Symplectic Numerical Methods

Yousaf Habib

Supervisor : Prof. John Butcher

Hamiltonian mechanics is a reformulation of classical mechanics invented by Hamilton (1833). In Hamiltonian mechanics, the equations of motion are based on generalised co-ordinates q_i and generalised momenta p_i. The Hamiltonian H is a function of $\mathbf{p} = (p_1, p_2, , , , , p_n)$ and $\mathbf{q} = (q_1, q_2, , , , , q_n)$ and defines the differential equation system,

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \qquad \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \qquad i = 1, ..., n.$$

H usually corresponds to the total energy of the underlying mechanical system.
Let $\phi_H(t, t_0)$ denote the solution operator of the Hamiltonian system.

$$(\mathbf{p}, \mathbf{q}) = \phi_H(t, t_0)(\mathbf{p}_0, \mathbf{q}_0).$$

It is the property of Hamiltonian systems that ϕ_H is symplectic. This means that if $(\mathbf{p}_0, \mathbf{q}_0)$ on some domain Ω possess certain properties, then $(\mathbf{p}, \mathbf{q})$ retain those properties after the transformation through ϕ_H. Since symplecticness is a characteristic property of Hamiltonian systems in terms of their solutions, it is natural to look for numerical methods that share this property.
Pioneering work in this regard is due to Ruth (1983) and Feng Kang (1985). Later, Sanz-Serna (1988) and Suris (1988) systematically developed symplectic Runge-Kutta methods. Their idea is based on features of algebraic stability introduced, in connection with stiff systems, by Burrage and Butcher (1979) and Crouzeix (1979).
A Runge-Kutta method of order s is symplectic if the coefficients $[a, b, c]$ of the Runge-Kutta method satisfy

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \qquad i, j = 1, ..., s.$$

The order conditions for classical Runge-Kutta methods consists of a complex system of algebraic equations. To study order conditions, the idea of rooted trees is usually employed as developed by Butcher (1963). Each rooted tree corresponds to an order condition for an RK method. It is a remarkable property of symplectic Runge-Kutta methods that if the order condition for one rooted tree is satisfied then the same is true for *all* rooted trees which have the same underlying tree. Furthermore, for some trees, known as "superfluous trees" the order conditions are satisfied automatically.
Another way of constructing symplectic Runge-Kutta methods is through the Vandermonde transformation of the matrix given by the symplectic condition above. The idea is to pre and post multiply the matrix of symplectic condition by a Vandermonde matrix and get the order conditions for a particular symplectic Runge-Kutta method.