Construction of symplectic (partitioned) Runge-Kutta methods with continuous stage

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Abstract

Hamiltonian systems are one of the most important class of dynamical systems with a geometric structure called symplecticity and the numerical algorithms which can preserve such geometric structure are of interest. In this article we study the construction of symplectic (partitioned) Runge-Kutta methods with continuous stage, which provides a new and simple way to construct symplectic (partitioned) Runge-Kutta methods in classical sense. This line of construction of symplectic methods relies heavily on the expansion of orthogonal polynomials and the simplifying assumptions for (partitioned) Runge-Kutta type methods.

Keywords: Hamiltonian system; Symplectic method; Continuous-stage Runge-Kutta method; Continuous-stage partitioned Runge-Kutta method.

1. Introduction

Geometric numerical integration is a subfield of the numerical solution of differential equations, and it turn out to be very efficient for long-time simulating the dynamical behavior of those systems with special structures [14]. For Hamiltonian systems, it is known that symplecticity of the flow is an important characteristic property of such systems [1] and to correctly reproduce this property, the numerical algorithms called symplectic methods have been proposed and extensively studied (see [9, 21, 14] and references therein), among of which symplectic (partitioned) Runge-Kutta methods are one of the most important subclass of such algorithms [20, 24, 22, 23]. In this article, we focus on a new and simple way to construct these methods.

Runge-Kutta (RK) method with continuous stage has been discussed and investigated by several authors recently [15, 25, 26, 28, 18], the idea of which was firstly presented by Butcher in 1970s [4, 6]. There are few literatures involving this kind of methods since Butcher's seminal work, until recently, [15] exploits it to interpret the energy-preserving collocation methods. Subsequently, [25] investigates four kinds of time finite element methods and relates them to Runge-Kutta methods with continuous stage. Moreover, it is shown in [25] that some energy-preserving RK methods including s-stage trapezoidal method [16], Hamiltonian boundary value methods [2, 3], average

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vector field method [19, 7] can also be related to such methods. [26, 28] discuss the construction of Runge-Kutta methods with continuous stage and present the characterizations for several geometric-structure preserving methods including symplectic methods, symmetric methods and energy-preserving methods. Exponentially-fitted continuous-stage Runge-Kutta methods with energy-preserving property for Hamiltonian systems are also presented in [18]. In this paper, we aim at further investigation of construction of symplectic (partitioned) Runge-Kutta methods, along the line of expansion of orthogonal polynomials and with the help of simplifying assumptions for (partitioned) Runge-Kutta type methods. This approach can naturally provides a simple way to construct symplectic (partitioned) Runge-Kutta methods in classical sense.

The outline of the paper is as follows. In Section 2, we provide some preliminaries for (partitioned) Runge-Kutta methods with continuous stage and review some existing results for the construction of general RK type methods with continuous stage. In section 3, we discuss the construction of symplectic (partitioned) Runge-Kutta methods with continuous stage as well as the symplectic (partitioned) Runge-Kutta methods in classical sense. At last, we conclude this paper.

2. Construction of (P)RK type methods

In this section, we first introduce the definition of (partitioned) Runge-Kutta method with continuous stage by following the formulation proposed in [15], then show some results which are useful in constructing (P)RK type methods.

2.1. Continuous-stage RK method

Consider a first-order system of ordinary differential equations (ODEs)

$$
\begin{cases}
\dot{\boldsymbol{z}} = \boldsymbol{f}(t, \boldsymbol{z}), \\
\boldsymbol{z}(t_0) = \boldsymbol{z}_0 \in \mathbb{R}^d,
\end{cases}
\tag{2.1}
$$

where the upper dot indicates differentiation with respect to t and $\boldsymbol{f} : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ is a sufficiently smooth vector function.

Definition 2.1. [15, 28] Let $A_{\tau, \sigma}$ be a function of two variables $\tau, \sigma \in [0, 1]$, B_τ be a function of $\tau \in [0, 1]$. Define $C_\tau = \int_0^1 A_{\tau, \sigma} \, d\sigma$. The one-step method $\Phi_h : \boldsymbol{z}_0 \mapsto \boldsymbol{z}_1$ given by

$$
\begin{aligned}
\boldsymbol{Z}_\tau &= \boldsymbol{z}_0 + h \int_0^1 A_{\tau, \sigma} \boldsymbol{f}(t_0 + C_\sigma h, \boldsymbol{Z}_\sigma) \, d\sigma, \ \tau \in [0, 1], \\
\boldsymbol{z}_1 &= \boldsymbol{z}_0 + h \int_0^1 B_\tau \boldsymbol{f}(t_0 + C_\tau h, \boldsymbol{Z}_\tau) \, d\tau,
\end{aligned}
\tag{2.2}
$$

is called a continuous-stage Runge-Kutta (csRK) method, where $\boldsymbol{Z}_\tau \approx \boldsymbol{z}(t_0 + C_\tau h)$, $\boldsymbol{z}_1 \approx \boldsymbol{z}(t_0 + h)$.

In this paper, the construction of csRK methods mainly relies on the following simplifying assumptions of order conditions [15]

$$
\mathfrak{B}(\xi): \quad \int_0^1 B_\tau C_\tau^{\kappa-1} \, d\tau = \frac{1}{\kappa}, \quad \kappa = 1, \dots, \xi,
$$

$$
\mathfrak{C}(\eta): \quad \int_0^1 A_{\tau, \sigma} C_\sigma^{\kappa-1} \, d\sigma = \frac{1}{\kappa} C_\tau^\kappa, \quad \kappa = 1, \dots, \eta,
$$

$$
\mathfrak{D}(\zeta): \quad \int_0^1 B_\tau C_\tau^{\kappa-1} A_{\tau, \sigma} \, d\tau = \frac{1}{\kappa} B_\sigma (1 - C_\sigma^\kappa), \quad \kappa = 1, \dots, \zeta.
$$

2

Analogously to the classical result [5] given by Butcher in 1964, we can determine the order of a csRK method with the help of these simplifying assumptions.

Theorem 2.1. *If a csRK method* (2.2) *with coefficients* $(A_{\tau,\sigma}, B_\tau, C_\tau)$ *satisfies* $\mathfrak{B}(\rho)$, $\mathfrak{C}(\alpha)$ *and* $\mathfrak{D}(\beta)$, *then it is at least of order*

$$\min(\rho, 2\alpha + 2, \alpha + \beta + 1).$$

Proof. This statement can be proved by using the similar idea to the one used in Theorem 7.4 [12]. $\qquad\square$

According to Proposition 2.1 shown in [28], we assume $B_\tau = 1$ in the current paper and to proceed conveniently, hereafter we also assume $C_\tau = \tau$. In such a case, $\mathfrak{B}(\xi)$ is reduced to

$$\int_0^1 \tau^{\kappa-1}\,\mathrm{d}\tau = \frac{1}{\kappa}, \quad \kappa = 1,\dots,\xi$$

which implies $\mathfrak{B}(\xi)$ holds with $\xi = \infty$. Now we introduce the ι-degree normalized shifted Legendre polynomial denoted by $P_\iota(x)$, which can be explicitly computed by the Rodrigues formula

$$P_0(x) = 1, \; P_\iota(x) = \frac{\sqrt{2\iota+1}}{\iota!}\frac{\mathrm{d}^\iota}{\mathrm{d}x^\iota}\Big(x^\iota(x-1)^\iota\Big), \quad \iota = 1,2,3,\cdots.$$

A well-known property of Legendre polynomials is that they are orthogonal to each other with respect to the L^2 inner product on $[0, 1]$

$$\int_0^1 P_\iota(t)P_\kappa(t)\,\mathrm{d}t = \delta_{\iota\kappa}, \quad \iota,\,\kappa = 0,1,2,\cdots,$$

and they as well satisfy the following integration formulae

$$
\begin{aligned}
\int_0^x P_0(t)\,\mathrm{d}t &= \xi_1 P_1(x) + \frac{1}{2}P_0(x),\\
\int_0^x P_\iota(t)\,\mathrm{d}t &= \xi_{\iota+1}P_{\iota+1}(x) - \xi_\iota P_{\iota-1}(x), \quad \iota = 1,2,3,\cdots,\\
\int_x^1 P_\iota(t)\,\mathrm{d}t &= \delta_{\iota 0} - \int_0^x P_\iota(t)\,\mathrm{d}t, \quad \iota = 0,1,2,\cdots,
\end{aligned}
\tag{2.3}
$$

where $\xi_\iota = \frac{1}{2\sqrt{4\iota^2-1}}$ and δ_{ij} is the Kronecker symbol.

With the help of (2.3), by exploiting the expansion of Legendre polynomials for the coefficients of a csRK method and the corresponding simplifying assumptions, we have the following result for construction of csRK methods (more details see [27, 28]).

Lemma 2.1. *[27] For a csRK method with* $B_\tau \equiv 1$ *and* $C_\tau = \tau$, *we have the following statements:*

(a) $\mathfrak{C}(\alpha)$ *is equivalent to the fact that* $A_{\tau,\sigma}$ *takes the form*

$$A_{\tau,\sigma} = \sum_{\iota=0}^{\alpha-1}\int_0^\tau P_\iota(x)\,\mathrm{d}x\,P_\iota(\sigma) + \sum_{\iota=\alpha}^\infty \gamma_\iota(\tau)P_\iota(\sigma),$$

where $\gamma_\iota(\tau)$, $\iota \geq \alpha$ *are arbitrary functions;*

3

(b) $\mathfrak{D}(\beta)$ is equivalent to the fact that $A_{\tau,\sigma}$ takes the form

$$A_{\tau,\sigma} = \sum_{\iota=0}^{\beta-1} \int_{\sigma}^{1} P_\iota(x)\,\mathrm{d}x\, P_\iota(\tau) + \sum_{\iota=\beta}^{\infty} \lambda_\iota(\sigma) P_\iota(\tau),$$

where $\lambda_\iota(\sigma)$, $\iota \geq \beta$ are arbitrary functions.

Theorem 2.2. *[28] For a csRK method with $B_\tau \equiv 1$ and $C_\tau = \tau$ (then $\mathfrak{B}(\infty)$ holds), the following two statements are equivalent:*

(a) *Both $\mathfrak{C}(\alpha)$ and $\mathfrak{D}(\beta)$ hold;*

(b) *The coefficient $A_{\tau,\sigma}$ has the form*

$$A_{\tau,\sigma} = \frac{1}{2} + \sum_{\iota=0}^{N_1} \xi_{\iota+1} P_{\iota+1}(\tau) P_\iota(\sigma) - \sum_{\iota=0}^{N_2} \xi_{\iota+1} P_{\iota+1}(\sigma) P_\iota(\tau) + \sum_{\substack{i \geq \beta \\ j \geq \alpha}} \gamma_{ij} P_i(\tau) P_j(\sigma), \qquad (2.4)$$

where $N_1 = \max(\alpha-1, \beta-2)$, $N_2 = \max(\alpha-2, \beta-1)$, $\xi_\iota = \frac{1}{2\sqrt{4\iota^2-1}}$ and γ_{ij} are arbitrary real numbers.

By combining Theorem 2.1 and Theorem 2.2 we can easily construct lots of csRK methods, the order of which are given by $\min(\infty, 2\alpha+2, \alpha+\beta+1) = \min(2\alpha+2, \alpha+\beta+1)$.

2.2. Continuous-stage PRK method

For a partitioned ODEs given by

$$\begin{cases} \dot{\boldsymbol{y}} = \boldsymbol{f}(t, \boldsymbol{y}, \boldsymbol{z}), \ \boldsymbol{y}(t_0) = \boldsymbol{y}_0 \in \mathbb{R}^d, \\ \dot{\boldsymbol{z}} = \boldsymbol{g}(t, \boldsymbol{y}, \boldsymbol{z}), \ \boldsymbol{z}(t_0) = \boldsymbol{z}_0 \in \mathbb{R}^s, \end{cases} \qquad (2.5)$$

we can consider methods that deal with the $\boldsymbol{y}$ and $\boldsymbol{z}$ variables by two different csRK methods, which then produce the following definition.

Definition 2.2. *[27, 28] Assume that $C_\tau = \int_0^1 A_{\tau,\sigma}\,\mathrm{d}\sigma$ and $\widehat{C}_\tau = \int_0^1 \widehat{A}_{\tau,\sigma}\,\mathrm{d}\sigma$. The following one-step method*

$$\boldsymbol{Y}_\tau = \boldsymbol{y}_0 + h \int_0^1 A_{\tau,\sigma} \boldsymbol{f}(t_0 + C_\sigma h, \boldsymbol{Y}_\sigma, \boldsymbol{Z}_\sigma)\,\mathrm{d}\sigma, \ \ \tau \in [0,1],$$

$$\boldsymbol{Z}_\tau = \boldsymbol{z}_0 + h \int_0^1 \widehat{A}_{\tau,\sigma} \boldsymbol{g}(t_0 + C_\sigma h, \boldsymbol{Y}_\sigma, \boldsymbol{Z}_\sigma)\,\mathrm{d}\sigma, \ \ \tau \in [0,1],$$

$$\boldsymbol{y}_1 = \boldsymbol{y}_0 + h \int_0^1 B_\tau \boldsymbol{f}(t_0 + C_\tau h, \boldsymbol{Y}_\tau, \boldsymbol{Z}_\tau)\,\mathrm{d}\tau,$$

$$\boldsymbol{z}_1 = \boldsymbol{z}_0 + h \int_0^1 \widehat{B}_\tau \boldsymbol{g}(t_0 + C_\tau h, \boldsymbol{Y}_\tau, \boldsymbol{Z}_\tau)\,\mathrm{d}\tau.$$

(2.6)

is referred to as continuous-stage partitioned Runge-Kutta (csPRK) method.

Similarly as those order conditions considered for classical PRK method [8], we propose the following simplifying assumptions of order conditions for the csPRK method

$$\mathcal{B}(\xi): \int_0^1 B_\tau C_\tau^{\kappa-1}\widehat{C_\tau}^\iota\, \mathrm{d}\tau = \frac{1}{\kappa+\iota},\ \ 1 \leq \kappa+\iota \leq \xi;$$

$$\mathcal{C}(\eta): \int_0^1 A_{\tau,\sigma} C_\sigma^{\kappa-1}\widehat{C_\sigma}^\iota\, \mathrm{d}\sigma = \frac{C_\tau^{\kappa+\iota}}{\kappa+\iota},\ \ 1 \leq \kappa+\iota \leq \eta,\ \ \tau \in [0,1];$$

$$\widehat{\mathcal{C}}(\widehat{\eta}): \int_0^1 \widehat{A}_{\tau,\sigma} C_\sigma^{\kappa-1}\widehat{C_\sigma}^\iota\, \mathrm{d}\sigma = \frac{\widehat{C_\tau}^{\kappa+\iota}}{\kappa+\iota},\ \ 1 \leq \kappa+\iota \leq \widehat{\eta},\ \ \tau \in [0,1]; \qquad (2.7)$$

$$\mathcal{D}(\zeta): \int_0^1 B_\tau C_\tau^{\kappa-1}\widehat{C_\tau}^\iota A_{\tau,\sigma}\, \mathrm{d}\tau = \frac{B_\sigma(1-\widehat{C_\sigma}^{\kappa+\iota})}{\kappa+\iota},\ \ 1 \leq \kappa+\iota \leq \zeta,\ \ \sigma \in [0,1];$$

$$\widehat{\mathcal{D}}(\widehat{\zeta}): \int_0^1 \widehat{B}_\tau C_\tau^{\kappa-1}\widehat{C_\tau}^\iota \widehat{A}_{\tau,\sigma}\, \mathrm{d}\tau = \frac{\widehat{B}_\sigma(1-\widehat{C_\sigma}^{\kappa+\iota})}{\kappa+\iota},\ \ 1 \leq \kappa+\iota \leq \widehat{\zeta},\ \ \sigma \in [0,1].$$

Theorem 2.3. *If a csPRK method* (2.6) *with coefficients* $(A_{\tau,\sigma},\, B_\tau,\, C_\tau;\, \widehat{A}_{\tau,\sigma},\, \widehat{B}_\tau,\, \widehat{C}_\tau)$ *satisfies* $\widehat{B}_\tau \equiv B_\tau$ *for* $\tau \in [0,1]$, *and moreover, all* $\mathcal{B}(\rho),\, \mathcal{C}(\alpha),\, \widehat{\mathcal{C}}(\alpha),\, \mathcal{D}(\beta),\, \widehat{\mathcal{D}}(\beta)$ *hold, then it is at least of order*

$$\min(\rho, 2\alpha + 2,\, \alpha + \beta + 1).$$

Proof. The proof is the same as that for classical (non-partitioned) Runge-Kutta methods (see [12]), in which the bi-colored trees have to be considered instead of trees. $\square$

If we let $B_\tau = \widehat{B}_\tau \equiv 1$ and $C_\tau = \widehat{C}_\tau = \tau$, then by using Theorem 2.2 it is easy to design $A_{\tau,\sigma}$ and $\widehat{A}_{\tau,\sigma}$ such that all the conditions described in Theorem 2.3 are fulfilled. This allows us to construct lots of csPRK methods of arbitrarily high order.

2.3. Classical (P)RK method retrieved

Though we have discussed the construction of csRK and csPRK methods above, it should be noticed that in general the practical implementation of cs(P)RK methods needs the use of numerical quadrature formula. Therefore, next we present classical (P)RK methods retrieved by using quadrature formulae.

2.3.1. RK method retrieved

Applying a quadrature formula denoted by $(b_i, c_i)_{i=1}^r$ to (2.2), we derive an r-stage classical RK method

$$\overline{\boldsymbol{Z}}_i = \boldsymbol{z}_0 + h\sum_{j=1}^r (b_j A_{c_i,c_j})\boldsymbol{f}(t_0 + c_j h, \overline{\boldsymbol{Z}}_j),\quad i = 1,\cdots,r,$$

$$\boldsymbol{z}_1 = \boldsymbol{z}_0 + h\sum_{i=1}^r b_i \boldsymbol{f}(t_0 + c_i h, \overline{\boldsymbol{Z}}_i), \qquad (2.8)$$

where $A_{c_i,c_j} = (A_{\tau,\sigma})|_{\tau=c_i,\sigma=c_j}$ and $\overline{\boldsymbol{Z}}_i \approx \boldsymbol{Z}_{c_i} = (\boldsymbol{Z}_\tau)|_{\tau=c_i}$. The scheme (2.8) can also be formulated by the following Butcher tableau

$$\begin{array}{c|c} c & (b_j A_{c_i,c_j})_{r\times r} \\ \hline & b^T \end{array}$$

where $c = (c_1, \cdots, c_r)^T$, $b = (b_1, \cdots, b_r)^T$.

Theorem 2.4. *Assume $A_{\tau,\sigma}$ is a bivariate polynomial of degree d^τ in τ and degree d^σ in σ, and the quadrature formula $(b_i, c_i)_{i=1}^r$ is of order[1] p. If a csRK method (2.2) with coefficients $(A_{\tau,\sigma}, B_\tau, C_\tau)$ satisfies $B_\tau \equiv 1$, $C_\tau = \tau$ (then $\mathfrak{B}(\infty)$ holds) and both $\mathfrak{C}(\eta)$, $\mathfrak{D}(\zeta)$ hold, then the classical RK method with coefficients $(b_j A_{c_i,c_j}, b_i, c_i)$ is at least of order*

$$\min(p, 2\alpha + 2, \alpha + \beta + 1),$$

where $\alpha = \min(\eta, p - d^\sigma)$ and $\beta = \min(\zeta, p - d^\tau)$.

Proof. Since $\int_0^1 f(x)\,\mathrm{d}x = \sum\limits_{i=1}^r b_i f(c_i)$ holds exactly for any polynomial $f(x)$ of degree up to $p - 1$, using the quadrature formula $(b_i, c_i)_{i=1}^r$ to compute the integrals of $\mathfrak{B}(\xi)$, $\mathfrak{C}(\eta)$, $\mathfrak{D}(\zeta)$ it gives

$$\sum_{i=1}^r b_i c_i^{\kappa-1} = \frac{1}{\kappa}, \ \kappa = 1, \cdots, p,$$

$$\sum_{j=1}^r (b_j A_{c_i,c_j}) c_j^{\kappa-1} = \frac{c_i^\kappa}{\kappa}, \ i = 1, \cdots, r, \ \kappa = 1, \cdots, \alpha,$$

$$\sum_{i=1}^r b_i c_i^{\kappa-1} (b_j A_{c_i,c_j}) = \frac{b_j}{\kappa}(1 - c_j^\kappa), \ j = 1, \cdots, r, \ \kappa = 1, \cdots, \beta.$$

where $\alpha = \min(\eta, p - d^\sigma)$ and $\beta = \min(\zeta, p - d^\tau)$. Note that in the last formula, we have multiplied a factor b_j afterwards from both sides of the original identity. These formulae imply that the RK method with coefficients $(b_j A_{c_i,c_j}, b_i, c_i)$ satisfies $B(p)$, $C(\alpha)$ and $D(\beta)$ (i.e., the classical simplifying assumptions for RK method, see [5, 13]), which provides the order of the method from a classical result by Butcher [5]. □

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[1] The numerical quadrature formula denoted by $(b_i, c_i)_{i=1}^r$ is called order p if and only if $\int_0^1 f(x)\,\mathrm{d}x = \sum\limits_{i=1}^r b_i f(c_i)$ exactly holds for any polynomial $f(x)$ of degree up to $p - 1$.

2.3.2. PRK method retrieved

Assume that $B_\tau = \widehat{B}_\tau \equiv 1$ and $C_\tau = \widehat{C}_\tau = \tau$, applying a quadrature formula denoted by $(b_i, c_i)_{i=1}^r$ to (2.6), we then derive a r-stage classical PRK method

$$\overline{\boldsymbol{Y}}_i = \boldsymbol{y}_0 + h \sum_{j=1}^r (b_j A_{c_i, c_j}) \boldsymbol{f}(t_0 + c_j h, \overline{\boldsymbol{Y}}_j, \overline{\boldsymbol{Z}}_j), \quad i = 1, \cdots, r,$$

$$\overline{\boldsymbol{Z}}_i = \boldsymbol{z}_0 + h \sum_{j=1}^r (b_j \widehat{A}_{c_i, c_j}) \boldsymbol{g}(t_0 + c_j h, \overline{\boldsymbol{Y}}_j, \overline{\boldsymbol{Z}}_j), \quad i = 1, \cdots, r,$$

$$\boldsymbol{y}_1 = \boldsymbol{y}_0 + h \sum_{i=1}^r b_i \boldsymbol{f}(t_0 + c_i h, \overline{\boldsymbol{Y}}_i, \overline{\boldsymbol{Z}}_i), \tag{2.9}$$

$$\boldsymbol{z}_1 = \boldsymbol{z}_0 + h \sum_{i=1}^r b_i \boldsymbol{g}(t_0 + c_i h, \overline{\boldsymbol{Y}}_i, \overline{\boldsymbol{Z}}_i),$$

which can be formulated by a pair of Butcher tableaux below

$$
\begin{array}{c|c}
c & (b_j A_{c_i, c_j})_{r \times r} \\
\hline
 & b^T
\end{array}
\qquad\qquad
\begin{array}{c|c}
c & (b_j \widehat{A}_{c_i, c_j})_{r \times r} \\
\hline
 & b^T
\end{array}
$$

where $c = (c_1, \cdots, c_r)^T$, $b = (b_1, \cdots, b_r)^T$.

Theorem 2.5. *Assume $A_{\tau, \sigma}$ is a bivariate polynomial of degree d^τ in τ and degree d^σ in σ, $\widehat{A}_{\tau, \sigma}$ is a bivariate polynomial of degree $\widehat{d^\tau}$ in τ and degree $\widehat{d^\sigma}$ in σ, and the quadrature formula $(b_i, c_i)_{i=1}^r$ is of order p. If $(A_{\tau, \sigma}, B_\tau, C_\tau; \widehat{A}_{\tau, \sigma}, \widehat{B}_\tau, \widehat{C}_\tau)$ satisfies $B_\tau = \widehat{B}_\tau \equiv 1$, $C_\tau = \widehat{C}_\tau = \tau$ (then $\mathcal{B}(\infty)$ holds) and all $\mathcal{C}(\alpha)$, $\widehat{\mathcal{C}}(\alpha)$, $\mathcal{D}(\beta)$, $\widehat{\mathcal{D}}(\beta)$ hold, then the classical PRK method with coefficients $(b_j A_{c_i, c_j}, b_i, c_i; b_j \widehat{A}_{c_i, c_j}, b_i, c_i)$ is of order*

$$\min(p, 2\eta + 2, \eta + \zeta + 1),$$

where $\eta = \min(\alpha, p - d^\sigma, p - \widehat{d^\sigma})$ and $\zeta = \min(\beta, p - d^\tau, p - \widehat{d^\tau})$.

Proof. The proof of the current theorem is similar to that of Theorem 2.4, and one needs using a known result presented in [8] (see Theorem 4.1, Page 97). $\square$

3. Construction of symplectic (P)RK methods

We consider Hamiltonian differential equations written in the following form

$$\begin{cases} \dot{\boldsymbol{p}} = -\nabla_{\boldsymbol{q}} \mathbf{H}(\boldsymbol{p}, \boldsymbol{q}), \\ \dot{\boldsymbol{q}} = \nabla_{\boldsymbol{p}} \mathbf{H}(\boldsymbol{p}, \boldsymbol{q}), \end{cases} \tag{3.1}$$

where the Hamiltonian namely the total energy $\mathbf{H}(\boldsymbol{p}, \boldsymbol{q})$ is a smooth scalar function of position coordinates $\boldsymbol{p} \in \mathbb{R}^d$ and momenta $\boldsymbol{q} \in \mathbb{R}^d$, and we specify the initial condition as $(\boldsymbol{p}(t_0), \boldsymbol{q}(t_0)) = (\boldsymbol{p}_0, \boldsymbol{q}_0) \in \mathbb{R}^d \times \mathbb{R}^d$. It is well-known that the energy of the system (3.1) is a conserved quantity along

the analytic solution of the system, and the system has a geometric structure called symplecticity [1, 9, 10, 11], i.e., the flow φ_t of the system satisfies

$$(\varphi_t')^T J \varphi_t' = J,$$

where J is a canonical structure matrix [14] and φ_t' denotes the derivative of φ_t with respect to initial values. An important numerical integrator for this special system is the so-called symplectic method [9, 10, 14], which has an excellent long-time behavior in simulating the exact flow of the system. A one-step method $\Phi_h : (\boldsymbol{p}_0, \boldsymbol{q}_0) \mapsto (\boldsymbol{p}_1, \boldsymbol{q}_1)$ for solving Hamiltonian systems is called symplectic if

$$(\Phi_h')^T J \Phi_h' = J.$$

More surveys and discussions about this special class of algorithms can be found in [11, 14, 21] and references therein.

It is known that for an r-stage RK method with coefficients (a_{ij}, b_i, c_i), when applied to the Hamiltonian system (3.1), it can preserve the symplecticity of the system only if the RK coefficients satisfy [20, 17, 24]

$$b_i a_{ij} + b_j a_{ji} = b_i b_j, \ i, j = 1, \cdots, r, \tag{3.2}$$

and for an r-stage PRK method with coefficients $(a_{ij}, b_i, c_i; \widehat{a}_{ij}, \widehat{b}_i, \widehat{c}_i)$, the conditions for symplecticity are [23, 14]

$$b_i \widehat{a}_{ij} + \widehat{b}_j a_{ji} = b_i \widehat{b}_j, \ i, j = 1, \cdots, r,$$
$$b_i = \widehat{b}_i, \ i = 1, \cdots, r. \tag{3.3}$$

Analogously to the classical results above, for a csRK method with $B_\tau \equiv 1$, $C_\tau = \tau$, it is symplectic if

$$A_{\tau, \sigma} + A_{\sigma, \tau} = 1, \quad \tau, \sigma \in [0, 1], \tag{3.4}$$

while for a csPRK method with $B_\tau = \widehat{B}_\tau \equiv 1$, $C_\tau = \widehat{C}_\tau = \tau$, it is symplectic if

$$\widehat{A}_{\tau, \sigma} + A_{\sigma, \tau} = 1, \quad \tau, \sigma \in [0, 1]. \tag{3.5}$$

Next, let us proceed by considering the construction of symplectic RK and symplectic PRK type schemes, separately for both non-classical and classical cases.

3.1. Symplectic RK type method

Theorem 3.1. *The csRK method (2.2) with $B_\tau = 1$, $C_\tau = \tau$ is symplectic if $A_{\tau, \sigma}$ has the form*

$$A_{\tau, \sigma} = \frac{1}{2} + \sum_{0 < i + j \in \mathbb{Z}} \alpha_{ij} P_i(\tau) P_j(\sigma), \quad \alpha_{ij} \in \mathbb{R}, \tag{3.6}$$

where α_{ij} is skew-symmetric, i.e., $\alpha_{ij} = -\alpha_{ji}$, $i + j > 0$.

Proof. Assume $A_{\tau, \sigma}$ can be expanded as a series in terms of basis $\{P_i(\tau) P_j(\sigma)\}_{i,j=0}^{\infty}$, written in the form

$$A_{\tau, \sigma} = \sum_{0 \le i, j \in \mathbb{Z}} \alpha_{ij} P_i(\tau) P_j(\sigma), \quad \alpha_{ij} \in \mathbb{R},$$

8

and thus we have

$$A_{\sigma,\tau} = \sum_{0 \le i,j \in \mathbb{Z}} \alpha_{ij} P_i(\sigma) P_j(\tau) = \sum_{0 \le i,j \in \mathbb{Z}} \alpha_{ji} P_j(\sigma) P_i(\tau).$$

Substituting the above two expressions into (3.4) and collecting the like basis, it gives

$$\alpha_{00} = \frac{1}{2}; \ \alpha_{ij} = -\alpha_{ji}, \ i + j > 0,$$

which completes the proof. $\square$

It is evident that combing Theorem 3.1 with Theorem 2.2, we can construct symplectic csRK methods of arbitrary order. Moreover, when consider using a quadrature formula, we have the following corollary.

Corollary 3.1. *If the coefficient $A_{\tau,\sigma}$ of a csRK method with $B_\tau = 1$, $C_\tau = \tau$ are given by (3.6), then the RK scheme $(b_j A_{c_i,c_j}, b_i, c_i)$ obtained by using a quadrature formula $(b_i, c_i)_{i=1}^r$ is always symplectic and the order of the method can be determined by Theorem 2.4.*

Proof. When applying a quadrature formula $(b_i, c_i)_{i=1}^r$ to calculate the integrals of the associated csRK method, it can be seen that

$$A_{c_i,c_j} + A_{c_j,c_i} = 1, \ \ i, j = 1, \cdots, r,$$

thus

$$b_i(b_j A_{c_i,c_j}) + b_j(b_i A_{c_j,c_i}) = b_i b_j, \ \ i, j = 1, \cdots, r,$$

which implies that the conditions for symplecticity, namely (3.2), are fulfilled. $\square$

Example 3.1. *Let $B_\tau = 1$, $C_\tau = \tau$ and take*

$$A_{\tau,\sigma} = \frac{1}{2} + \sum_{\iota=0}^{s-1} \xi_{\iota+1} \Big(P_{\iota+1}(\tau) P_\iota(\sigma) - P_{\iota+1}(\sigma) P_\iota(\tau) \Big), \tag{3.7}$$

by using some suitable quadrature formulae, we can retrieve a lot of classical symplectic RK methods including $(s+1)$-stage Lobatto IIIE, Radau IB, Radau IIB and Gauss-Legendre RK schemes, and the orders are $2s, 2s+1, 2s+1, 2s+2$ respectively.

If we introduce a parameter λ by adding a term $\lambda \xi_{s+1} \big(P_{s+1}(\tau) P_s(\sigma) - P_{s+1}(\sigma) P_s(\tau) \big)$ to (3.7), and consider $s = 1$, then by using 3-point Gaussian quadrature formula it produces a new class of symplectic RK methods, which is shown in Table 3.1.

3.2. Symplectic PRK type method

For convenience, we first give the following lemma.

Lemma 3.1. *Assume $B_\tau \equiv 1$ and $C_\tau = \tau$. If $(A_{\tau,\sigma}, B_\tau, C_\tau)$ satisfies $\mathfrak{C}(\eta)$ and $\mathfrak{D}(\zeta)$, define $\widehat{A}_{\tau,\sigma} := 1 - A_{\sigma,\tau}$, then $(\widehat{A}_{\tau,\sigma}, B_\tau, C_\tau)$ satisfies $\mathfrak{C}(\zeta)$ and $\mathfrak{D}(\eta)$.*

Proof. The proof can be directly deduced from Theorem 2.2. $\square$

$$
\begin{array}{c|ccc}
\frac{1}{2}-\frac{\sqrt{15}}{10} & \frac{5}{36} & \frac{2}{9}-\frac{(2+\lambda)\sqrt{15}}{45} & \frac{5}{36}-\frac{(5-2\lambda)\sqrt{15}}{90} \\
\frac{1}{2} & \frac{5}{36}+\frac{(2+\lambda)\sqrt{15}}{72} & \frac{2}{9} & \frac{5}{36}-\frac{(2+\lambda)\sqrt{15}}{72} \\
\frac{1}{2}+\frac{\sqrt{15}}{10} & \frac{5}{36}+\frac{(5-2\lambda)\sqrt{15}}{90} & \frac{2}{9}+\frac{(2+\lambda)\sqrt{15}}{45} & \frac{5}{36} \\
\hline
& \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array}
$$

Table 3.1: A class of symplectic RK methods of order 4 retrieved by Gaussian quadrature.

Theorem 3.2. *If a csPRK method* (2.6) *with coefficients* $(A_{\tau,\sigma},\ B_\tau,\ C_\tau;\ \widehat{A}_{\tau,\sigma},\ \widehat{B}_\tau,\ \widehat{C}_\tau)$ *satisfying*

$$B_\tau = \widehat{B}_\tau \equiv 1,$$

$$C_\tau = \widehat{C}_\tau = \tau,$$

$$\widehat{A}_{\tau,\sigma} = 1 - A_{\sigma,\tau},$$

and $A_{\tau,\sigma}$ *is given such that both* $\mathfrak{C}(\eta)$ *and* $\mathfrak{D}(\zeta)$ *hold, then this csPRK method is symplectic and of order at least*

$$2\min(\eta,\ \zeta) + 1.$$

Proof. Since $B_\tau = \widehat{B}_\tau \equiv 1, C_\tau = \widehat{C}_\tau = \tau$, this implies that $\mathcal{B}(\infty)$ holds. In such a case, note that $\mathfrak{C}(\eta)$ and $\mathfrak{D}(\zeta)$ are equivalent to $\mathcal{C}(\eta)$ and $\mathcal{D}(\zeta)$, respectively. Next, by combining Theorem 2.3 and Lemma 3.1 it gives the final result. $\qquad\square$

One can then easily construct symplectic PRK methods by means of Theorem 3.2 and Theorem 2.5 based on numerical quadrature formulae. we provide the following corollary.

Corollary 3.2. *Assume* $A_{\tau,\sigma}$ *is a bivariate polynomial of degree* d^τ *in* τ *and degree* d^σ *in* σ, $\widehat{A}_{\tau,\sigma} = 1 - A_{\sigma,\tau}$, *and the quadrature formula* $(b_i, c_i)_{i=1}^r$ *is of order* p. *If* $(A_{\tau,\sigma},\ B_\tau,\ C_\tau)$ *satisfies* $B_\tau \equiv 1,\ C_\tau = \tau$ *(then* $\mathfrak{B}(\infty)$ *holds) and both* $\mathfrak{C}(\eta)$, $\mathfrak{D}(\zeta)$ *hold, then the classical PRK method with coefficients* $(b_j A_{c_i,c_j}, b_i, c_i;\ b_j \widehat{A}_{c_i,c_j}, b_i, c_i)$ *is symplectic and of order at least*

$$\min(p, 2\alpha + 1),$$

where $\alpha = \min(\eta,\ \zeta,\ p - d^\tau,\ p - d^\sigma)$.

Proof. The symplecticity-preserving property of the associated PRK method can be easily seen from the following fact

$$b_i(b_j \widehat{A}_{c_i,c_j}) + b_j(b_i A_{c_j,c_i}) = b_i b_j,\ \ i,j = 1,\cdots,r.$$

Note that $\widehat{A}_{\tau,\sigma} = 1 - A_{\sigma,\tau}$ is a bivariate polynomial of degree d^σ in τ and degree d^τ in σ, thus inserting $\widehat{d^\tau} = d^\sigma$ and $\widehat{d^\sigma} = d^\tau$ into the formula given in Theorem 2.5 gives the final result. $\qquad\square$

Example 3.2. *Let* $B_\tau = \widehat{B}_\tau \equiv 1,\ C_\tau = \widehat{C}_\tau = \tau$ *and take*

$$
\begin{aligned}
A_{\tau,\sigma} &= \frac{1}{2} + \sum_{\iota=0}^{s-1} \xi_{\iota+1} P_{\iota+1}(\tau) P_\iota(\sigma) - \sum_{\iota=0}^{s-2} \xi_{\iota+1} P_{\iota+1}(\sigma) P_\iota(\tau), \\
\widehat{A}_{\tau,\sigma} &= 1 - A_{\sigma,\tau} = \frac{1}{2} + \sum_{\iota=0}^{s-2} \xi_{\iota+1} P_{\iota+1}(\tau) P_\iota(\sigma) - \sum_{\iota=0}^{s-1} \xi_{\iota+1} P_{\iota+1}(\sigma) P_\iota(\tau),
\end{aligned}
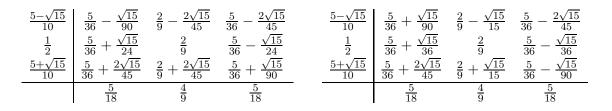\tag{3.8}
$$

$$
\begin{array}{c|ccc}
\frac{5-\sqrt{15}}{10} & \frac{5}{36} - \frac{\sqrt{15}}{90} & \frac{2}{9} - \frac{2\sqrt{15}}{45} & \frac{5}{36} - \frac{2\sqrt{15}}{45} \\
\frac{1}{2} & \frac{5}{36} + \frac{\sqrt{15}}{24} & \frac{2}{9} & \frac{5}{36} - \frac{\sqrt{15}}{24} \\
\frac{5+\sqrt{15}}{10} & \frac{5}{36} + \frac{2\sqrt{15}}{45} & \frac{2}{9} + \frac{2\sqrt{15}}{45} & \frac{5}{36} + \frac{\sqrt{15}}{90} \\
\hline
 & \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array}
\qquad
\begin{array}{c|ccc}
\frac{5-\sqrt{15}}{10} & \frac{5}{36} + \frac{\sqrt{15}}{90} & \frac{2}{9} - \frac{\sqrt{15}}{15} & \frac{5}{36} - \frac{2\sqrt{15}}{45} \\
\frac{1}{2} & \frac{5}{36} + \frac{\sqrt{15}}{36} & \frac{2}{9} & \frac{5}{36} - \frac{\sqrt{15}}{36} \\
\frac{5+\sqrt{15}}{10} & \frac{5}{36} + \frac{2\sqrt{15}}{45} & \frac{2}{9} + \frac{\sqrt{15}}{15} & \frac{5}{36} - \frac{\sqrt{15}}{90} \\
\hline
 & \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array}
$$

Table 3.2: A new symplectic PRK method of order 4 retrieved by Gaussian quadrature.

$$
\begin{array}{c|ccc}
0 & 0 & 0 & 0 \\
\frac{6-\sqrt{6}}{10} & \frac{19}{150} - \frac{\sqrt{6}}{225} & \frac{1}{4} + \frac{\sqrt{6}}{72} & \frac{67}{300} - \frac{197\sqrt{6}}{1800} \\
\frac{6+\sqrt{6}}{10} & \frac{19}{150} + \frac{\sqrt{6}}{225} & \frac{67}{300} + \frac{197\sqrt{6}}{1800} & \frac{1}{4} - \frac{\sqrt{6}}{72} \\
\hline
 & \frac{1}{9} & \frac{16+\sqrt{6}}{36} & \frac{16-\sqrt{6}}{36}
\end{array}
\qquad
\begin{array}{c|ccc}
0 & \frac{1}{9} & -\frac{1}{18} + \frac{\sqrt{6}}{72} & -\frac{1}{18} - \frac{\sqrt{6}}{72} \\
\frac{6-\sqrt{6}}{10} & \frac{1}{9} & \frac{7}{36} + \frac{\sqrt{6}}{72} & \frac{53}{180} - \frac{41\sqrt{6}}{360} \\
\frac{6+\sqrt{6}}{10} & \frac{1}{9} & \frac{53}{180} + \frac{41\sqrt{6}}{360} & \frac{7}{36} - \frac{\sqrt{6}}{72} \\
\hline
 & \frac{1}{9} & \frac{16+\sqrt{6}}{36} & \frac{16-\sqrt{6}}{36}
\end{array}
$$

Table 3.3: A new symplectic PRK method of order 4 retrieved by Radau-Left quadrature.

$$
\begin{array}{c|ccc}
\frac{4-\sqrt{6}}{10} & \frac{14-\sqrt{6}}{72} & \frac{398-147\sqrt{6}}{1800} & \frac{-7-2\sqrt{6}}{450} \\
\frac{4+\sqrt{6}}{10} & \frac{398+147\sqrt{6}}{1800} & \frac{14+\sqrt{6}}{72} & \frac{-7+2\sqrt{6}}{450} \\
1 & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9} \\
\hline
 & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9}
\end{array}
\qquad
\begin{array}{c|ccc}
\frac{4-\sqrt{6}}{10} & \frac{1}{4} - \frac{\sqrt{6}}{72} & \frac{3}{20} - \frac{31\sqrt{6}}{360} & 0 \\
\frac{4+\sqrt{6}}{10} & \frac{3}{20} + \frac{31\sqrt{6}}{360} & \frac{1}{4} + \frac{\sqrt{6}}{72} & 0 \\
1 & \frac{1}{2} - \frac{\sqrt{6}}{72} & \frac{1}{2} + \frac{\sqrt{6}}{72} & 0 \\
\hline
 & \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9}
\end{array}
$$

Table 3.4: A new symplectic PRK method of order 4 retrieved by Radau-Right quadrature.

$$
\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
\frac{5-\sqrt{5}}{10} & \frac{11-\sqrt{5}}{120} & \frac{25+\sqrt{5}}{120} & \frac{25-11\sqrt{5}}{120} & \frac{-1-\sqrt{5}}{120} \\
\frac{5+\sqrt{5}}{10} & \frac{11+\sqrt{5}}{120} & \frac{25+11\sqrt{5}}{120} & \frac{25-\sqrt{5}}{120} & \frac{-1+\sqrt{5}}{120} \\
1 & \frac{1}{12} & \frac{5}{12} & \frac{5}{12} & \frac{1}{12} \\
\hline
 & \frac{1}{12} & \frac{5}{12} & \frac{5}{12} & \frac{1}{12}
\end{array}
\qquad
\begin{array}{c|cccc}
0 & \frac{1}{12} & \frac{-1+\sqrt{5}}{24} & \frac{-1-\sqrt{5}}{24} & 0 \\
\frac{5-\sqrt{5}}{10} & \frac{1}{12} & \frac{25-\sqrt{5}}{120} & \frac{25-11\sqrt{5}}{120} & 0 \\
\frac{5+\sqrt{5}}{10} & \frac{1}{12} & \frac{25+11\sqrt{5}}{120} & \frac{25+\sqrt{5}}{120} & 0 \\
1 & \frac{1}{12} & \frac{11+\sqrt{5}}{24} & \frac{11-\sqrt{5}}{24} & 0 \\
\hline
 & \frac{1}{12} & \frac{5}{12} & \frac{5}{12} & \frac{1}{12}
\end{array}
$$

Table 3.5: A new symplectic PRK method of order 4 retrieved by Lobatto quadrature.

$$
\begin{array}{c|ccc}
\frac{5-\sqrt{15}}{10} & \frac{2}{9} & \frac{2}{9} - \frac{2\sqrt{15}}{45} & \frac{1}{18} - \frac{\sqrt{15}}{18} \\
\frac{1}{2} & \frac{5}{36} + \frac{\sqrt{15}}{36} & \frac{2}{9} & \frac{5}{36} - \frac{\sqrt{15}}{36} \\
\frac{5+\sqrt{15}}{10} & \frac{1}{18} + \frac{\sqrt{15}}{18} & \frac{2}{9} + \frac{2\sqrt{15}}{45} & \frac{2}{9} \\
\hline
 & \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array}
\qquad
\begin{array}{c|ccc}
\frac{5-\sqrt{15}}{10} & \frac{1}{18} & \frac{2}{9} - \frac{2\sqrt{15}}{45} & \frac{2}{9} - \frac{\sqrt{15}}{18} \\
\frac{1}{2} & \frac{5}{36} + \frac{\sqrt{15}}{36} & \frac{2}{9} & \frac{5}{36} - \frac{\sqrt{15}}{36} \\
\frac{5+\sqrt{15}}{10} & \frac{2}{9} + \frac{\sqrt{15}}{18} & \frac{2}{9} + \frac{2\sqrt{15}}{45} & \frac{1}{18} \\
\hline
 & \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
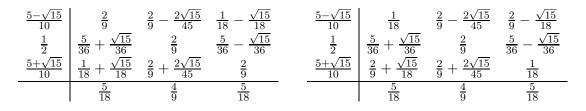\end{array}
$$

Table 3.6: A new symplectic PRK method of order 3 retrieved by Gaussian quadrature.

by using some suitable quadrature formulae with s quadrature points, we can retrieve a lot of classical high order symplectic PRK methods including s-stage Lobatto IIIA-IIIB, Radau IA-I$\bar{A}$, Radau IIA-II$\bar{A}$ and Gauss-Legendre schemes, and the orders are $2s - 2, 2s - 1, 2s - 1, 2s$ respectively.

If we use more quadrature points, then we can get lots of new symplectic PRK schemes which are not found in the literature. For instance, consider $s = 2$, it gives the symplectic PRK schemes shown in Table 3.2-3.5.

Example 3.3. *Let $B_\tau = \widehat{B}_\tau \equiv 1$, $C_\tau = \widehat{C}_\tau = \tau$ and take*

$$
\begin{aligned}
A_{\tau,\sigma} &= \frac{1}{2} + \sum_{\iota=0}^{s-1} \xi_{\iota+1}\Big(P_{\iota+1}(\tau)P_\iota(\sigma) - P_{\iota+1}(\sigma)P_\iota(\tau)\Big) + \frac{1}{2(2s+1)}P_s(\tau)P_s(\sigma), \\
\widehat{A}_{\tau,\sigma} &= 1 - A_{\sigma,\tau} = \frac{1}{2} + \sum_{\iota=0}^{s-1} \xi_{\iota+1}\Big(P_{\iota+1}(\tau)P_\iota(\sigma) - P_{\iota+1}(\sigma)P_\iota(\tau)\Big) - \frac{1}{2(2s+1)}P_s(\tau)P_s(\sigma),
\end{aligned}
\tag{3.9}
$$

by using suitable quadrature formulae with $s+1$ quadrature points, we can retrieve a lot of classical high order symplectic PRK methods including $(s+1)$-stage Lobatto IIIC-III$\bar{C}$, Radau IA-I$\bar{A}$, Radau IIA-II$\bar{A}$ and Gauss IA-I$\bar{A}$ schemes[2], and the orders are $2s, 2s + 1, 2s + 1, 2s + 1$ respectively.

If we use more quadrature formulae with different number of quadrature points, then we can get more new symplectic PRK schemes. Table 3.6 provides a symplectic PRK scheme based on Gaussian quadrature for the case $s = 1$.

4. Conclusions

This paper investigates the construction of symplectic (P)RK type methods based on continuous-stage (P)RK methods. In the process of construction, we first discuss the general continuous-stage (P)RK methods with the help of the simplifying assumptions and the expansion technique of orthogonal polynomials (i.e., Legendre polynomials), and then establish (P)RK methods in classical sense by means of numerical quadrature formulae. The newly obtained results are then directly applied to construct a special class of (P)RK methods which have symplecticity-preserving property for solving Hamiltonian systems. The line of construction of numerical algorithms combines the continuous and discrete mathematical theory, which forms a new and simple way for numerical integration of ODEs especially for Hamiltonian systems with a symplectic structure.

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