Note

A Numerical Algorithm for Hamiltonian Systems

1. Introduction

A frequent problem in numerical analysis is that of computing particle trajectories for Hamiltonian (conservative) systems. A number of distinct algorithms are known and the one discussed below is not new, but is chosen to illustrate the general procedure. By a *reinterpretation* of the algorithm a more accurate solution to the problem, as judged by the constancy of the energy, is obtained. In brief, rather than try to find the best algorithm for a particular Hamiltonian, the procedure is to choose an algorithm and ask what Hamiltonian system it best represents. The basic method is straightforward and is illustrated in the next section with respect to a simple system. Some generalization are discussed in Section 3.

2. General Method

We consider a Hamiltonian system and write the equations of motion in the form

$$\frac{dq}{dt} = p, \qquad \frac{dp}{dt} = -\frac{\partial \Phi}{\partial q} \equiv F(q) \tag{1}$$

which corresponds to the Hamiltonian

$$H = p^2/2 + \Phi(q). \tag{2}$$

The simplest Euler finite difference scheme is

$$q_{n+1} = q_n + hp_n, \tag{3}$$

$$p_{n+1} = p_n + hF(q_n), \tag{4}$$

where h is the time step length. This scheme suffers from three major disadvantages:

(a) The Jacobian J defined by the determinant

$$J = \begin{vmatrix} \dfrac{\partial p_{n+1}}{\partial p_n}, & \dfrac{\partial q_{n+1}}{\partial p_n} \\[2ex] \dfrac{\partial p_{n+1}}{\partial q_n}, & \dfrac{\partial q_{n+1}}{\partial q_n} \end{vmatrix},$$

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is equal to $1 - h^2 F'(q_n)$, where the dash denotes differentiation with respect to the argument. A value of $J < 1$ (>1) leads to a volume contraction (expansion) in phase space, neither being a property of Hamiltonian systems.

(b)   The above set of equations can be rewritten in the form

$$q_n = q_{n+1} - hp_n,$$
$$p_n = p_{n+1} - hF(q_n).$$

Comparison with (3) and (4) shows that this set is not time-reversal-invariant, that is, not of the same form with the interchange of n and $n+1$ and $+h$ and $-h$. (For invariance one would need $F(q_{n+1})$ in the above set.)

(c)   The energy, defined by

$$E_n = p_n^2/2 + \Phi(q_n) \tag{5}$$

is not independent of n, and in fact, as is readily shown

$$E_{n+1} - E_n = \frac{h^2}{2} [F^2(q_n) - p_n^2 F'(q_n)] + O(h^3). \tag{6}$$

The energy E ($\equiv H$) of a Hamiltonian system is of course constant.

The first two disadvantages, (a) and (b), can be overcome by considering the finite difference equations

$$q_{n+1} = q_n + \frac{h}{2}(p_n + p_{n+1}) \tag{7}$$

$$p_{n+1} = p_n hF(q_n + hp_n/2). \tag{8}$$

The energy is still not constant, but since

$$E_{n+1} - E_n = -\frac{h^3 p_n}{4}\left(\frac{p_n^2 F''}{6} + FF'\right) + O(h^4), \tag{9}$$

the error is one order less in h than the original scheme.

The difference scheme given by (7) and (8) is fairly standard and in fact Ruth [1] has drawn attention to the fact that it satisfies the canonical character of Hamiltonian systems, namely $J = 1$.

Although the finite difference scheme (7), (8) does not solve the original Hamiltonian it is time-reversal-invariant and the Jacobian is unity. Thus it is interesting to ask what *continuous* systems of equations it most *closely* represents. To help answer this we consider a continuous approximation to the equations by writing $q_n \equiv q(nh) = q(\tau)$ and making a Taylor series of q_{n+1} about $q(\tau)$. In this manner (7), (8) reduce to

$$\frac{dq}{d\tau} = p(1 + h^2 F_q/12) + O(h^4) \tag{10}$$

and

$$\frac{dp}{d\tau} = F - h^2(FF_q/6 + p^2F_{qq}/24) + O(h^4), \qquad (11)$$

where $F_q \equiv \partial F/\partial q$. To $O(h^4)$ these are equivalent to a Hamiltonian system with

$$H(p, q) = (p^2/2)(1 + h^2F_q/12) + \Phi(q) + h^2F^2/12. \qquad (12)$$

In this form the system is equivalent to one with a spatially variable mass. This undesirable feature may be removed by making a contact transformation defined by a change of variables from (q, p) to $(\bar{q}, \bar{p})$, where

$$p = \bar{p}(1 - h^2F_q(q)/24) \qquad (13)$$

and

$$\bar{q} = q - h^2F(q)/24. \qquad (14)$$

The new Hamiltonian is then

$$\bar{H} = \bar{p}^2/2 + \bar{\Phi}(\bar{q}) \qquad (15)$$

with

$$\bar{\Phi}(q) = \Phi(q) + h^2F^2(q)/24. \qquad (16)$$

To $O(h^2)$, the finite difference scheme (7) and (8) is equivalent to the original Hamiltonian system defined by (2). However to $O(h^4)$ this *same* finite difference scheme is equivalent to a Hamiltonian system defined by $\bar{H}$ and not by H.

Thus to obtain increased accuracy, but still use (7) and (8) with the same value of h, we must identify $\bar{\Phi}$, and not Φ, with the real potential (the problem we really want to solve) and $\bar{q}$, $\bar{p}$ with real physical position and momentum variables. This means that the potential Φ, that appears in (7) and (8), is an effective potential; it is expressed in terms of $\bar{\Phi}$, the real potential, using (16). To $O(h^4)$ we have

$$\Phi(q) = \bar{\Phi}(q) - h^2\bar{\Phi}_q^2/24. \qquad (17)$$

Once the finite difference equations are solved the real coordinates $\bar{q}$, $\bar{p}$ are obtained from (13) and (14). Again to $O(h^4)$, we have ($\bar{\Phi}_q \equiv \partial\bar{\Phi}/\partial q$)

$$\bar{q} = q + h^2\bar{\Phi}_q/24 \qquad (18)$$

and

$$\bar{p} = p(1 - h^2\bar{\Phi}_{qq}/24). \qquad (19)$$

Most importantly it is found that the true energy $\bar{E} = \bar{p}^2/2 + \bar{\Phi}(\bar{q})$ is constant to $O(h^5)$.

The whole procedure is illustrated (in the Appendix) by considering the harmonic oscillator.

3. Generalization

An obvious extension is to include explicitly the terms of $O(h^4)$ in (10) and (11). This produces, after a suitable contact transformation, an effective Hamiltonian which may be identified with the real Hamiltonian. In this way it is possible to find a finite difference scheme in which the energy is conserved to $O(h^7)$.

Another extension is to treat a $2N$-dimensional system with coordinates (q_i, p_i) for $i = 1, 2, ..., N$. The difference scheme, chosen in analogy to (7) and (8), is

$$q_{i,n+1} = q_{i,n} + \frac{h}{2}(p_{i,n} + p_{i,n+1}) \tag{20}$$

and

$$p_{i,n+1} = p_{i,n} - h\Phi_{q_i}(q_{j,n} + hp_{j,n}/2), \tag{21}$$

where Φ_{q_i} denotes differentiation with respect to q_i. The potential Φ is related to the real potential $\bar{\Phi}$ by

$$\Phi = \bar{\Phi} - (h^2/24)\sum_{i}^{N}(\bar{\Phi}_{q_i})^2$$

and the contact transformation between the variables is such that

$$\bar{q}_i = q_i + (h^2/24)\bar{\Phi}_{q_i} \tag{22}$$

and

$$\bar{p}_i = p_i - (h^2/24)\sum_{j} p_j \bar{\Phi}_{q_i p_j}. \tag{23}$$

The energy is constant to $O(h^5)$.

In this paper a simple difference scheme, namely (7) and (8), has been used to illustrate the procedure of introducing an effective potential and coordinates, related to the real potential and coordinates by a canonical transformation. However, since the procedure only relies on the finite difference scheme being time-reversal-invariant with a Jacobian of unity, it is readily applicable to other difference schemes sharing these properties.

Appendix

To illustrate the above procedure, consider the problem of solving the time evolution of a harmonic oscillator. The appropriate potential that appears in (2) is given by $\Phi = \omega^2 q^2/2$, where ω is a constant. The exact solution of this problem is of course well known and takes the form

$$q = A\cos(\omega t + \Psi), \tag{20}$$

where A and Ψ are constants. The corresponding energy $E = A^2\omega^2/2$ and is independent of time.

Equations (3) and (4) may also be solved $(F(q) = -\omega^2 q)$ to give

$$q = Ar^n\cos(\hat{\omega}t + \Psi) \qquad \text{and} \qquad E = A^2r^{2n}\omega^2/2,$$

where $r^2 = 1 + h^2\omega^2$, $\cos(h\hat{\omega}) = 1/\sqrt{1 + h^2\omega^2}$ with $t = nh$. This gives the effective frequency of oscillation to be $\hat{\omega}$, not ω, where to $O(h^4)$, $\hat{\omega} = \omega(1 - h^2\omega^2/3)$. As is well known the weakness of this algorithm is that the energy E steadily increases with the number of iterates.

The solution of (7) and (8) is of the form $q = A\cos(\hat{\omega}t + \Psi)$, where $\cos(h\hat{\omega}) = 1 - h^2\omega^2/2$ so that to $O(h^4)$, $\hat{\omega} = \omega(1 - 7h^2\omega^2/24)$. The energy $E = (A^2\omega^2/2)$ $(1 + (h^2\omega^2/4)\sin(\hat{\omega}t + \Psi))$ which, although a function of time, is now bounded.

To use the procedure suggested in this paper it is first necessary to identify $\bar{\Phi}$ as the true potential $(= \omega^2 q^2/2)$ and use (17) to construct the effective potential Φ which appears in the algorithm. Then to $O(h^4)$, $\Phi = (\omega^2 q^2/2)(1 - h^2\omega^2/12)$. With this form for Φ in (7) and (8) the equations may be solved for q and p to give $q = A_0\cos(\hat{\omega}t + \Psi)$, where $\cos(h\hat{\omega}) = 1 - h^2\omega^2/2 + h^4\omega^4/24$, so that to $O(h^4)$, $\hat{\omega} = \omega$. From (18) it is found that $\bar{q} = (1 + h^2\omega^2/24)q$ so that q is also a harmonic function. The energy, defined by (5) (but in terms of $\bar{q}$ and $\bar{p}$) is readily calculated and found to be constant to $O(h^5)$, and equal to $A^2\omega^2/2$.

Thus the procedure advocated in this paper gives, for the particular case of the harmonic oscillator, an exact solution with constant energy to $O(h^5)$.

REFERENCE

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