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SYMPLECTIC PARTITIONED RUNGE-KUTTA METHODS*[1)]

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

Abstract

For partitioned Runge-Kutta methods, in the integration of Hamiltonian systems, a condition for symplecticness and its characterization which is based on the W-transformation of Hairer and Wanner are presented. Examples for partitioned Runge-Kutta methods which satisfy the symplecticness condition are given. A special class of symplectic partitioned Runge-Kutta methods is constructed.

1. Introduction

Let Ω be a domain (i.e. a non-empty, open, simply connected set) in the oriented Euclidean space $I\!R^{2d}$ of the point $(p,q)=(p_1,\cdots,p_d;q_1,\cdots,q_d)$. If H is a sufficiently smooth real function defined in Ω, then the Hamiltonian system of differential equations with Hamiltonian H is given by

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

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.

A smooth transformation $(p,q)=\psi(p^*,q^*)$ defined in Ω is said to be symplectic(with respect to symplectic matrix J) if the Jacobian $\psi'=\dfrac{\partial(p,q)}{\partial(p^*,q^*)}$ satisfies

$$\psi'^TJ\psi'=\frac{\partial(p,q)^T}{\partial(p^*,q^*)}J\frac{\partial(p,q)}{\partial(p^*,q^*)}=J,\qquad \forall(p^*,q^*)\in\Omega,$$

where $J=\begin{pmatrix}0 & I_d\\ -I_d & 0\end{pmatrix}$ is the standard symplectic matrix. This property is the hallmark of Hamiltonian systems.

In this paper we restrict our interest to one-step methods. If h denotes the steplength and (p^n,q^n) denotes the numerical approximations at time $t_n=nh$ to the value $(p(t_n),q(t_n))$ of a solution of (1.1), the one-step method is specified by a smooth mapping

$$(p^{n+1},q^{n+1})=\psi_{h,H}(p^n,q^n)$$

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and $\psi_{h,H}$ is assumed to depend only smoothly on h and H. In numerically solving the Hamiltonian systems of differential equations (1.1), it is natural to require that numerical solutions should preserve the property of symplecticness. Then the numerical method

$$(p^{n+1}, q^{n+1}) = \psi_{h,H}(p^n, q^n)$$

should be a symplectic transformation. Consequently we may give the following definitions.

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* $(p^{n+1}, q^{n+1}) = \psi_{h,H}(p^n, q^n)$ *is a symplectic transformation, that is ,*

$$\psi_{h,H}'^T J \psi_{h,H}' = \frac{\partial(p^{n+1}, q^{n+1})^T}{\partial(p^n, q^n)} J \frac{\partial(p^{n+1}, q^{n+1})}{\partial(p^n, q^n)} = J, \qquad \forall (p^n, q^n) \in \Omega, \tag{1.2}$$

where $\psi_{h,H}' = \partial \frac{(p^{n+1}, q^{q^{n+1}})^T}{\partial(p^n, q^n)}$ *is the Jacobian matrix of the transformation.*

At least three authors ([5],[6]and [9]) discovered independently the fact that the Runge-Kutta method with tableau

$$\begin{array}{c|ccc}
c_1 & a_{11} & \cdots & a_{1s} \\
c_2 & a_{21} & \cdots & a_{2s} \\
\vdots & \vdots & \cdots & \vdots \\
c_s & a_{s1} & \cdots & a_{ss} \\
\hline
 & b_1 & \cdots & b_s
\end{array} \tag{1.3}$$

applied to the Hamiltonian system (1.1), if its coefficients (1.3) satisfy the relation

$$M = BA + A^T B - bb^T = 0 \text{ or } m_{ij} = b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \quad 1 \le i, j \le s, \tag{1.4}$$

where $B =$ diag $(b_1, b_2, \cdots, b_s)$, then the Runge-Kutta method is symplectic.

In the integration of systems of differential equations it is possible to integrate some components of an unknown vector with a numerical method and the remaining components with an other one, as in dealing with some stiff systems including both stiff and nonstiff components. In Section 2, for Hamiltonian systems we shall integrate the p equations with an RK formula and the q equations with a different RK formula. The overall scheme is called a partitioned Runge-Kutta (PRK) scheme. For PRK scheme we shall give the conditions for symplecticness and its characterization which is based on the W-transformation of Hairer and Wanner[3],[4]. Besides, some examples are presented. In Section 3, a special class of symplectic PRK methods is constructed.

2. Conditions for symplecticness and its Characterization

In this section first of all we derive the conditions of symplecticness for PRK methods. For notational simplicity we shall assume $d = 1$ in the following.

A partitioned Runge-Kutta method with tableaux

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ c_2 & a_{21} & \cdots & a_{2s} \\ \vdots & \vdots & \cdots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array} \tag{2.1}$$

and

$$\begin{array}{c|ccc} \bar{c}_1 & \bar{a}_{11} & \cdots & \bar{a}_{1s} \\ \bar{c}_2 & \bar{a}_{21} & \cdots & \bar{a}_{2s} \\ \vdots & \vdots & \cdots & \vdots \\ \bar{c}_s & \bar{a}_{s1} & \cdots & \bar{a}_{ss} \\ \hline & \bar{b}_1 & \cdots & \bar{b}_s \end{array} \tag{2.1$'$}$$

applied to the Hamiltonian system (1.1), may have the relation

$$P_i = p^n + h\sum_{j=1}^{s} a_{ij}f(P_j, Q_j), \quad Q_i = q^n + h\sum_{j=1}^{s} \bar{a}_{ij}g(P_j, Q_j), \quad 1 \le i \le s, \tag{2.2}$$

$$p^{n+1} = p^n + h\sum_{i=1}^{s} b_i f(P_i, Q_i), \quad q^{n+1} = q^n + h\sum_{i=1}^{s} \bar{b}_i g(P_i, Q_i). \tag{2.3}$$

By virtue of the relation

$$\frac{\partial(f,g)^T}{\partial(p,q)}J + J\frac{\partial(f,g)}{\partial(p,g)} = 0 \tag{2.4}$$

which exist in Hamiltonian eystems, we can obtain the following result:

Theorem 2.1a. *If the coefficients of an s-stage PRK-method* (2.1) *satisfy the relation*

$$\overline{M} = BA + \bar{A}^T B - bb^T = 0$$

or

$$\bar{m}_{ij} = b_i a_{ij} + b_j \bar{a}_{ji} - b_i b_j = 0, \quad b_i = \bar{b}_i, \quad 1 \le i, j \le s, \tag{2.5}$$

then the method is symplectic.

Proof. By (2.3), inserting

$$\frac{\partial(p^{n+1}, q^{n+1})}{\partial(p^n, q^n)} = I + h\sum_{i=1}^{s} \operatorname{diag}(b_i, \bar{b}_i)\frac{\partial(f_i, g_i)}{\partial(p^n, q^n)}$$

into (1.2) yields

$$\frac{\partial(p^{n+1}, q^{n+1})^T}{\partial(p^n, q^n)}J\frac{\partial(p^{n+1}, q^{n+1})}{\partial(p^n, q^n)} = J + h\sum_{j=1}^{s}\left(\operatorname{diag}(b_j, \bar{b}_j)\frac{\partial(f_j, g_j)}{\partial(p^n, q^n)}\right)^T J$$

$$+h\sum_{i=1}^{s} J \operatorname{diag}(b_i, \bar{b}_i)\frac{\partial(f_i, g_i)}{\partial(p^n, q^n)}$$

$$+h^2 \sum_{i,j=1}^{s} \left(\operatorname{diag}(b_i, \bar{b}_i) \frac{\partial(f_i, g_i)}{\partial(p^n, q^n)} \right)^T J \operatorname{diag}(b_j, \bar{b}_j) \frac{\partial(f_j, g_j)}{\partial(p^n, q^n)}. \tag{2.6}$$

By (2.2)

$$\frac{\partial(P_i, Q_i)}{\partial(p^n, q^n)} = I + h \sum_{j=1}^{s} \operatorname{diag}(a_{ij}, \bar{a}_{ij}) \frac{\partial(f_j, g_j)}{\partial(p^n, q^n)}, \tag{2.7}$$

thus

$$hJ \sum_{i=1}^{s} \operatorname{diag}(b_i, \bar{b}_i) \frac{\partial(f_i, g_i)}{\partial(p^n, q^n)} = hJ \sum_{i=1}^{s} \operatorname{diag}(b_i, \bar{b}_i) \frac{\partial(f_i, g_i)}{\partial(P_i, Q_i)} \frac{\partial(P_i, Q_i)}{\partial(p^n, q^n)}$$

$$= hJ \sum_{i=1}^{s} \operatorname{diag}(b_i, \bar{b}_i) \frac{\partial(f_i, g_i)}{\partial(P_i, Q_i)} + h^2 J \sum_{i,j=1}^{s} \operatorname{diag}(b_i, \bar{b}_i) \frac{\partial(f_i, g_i)}{\partial(P_i, Q_i)} \operatorname{diag}(a_{ij}, \bar{a}_{ij}) \frac{\partial(f_j, g_j)}{\partial(p^n, q^n)}$$

$$= hJ \sum_{i=1}^{s} \operatorname{diag}(b_i, \bar{b}_i) \frac{\partial(f_i, g_i)}{\partial(P_i, Q_i)} + h^2 \sum_{i,j=1}^{s} \operatorname{diag}(\bar{b}_i, b_i) J \frac{\partial(f_i, g_i)}{\partial(P_i, Q_i)} \operatorname{diag}(a_{ij}, \bar{a}_{ij}) \frac{\partial(f_j, g_j)}{\partial(p^n, q^n)}$$

$$= hJ \sum_{i=1}^{s} \operatorname{diag}(b_i, \bar{b}_i) \frac{\partial(f_i, g_i)}{\partial(P_i, Q_i)} - h^2 \sum_{i,j=1}^{s} \operatorname{diag}(\bar{b}_i, b_i) \frac{\partial(f_i, g_i)^T}{\partial(P_i, Q_i)} J \operatorname{diag}(a_{ij}, \bar{a}_{ij}) \frac{\partial(f_j, g_j)}{\partial(p^n, q^n)}$$

$$= hJ \sum_{i=1}^{s} \operatorname{diag}(b_i, \bar{b}_i) \frac{\partial(f_i, g_i)}{\partial(P_i, Q_i)} - h^2 \sum_{i,j=1}^{s} \operatorname{diag}(\bar{b}_i, b_i) \left(\frac{\partial(f_i, g_i)}{\partial(P_i, Q_i)} \left(\frac{\partial(P_i, Q_i)}{\partial(p^n, q^n)} \right.\right.$$

$$\left.\left. - h \sum_{k=1}^{s} \operatorname{diag}(a_{ik}, \bar{a}_{ik}) \frac{\partial(f_k, g_k)}{\partial(p^n, q^n)} \right) \right)^T J \operatorname{diag}(a_{ij}, \bar{a}_{ij}) \frac{\partial(f_j, g_j)}{\partial(p^n, q^n)}$$

$$= hJ \sum_{i=1}^{s} \operatorname{diag}(b_i, \bar{b}_i) \frac{\partial(f_i, g_i)}{\partial(P_i, Q_i)} - h^2 \sum_{i,j=1}^{s} \operatorname{diag}(\bar{b}_i, b_i) \frac{\partial(f_i, g_i)^T}{\partial(p^n, q^n)} J \operatorname{diag}(a_{ij}, \bar{a}_{ij}) \frac{\partial(f_j, g_j)}{\partial(p^n, q^n)}$$

$$+ h^3 \sum_{ijk=1}^{s} \operatorname{diag}(\bar{b}_i, b_i) \left(\frac{\partial(f_i, g_i)}{\partial(P_i, Q_i)} \operatorname{diag}(a_{jk}, \bar{a}_{jk}) \frac{\partial(f_k, g_k)}{\partial(p^n, q^n)} \right)^T J \operatorname{diag}(a_{ij}, \bar{a}_{ij}) \frac{\partial(f_j, g_j)}{\partial(p^n, q^n)}$$

$$= hJ \sum_{i=1}^{s} \operatorname{diag}(b_i, \bar{b}_i) \frac{\partial(f_i, g_i)}{\partial(P_i, Q_i)} - h^2 \sum_{i,j=1}^{s} \operatorname{diag}(\bar{b}_i, b_i) \frac{\partial(f_i, g_i)^T}{\partial(p^n, q^n)} J \operatorname{diag}(a_{ij}, \bar{a}_{ij}) \frac{\partial(f_j, g_j)}{\partial(p^n, q^n)}$$

$$+ h^3 \sum_{ijk=1}^{s} \operatorname{diag}(\bar{b}_i, b_i) \frac{\partial(f_k, g_k)^T}{\partial(p^n, q^n)} \operatorname{diag}(a_{ik}, \bar{a}_{ik}) \frac{\partial(f_i, g_i)^T}{\partial(P_i, Q_i)} J \operatorname{diag}(a_{ij}, \bar{a}_{ij}) \frac{\partial(f_j, g_j)}{\partial(p^n, q^n)}.$$

On the other hand,

$$h\left(\operatorname{diag}(b_j, \bar{b}_j) \frac{\partial(f_j, g_j)}{\partial(p^n, q^n)} \right)^T J = -h\left(J \operatorname{diag}(b_j, \bar{b}_j) \frac{\partial(f_j, g_j)}{\partial(p^n, q^n)} \right)^T$$

$$= h \sum_{j=1}^{s} \frac{\partial(f_j, g_j)^T}{\partial(P_j, Q_j)} \operatorname{diag}(b_j, \bar{b}_j) J - h^2 \sum_{ji=1}^{s} \frac{\partial(f_i, g_i)^T}{\partial(p^n, q^n)} J \operatorname{diag}(\bar{a}_{ji}, a_{ji}) \frac{\partial(f_j, g_j)}{\partial(p^n, q^n)} \operatorname{diag}(\bar{b}_j, b_j)$$

$$+h^3\sum_{ijk=1}^{s}\frac{\partial(f_k,g_k)^T}{\partial(p^n,q^n)}\operatorname{diag}(a_{ik},\bar a_{ik})J\frac{\partial(f_i,g_i)}{\partial(P_i,Q_i)}\operatorname{diag}(a_{ij},\bar a_{ij})\frac{\partial(f_j,g_j)}{\partial(p^n,q^n)}\operatorname{diag}(\bar b_i,b_i).$$

For non separable Hamiltonian systems, if and only if $b_i=\bar b_i$ $(i=1,2,\cdots,s)$ there is

$$\sum_{i=1}^{s}\Big(\operatorname{diag}(\bar b_i,b_i)J\frac{\partial(f_i,g_i)}{\partial(P_i,Q_i)}+\frac{\partial(f_i,g_i)^T}{\partial(P_i,Q_i)}J\operatorname{diag}(\bar b_i,b_i)\Big)=0.$$

Now inserting the above two formulas into (2.6) and leting $b_i=\bar b_i$ $(i=1,2,\cdots,s)$ we may obtain

$$\frac{\partial(p^{n+1},q^{n+1})^T}{\partial(p^n,q^n)}J\frac{\partial(p^{n+1},q^{n+1})}{\partial(p^n,q^n)}=J-h^2*$$

$$\sum_{ij=1}^{s}\frac{\partial(f_i,g_i)^T}{\partial(p^n,q^n)}J\Big(b_i\operatorname{diag}(a_{ij},\bar a_{ij})+b_j\operatorname{diag}(\bar a_{ji},a_{ji})-b_ib_j\Big)\frac{\partial(f_j,g_j)}{\partial(p^n,q^n)}.$$

Therefore

$$\bar m_{ij}=b_ia_{ij}+b_j\bar a_{ji}-b_ib_j=0,\quad b_i=\bar b_i,\quad 1\le i,j\le s$$

or

$$\overline{M}=BA+\bar A^TB-bb^T=0,$$

the PRK method is symplectic.

Of course, an RK method is a particular instance of Theorem 2.1a, where $A=\bar A$. Therefore, for an irreducible PRK method, condition (2.5) is also necessary and there must be $b_i\neq 0$, $(i=1,2,\cdots,s)$ just as for an RK method.

In the following we give examples of symplectic PRK methods and its characterization which is based on the W-transformation of Hairer and Wanner[3],[4].

Example 1. One stage, order 1:

$$P_1=p^n+hf(P_1,Q_1),\qquad Q_1=q^n,$$
$$p^{n+1}=p^n+hf(P_1,Q_1),\qquad q^{n+1}=q^n+hg(P_1,Q_1).$$

In implementation only d-nonlinear algebraic equations are solved per step.

For an s-stage PRK method generated by $(A,\bar A,b,c)$ with distinct nodes c_i and $b_i\neq 0$ $(i=1,2,\cdots,s)$, we consider the transformation (see [7], [2] and [4])

$$X=W^TBAW.$$

Thus, Theorem 2.1a can be rewritten in the following form:

Theorem 2.1b. *If an s-stage PRK method generated by $(A,\bar A,b,c)$ with distinct nodes c_i and $b_i\neq 0$ $(i=1,2,\cdots,s)$ satisfies*

$$W^T\overline{M}W=X+\bar X^T-e_1e_1^T=0,\tag{2.8}$$

then the method is symplectic.

From Theorem 2.1b. we may construct a lot of symplectic PRK methods. For example, all the s-stage PRK methods with order $(2s-2)$:

1) s-stage Lobatto III A method and Lobatto III B method,

2) s-stage Radau I C method and Radau I D method[8],

3) s-stage Radau II C method and Radau II D method[8],

4) s-stage Gauss-type methods with $B(2s), C(s-1)$ and $D(s-2)$ and with $B(2s)$, $C(s-2)$ and $D(s-1)$ [8] are symplectic. Furthermore, we have the following result:

Corollary 1. For an s-stage RK method with distinct nodes c_i and $b_i \neq 0 \quad (i = 1, 2, \cdots, s)$ satisfying $B(p), C(\eta)$ and $D(\zeta)$, if its transformation matrix X takes the following form :

$$X = W^T BAW = \begin{pmatrix} 1/2 & -\xi_1 & & & \\ \xi_1 & \ddots & \ddots & & \\ & \ddots & 0 & -\xi_\nu & \\ & & \xi_\nu & \multicolumn{2}{|c}{R_\nu} \end{pmatrix}, \text{ where } \nu = \min(\eta, \zeta), \tag{2.9}$$

then the PRK method generated by the transformation X and

$$\bar{X} = (e_1 e_1^T - X^T) = \begin{pmatrix} 1/2 & -\xi_1 & & & \\ \xi_1 & \ddots & \ddots & & \\ & \ddots & 0 & -\xi_\nu & \\ & & \xi_\nu & \multicolumn{2}{|c}{-R_\nu^T} \end{pmatrix} \tag{2.10}$$

with $p \leq \eta + \zeta + 1$ and $p \leq 2\nu + 2$, is symplectic and of order p (see [1] and [4]).

3. A special class of symplectic PRK methods

In this section we give a special class of symplectic PRK methods. In fact, from a known RK method generated by $(\bar{A}, b, c)$ with $b_i \neq 0 \quad (i = 1, 2, \cdots, s)$, by the symplecticness condition (2.5) it is very easy to construct an associated symplectic PRK method. By symplecticness condition (2.5) there is

$$a_{ij} = b_j \left(1 - \frac{\bar{a}_{ji}}{b_i}\right), \quad 1 \leq i, j \leq s. \tag{3.1}$$

Now we consider the known RK methods generated by $(\bar{A}, b, c)$ with $b_i \neq 0$, $i = 1, 2, \cdots, s$, which are explicit. A special class of symplectic PRK methods can be given as

Table 3.1. One stage, order 1

$$\begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array} \qquad \begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}$$

Table 3.2. Two stages, order 2

$$
\begin{array}{c|cc}
0 & \frac{1}{2} & -\frac{1}{2} \\
1 & \frac{1}{2} & \frac{1}{2} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
\qquad
\begin{array}{c|cc}
0 & 0 & 0 \\
1 & 1 & 0 \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
$$

Table 3.3. Three stages, order 3

$$
\begin{array}{c|ccc}
0 & \frac{1}{6} & -\frac{4}{3} & \frac{7}{6} \\
\frac{1}{2} & \frac{1}{6} & \frac{2}{3} & -\frac{1}{3} \\
1 & \frac{1}{6} & \frac{4}{6} & \frac{1}{6} \\
\hline
 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{array}
\qquad
\begin{array}{c|ccc}
0 & 0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & 0 & 0 \\
1 & -1 & 2 & 0 \\
\hline
 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{array}
$$

Table 3.4. Four stages, order 4

$$
\begin{array}{c|cccc}
0 & b_1 & b_2(1-\frac{\bar{a}_{21}}{b_1}) & b_3(1-\frac{\bar{a}_{31}}{b_1}) & b_4(1-\frac{\bar{a}_{41}}{b_1}) \\
c_2 & b_1 & b_2 & b_3(1-\frac{\bar{a}_{32}}{b_2}) & b_4(1-\frac{\bar{a}_{42}}{b_2}) \\
c_3 & b_1 & b_2 & b_3 & b_4(1-\frac{\bar{a}_{43}}{b_3}) \\
1 & b_1 & b_2 & b_3 & b_4 \\
\hline
 & b_1 & b_2 & b_3 & b_4
\end{array}
$$

$$
\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
c_2 & c_2 & 0 & 0 & 0 \\
c_3 & \dfrac{c_3(3c_2-c_3-4c_2^2)}{2c_2(1-2c_2)} & \dfrac{c_3(c_3-c_2)}{2c_2(1-2c_2)} & 0 & 0 \\
1 & \bar{a}_{41} & \bar{a}_{42} & \bar{a}_{43} & 0 \\
\hline
 & b_1 & b_2 & b_3 & b_4
\end{array}
$$

where

$$b_1 = \frac{1-2(c_2+c_3)+6c_2c_3}{12c_2c_3}, \qquad b_2 = \frac{2c_3-1}{12c_2(c_3-c_2)(1-c_2)},$$

$$b_3 = \frac{1-2c_2}{12c_3(c_3-c_2)(1-c_3)}, \qquad b_4 = \frac{3-4(c_2+c_3)+6c_2c_3}{12(1-c_2)(1-c_3)},$$

$$\bar{a}_{41} = \frac{c_3^2(12c_2^2-12c_2+4)-c_3(12c_2^2-15c_2+5)+(4c_2^2-6c_2+2)}{2c_2c_3[3-4(c_2+c_3)+6c_2c_3]},$$

$$\bar{a}_{42} = \frac{(-4c_3^2+5c_3+c_2-2)(1-c_2)}{2c_2(c_3-c_2)[3-4(c_2+c_3)+6c_2c_3]},$$

$$\bar{a}_{43} = \frac{(1-2c_2)(1-c_3)(1-c_2)}{c_3(c_3-c_2)[3-4(c_2+c_3)+6c_2c_3]}(see[2]).$$

Motivated by the above low-order methods, we may conjecture that, if an s-stage explicit RK method generated by $(\bar{A}, b, c)$ with $b_i \neq 0 \quad (i = 1, 2, \cdots, s)$ is of order p, then the PRK method constituted by (A, b, c) with (3.1) and $(\bar{A}, b, c)$ is symplectic and of order p.

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