= m\mathbf{x}(t) + m\Delta t\, \mathbf{v}(t+\Delta t)\,, \\ m\mathbf{v}(t+\Delta t) &= m\mathbf{v}(t) - \left[m\Delta t \frac{\partial U}{\partial \mathbf{x}}(\mathbf{x}(t)) \right], \end{aligned} \tag{3}$$

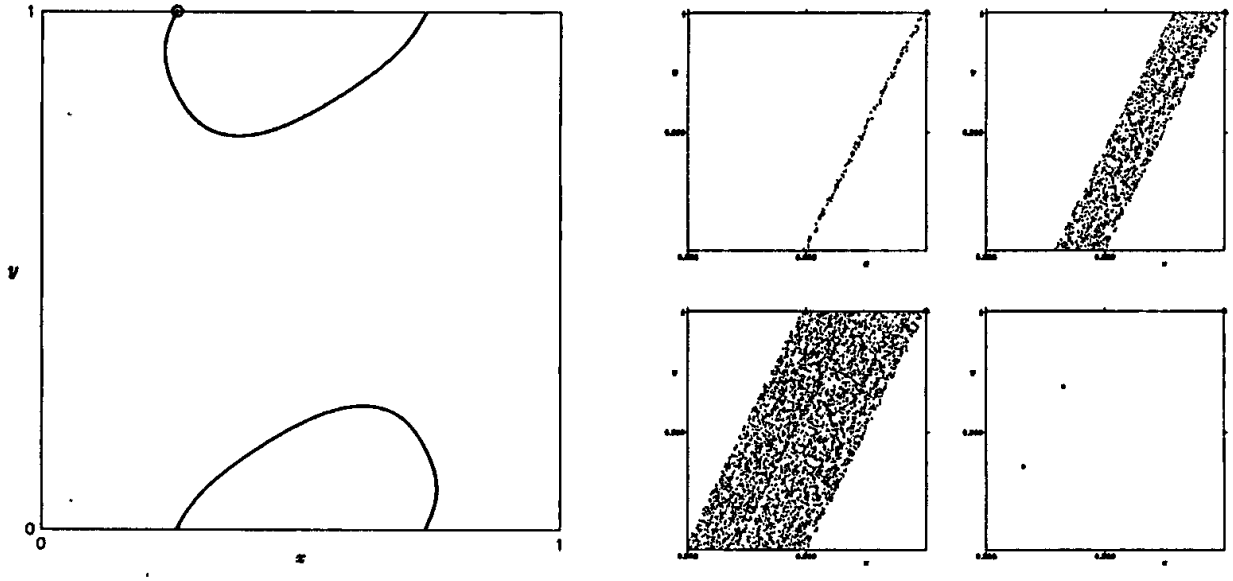

Figure 1. (a) A typical "regular" phase trajectory of the map obtained by applying ordinary leapfrog (with REAL*4 floating-point arithmetic) to evolve the motion of a particle in the potential $U(x) = (2\pi)^{-2}\cos 2\pi x$. The complete phase trajectory is shown; it appears to remain on an invariant curve but the following enlargements at various times reveal that the motion is more complicated. (b) 10^5 iterations. (c) 10^6 iterations. (d) 2 150 019 iterations. The limit circuit has been reached by this time and the plot has been terminated after one completion of the limit circuit. (e) The limit circuit alone (1622 iterations). Only two points of the limit circuit appear in this enlargement, which is of the same region as (b), (c), and (d). The phenomenon observed here, attraction of a trajectory onto a limit circuit that does not contain the initial point of the trajectory, cannot occur in a Hamiltonian system.

where square brackets denote the nearest integer vector. Provided that we choose initial conditions $(\mathbf{x}(0), \mathbf{v}(0))$ such that $mx_i(0)$ and $mv_i(0)$ are integers for each i, $(m\mathbf{x}(n\Delta t), m\mathbf{v}(n\Delta t))$ can be determined exactly for all n. Thus (3) yields the exact solution of the problem with Hamiltonian $\tilde{H} = \frac{1}{2}\mathbf{v}^2 + \tilde{U}(\mathbf{x})\sum_n \delta(t - n\Delta t)$. (A precise discussion of $\tilde{U}$, including a proof that it exists, is given elsewhere (Earn and Tremaine 1991), but equations (3) are all that is needed to carry out the computations.)

3. The Standard Map

To illustrate the bad effects of roundoff error and how these are overcome using lattice maps, we have applied both ordinary leapfrog (eqs. 2 with single-precision floating-point arithmetic) and integerized leapfrog (eqs. 3) to the motion of a particle in the one-dimensional potential $U(x) = K/(2\pi)^2\cos 2\pi x$, where K is a constant. Inserting

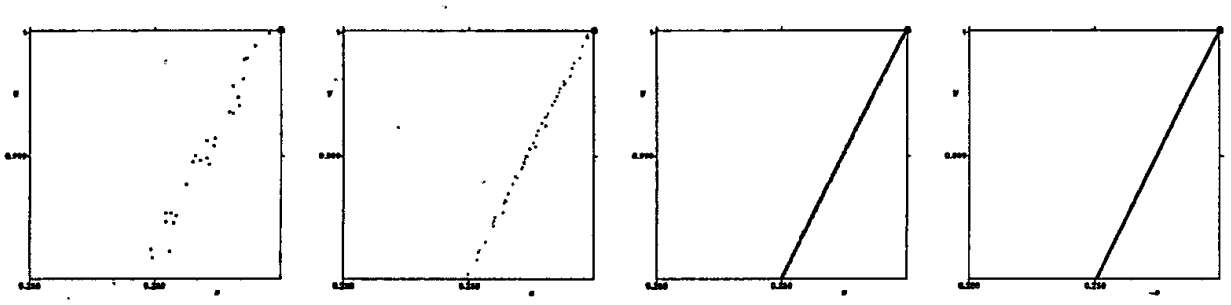

Figure 2. Complete trajectories obtained using integerized leapfrog, starting from the same point as the plots in Figure 1. The scale is the same as in Figure 1(b–d). (a) $m = 10^5$, cycle length $L = 16\,728$. (b) $m = 10^6$, $L = 34\,756$. (c) $m = 10^7$, $L = 1\,689\,794$. (d) $m = 10^8$, $L = 130\,141\,384$. In a Hamiltonian system on a finite lattice, such as this one, all trajectories are periodic.

this potential in (2) we obtain

$$\begin{aligned} x_{n+1} &= x_n + v_{n+1}\,, \\ v_{n+1} &= v_n + \frac{K}{2\pi}\sin(2\pi x_n)\,. \end{aligned} \tag{4}$$

where $x_n \equiv x(n\Delta t)$, $v_n \equiv v(n\Delta t)$ and time units are chosen so that $\Delta t = 1$. This is the well-known "standard map". K is known as the "stochasticity parameter". This map is periodic in both x and v with period 1.

Since computers can only represent a finite number of states, repeated iteration of (4) eventually leads to a cycle, which we call the *limit circuit*. This is true whether we use ordinary or integerized leapfrog. The advantage of integerized leapfrog is that it is exactly Hamiltonian; thus phase trajectories do not intersect and initial points always lie on the limit circuit. An integerized version of the standard map was first investigated by Rannou (1974).

The figures show the results of a number of experiments investigating the differences between trajectories calculated using ordinary leapfrog and integerized leapfrog. Ordinary leapfrog allows "regular" trajectories to cross invariant curves, and it allows "chaotic" trajectories to be trapped indefinitely by a "regular" attractor. These effects are simply wrong and do not occur if integerized leapfrog is used instead.

4. Concluding Remarks

The effects of roundoff error and the benefits of lattice maps are discussed in greater detail in Earn and Tremaine (1991). The use of lattice maps to design exactly symplectic integration algorithms of arbitrary order for general Hamiltonians is discussed by Scovel (1991).

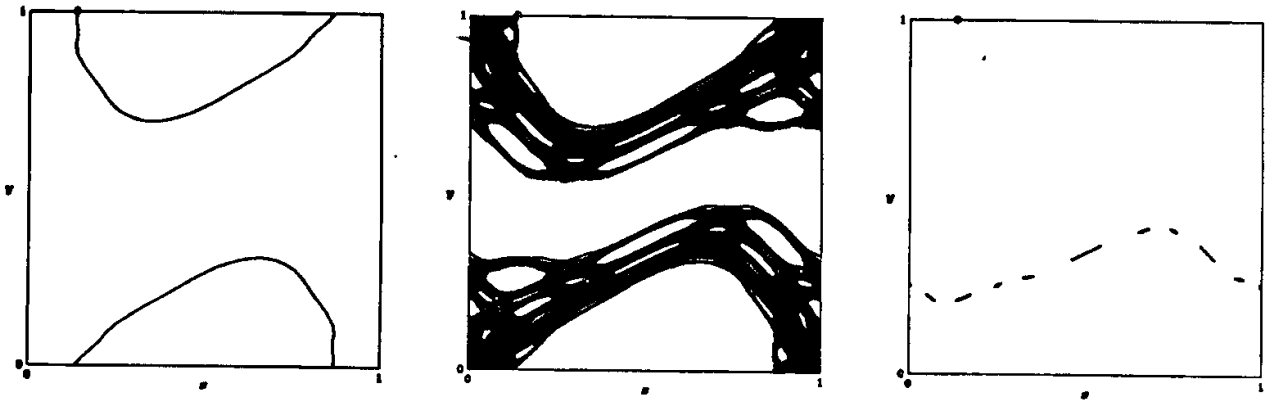

Figure 3. Another example of unsatisfactory behaviour found when using ordinary leapfrog with REAL*4 floating-point arithmetic. (a) The first 40 000 iterations display an apparently regular trajectory. (b) The next 1 730 000 iterations show an apparently chaotic trajectory. The limit circuit is reached near the end of this interval. (c) The limit circuit has length only 37 310 iterations and appears to be a regular trajectory (a chain of islands).

The use of lattice maps has practical value mostly for systems that are studied over long time scales. Thus the use of lattice maps is likely to be more important for Solar System simulations lasting for millions of orbital times, than for galaxy simulations lasting for hundreds of orbital times.

References

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