Journal of Computational Mathematics, Vol.13, No.1, 1995, 64–69.

ON STABILITY OF SYMPLECTIC ALGORITHMS*[1)]

Li Wang-yao
(*Computing Center, Academia Sinica, Beijing, China*)

Abstract

The stability of symplectic algorithms is discussed in this paper. There are following conclusions.

1. Symplectic Runge-Kutta methods and symplectic one-step methods with high order derivative are unconditionally critically stable for Hamiltonian systems. Only some of them are A-stable for non-Hamiltonian systems. The criterion of judging A-stability is given.

2. The hopscotch schemes are conditionally critically stable for Hamiltonian systems. Their stability regions are only a segment on the imaginary axis for non-Hamiltonian systems.

3. All linear symplectic multistep methods are conditionally critically stable except the trapezoidal formula which is unconditionally critically stable for Hamiltonian systems. Only the trapezoidal formula is A-stable, and others only have segments on the imaginary axis as their stability regions for non-Hamiltonian systems.

1. Fundamental Definitions

Lemma 1. *The solution of a linear ordinary differential equation with constant coefficient $\dot{Y} = AY$ is stable if all eigenvalues of A have nonpositive real parts and the eigenvalues with null real part are single roots of the minimal polynomial.*

The linear Hamiltonian system can be denoted as $\dot{Z} = JSZ$ where $Z = (\,pq)$, $J = (\,0 - EE0)$, and the Hamiltonian function $H(z) = z'sz2$.

Lemma 2. *The solutions of linear Hamiltonian systems are critically stable if all eigenvalues of JS have null real part and are single roots of the minimal polynomial.*

Definition 1. *When the model equation $\dot{Y} = AY$ is solved using a numerical method, the method is A-stable if its stability region involves the whole left half plane.*

Definition 2. *When the linear Hamiltonian system $\dot{Z} = JSZ$ is solved using a one-step method, the one-step method is critically stable if all eigenvalues of the amplification matrix have module 1 and are single roots of the minimal polynomial.*

---

* Received July 19, 1993.
1) The Project Supported by National Natural Science Foundation of China.

Definition 3. *When the linear Hamiltonian system $\dot{Z} = JSZ$ is solved using a multistep method, the multistep method is critically stable if all roots of the characteristic equation are on the unit circle and are single roots.*

2. The Stability of One-Step Symplectic Algorithms

When the one-step symplectic algorithms (such as symplectic Runge-Kutta methods, the one-step symplectic methods with higher order derivative) are used to solved the model equation $\dot{Y} = AY$, in most cases the characteristic equation always has the following form[1−2]:

$$\xi(\mu) = P(\mu)P(-\mu)$$

where $\mu = h\lambda$, λ stands for the eigenvalues of the matrix A and P is a polynomial with real coefficient.

Theorem 1. *The one-step method is unconditionally critically stable if the corresponding characteristic equation can be expressed as $\xi(\mu) = P(\mu)P(-\mu)$.*

Proof. When $\lambda = iy$, we have

$$\xi = P(\mu)P(-\mu) = P(ihy)P(-ihy) = P(ihy)P(\overline{ihy}) = P(ihy)\bar{P}(ihy)$$

and

$$\overline{\xi} = \bar{P}(ihy)\bar{P}(-ihy) = \bar{P}(ihy)P(ihy).$$

Therefore $\xi \cdot \overline{\xi} = 1$. The above relationship holds as long as λh is on the imaginary axis, so there is no restriction on h.

Theorem 2. *If all poles of $\xi(w)$ are on the right half plane, then the corresponding one-step symplectic method is A-stable.*

Proof. .Unconditional critical stability means $\xi = P(\mu)P(-\mu) = 1$ as long as $\mu = \lambda h = iyh$, where $-\infty < y < \infty$.

If all poles of ξ are on the right half plane, then ξ is an analytical function on the left half plane. According to the maximum module principle we have $\xi(\mu) < 1$ as long as $\mathrm{Re}(\mu) < 0$.

Example 1. The midpoint formula $y_{n+1} = y_n + hf(y_n + y_{n+1}2)$ and trapezoidal formula $y_{n+1} = y_n + h2(f(y_n) + f(y_{n+1}))$ have the same characteristic equation $\xi = 1 + \mu 1 - \mu$, so they are unconditionally critically stable and A-stable. The symplectic schemes, whose characteristic equations are diagonal Pade approximation, are the same (such as s-stage Runge-Kutta methods with order $2s + 2$).

Example 2. The composite symplectic schemes of order 4.[3]

$$\Big\{y_{n+\frac{1}{3}} = y_n + c_1 h2(f(y_n) + f(y_{n+\frac{1}{3}})), y_{n+\frac{2}{3}} = y_{n+\frac{1}{3}} + c_2 h2(f(y_{n+\frac{1}{3}}) + f(y_{n+\frac{2}{3}})), y_{n+1} = y_{n+\frac{2}{3}} + c_1 h2(f(y_{n+\frac{2}{3}}) + f$$

and

$$\Big\{y_{n+\frac{1}{3}} = y_n + c_1 hf\Big(y_n + y_{n+\frac{1}{3}}2\Big), y_{n+\frac{2}{3}} = y_{n+\frac{1}{3}} + c_2 hf\Big(y_{n+\frac{1}{3}} + y_{n+\frac{2}{3}}2\Big), y_{n+1} = y_{n+\frac{2}{3}} + c_1 hf\Big(y_{n+\frac{2}{3}} + y_{n+1}2\Big)$$

where $c_1 = 12 - 2^{\frac{1}{3}}$, $c_2 = -2^{\frac{1}{3}}2 - 2^{\frac{1}{3}}$, have a characteristic equation $\xi = \{(1+c_1\mu)(1+c_2\mu)(1+c_1\mu)\}\{(1-c_1\mu)(1-c_2\mu)(1-c_1\mu)\}^{-1}$ and a pole $2 - 2^{\frac{1}{3}} - 2^{\frac{1}{3}}$ which is on the left half plane, so they are not A-stable and have an unstability region around the point $2 - 2^{\frac{1}{3}} - 2^{\frac{1}{3}}$.

3. The Hopscotch Schemes for Separable Hamiltonian Systems[4−6]

The separable Hamiltonian systems extensively arise in astronomical mechanics, so research of the numerical methods for them is significant. Because the hopscotch schemes are explicit, they have important practical value. For separable linear Hamiltonian systems

$$ddt\,(\,pq) = (\,0 - uv0)\,(\,pq)\,,$$

where $u' = u,\ v' = v$, the characteristic equation of the coefficient matrix is

$$|\,\lambda Euv\lambda E| = |\lambda E + uv| = 0.$$

If $T^{-1}uvT = \mathrm{diag}(K_1, \cdots, K_n),\ K_i > 0$ and they are different from each other, then the eigenvalues of the coefficient matrix are $\lambda_i = \pm i\sqrt{k}$. It follows that the solutions of the separable linear Hamiltonian systems are critically stable. The fundamental form of a hopscotch scheme is

$$(\,p_{k+1}q_{k+1}) = \Big(\,I - huhvI - h^2uv\Big)\,(\,p_kq_k)\,.$$

The characteristic equation of the amplification matrix may be expressed as

$$\Big|\,(\lambda-1)Ehu - hv(\lambda-1)E + h^2uv\Big| = |\lambda^2E - \lambda(2E - h^2uv) + E| = 0.$$

We have $\lambda_i = 12(2 - h^2k_i \pm h\sqrt{k_i(h^2k_i - 4)})$. When $h^2k_i > 4$, the eigenvalues $\lambda_{i1}, \lambda_{i2}$ are a couple of real roots and $\lambda_{i1}\lambda_{i2} = 1$, so the method is unstable. When $h^2k_i < 4$, the eigenvalues λ_i are a couple of conjugate imaginary roots and have module 1, so the method is conditionally critically stable. The stability region of the method is shown in Fig.1 and Fig.2.

4. Multistep Symplectic Methods

Three classes of linear symplectic multistep methods are shown in [7].

1. Implicit linear symplectic k(even)-step methods of order $k+2$ (optimal methods). Some examples are as follows:

$l \quad lk = 2, y_{n+2} - y_n = h(2f_{n+1} - 13\nabla^2 f_{n+2})$ Milne-Simpson formula$k = 4, y_{n+4} - y_n = h(4f_{n+2} + 83\nabla^2 f_{n+3} + 1$

2. Explicit linear symplectic k(even)-step methods of order k. Some examples are below:

$l \quad lk = 2, y_{n+2} - y_n = 2hf_{n+1}$ leap-frog formula$k = 4, y_{n+4} - y_n = h(4f_{n+2} + 83\nabla^2 f_{n+3})k = 6, y_{n+6} - y_{n+5} + y_n$

3. Implicit linear symplectic k(odd)-step methods of order $k+1$. Some examples are as follows:

l $\quad lk = 1, y_{n+1} - y_n = h2(f_{n+1} + f_n)$ $\quad$ trapeizoidal formula, $k = 3, y_{n+3} - y_{n+2} + y_{n+1} - y_n = h12(5f_{n+3} + 7f_{n+2} +$

Theorem 3. *The linear symplectic multistep methods are critically stable.*

Proof. Theorem 3 in [7] shows that there exists an interval $D : [-hi, hi]$ on the imaginary axis of λh-plane such that all roots of the characteristic equation of linear symplectic multistep methods lie on the circle $\xi = 1$ as long as $\lambda h \in D$. This means the conclusion of our theorem holds.

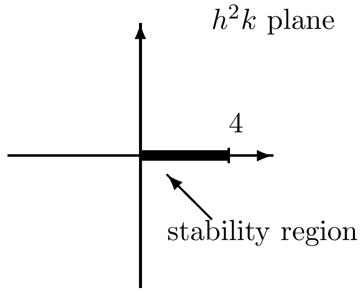

Fig. 1.

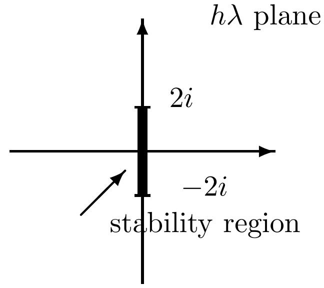

Fig. 2.

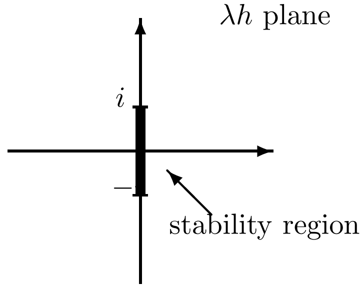

Fig. 3.

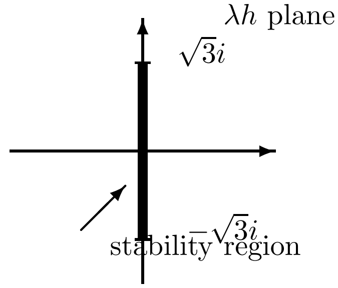

Fig. 4.

Theorem 4. *All linear symplectic multistep methods are conditionally critically stable except the trapezoidal formula and their stability regions are only segments symmetric to the null point. The trapezoidal formula is unconditionally critically stable and A-stable.*

Proof. First we prove that unconditionally critically stable linear multistep methods are A-stable. Let

$$r(z) = (1-z)^k \rho(1 + z1 - z) = \sum_{i=1}^{k} a_i z^i, \qquad s(z) = (1-z)^k \sigma(1 + z1 - z) = \sum_{i=1}^{k} b_i z^i.$$

If the linear multistep method $M(\rho, \sigma)$ is unconditionally critically stable, all the roots of the characteristic equation corresponding to infinity on the λh plane, are on the unit circle of ξ plane. i.e., all null points of $s(z)$ are on the imaginary axis of z-plane and $r(z)$ are the same (because all roots of $\rho(\xi)$ are on the unit circle). Because $r(z)$ and $s(z)$ are polynomials with real coefficients, their roots are conjugate. We conclude that $a_i \geq 0, b_i \geq 0$ $(i = 1, 2, \cdots, k)$. The multistep method $M(\rho, \sigma)$ is unconditionally critically stable, thus all roots of the characteristic equation corresponding to all points on the imaginary axis of λh-plane are on the imaginary axis of the z-plane and all poles of $r(z)s(z)$ are the same. If $\mathrm{Re}\, z \neq 0, r(z)s(z)$ is analytic and $\mathrm{Re}\, r(z)s(z) \neq 0$. It follows that $\mathrm{Re}(r(z)s(z))$ has the same sign when $\mathrm{Re} z > 0$. Since $a_i \geq 0$ and $b_i \geq 0$, we have $\mathrm{Re}(r(z)s(z)) > 0$, i.e., when $|\xi| > 0$, $\mathrm{Re}(\rho(\xi)\sigma(\xi)) > 0$. This means A-stability.

It has been shown by Dahlquist [8] that an explicit linear multistep method cannot be A-stable and the order of an A-stable linear multistep method cannot exceed 2. Therefore all linear symplectic multistep methods are conditionally critically stable except the trapezoidal formula and their stability regions are only segments symmetric to the null point.

Example. 1. The stability region of the leap-frog formula is shown in Fig.3.

2. The stability region of Milne-Simpson formula is shown in Fig.4.

References

[1] Feng Kang, On difference schemes and symplectic geometry, Proceedings of the 1984 Beijing symposium on differential geometry and differential equations.

[2] Feng Kang, On approximation by algebraic functions, Proceeding of the annual meeting on computational mathematics in Tianjing, China,1990.

[3] Qin Meng-zhao and Zhu Wen-jie, A note on stability of a three-stage difference scheme for ordinary differential equations, Computers Math. Applic.

[4] R. D. Ruth, An canonical integration technique, *IEEE Trans. Nucl. Sci.*, 30(1983), 2669–2671.

[5] H. Yoshida, Construction of higher order symplectic integrators, Phys. Letters A, 150, 1990, 262–265.

[6] Qin Meng-zhao, Wang Dao-liu and Zhang Mei-qing, Explicit symplectic difference schemes for separable Hamiltonian systems, *J. Comp. Math.*, 9:3(1991), 211–221.

[7] Li Wang-yao, Symplectic multistep methods for linear Hamiltonian systems, to appear.

[8] G. Dahlquist, A special stability problem for linear multistep methods, *BIT*, 3(1963), 27–43.