Journal of Computational Mathematics, Vol.18, No.6, 2000, 645–656.

ORDER PROPERTIES AND CONSTRUCTION OF SYMPLECTIC RUNGE-KUTTA METHODS*1)

Shou-fu Li
(*Institute for Computational and Applied Mathematics, Xiangtan University, Xiangtan 411105, China*)

Abstract

The main results of this paper are as follows: (1) Suppose an s stage Runge-Kutta method is consistent, irreducible, non-confluent and symplectic. Then this method is of order at least $2p+l(1 \le p \le s-1)$ provided that the simplifying conditions $C(p)$ (or $D(p)$ with non-zero weights) and $B(2p+l)$ hold, where $l = 0,1,2$. (2) Suppose an s stage Runge-Kutta method is consistent, irreducible and non-confluent, and satisfies the simplifying conditions $C(p)$ and $D(p)$ with $0 < p \le s$. Then this method is symplectic if and only if either $p = s$ or the nonlinear stability matrix M of the method has an $(s-p)\times(s-p)$ chief submatrix $\hat{M} = 0$. (3) Using the results (1) and (2) as bases, we present a general approach for the construction of symplectic Runge-Kutta methods, and a software has been designed, by means of which, the coefficients of s stage symplectic Runge-Kutta methods satisfying $C(p), D(p)$ and $B(2p+l)$ can be easily computed, where $1 \le p \le s, 0 \le l \le 2, s \le 2p+l \le 2s$.

Key words: Numerical analysis, Symplectic Runge-Kutta methods, Simplifying conditions, Order results.

1. Introduction

For a given s stage Runge-Kutta method

$$\begin{array}{c|c} \mu & A \\ \hline & \gamma^T \end{array} \tag{1.1}$$

with $A = [a_{ij}], \mu = [\mu_1, \mu_2, \cdots, \mu_s]^T$ and $\gamma = [\gamma_1, \gamma_2, \cdots, \gamma_s]^T \neq 0$, we introduce the following simplifying conditions as in Butcher [1]

$$\begin{cases} B(p): \ i\gamma^T\mu^{i-1} = 1, & i = 1,2,\cdots,p, \\ C(p): \ iA\mu^{i-1} = \mu^i, & i = 1,2,\cdots,p, \\ D(p): \ iA^T\mathrm{diag}(\gamma)\mu^{i-1} = \gamma - \mathrm{diag}(\gamma)\mu^i, & i = 1,2,\cdots,p, \end{cases}$$

and make the notational convension

$$\begin{cases} M = [m_{ij}] := \mathrm{diag}(\gamma)A + A^T\mathrm{diag}(\gamma) - \gamma\gamma^T, \\ U_{lm} := [\rho_l(\mu), \rho_{l+1}(\mu), \cdots, \rho_m(\mu)], \\ V_{lm} := [\rho'_l(\mu), \rho'_{l+1}(\mu), \cdots, \rho'_m(\mu)], \\ B_{lm} := [b_l, b_{l+1}, \cdots, b_m], \ \ C_{lm} := [c_l, c_{l+1}, \cdots, c_m], \\ D_{lm} := [d_l, d_{l+1}, \cdots, d_m], \end{cases}$$

* Received February 15, 1998.
1)Project supported by the National Natural Science Foundation of China.

where $l \leq m, \rho_i(x), i = 1, 2, 3, \cdots$, are arbitrarily given i-th polynomials with the property that $\rho_i(0) = 0$,

$\rho_i(\nu) := [\rho_i(\nu_1), \rho_i(\nu_2), \cdots, \rho_i(\nu_N)]^T$,
$\rho_i'(\nu) := [\rho_i'(\nu_1), \rho_i'(\nu_2), \cdots, \rho_i'(\nu_N)]^T$, for $\nu = [\nu_1, \nu_2, \cdots, \nu_N]^T \in \mathbf{R}^N$,
$b_i := \gamma^T \rho_i'(\mu) - \rho_i(1)$,
$c_i := A\rho_i'(\mu) - \rho_i(\mu)$,
$d_i := A^T \mathrm{diag}(\gamma)\rho_i'(\mu) - \gamma\rho_i(1) + \mathrm{diag}(\gamma)\rho_i(\mu)$, for $i = 1, 2, 3, \cdots$.

Note that $B(p), C(p)$ and $D(p)$ are equivalent to $B_{1,p} = 0, C_{1,p} = 0$ and $D_{1,p} = 0$ respectively. We shall always denote $B_{1,s}, C_{1,s}, D_{1,s}$ and $V_{1,s}$ by B, C, D and V respectively, and frequently refer the following two theorems in the sequel.

Theorem 1.1. *(cf. Butcher* [1]*)* $B(p), C(\eta)$ *and* $D(\xi)$ *with* $\min\{\eta+\xi+1, 2\eta+2\} \geq p$ *implies that the method has order at least* p.

Theorem 1.2. *(cf. Sanz-Serna* [2] *and Lasagni* [3]*) An irreducible Runge-Kutta method is symplectic if and only if* $M = 0$.

2. Order Properties

Lemma 2.1. *Suppose* $B(q)$ *holds. Then we have*

$$d_i^T \rho_j'(\mu) - c_j^T \mathrm{diag}(\gamma)\rho_i'(\mu) = 0 \qquad \textit{for} \quad i + j \leq q. \tag{2.1}$$

Lemma 2.2. *Suppose that*

$$d_{i_k}^T \rho_{j_k}'(\mu) - c_{j_k}^T \mathrm{diag}(\gamma)\rho_{i_k}'(\mu) = 0, \ \ i_k + j_k = k \quad \textit{for} \quad k = 2, 3, \cdots, q. \tag{2.2}$$

Then $B(1)$ implies $B(q)$.

Corollary 2.3. *The following implications hold.*

(1) $B(q)$ *and* $C(p) \Longrightarrow d_i^T \rho_j'(\mu) = 0$ *for* $j \leq p,\ i + j \leq q$,
(2) $B(q)$ *and* $D(p) \Longrightarrow c_i^T \mathrm{diag}(\gamma)\rho_j'(\mu) = 0$ *for* $j \leq p,\ i + j \leq q$,
(3) $B(p + q)$ *and* $C(p) \Longrightarrow D_{1,q}^T V_{1,p} = 0$,
(4) $B(p + q)$ *and* $D(p) \Longrightarrow C_{1,q}^T \mathrm{diag}(\gamma) V_{1,p} = 0$,
(5) $B(1)$, $C_{1,p}^T \mathrm{diag}(\gamma) V_{1,q} = 0$ *and* $D_{1,q}^T V_{1,p} = 0 \Longrightarrow B(p + q)$,
(6) $B(1)$, $C(p)$ *and* $D(q) \Longrightarrow B(p + q)$.

Proof. Corollary 2.3 follows directly from Lemmas 2.1 and 2.2. Lemmas 2.1 and 2.2 can be easily verified by using the following identity and simple induction.

$$d_i^T \rho_j'(\mu) - c_j^T \mathrm{diag}(\gamma)\rho_i'(\mu) = b_{i+j}^{(i,j)} - \rho_i(1) b_j, \quad i, j = 1, 2, 3, \cdots, \tag{2.3}$$

where

$$b_{i+j}^{(i,j)} = \gamma^T \frac{d}{dx}(\rho_i(x)\rho_j(x))_{x=\mu} - \rho_i(1)\rho_j(1).$$

Theorem 2.4. *Suppose the method (1.1) is irreducible and symplectic. Then we have the following implications for* $1 \leq p \leq s$.

(1) $B(1)$ *and* $C(p) \Longrightarrow B(2p)$;
(2) $B(1)$ *and* $D(p) \Longrightarrow B(2p)$;
(3) $B(1)$ *and* $C(p)$ *with distinct abscissae* $\Longrightarrow B(2p)$ *and* $D(p)$;
(4) $B(1)$ *and* $D(p)$ *with distinct abscissae and nonzero weights* $\Longrightarrow B(2p)$ *and* $C(p)$;
(5) $C(1)$ *and* $D(p)$ *with distinct abscissae* $\Longrightarrow B(2p)$;
(6) $D(1)$ *and* $C(p)$ *with distinct abscissae* $\Longrightarrow B(2p)$ *and* $D(p)$;