A class of symplectic partitioned Runge–Kutta methods

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ABSTRACT

This paper deals with some relevant properties of Runge–Kutta (RK) methods and symplectic partitioned Runge–Kutta (PRK) methods. First, it is shown that the arithmetic mean of a RK method and its adjoint counterpart is symmetric. Second, the symplectic adjoint method is introduced and a simple way to construct symplectic PRK methods via the symplectic adjoint method is provided. Some relevant properties of the adjoint method and the symplectic adjoint method are discussed. Third, a class of symplectic PRK methods are proposed based on Radau IIA, Radau IIB and their adjoint methods. The structure of the PRK methods is similar to that of Lobatto IIIA–IIIB pairs and is of block forms. Finally, some examples of symplectic partitioned Runge–Kutta methods are presented.

1. Introduction

Let Ω be a domain in the Euclidean space ℝ 2d with coordinates (p, q) = (p1, . . . , p d; q1, . . . , q d). Let H(p, q) be a sufficiently smooth real function defined on Ω. Consider the following Hamiltonian system of differential equations of d degrees of freedom:

\[
\frac{dp_i}{dt} = - \frac{\partial H}{\partial q_i} =: f_i(p, q), \quad \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} =: g_i(p, q), \quad i = 1, 2, \ldots, d. \tag{1.1}
\]

Consider a partitioned Runge–Kutta (PRK) method with tableaux

\[
\begin{pmatrix} c \\ A \\ \bar{c} \\ \bar{A} \end{pmatrix}, \quad \begin{pmatrix} b^T \\ b^T \end{pmatrix}, \quad c = (c_1, \ldots, c_s)^T, \quad \bar{c} = (\bar{c}_1, \ldots, \bar{c}_s)^T, \quad A = (a_{ij}), \quad \bar{A} = (\bar{a}_{ij}) \text{ are } s \times s \text{ matrices, } \end{pmatrix}
\]

where A = (a ij) and \(\bar{A} = (\bar{a}_{ij})\) are s × s matrices, c = (c 1, . . . , c s)^T, b = (b 1, . . . , b s)^T, \(\bar{c} = (\bar{c}_1, \ldots, \bar{c}_s)^T\) and \(\bar{b} = (\bar{b}_1, \ldots, \bar{b}_s)^T\) are s-dimensional vectors.

Application of the PRK method (1.2) to the systems (1.1) leads to the following numerical scheme:

\[
P_i = p^n + h \sum_{j=1}^{s} a_{ij} f(P_j, Q_j), \quad Q_i = q^n + h \sum_{j=1}^{s} \bar{a}_{ij} g(P_j, Q_j), \quad i = 1, \ldots, s, \tag{1.3a}
\]

\[
p^{n+1} = p^n + h \sum_{i=1}^{s} b_i f(P_i, Q_i), \quad q^{n+1} = q^n + h \sum_{i=1}^{s} \bar{b}_i g(P_i, Q_i). \tag{1.3b}
\]

The following theorem gives a characterization of symplectic partitioned Runge–Kutta methods.
Theorem 1.1 ([1–3]). If the coefficients of (1.3) satisfy
\begin{equation}
\begin{aligned}
b_i \bar{a}_{ij} + \bar{b}_j a_{ij} - b_i \bar{b}_j &= 0, \quad i, j = 1, \ldots, s, \\
b_i &= \bar{b}_i, \quad i = 1, \ldots, s,
\end{aligned}
\end{equation}
that is,
\begin{equation}
\bar{B} \Lambda + \Lambda^T B - bb^T = 0,
\end{equation}
then the method (1.3) is symplectic, where \( B = \text{diag}(b_1, b_2, \ldots, b_s) \).

For an \( s \)-stage RK method \((A, b, c)\) with distinct abscissae \( c_i \), we consider the following transformation (see [4–6])
\begin{equation}
X = W^T BAW,
\end{equation}
where
\begin{equation}
W = (P_0(c), P_1(c), \ldots, P_{s-1}(c))
\end{equation}
and the normalized shifted Legendre polynomials are defined by
\begin{equation}
P_k(x) = \frac{\sqrt{2k+1}}{k!} \frac{d^k}{dx^k} (x^k(x-1)^k) = \sqrt{2k+1} \sum_{i=0}^{k} (-1)^{k+i} \binom{k+i}{i} x^i, \quad k = 0, 1, \ldots.
\end{equation}

Using the transformation (1.6), we can rewrite Theorem 1.1 as the following form.

Theorem 1.2 ([2]). If an \( s \)-stage PRK method generated by \((A, \tilde{A}, b, c)\) with distinct abscissae \( c_i \) and \( b_i \neq 0 \) \((i = 1, \ldots, s)\) satisfies
\begin{equation}
W^T \tilde{M} W = \bar{X} + X^T - e_1 e_1^T = 0,
\end{equation}
then the PRK method is symplectic, where
\begin{equation}
\tilde{M} = B \Lambda + \Lambda^T B - bb^T, \quad \bar{X} = W^T B \Lambda W,
\end{equation}
\( e_1 = (1, 0, \ldots, 0)^T \in \mathbb{R}^s \).

It is very easy to construct symplectic PRK methods starting from a known RK method with \( b_i \neq 0 \) \((i = 1, \ldots, s)\) as follows.

Theorem 1.3 ([2,7]). Suppose that an \( s \)-stage RK method generated by \((A, b, c)\) with distinct abscissae \( c_i \) and \( b_i \neq 0 \) \((i = 1, \ldots, s)\) satisfies the order conditions \( B(p), C(\eta) \) and \( D(\zeta) \), then the PRK method generated by the coefficients \((a_{ij}, \tilde{a}_{ij} = b_j(1 - \frac{a_{ij}}{b_i}), b_i, c_i)\) is symplectic and of order \( q = \min(p, 2\eta + 2, 2\zeta + 2, \eta + \zeta + 1) \).

2. Adjoint methods and symplectic adjoint methods

For an \( s \)-stage RK method \((A, b, c)\) with distinct abscissae \( c_i \) and \( b_i \neq 0 \) \((i = 1, \ldots, s)\), by condition (1.4), we can obtain an associated RK method \((\tilde{A}, b, c)\) with
\begin{equation}
\tilde{a}_{ij} = b_j \left(1 - \frac{a_{ij}}{b_i}\right), \quad i, j = 1, \ldots, s.
\end{equation}

Definition 2.1. An RK method \((\tilde{A}, b, c)\) defined by (2.1) is called a symplectic adjoint method of the underlying RK method \((A, b, c)\).

Definition 2.2 ([8–10]). An RK method \((A^*, b^*, c^*)\) defined by
\begin{equation}
A^* = \tilde{P}(eb^T - A)\tilde{P}^T, \quad b^* = \tilde{P} b, \quad c^* = e - \tilde{P} c,
\end{equation}
is called an adjoint method of the underlying RK method \((A, b, c)\), where \(e = (1, \ldots, 1)^T \in \mathbb{R}^s\), \(\tilde{P}\) is a permutation matrix, the \((i, j)\)-th element of the matrix is the Kronecker \(\delta_{i+s+1-j}\).

Let \(\Phi\) denote a given RK method \((A, b, c)\), \(\Phi^*\) the adjoint method \((A^*, b^*, c^*)\) of \(\Phi\) and \(\Phi^{sym}\) the symplectic adjoint method \((\tilde{A}, b, c)\) of \(\Phi\).
Definition 2.3 ([8–10]). An RK method $\Phi$ is called symmetric if $\Phi^* = \Phi$, i.e.,

$$A = \tilde{\Phi}(eb^T - A)\tilde{\Phi}^T, \quad b = \tilde{\Phi}b, \quad c = e - \tilde{\Phi}c.$$ 

Suppose that $c_i$ ($i = 1, \ldots, s$) are distinct and $b_i \neq 0$. $\Phi^*$ and $\tilde{\Phi}^*s$ have the following properties.

Proposition 2.4. 1. $(\tilde{\Phi}^*)^s = \Phi$.

2. If $\tilde{\Phi}^s = \Phi$, then $\Phi$ is symplectic. In other words, the symplectic RK method is a special case of symplectic PRK with $\tilde{A} = A$. (See [2]).

3. $\Phi^s$ is symmetric if and only if $\Phi$ is symmetric.

Proof. The result follows from Theorem 2.4 of [6] and Theorem 2.1b of [2].

4. Suppose that $\Phi$ satisfies the simplifying assumptions $B(p), C(\eta)$, and $D(\xi)$; then $\tilde{\Phi}^s$ satisfies the simplifying assumptions $B(p), C(\zeta)$ and $D(\eta)$.

Proof. The result follows from the symplectic condition (1.7) and Theorem 4.5.11 of [5].

5. If $\Phi$ satisfies the simplifying assumptions $B(p), C(\eta)$, and $D(\xi)$, then the arithmetic mean of the coefficients of $\Phi$ and $\Phi^s$, i.e., the RK method $(\frac{1}{2}(A + A), b, c)$, is symplectic and satisfies at least $B(p), C(\xi)$ and $D(\xi)$, where $\xi = \min(\eta, \xi)$. (See [11].)

Proposition 2.5. 1. $\Phi^* = \Phi$.

2. $\Phi^*$ has the same order as $\Phi$. If the principal error term of $\Phi$ is $d_{p+1}(t)h^{p+1}$, then that of $\Phi^*$ is $-d_{p+1}(t)h^{p+1}$. (See [8]).

3. Both of the composition methods $\Phi^* (\frac{1}{2}) \circ \Phi (\frac{1}{2})$ and $\Phi (\frac{1}{2}) \circ \Phi^* (\frac{1}{2})$ are symmetric. In addition, if $\Phi(h)$ is of order $p$ with odd $p$, then both of the composition methods $\Phi^* (\frac{1}{2}) \circ \Phi (\frac{1}{2})$ and $\Phi (\frac{1}{2}) \circ \Phi^* (\frac{1}{2})$ are of order $p + 1$. (See p. 41 of [12]).

4. (a) $\Phi^*$ is symplectic if and only if $\Phi$ is symplectic.

(b) Composition methods $\Phi^* (\frac{1}{2}) \circ \Phi (\frac{1}{2})$ and $\Phi (\frac{1}{2}) \circ \Phi^* (\frac{1}{2})$ are symplectic if $\Phi$ is symplectic.

Proof. The results follow immediately from the definitions of symmetry and symplecticity.

5. The pair of Radau I-type and Radau II-type:

(a) If an $s$-stage Radau IA method with order $2s - 1$ and distinct $c_i$, satisfies the simplifying assumptions $B(2s - 1), C(s)$ and $D(s - 1)$, then its adjoint method is an $s$-stage Radau I-type method with order $2s - 1$ and distinct $c^*_i = 1 - c_{s+1-i}$ and satisfies the simplifying assumptions $B(2s - 1), C(s)$ and $D(s - 1)$.

(b) If an $s$-stage Radau IA method with order $2s - 1$ and distinct $c_i$ satisfies the simplifying assumptions $B(2s - 1), C(s - 1)$ and $D(s)$, then its adjoint method is an $s$-stage Radau II-type method with order $2s - 1$ and distinct $c^*_i = 1 - c_{s+1-i}$ and satisfies the simplifying assumptions $B(2s - 1), C(s - 1)$ and $D(s)$.

Proposition 2.6. The arithmetic mean of $\Phi$ and $\Phi^*$ is symmetric, that is, the RK method $(\frac{\Phi + \Phi^*}{2}, \frac{b + b^*}{2}, \frac{c + c^*}{2})$ is symmetric.

Proof. The result follows immediately from (2.2) and the definition of symmetry. $\square$

Remark 2.7. Proposition 2.6 tells us a simple way to construct symmetric RK methods.

3. Construction of a class of symplectic PRK methods

For simplicity, we introduce the following notations which are used to denote the specific RK methods.

$\Phi_{RIA}$ or $(A_i, b_i, c_i)$: $s$-stage Radau IA method.

$\Phi_{RIA}$ or $(A_{IA}, b_{IA}, c_{IA})$: $s$-stage Radau IA method.

$\Phi_{RIA}^*$ or $(A_{IA}^*, b_{IA}^*, c_{IA}^*)$: adjoint method of $\Phi_{RIA}$.

$\Phi_{RIA}^{*s}$ or $(A_{IA}^{*s}, b_{IA}^{*s}, c_{IA}^{*s})$: adjoint method of $\Phi_{RIA}$.

$\Phi_{RIA}^*$ or $(\tilde{A}_{IA}, \tilde{b}_{IA}, \tilde{c}_{IA})$: symplectic adjoint method of $\Phi_{RIA}$.

$\Phi_{RIA}^{*s}$ or $(\tilde{A}_{IA}^{*s}, \tilde{b}_{IA}^{*s}, \tilde{c}_{IA}^{*s})$: symplectic adjoint method of $\Phi_{RIA}$.

It is well known that $\Phi_{RIA}$ and $\Phi_{RIA}^*$ have the same transformation matrix (1.6) (see [6])

$$X = \begin{pmatrix}
\frac{1}{2} & -\xi_1 \\
\xi_1 & 0 & -\xi_2 \\
\xi_2 & \ddots & \ddots \\
\vdots & \ddots & 0 & -\xi_{s-1} \\
\xi_{s-1} & & & 1 \\
\frac{1}{4s - 1} & & & \\
\end{pmatrix}$$

(3.1)
where $\xi_k = \frac{1}{2\sqrt{4k^2-1}}$, $k = 1, \ldots, s - 1$. It is easy to verify that the adjoint methods $\Phi^*_{RIA_n}$ and $\Phi^*_{RIA_s}$ have the same transformation matrix

$$
\begin{pmatrix}
\frac{1}{2} & -\xi_1 \\
\xi_1 & 0 & -\xi_2 \\
& \ddots & \ddots \\
& & \xi_{s-1} & 0 & -\xi_s \\
& & & \xi_s & -\frac{1}{4s-1}
\end{pmatrix}
$$

(3.2)

and (3.2) is also the transformation matrix of the symplectic adjoint methods $\bar{\Phi}_{RIA_n}^*$ and $\bar{\Phi}_{RIA_s}^*$. Matrices (3.1) and (3.2) play important roles in deriving the main results of this paper.

**Definition 3.1.** $\bar{\Phi}_{RIA_n}^*$ and $\bar{\Phi}_{RIA_s}^*$ are called Radau IC-type method and Radau IIC-type method, respectively.

**Theorem 3.2.**
1. $\Phi_{RIA_n}^*$ satisfies $c_1^* = 0$, $a_{ij}^* = 0$ $(j = 1, \ldots, s)$ and

$$
\Phi_{RIA_n}^* = \bar{\Phi}_{RIA_n}^*.
$$

In other words, the adjoint method of an s-stage Radau IIA method is an s-stage Radau IC-type method.

2. $\Phi_{RIA_s}^*$ satisfies $c_1^* = 1$, $a_{ij}^* = 0$ $(i = 1, \ldots, s)$ and

$$
\Phi_{RIA_s}^* = \bar{\Phi}_{RIA_s}^*.
$$

In other words, the adjoint method of an s-stage Radau IAA method is an s-stage Radau IIC-type method.

**Proof.**
1. $a_{ij}^* = 0$ $(j = 1, \ldots, s)$ follows from the fact that $\Phi_{RIA_n}$ satisfies $a_{ij} = b_j$ $(j = 1, \ldots, s)$. The relationship between the Radau IA methods and the Radau IAA methods given in Proposition 2.5 and (3.2) imply that (3.3) holds.

2. The proof is similar to that of the first part of the theorem. $\square$

Based on the Radau IA methods, the Radau IIA methods and their adjoint methods, we will construct composition methods and present their properties.

Composition methods $\Phi_{RIA_n}(h/2) \circ \Phi_{RIA_n}^*(h/2)$ and $\Phi_{RIA_s}(h/2) \circ \Phi_{RIA_s}^*(h/2)$ are all 2s-stage Runge–Kutta methods. Butcher’s tableaux of $\Phi_{RIA_n}(h/2) \circ \Phi_{RIA_n}^*(h/2)$ and $\Phi_{RIA_s}(h/2) \circ \Phi_{RIA_s}^*(h/2)$ are as given in Tables 1 and 2.

**Theorem 3.3.**
1. $\Phi_{RIA_n}(h/2) \circ \Phi_{RIA_n}^*(h/2) = \Phi_{RIA_n}(h/2) \circ \bar{\Phi}_{RIA_n}^*(h/2)$ is a symmetric and A-stable block method with order 2s. The coefficients of the block method satisfy

$$
a_{11} = b_1, \quad a_{ij} = b_j, \quad j = 1, \ldots, s.
$$

(3.5)

Therefore, the structure of the block method is the same as that of the Lobatto IIIA method in the sense of (3.5).

2. $\Phi_{RIA_s}(h/2) \circ \Phi_{RIA_s}^*(h/2) = \bar{\Phi}_{RIA_s}^*(h/2) \circ \Phi_{RIA_s}(h/2)$ is a symmetric and A-stable block method with order 2s. The coefficients of the block method satisfy

$$
a_{11} = b_1, \quad a_{ii} = 0, \quad i = 1, \ldots, s.
$$

(3.6)

Therefore, the structure of the block method is the same as that of Lobatto IIIB method in the sense of (3.6).
The PRK methods are to be discussed. This is our future work. Theorem 3.4 tells us a new way to construct symplectic PRK methods. It is clear that the structure of the abscissae. It is easy to verify that \( \Phi \) proof. It follows from Tables 1 and 2 that \( \Phi \) pair satisfies the condition (1.4). Therefore, the partitioned Runge–Kutta method composed of \( \Phi \) and \( \Phi \) is symplectic.

Remark 3.5. Theorem 3.4 tells us a new way to construct symplectic PRK methods. It is clear that the structure of the proposed symplectic PRK methods is similar to that of Lobatto IIIA–IIIB pairs and is of block forms. The other properties of the PRK methods are to be discussed. This is our future work.

4. Examples

Now we present examples of symplectic block methods based on the composition methods, \( \Phi \) and \( \Phi \) with \( s = 1, 2, 3 \) are listed below.

\[
\begin{array}{cccccc}
1. & s = 1, & & & & \\
 & 0 & 1 & 2 & 0 & 0 \\
 & 0 & 1 & 2 & 0 & 0 \\
& & & & & \\
2. & s = 2, & & & & \\
 & 0 & 1 & 2 & 0 & 0 \\
 & 0 & 1 & 2 & 0 & 0 \\
& & & & & \\
3. & s = 3, & & & & \\
 & 0 & 1 & 2 & 0 & 0 \\
 & 0 & 1 & 2 & 0 & 0 \\
& & & & & \\
\end{array}
\]

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