Journal of Computational Mathematics, Vol.18, No.1, 2000, 61–68.

A SIMPLE WAY CONSTRUCTING SYMPLECTIC RUNGE-KUTTA METHODS*

Geng Sun
(*Institute of Mathematics, Academia Sinica, Beijing 100080, China*)

Abstract

With the help of symplecticity conditions of Partitioned Runge-Kutta methods, a simple way constructing symplectic methods is derived. Examples including several classes of high order symplectic Runge-Kutta methods are given, and showed up the relationship between existing high order Runge-Kutta methods.

Key words: Symplecticity condition, Partitioned Runge-Kutta method.

1. Introduction and Preliminaries

Let Ω be a demain in the oriented Euclidean space $\mathbb{R}^{2d}$ of point $(p,q)=((p_1,\cdots,p_d)^T,(q_1,\cdots,q_d)^T)$. If $H(p,q)$ is a sufficiently smooth real function defined in Ω, then the Hamiltonian system of differential equations with Hamiltonian $H(p,q)$ is given by

$$\frac{dp_i}{dt}=-\frac{\partial H}{\partial q_i}=:f_i(p,q),\quad \frac{dq_i}{dt}=\frac{\partial H}{\partial p_i}=:g_i(p,q), 1\le i\le d. \tag{1.1}$$

The integer d is called the number of degrees of freedom and Ω is the phase space. Here we assume that all Hamiltonians considered are autonomous, i.e., time- independent.

Definition 1.1. *A one-step method is called symplectic if, as applied to the Hamiltonian system* $(1,1)$, *the underlying formula generating numerical solutions* (p^{n+1},q^{n+1}) *is a symplectic transformation, that is,*

$$\frac{\partial(p^{n+1},q^{n+1})^T}{\partial(p^n,q^n)}J\frac{\partial(p^{n+1},q^{n+1})}{\partial(p^n,q^n)}=J,\quad \forall(p^n,q^n)\in\Omega, \tag{1.2}$$

Where $J=\begin{pmatrix}0 & I_d\\ -I_d & 0\end{pmatrix}$ *is the standard symplectic matrix.*

Definition 1.2. *One step of an s-stage Partitioned Runge-Kutta (PRK) method with stepsize h and initial values* (p^n,q^n) *applied to (1.1) reads*

$$P_i=p^n+h\sum_{j=1}^{s}a_{ij}F_j(P_j,Q_j),\quad Q_i=q^n+h\sum_{j=1}^{s}\overline{a}_{ij}G_j(P_j,Q_j), \tag{1.3a}$$

* Received October 16, 1996.

$$p^{n+1} = p^n + h\sum_{i=1}^{s} b_i F_i(P_i, Q_i), \quad q^{n+1} = q^n + h\sum_{i=1}^{s} \overline{b}_i G_i(P_i, Q_i), \tag{1.3b}$$

Where a_{ij}, b_i *and* $\overline{a}_{ij}, \overline{b}_i$ *represent two different Runge-Kutta schemes,* $F = (f_1, f_2, \cdots, f_d)^T$, $G = (g_1, g_2, \cdots, g_d)^T$.

Definition 1.3. *The local error of a PRK method (1.3) is defined by*

$$\delta_{p_h}(t_n) = p^{n+1} - p(t_n + h), \quad \delta_{q_h}(t_n) = q^{n+1} - q(t_n + h)$$

Where $(p(t), q(t))$ *is the exact solutions of (1.1) possing through* (p^n, q^n) *at* t_n.

By definition 1.1, an s-stage symplectic PRK method can be characterized as follows:[7],[9],[12]

Theorem 1.4. *If the coefficients of an s-stage PRK method (1.3) satisfy the relation*

$$b_i = \overline{b}_i \quad for \quad i = 1, \cdots, s \tag{1.4a}$$

$$b_i\overline{a}_{ij} + \overline{b}_j a_{ji} - b_i\overline{b}_j = 0 \quad for \quad i, j = 1, \cdots, s, \tag{1.4b}$$

then the PRK method is symplectic.

Remark 1. Symplectic Runge-Kutta methods are a special case of symplectic PRK methods with coefficients $\overline{a}_{ij} = a_{ij}, i, j = 1, \cdots, s$.

Starting from a known s-stage RK method with $b_i \neq 0 (i = 1, \cdots, s)$, an s-stage symplectic PRK method can be defined uniquely as follows:[9]

Theorem 1.5. *Suppose that an s-stage RK method with coefficients $a_{ij}, b_i \neq 0$ and distinct c_i, satisfies the following simplifying assumptions*

$$B(p): \sum_{i=1}^{s} b_i c_i^{k-1} = \frac{1}{k} \quad for \quad k = 1, 2, \cdots, p,$$
$$C(\eta): \sum_{j=1}^{s} a_{ij} c_j^{k-1} = \frac{c_i^k}{k} \quad for \quad i = 1, \cdots, s, k = 1, \cdots, \eta,$$
$$D(\zeta): \sum_{i=1}^{s} b_i c_i^{k-1} a_{ij} = \frac{b_j}{k}(1 - c_j^k) \quad for \quad j = 1, \cdots, s, k = 1, \cdots, \zeta,$$

then the s-stage PRK method with coefficients $a_{ij}, \overline{b}_i = b_i, \overline{c}_i = c_i$ and $\overline{a}_{ij} = b_j(1 - a_{ji}/b_i)$ is symplectic and satisfies

$$\delta_{p_h}(t_n) = O(h^{r+1}), \quad \delta_{q_h}(t_n) = O(h^{r+1}),$$

i.e., at least, order $r = \min(p, 2\eta + 2, 2\zeta + 2, \eta + \zeta + 1)$.

Remark 2. By using the W-transformation of Hairer and Wanner[5] it can be shown that the RK method with coefficients $\overline{a}_{ij} = b_j(1 - a_{ji}/b_i), b_i$ and c_i satisfies $B(p), C(\zeta)$ and $D(\eta)$.