A DIFFERENCE SCHEME FOR THE HAMILTONIAN EQUATION*

QIN MENG-ZHAO (秦孟兆)

(Computing Center, Academia Sinica, Beijing, China)

§ 1

In the recent DD-5 Beijing conference, Feng Kang proposed three types of difference schemes for the Hamiltonian equation from the viewpoint of symplectic geometry. In this paper, we give a further discussion on these schemes and propose another difference scheme suitable for the nonquadric Hamiltonian function of second order.

We consider the following system of canonical equations

$$\begin{cases}
\frac{dp_{\nu}}{dt} = \frac{-\partial H}{\partial q_{\nu}}, \\
\frac{dq_{\nu}}{dt} = \frac{\partial H}{\partial p_{\nu}},
\end{cases} \quad \nu = 1, 2, \dots, n$$
(1.1)

with Hamiltonian function $H(p_1, p_2, \dots, p_n, q_1, q_2, \dots, q_n)$. Let the space R^{2n} be equipped with a symplectic structure defined by the differential two form

$$\omega^2 = dp \wedge dq, \quad z = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix} = \begin{bmatrix} p \\ q \end{bmatrix}, \quad J = \begin{bmatrix} 0 & E_n \\ -E_n & 0 \end{bmatrix}.$$

$$E_{n} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad J^{-1} = J = -J = \begin{bmatrix} 0 & -E_{n} \\ E_{n} & 0 \end{bmatrix}. \tag{1.2}$$

(1.1) can be rewritten as

$$\frac{dz}{dt} = J^{-1}H_s = -JH_s \tag{1.3}$$

with solution z(t).

Assume that for each t, $z(0) \rightarrow z(t)$ defines a diffeomorphism g(t). Then its Jocobian G(t) is a symplectic matrix, i.e.

$$G'(t)JG(t)-J. (1.4)$$

Suppose H_s can be written as A(z)z. Then equation (1.3) has the form

$$\frac{dz}{dt} = -JA(z)z. \tag{1.5}$$

We call the first scheme investigated in [1] (one-leg C-N difference scheme) the

^{*} Received September 19, 1984

Euler scheme

$$\frac{z^{n+1}-z^n}{At} = -JA\frac{z^{n+1}+z^n}{2}. (1.6)$$

Multiplying (1.6) by $A = \frac{z^{n+1} + z^n}{2}$ and summing over all m and noting that J is antisymmetric, we have

$$\left(\frac{z^{n+1}-z^n}{\Delta t}, A\frac{z^{n+1}+z^n}{2}\right)=0.$$

If the matrix is a symmetric constant, we have

$$(z^{n+1}, Az^{n+1}) = (z^n, Az^n).$$
 (1.7)

Let $||H||^{n+1} = (z^{n+1}, Az^{n+1})$. Therefore we have

$$||H||^{n+1} = ||H||^n = \dots = ||H||^0. \tag{1.7}$$

The amplification of this scheme is $\left[I + \frac{\tau}{2}JA\right]^{-1}\left[I - \frac{\tau}{2}JA\right]$, which is a symplectic operator. When (1.5) is well posed, then this scheme is absolutely stable.

Now we consider the hopscotch method for the system of equation (1.5). The method requires that we combine the simple one-step processes

$$z^{n+1} = z^n - \Delta t J A z^n, \tag{1.8}$$

$$z^{n+1} = z^n - \Delta t J A z^{n+1} \tag{1.9}$$

using them at alternate node points on the t-axis. If (1.8) is used at those points with m even and (1.9) is used at those with m odd, and if we define

$$\theta^m = \begin{cases} 1, & \text{if } m \text{ is even,} \\ 0, & \text{otherwise,} \end{cases}$$

then the hopscotch method is

$$z^{n+1} + \Delta t \theta^{n+1} J A z^{n+1} = z^n - \Delta t \theta^n J A z^n.$$
 (1.10)

Writing (1.10) with (n+1) replacing n and eliminating z^{n+1} from this equation, we have

$$z^{n+2} = z^n - \Delta t \theta^n (J A z^{n+2} + J A z^n) - 2 \Delta t \theta^{n+1} J A z^{n+1}. \tag{1.11}$$

When n is odd, the above equation reduces to

$$z^{n+2} = z^n - 2\Delta t J A z^{n+1} \tag{1.12}$$

which is just the leap-frog scheme. Multiplying (1.12) by Az^{n+1} on both sides and summing over all space points, we have

$$(z^{n+2}, Az^{n+1}) = (z^{n+1}, Az^n).$$
 (1.13)

We first use the forward time difference scheme

$$\frac{z^1-z^0}{\Delta t}=-JAz^0. \tag{1.14}$$

We obtain

$$(z^1, Az^0) = (z^0, Az^0).$$

Therefore

$$(z^{n+2}, Az^{n+1}) = (z^{n+1}, Az^n) = \dots = (z^1, Az^0) = (z^0, Az^0).$$
 (1.15)

We call these schemes quasi-energy conservative. Let (1.12) be rewritten in form

$$z^{n+1} - z^{n-1} = -2\Delta t J A z^n. ag{1.16}$$

Multiplying (1.16) by $z^{n+1}+z^{n-1}$ and summing over all space points yield

$$||z^{n+1}||^2 - ||z^{n-1}||^2 = -2\Delta t(z^{n+1} + z^{n-1}, JAz^n). \tag{1.17}$$

We define s, by

$$s_n = ||z^n||^2 + ||z^{n+1}||^2 + 2\Delta t(z^{n+1}, JAz^n).$$

Hence

$$s_n - s_{n-1} = ||z^{n+1}||^2 - ||z^{n-1}||^2 + 2\Delta t(z^{n+1}, JAz^n) - 2\Delta t(z^n, JAz^{n-1}).$$
 (1.18)

Then $s_n - s_{n-1} = -2\Delta t(z^{n-1}, JAz^n) - 2\Delta t(z^n, JAz^{n-1})$ and we have

$$s_{n}-s_{n-1} \leq +2\Delta t \lambda (\|z^{n}\|^{2}+\|z^{n-1}\|^{2}). \tag{1.19}$$

Further,

$$2|(z^{n+1}, JAz^n)| \leq \lambda(||z^{n+1}||^2 + ||z^n||^2), \qquad (1.20)$$

where λ is the maximal eigenvalue of matrix JA. So if $\lambda \Delta t < 1$, which is in fact the Courant condition, we have

$$K^*(\|z^n\|^2 + \|z^{n+1}\|^2) \leq s_n \leq K(\|z^n\|^2 + \|z^{n+1}\|^2)$$
(1.21)

for some constant K>0. Stability in the norm s_n is easily obtained from (1.19) and (1.21) as follows:

$$s_n - s_{n-1} \leq 2\Delta t \lambda / K^* s_n,$$

$$s_n \leq s_0 \exp(2\lambda n \Delta t / K^*).$$
(1.22)

Thus, it is clear from the equivalency of s_n and $||z^{n+1}||^2 + ||z^n||^2$ that

$$||z^{n+1}||^2 + ||z^n||^2 \le C \cdot (||z^0||^2 + ||z^1||^2).$$

We can summarize this discussion in

Theorem. When matrix A is a symmetric constant, the hopscotch scheme is stable. When $\lambda \Delta t < 1$, this scheme is quasi-energy conservative.

Next we describe a self-adaptive procedure based on the conservation of discrete energy

$$\frac{z^{n+1}-z^{n-1}}{2\Delta t_n} = -JAz^n,$$

$$\Delta t_n = A(z^n - z^{n-1})JAz^n/(JAz^n, JAz^n),$$

where the values of Δt_n are computed recursively according to

$$t_{n+1} - t_{n-1} = 2\Delta t_n$$
.

This scheme is still explicit and is of second order, and is in the energy conservation form. Denote JAz^n by f:

$$\begin{aligned} (z^{n+1}, Az^{n+1}) &= (z^{n-1} + 2\Delta t_n f, A(z^{n-1} + 2\Delta t_n f)) \\ &= (z^{n-1}, Az^{n-1}) + \frac{2(f, A(z^n - z^{n-1}))}{(f, Af)} (Az^{n-1}, f) \\ &+ \frac{2(f, A(z^n - z^{n-1}))}{(f, Af)} (Af, z^{n-1}) + 4 \left[\frac{(f, A(z^n - z^{n-1}))}{(f, Af)} \right]^2 (f, Af) \\ &= (z^{n-1}, Az^{n-1}). \end{aligned}$$

[1] proposed energy conservative schemes by Hamiltonian differencing which have first order accuracy only. Here we propose another more symmetric form, which possesses second order accuracy.

For simplicity, only the case n=2 is given:

From the above first two equations, we have

$$\frac{1}{2}(H(\bar{p}_1p_2\bar{q}_1q_2)+H(\bar{p}_1\bar{p}_2\bar{q}_1\bar{q}_2))=\frac{1}{2}(H(p_1\bar{p}_2q_1\bar{q}_2)+H(p_1p_2q_1q_2)).$$

From the last two equations, we have

$$\frac{1}{2}(H(\bar{p}_1\bar{p}_2\bar{q}_1\bar{q}_2) + H(p_1\bar{p}_2q_1\bar{q}_2)) = \frac{1}{2}(H(\bar{p}_1p_2\bar{q}_1q_2) + H(p_1p_2q_1q_2)).$$

Combining these equations, we observe that these schemes have exact conservation of the Hamiltonian $H_{\scriptscriptstyle{\bullet}}$.

§ 2

In direct analog with the finite dimensional case of ordinary differential equations, a system of evolution equations involving the dependent variables $u = (u_1, \dots, u_n)$ is called Hamiltonian, if it can be written in the special form

$$u_i = J_{\mathcal{S}}(H), \tag{2.1}$$

where H is a Hamiltonian functional, ε denotes the Euler operator, and J is a skew-adjoint matrix of differential or pseudo-differential operators.

For simplicity, we suppose that the Hamiltonian density has the form $H(u, u_s)$, so that its n Euler derivatives are

$$\varepsilon_{i}H = \frac{\partial H}{\partial u_{i}} - \frac{\partial}{\partial x} \left(\frac{\partial H}{\partial u_{i,s}} \right) \tag{2.2}$$

and the symplectic operator has the form

$$J = (J_{ij}) = (a_{ij}\partial x), \qquad (2.3)$$

where (a_{ij}) is an $n \times n$ symmetric matrix of real constants with $\det(a_{ij}) \neq 0$.

The n equations of motion are

$$(u_i)_t = J_{ij} \varepsilon_j H = (a_{ij} \varepsilon_j H)_{\sigma}. \tag{2.4}$$

For example, the wave equations are

$$(a_{ij}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (J_{ij}) = \begin{pmatrix} 0 & \frac{\partial}{\partial x} \\ \frac{\partial}{\partial x} & 0 \end{pmatrix},$$

$$u = \binom{v}{w}, \quad H = \frac{1}{2} \int (v^2 + w^2) dx.$$

The boundary condition, if any, will be periodic. Its equations of motion are

$$\begin{pmatrix} v \\ w \end{pmatrix}_{t} = \begin{pmatrix} 0 & \partial x \\ \partial x & 0 \end{pmatrix} \begin{pmatrix} v \\ w \end{pmatrix}.$$
 (2.5)

The discretization of the difference equation of PDE should retain the symplectic property not only in time t but also in space variable. Here ∂x must take central difference Δ_0 , or it will not retain the symplectic property. So, for the wave equation, we have, similar to (2.5),

$$\begin{pmatrix} v \\ w \end{pmatrix}_{t} = \begin{pmatrix} 0 & \Delta_{0} \\ \Delta_{0} & 0 \end{pmatrix} \begin{pmatrix} v \\ w \end{pmatrix}. \tag{2.6}$$

Evidently

$$(\dot{u}, \, \varepsilon H) - (J\varepsilon H, \, \varepsilon H) = 0. \tag{2.7}$$

For (2.6) we take the first type of difference scheme

$$\begin{pmatrix}
\frac{v^{n+1}-v^n}{\Delta t} \\
\frac{w^{n+1}-w^n}{\Delta t}
\end{pmatrix} = \begin{pmatrix} 0 & \Delta_0 \\ \Delta_0 & 0 \end{pmatrix} \begin{pmatrix} \frac{v^{n+1}+v^n}{2} \\ \frac{w^{n+1}+w^n}{2} \end{pmatrix}.$$
(2.8)

From (2.8), taking inner products with $\left(\frac{\frac{v^{n+1}+v^n}{2}}{\frac{w^{n+1}+w^n}{2}}\right)$, and noticing the periodic

boundary condition, we get

$$\frac{1}{2} \Sigma (v^{n+1})^2 + (w^{n+1})^2 = \frac{1}{2} \Sigma (v^n)^2 + (w^n)^2. \tag{2.9}$$

From here, we can see that the total energy is conservative.

It is well known that the equation of compressible fluid has the form

$$\frac{Ds}{Dt} = 0, \quad \rho \frac{Du}{Dt} + \nabla p = 0, \quad \frac{D\rho}{Dt} + \rho \nabla u = 0. \tag{2.10}$$

Here s is entropy, ρ is density, p is pressure, and u(u, v, w) are velocity. It has been shown that the Clebsch transformation of the velocity field results in Hamilton's form for compressible fluid dynamics.

The Clebsch representation of fluid velocity is

$$\boldsymbol{u} = \nabla \varphi + \lambda \nabla \mu + s \nabla \nu \tag{2.11}$$

in which φ , λ , μ , s, ν are scalar functions of $x \in D$ and t, φ , μ , ν are Clebsch potentials. Writing $\tilde{\lambda} = \rho \lambda$, $\tilde{s} = \rho s$, we have three densities ρ , $\tilde{\lambda}$, \tilde{s} , and three gauge potentials φ , μ , ν and Hamiltonian density

$$H = \rho \left(\frac{1}{2} |\boldsymbol{u}|^2 + \epsilon\right) = \rho \left\{\frac{1}{2} \left| \nabla \varphi + \left(\frac{\tilde{\lambda}}{\rho}\right) \nabla \mu + \left(\frac{\tilde{s}}{\rho} \nabla \nu\right) \right|^2 + \epsilon \left(\rho, \frac{\tilde{s}}{\rho}\right) \right\}$$
(2.12)

whose Euler derivatives are found by thermodynamic relation to be

$$egin{aligned} egin{aligned} egin{aligned} eta_{
ho}H = -m{u}(\lambda
abla\mu + s
abla
u) + rac{1}{2}|m{u}|^2 + h - sT, \ & \varepsilon_{\overline{\lambda}}H = -m{u}
abla\mu, \ & \varepsilon_{\overline{\lambda}}H = -m{u}
abla
u - T, \ & \varepsilon_{\overline{\lambda}}H = -m{v}\cdot(\rhom{u}), \ & \varepsilon_{\mu}H =
abla\cdot(\hat{\lambda}m{u}), \ & \varepsilon_{\mu}H =
abla\cdot(\tilde{\lambda}m{u}), \ & \varepsilon_{\nu}H =
abla\cdot(\tilde{s}m{u}). \end{aligned}$$

Here h is enthalpy and T is absolute temperature. Thus we get Hamilton's canonical equation for compressible fluid dynamics (2.10)

$$U_t = Js(H) \tag{2.14}$$

in which

$$J = \begin{pmatrix} 0 & E \\ -E & 0 \end{pmatrix}$$
.

Here U is a column vector $U = [\rho, \tilde{\lambda}, \tilde{s}, \varphi, \mu, \nu]^T$ and E is a 3×3 identity matrix. We write (2.14) in concrete form

$$\frac{\partial \rho}{\partial t} = \frac{-\partial H}{\partial \varphi} = -\nabla(\rho \boldsymbol{u}), \quad \frac{\partial \phi}{\partial t} = \frac{\partial H}{\partial \rho} = -\boldsymbol{u}(\lambda \nabla \mu + s \nabla \nu) + \frac{1}{2} |\boldsymbol{u}|^2 - sT,$$

$$\frac{\partial \tilde{\lambda}}{\partial t} = \frac{-\partial H}{\partial \mu} = -\nabla(\tilde{\lambda}\boldsymbol{u}), \quad \frac{\partial \mu}{\partial t} = \frac{\partial H}{\partial \tilde{\lambda}} = -\boldsymbol{u}\nabla\mu,$$

$$\frac{\partial \tilde{s}}{\partial t} = -\frac{\partial H}{\partial \nu} = -\nabla\cdot(\tilde{s}\boldsymbol{u}), \quad \frac{\partial \nu}{\partial t} = \frac{\partial H}{\partial s} = -\boldsymbol{u}\nabla\nu - T.$$
(2.15)

In the above ρ , $\tilde{\lambda}$, \tilde{s} are called densities, and φ , μ , ν "potentials".

Because the state variables fall into two groups: potentials (φ, μ, ν) and densities $(\rho, \tilde{\lambda}, \tilde{s})$, this description of compressible flow has the advantage of keeping the conservation of energy. Multiplying both sides of (2.14) by sH we get

$$(U_t, \varepsilon H) = (J \varepsilon H, \varepsilon H) = 0. \tag{2.16}$$

We know

$$\frac{dH}{dt} = (U_t, \ \varepsilon H) = 0. \tag{2.17}$$

First we rewrite (2.15) in form

$$U_t = -JA(U)U, \qquad (2.18)$$

where A(U) is a differential operator with respect to the space variable. Using the mean value theorem, we discretize (2.18)

$$\frac{H^{n+1}-H^n}{\Delta t} = \int_{t^n}^{t^{n+1}} \dot{U}A(U)Udt = \dot{U}A(U^*)U^* = \frac{U^{n+1}-U^n}{\Delta t} A(U^*)U^* = 0, \quad (2.19)$$

where $U^* \in (U(t^n), U(t^{n+1}))$.

Thus we get a scheme with exact conservation of energy

$$H^{n+1}-H^n=U^{n+1}A(U^*)U^*-U^nA(U^*)U^*=0. (2.20)$$

But in the real case, the mean value U^* is difficult to be defined. First we discuss the one-leg C-N difference scheme

$$\frac{U^{n+1}-U^n}{\Delta t}=-JA\left(\frac{U^{n+1}+U^n}{2}\right)\left(\frac{U^{n+1}+U^n}{2}\right),\qquad (2.21)$$

Multiplying (2.21) by $A\left(\frac{U_m^{n+1}+U_m^n}{2}\right)\frac{U_m^{n+1}+U_m^n}{2}$ on both sides and summing over all m we have

$$\left(\frac{\overline{U_m^{n+1}} - \overline{U_m^n}}{\Delta t}, A\left(\frac{\overline{U_m^{n+1}} + \overline{U_m^n}}{2}\right) \frac{\overline{U_m^{n+1}} + \overline{U_m^n}}{2}\right) = 0$$

or

$$\left(U_m^{n+1}, A\left(\frac{U_m^{n+1}+U_m^n}{2}\right)\frac{U_m^{n+1}+U_m^n}{2}\right) = \left(U_m^n, A\left(\frac{U_m^{n+1}+U_m^n}{2}\right)\frac{U_m^{n+1}+U_m^n}{2}\right).$$

We know

$$\frac{dH}{dt} = (\dot{U}A(U)U).$$

Using the trapezoid formula, we get

$$H^{n+1} = H^{n+1} \int_{t^n}^{t^{n+1}} \dot{U}A(U)Udt = H^n + \Delta t \dot{U}A\left(\frac{U^{n+1} + U^n}{2}\right) \left(\frac{U^{n+1} + U^n}{2}\right) + O(\Delta t^8).$$

Then

$$\begin{split} H^{n+1} &= H^n + (U^{n+1} - U^n) A \left(\frac{U^{n+1} + U^n}{2} \right) \frac{U^{n+1} + U^n}{2} + O(\Delta t^3), \\ H^n &= H^{n-1} + (U^n - U^{n-1}) A \left(\frac{U^n + U^{n-1}}{2} \right) \frac{U^n + U^{n-1}}{2} + O(\Delta t^3), \\ &\vdots \\ &\| H^{n+1} \| = \| H^0 \| + O(\Delta t^2). \end{split}$$

Equation (2.21) is nonlinear. We can apply the predictor-corrector procedure

$$U^* = U^n - \Delta t J A(U^*) U^n,$$

$$U^{n+1} = U^n - \Delta t J A(U^*) \frac{U^{n+1} + U^n}{2}.$$
(2.23)

Next, for (2.15) we can apply time staggered explicit schemes described in [2]. Here we propose a leap-frog scheme as distinguished from [2]

$$\frac{z^{n+1}-z^{n-1}}{2At} = -JA(z^n)z^n. (2.24)$$

This scheme also has

$$H^n = H^0 + O(\Delta t^2).$$

Scheme (2.21) is a canonical difference scheme, which will be Remark. discussed in a subsequent paper.

References

- Feng Kang, On difference schemes and symplectic geometry, Proceedings of the 1984 Beijing Symposium on Differential Geometry and Differential Equations, 42-58.
- O. Buneman, Compressible Flow Simulation Using Hamilton's Eqs. and Clebsch-type Vortex Parameters, Proc. 5th Int. Conf. on Numerical Methods in Fluid Dynamics, 103-106.