

A note on continuous-stage Runge-Kutta methods

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Abstract

We provide a note on continuous-stage Runge-Kutta methods (csRK) for solving initial value problems of first-order ordinary differential equations. Such methods, as an interesting and creative extension of traditional Runge-Kutta (RK) methods, can give us a new perspective on RK discretization and it may enlarge the application of RK approximation theory in modern mathematics and engineering fields. A highlighted advantage of investigation of csRK methods is that we do not need to study the tedious solution of multi-variable nonlinear algebraic equations associated with order conditions. In this note, we will discuss and promote the recently-developed csRK theory. In particular, we will place emphasis on geometric integrators including symplectic methods, symmetric methods and energy-preserving methods which play a central role in the field of geometric numerical integration.

Keywords: Continuous-stage Runge-Kutta methods; Hamiltonian systems; Symplectic methods; Conjugate-symplectic methods; Energy-preserving methods; Symmetric methods.

1. Introduction

Since the pioneering work of Runge in 1895 [27] and Kutta in 1901 [21], Runge-Kutta (RK) methods have been developed very well for over a hundred and twenty years [6, 7, 15, 16]. However, continuous-stage Runge-Kutta (csRK) methods, as an interesting and creative extension of traditional RK methods, begin entering people's horizons only in recent years. As far as we know, the most original idea of such methods can be dated back to the early work by Butcher in 1972 [5] (see also [7]), in which RK methods were generalized by allowing the schemes to be "continuous" with "infinitely many stages". It is surprising that there was a very long period of quiescence without any development. Until the year 2010, Hairer pulled the idea back by exploiting it to explain and analyze energy-preserving collocation

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methods he proposed in [18]. Subsequently, Tang & Sun [33, 35] found that some Galerkin time-discretization methods for ordinary differential equations (ODEs) can be equivalently transformed into csRK methods, which implies that RK-type methods bear a close relationship to Galerkin variational methods. Based on these previous studies, Tang & Sun further went deep into the discussion of constructive theory of csRK methods in [32, 34], where orthogonal polynomial expansion techniques combined with order theory were firstly utilized. These studies show that an interesting and highlighted advantage of considering csRK methods is that we do not need to study the tedious solution of multi-variable nonlinear algebraic equations associated with order conditions. More recently, Tang et al have derived some extensions of csRK methods by using similar techniques, see [36, 37, 38], in which continuous-stage partitioned Runge-Kutta methods and Runge-Kutta-Nyström methods are being proposed and investigated. Miyatake & Butcher [24, 25] investigate an energy-preserving condition in terms of the coefficients of csRK methods for solving Hamiltonian systems, and extend the theory of exponentially-fitted RK methods in the context of csRK methods. Besides, Li & Wu [23] proposed functionally fitted energy-preserving methods for oscillatory nonlinear Hamiltonian systems and showed that they can be transformed into a class of csRK methods.

It is well known that geometric numerical integration has become a major thread in numerical mathematics since around 30 years ago [12, 13, 17, 29]. RK methods are greatly developed in such a promising field since 1988 [22, 28, 31]. By introducing a completely new framework, csRK methods opened up their own important but distinctive (compared with the traditional RK methods) avenues in the study of geometric numerical integration. For instance, some recent literatures show that there exists csRK methods which are structure-preserving including symplectic csRK methods [34, 32], conjugate-symplectic (up to a finite order) csRK methods [19, 34], symmetric csRK methods [18, 34, 32], energy-preserving csRK methods [3, 25, 8, 18, 26, 34, 32]. Particularly, there are fruitful energy-preserving methods being proposed from different approaches recently, e.g., energy-preserving trapezoidal methods [20], average vector field method (AVFM) (a kind of discrete gradient method) [26], Hamiltonian boundary value methods (HBVMs) [3], continuous time finite element methods (TFEMs) [2, 11, 33], energy-preserving collocation methods (EPCMs) [18]. However, all these methods can be unified in the framework of csRK methods [33]. In addition, csRK methods may promote the investigation of energy-preserving methods which are conjugate symplectic (up to a finite order) [19, 34].

It is worth mentioning that some special-purpose algorithms are impossible to exist in the classic context of RK methods but they can be created fruitfully within the new framework. For example, Celledoni et al [8] proved that there exists no energy-preserving RK methods for general non-polynomial Hamiltonian systems, but energy-preserving csRK methods obviously exist [25, 18, 26, 34, 32]. Furthermore, some numerical integrators can not be perfectly explained in the classic RK framework, but they can be clearly understood [33, 35] with the help of csRK methods (e.g., AVFM [26], ∞ -HBVMs [3], EPCMs [18], Galerkin TFEMs [2, 11] etc). Hence, it seems that continuous-stage methods provide us a new realm for

numerical solution of ODEs and it may produce new applications in various fields especially in geometric numerical integration [32, 34, 24, 25, 36, 37, 38].

This note is organized as follows. In Section 2, we contrive to investigate the construction of csRK methods. Based on polynomial expansion techniques, two effective ways to obtain csRK methods will be introduced. Section 3 is devoted to discussing the geometric numerical integration by csRK methods. Some algebraic conditions for geometric integration are presented, and the ideas of designing geometric integrators are sketched with the help of them. In the final section, we give some concluding remarks to end this note.

2. Construction of csRK methods

For an initial value problem of first-order system in the form

$$\dot{\mathbf{z}} = \mathbf{f}(t, \mathbf{z}), \quad \mathbf{z}(t_0) = \mathbf{z}_0 \in \mathbb{R}^d, \quad (2.1)$$

we introduce the following definition of csRK methods.

Definition 2.1. [18, 34] Let $A_{\tau, \sigma}$ be a function of two variables $\tau, \sigma \in [0, 1]$, and B_τ, C_τ be functions of $\tau \in [0, 1]$. The one-step method $\Phi_h : \mathbf{z}_0 \mapsto \mathbf{z}_1$ given by

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

is called a continuous-stage Runge-Kutta (csRK) method, where $\mathbf{Z}_\tau \approx \mathbf{z}(t_0 + C_\tau h)$. For the sake of internal consistency, here we often assume that

$$C_\tau = \int_0^1 A_{\tau, \sigma} d\sigma. \quad (2.3)$$

A csRK method is of order p , if as $h \rightarrow 0$, for all sufficiently regular problem (2.1) its *local error* satisfies

$$\mathbf{z}_1 - \mathbf{z}(t_0 + h) = \mathcal{O}(h^{p+1}).$$

The uniqueness and existence of the solution of csRK schemes are guaranteed by the following theorem.

Theorem 2.1. [33, 25] Assume \mathbf{f} is Lipschitz continuous with constant L . If step size h satisfies

$$h < \frac{1}{L \max_{\tau \in [0, 1]} \int_0^1 |A_{\tau, \sigma}| d\sigma},$$

then there exists a unique solution of (2.2).

Theorem 2.2. Assume a csRK method with coefficients $(A_{\tau, \sigma}, B_\tau, C_\tau)$ satisfies the following two conditions:

(a) $\chi(\xi) = \int_0^\xi B_\tau d\tau$, $\xi \in [0, 1]$ has an inverse function and B_τ is non-vanishing almost everywhere (e.g., if $B_\tau > 0$ in $[0, 1]$, then this condition is fulfilled);

(b) $\check{B}(\rho)$ holds for some integer $\rho \geq 1$, where¹

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

then the method can always be transformed into a new csRK method with $B_\tau \equiv 1$, $\tau \in [0, 1]$.

Proof. Note that the special case with $B_\tau > 0$ has been given in [34], and the more general case can be proved very similarly (cf. [34], Proposition 2.1, page 181). \square

In what follows, we attempt to construct csRK methods by using orthogonal polynomial expansion techniques. For convenience, we often assume $B_\tau \equiv 1$ (in view of Theorem 2.2) and let $C_\tau \equiv \tau$ for the following discussions. Firstly, we need to introduce the following ι -degree normalized shifted Legendre polynomial $P_\iota(x)$ by using the Rodrigues' formula

$$P_0(x) = 1, \quad P_\iota(x) = \frac{\sqrt{2\iota+1}}{\iota!} \frac{d^\iota}{dx^\iota} \left(x^\iota (x-1)^\iota \right), \quad \iota = 1, 2, 3, \dots$$

They are orthogonal to each other with respect to the L^2 inner product on $[0, 1]$

$$\int_0^1 P_\iota(t) P_\kappa(t) dt = \delta_{\iota\kappa}, \quad \iota, \kappa = 0, 1, 2, \dots,$$

and satisfy the following integration formulae [16]

$$\begin{aligned} \int_0^x P_0(t) dt &= \xi_1 P_1(x) + \frac{1}{2} P_0(x), \\ \int_0^x P_\iota(t) dt &= \xi_{\iota+1} P_{\iota+1}(x) - \xi_\iota P_{\iota-1}(x), \quad \iota = 1, 2, 3, \dots, \\ \int_x^1 P_\iota(t) dt &= \delta_{\iota 0} - \int_0^x P_\iota(t) dt, \quad \iota = 0, 1, 2, \dots, \end{aligned} \tag{2.4}$$

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

Since $\{P_i(\tau)P_j(\sigma)\}_{i,j=0}^\infty$ forms a complete orthogonal basis in function space $L^2([0, 1] \times [0, 1])$, we can expand $A_{\tau, \sigma}$ as

$$A_{\tau, \sigma} = \sum_{0 \leq i, j \in \mathbb{Z}} \alpha_{(i,j)} P_i(\tau) P_j(\sigma), \quad \alpha_{(i,j)} \in \mathbb{R}, \tag{2.5}$$

where $\alpha_{(i,j)}$ are real parameters to be determined.

¹This condition is always fulfilled for a csRK method of order at least 1 (cf., simplifying conditions in (2.9)).

By substituting (2.5) into (2.3), we have

$$C_\tau = \int_0^1 A_{\tau,\sigma} d\sigma = \int_0^1 \left(\sum_{0 \leq i,j \in \mathbb{Z}} \alpha_{(i,j)} P_i(\tau) P_j(\sigma) \right) d\sigma = \sum_{i \geq 0} \alpha_{(i,0)} P_i(\tau).$$

Note that the first formula of (2.4) implies

$$C_\tau \equiv \tau = \frac{1}{2} P_0(\tau) + \frac{\sqrt{3}}{6} P_1(\tau), \quad (2.6)$$

then, by comparing the two formulae above with each other, we get

$$\alpha_{(0,0)} = \frac{1}{2}, \quad \alpha_{(1,0)} = \frac{\sqrt{3}}{6}, \quad \alpha_{(i,0)} = 0, \quad i \geq 2.$$

2.1. Construction of csRK methods order by order

Analogously to the traditional case of RK-type methods [17], by B-series theory we have the following order conditions up to order 4 (under the condition (2.3)):

$$\left| \begin{array}{ll} (1) \int_0^1 B_\tau d\tau = 1; & (5) \int_0^1 B_\tau C_\tau^3 d\tau = \frac{1}{4}; \\ (2) \int_0^1 B_\tau C_\tau d\tau = \frac{1}{2}; & (6) (\int_0^1)^2 B_\tau C_\tau C_\sigma A_{\tau,\sigma} d\tau d\sigma = \frac{1}{8}; \\ (3) \int_0^1 B_\tau C_\tau^2 d\tau = \frac{1}{3}; & (7) (\int_0^1)^2 B_\tau C_\sigma^2 A_{\tau,\sigma} d\tau d\sigma = \frac{1}{12}; \\ (4) (\int_0^1)^2 B_\tau C_\sigma A_{\tau,\sigma} d\tau d\sigma = \frac{1}{6}; & (8) (\int_0^1)^3 B_\tau C_\rho A_{\tau,\sigma} A_{\sigma,\rho} d\tau d\sigma d\rho = \frac{1}{24}. \end{array} \right|$$

If the condition (1) holds, then the csRK method is of order 1; if conditions (1)-(2) hold, then the csRK method is of order 2; if conditions (1)-(4) hold, then the csRK method is of order 3; if conditions (1)-(8) hold, then the csRK method is of order 4.

By hypothesis (i.e., $B_\tau \equiv 1$ and $C_\tau \equiv \tau$), conditions (1)-(3) and (5) are automatically satisfied. Therefore, the remaining 4 conditions are to be considered. Our approach is to substitute the expansion formula (2.5) into the conditions one by one so as to get the requirements in terms of the expansion coefficients. In the following the orthogonality of Legendre polynomials and formula (2.6) will be used several times.

For condition (4):

$$\begin{aligned} \left(\int_0^1 \right)^2 B_\tau A_{\tau,\sigma} C_\sigma d\tau d\sigma &= \int_0^1 \left(\int_0^1 A_{\tau,\sigma} d\tau \right) \sigma d\sigma \\ &= \int_0^1 \left(\sum_{j \geq 0} \alpha_{(0,j)} P_j(\sigma) \right) \left(\frac{1}{2} P_0(\sigma) + \frac{\sqrt{3}}{6} P_1(\sigma) \right) d\sigma = \frac{1}{2} \alpha_{(0,0)} + \frac{\sqrt{3}}{6} \alpha_{(0,1)} = \frac{1}{6}, \end{aligned}$$

which then gives $\alpha_{(0,1)} = -\frac{\sqrt{3}}{6}$.

For condition (6):

$$\begin{aligned}
& \left(\int_0^1 \right)^2 B_\tau C_\tau C_\sigma A_{\tau,\sigma} d\tau d\sigma = \int_0^1 \left(\int_0^1 \tau A_{\tau,\sigma} d\tau \right) \sigma d\sigma \\
& = \int_0^1 \left(\int_0^1 \left(\frac{1}{2} P_0(\tau) + \frac{\sqrt{3}}{6} P_1(\tau) \right) \left(\sum_{0 \leq i, j \in \mathbb{Z}} \alpha_{(i,j)} P_i(\tau) P_j(\sigma) \right) d\tau \right) \sigma d\sigma \\
& = \int_0^1 \left(\frac{1}{2} \sum_{j \geq 0} \alpha_{(0,j)} P_j(\sigma) + \frac{\sqrt{3}}{6} \sum_{j \geq 0} \alpha_{(1,j)} P_j(\sigma) \right) \left(\frac{1}{2} P_0(\sigma) + \frac{\sqrt{3}}{6} P_1(\sigma) \right) d\sigma \\
& = \frac{1}{4} \alpha_{(0,0)} + \frac{\sqrt{3}}{12} \alpha_{(1,0)} + \frac{\sqrt{3}}{12} \alpha_{(0,1)} + \frac{1}{12} \alpha_{(1,1)} = \frac{1}{8},
\end{aligned}$$

which then gives $\alpha_{(1,1)} = 0$.

For condition (7):

$$\begin{aligned}
& \left(\int_0^1 \right)^2 B_\tau C_\sigma^2 A_{\tau,\sigma} d\tau d\sigma = \int_0^1 \left(\int_0^1 A_{\tau,\sigma} d\tau \right) \sigma^2 d\sigma \\
& = \int_0^1 \left(\sum_{j \geq 0} \alpha_{(0,j)} P_j(\sigma) \right) \left(\frac{1}{3} P_0(\sigma) + \frac{\sqrt{3}}{6} P_1(\sigma) + \frac{\sqrt{5}}{30} P_2(\sigma) \right) d\sigma \\
& = \frac{1}{3} \alpha_{(0,0)} + \frac{\sqrt{3}}{6} \alpha_{(0,1)} + \frac{\sqrt{5}}{30} \alpha_{(0,2)} = \frac{1}{12},
\end{aligned}$$

which then gives $\alpha_{(0,2)} = 0$. Here we used an identity

$$\sigma^2 = 2 \int_0^\sigma \left(\int_0^x P_0(t) dt \right) dx = \frac{1}{3} P_0(\sigma) + \frac{\sqrt{3}}{6} P_1(\sigma) + \frac{\sqrt{5}}{30} P_2(\sigma)$$

which is deduced from (2.4).

For condition (8):

$$\begin{aligned}
& \left(\int_0^1 \right)^3 B_\tau C_\rho A_{\tau,\sigma} A_{\sigma,\rho} d\tau d\sigma d\rho = \int_0^1 \left(\int_0^1 A_{\tau,\sigma} d\tau \right) \left(\int_0^1 \rho A_{\sigma,\rho} d\rho \right) d\sigma \\
& = \int_0^1 \left(\sum_{j \geq 0} \alpha_{(0,j)} P_j(\sigma) \right) \left(\frac{1}{2} \sum_{i \geq 0} \alpha_{(i,0)} P_i(\sigma) + \frac{\sqrt{3}}{6} \sum_{i \geq 0} \alpha_{(i,1)} P_i(\sigma) \right) d\sigma \\
& = \frac{1}{2} \sum_{i \geq 0} \alpha_{(0,i)} \alpha_{(i,0)} + \frac{\sqrt{3}}{6} \sum_{i \geq 0} \alpha_{(0,i)} \alpha_{(i,1)} = \frac{1}{24},
\end{aligned}$$

which then gives $\frac{1}{2} \sum_{i \geq 2} \alpha_{(0,i)} \alpha_{(i,0)} + \frac{\sqrt{3}}{6} \sum_{i \geq 2} \alpha_{(0,i)} \alpha_{(i,1)} = 0$. Take into account that $\alpha_{(0,2)} = 0$ and $\alpha_{(i,0)} = 0$, $i \geq 2$, and then it ends up with $\sum_{i \geq 3} \alpha_{(0,i)} \alpha_{(i,1)} = 0$.

Theorem 2.3. *Under the assumptions $B_\tau \equiv 1$ and $C_\tau \equiv \tau$, the csRK method (2.2) with $A_{\tau,\sigma}$ given by*

$$A_{\tau,\sigma} = \frac{1}{2} + \frac{\sqrt{3}}{6} P_1(\tau) + \sum_{i \geq 0, j \geq 1} \alpha_{(i,j)} P_i(\tau) P_j(\sigma), \quad \alpha_{(i,j)} \in \mathbb{R}, \quad (2.7)$$

is of order 2 at least. Moreover, if we additionally require $\alpha_{(0,1)} = -\frac{\sqrt{3}}{6}$, then the method is of order 3 at least; if we require, additionally,

$$\alpha_{(1,1)} = 0, \alpha_{(0,2)} = 0, \sum_{i \geq 3} \alpha_{(0,i)} \alpha_{(i,1)} = 0, \quad (2.8)$$

then the method is of order 4 at least.

2.2. Construction of high-order csRK methods

Although we can construct csRK methods of arbitrarily high order via the above technique order by order, it is not an easy task to derive higher order methods, seeing that the number of order conditions will increase dramatically [17, 15, 16] and one has to conduct more tedious and complicated computation. To overcome these difficulties, we have to use the following *simplifying assumptions* [18]

$$\begin{aligned} \check{B}(\rho) : \quad & \int_0^1 B_\tau C_\tau^{\kappa-1} d\tau = \frac{1}{\kappa}, \quad \kappa = 1, \dots, \rho, \\ \check{C}(\eta) : \quad & \int_0^1 A_{\tau,\sigma} C_\sigma^{\kappa-1} d\sigma = \frac{1}{\kappa} C_\tau^\kappa, \quad \kappa = 1, \dots, \eta, \\ \check{D}(\zeta) : \quad & \int_0^1 B_\tau C_\tau^{\kappa-1} A_{\tau,\sigma} d\tau = \frac{1}{\kappa} B_\sigma (1 - C_\sigma^\kappa), \quad \kappa = 1, \dots, \zeta. \end{aligned} \quad (2.9)$$

Actually, Tang & Sun [34] have investigated the construction of high-order methods by using these *simplifying assumptions*. Now we give a brief review of some existing results. The following result is completely similar to the classic result by Butcher in 1964 [4].

Theorem 2.4. [34] *If the coefficients $(A_{\tau,\sigma}, B_\tau, C_\tau)$ of method (2.2) satisfy $\check{B}(\rho)$, $\check{C}(\alpha)$ and $\check{D}(\beta)$, then the method is of order at least $\min(\rho, 2\alpha + 2, \alpha + \beta + 1)$.*

Theorem 2.5. [34] *For a csRK method with $B_\tau \equiv 1$ and $C_\tau = \tau$ (then $\check{B}(\infty)$ holds), the following two statements are equivalent to each other: (a) Both $\check{C}(\alpha)$ and $\check{D}(\beta)$ hold; (b) The coefficient $A_{\tau,\sigma}$ has the following form in terms of Legendre polynomials*

$$A_{\tau,\sigma} = \frac{1}{2} + \sum_{\iota=0}^{N_1} \xi_{\iota+1} P_{\iota+1}(\tau) P_\iota(\sigma) - \sum_{\iota=0}^{N_2} \xi_{\iota+1} P_{\iota+1}(\sigma) P_\iota(\tau) + \sum_{i \geq \beta, j \geq \alpha} \alpha_{(i,j)} P_i(\tau) P_j(\sigma), \quad (2.10)$$

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 $\alpha_{(i,j)}$ are any real parameters.

By combining Theorem 2.4 with Theorem 2.5 we can easily construct csRK methods of arbitrarily high order, the order of which are given by $\min(\infty, 2\alpha + 2, \alpha + \beta + 1) = \min(2\alpha + 2, \alpha + \beta + 1)$. For example, if we take $\alpha = 2, \beta = 1$ in Theorem 2.5, then we get a family of 4-order methods which can be retrieved by taking

$$\alpha_{(0,i)} = \alpha_{(i,1)} = 0, \quad i \geq 3, \quad \alpha_{(2,1)} = \xi_2 = \frac{\sqrt{15}}{30},$$

in Theorem 2.3. Note that methods constructed by Theorem 2.3 cover all the methods given by Theorem 2.5 (as we construct methods up to order 4). This implies that we will lose the opportunity to discover many other new csRK methods by using Theorem 2.5, even though it is much easier to construct high-order csRK methods compared with the approach shown in subsection 2.1.

To derive a practical csRK method, we need to get a finite form of $A_{\tau,\sigma}$ by truncating the series (2.10). In such a case, without loss a generality, we assume $A_{\tau,\sigma}$ is a bivariate polynomial of degree π_A^τ in τ and degree π_A^σ in σ . Applying a quadrature formula $(b_i, c_i)_{i=1}^s$ ($0 \leq c_i \leq 1$) to (2.2), we derive an s -stage RK method

$$\begin{aligned}\tilde{\mathbf{Z}}_i &= \mathbf{z}_0 + h \sum_{j=1}^s b_j A_{c_i, c_j} \mathbf{f}(t_0 + c_j h, \tilde{\mathbf{Z}}_j), \quad i = 1, \dots, s, \\ \mathbf{z}_1 &= \mathbf{z}_0 + h \sum_{i=1}^s b_i B_{c_i} \mathbf{f}(t_0 + c_i h, \tilde{\mathbf{Z}}_i),\end{aligned}\tag{2.11}$$

where $\tilde{\mathbf{Z}}_i \approx \mathbf{Z}_{c_i}$.

Theorem 2.6. [36] *Assume $A_{\tau,\sigma}$ is a bivariate polynomial of degree π_A^τ in τ and degree π_A^σ in σ , and the quadrature formula $(b_i, c_i)_{i=1}^s$ is of order² 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 $\check{B}(\infty)$ holds) and both $\check{C}(\eta)$, $\check{D}(\zeta)$ hold, then the classic RK method (2.11) with coefficients $(b_j A_{c_i, c_j}, b_i, c_i)$ is of order at least*

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

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

Theorem 2.6 tells us how to construct a traditional RK scheme based on csRK methods. The most highlighted advantage of such approach to construct RK-type methods is that we do not need to consider and study the tedious solution of nonlinear algebraic equations deduced from order conditions. It turns out that this approach [32, 34] is comparable to the W-transformation technique proposed by Hairer & Wanner [16].

3. Geometric numerical integration by csRK methods

In this section, we mainly focus on the geometric numerical integration of Hamiltonian problem

$$\dot{\mathbf{z}} = J^{-1} \nabla H(\mathbf{z}), \quad \mathbf{z}(t_0) = \mathbf{z}_0 \in \mathbb{R}^{2d},\tag{3.1}$$

where $J = \begin{pmatrix} \mathbf{0} & I_d \\ -I_d & \mathbf{0} \end{pmatrix}$ (with I_d the $d \times d$ identity matrix) is a standard structure matrix, $H : \mathbb{R}^{2d} \rightarrow \mathbb{R}$ is the Hamiltonian function which generally represents the total energy of the given system. The system (3.1) has two main geometric properties [1]:

²The quadrature formula is of order p iff $\int_0^1 f(x) dx = \sum_{i=1}^s b_i f(c_i)$ holds for any polynomial $f(x)$ of degree up to $p - 1$.

(a) Energy preservation: $H(\mathbf{z}(t)) \equiv H(\mathbf{z}(t_0))$ for $\forall t$;

(b) Symplecticity (Poincaré 1899): $d\mathbf{z}(t) \wedge Jd\mathbf{z}(t) = d\mathbf{z}(t_0) \wedge Jd\mathbf{z}(t_0)$ for $\forall t$.

It is known that property (b) is a characteristic property for Hamiltonian systems (see [17], Theorem 2.6, page 185) and it essentially implies (a). A well-known negative result given by Ge & Marsden [14] manifests that, generally, we can not have a numerical method which exactly preserves both properties at the same time³. It has been evidenced that symplectic methods possess a nearly energy-preserving property (exactly preserve a modified Hamiltonian) for long-term computation [17], while energy-preserving methods will lose the symplecticity in general—It may possibly lead to incorrect phase space behavior. Particularly, when symplectic methods are applied to integrable and near-integrable systems, they produce excellent numerical behaviors: linear error growth, long-time near-conservation of first integrals, existence of invariant tori [17, 30]. For these reasons, symplectic methods have been drawn more attentions in geometric integration. However, energy-preserving methods are also of interest in many fields, e.g., molecular dynamics, plasma physics etc [13, 17, 29]. An interesting result is that there exists an energy-preserving B-series integrator which is conjugate to a symplectic method [10], but it remains a challenge to construct a computational method owning such a symplectic-like property [19]. Besides, symmetric methods are popular for solving many time-reversible problems arising in various fields, and they share many similar excellent long-time properties with symplectic methods especially when they are applied to (near-)integrable systems [17]. In general, energy-preserving methods for time-reversible Hamiltonian system are often expected to be symmetric.

3.1. Symplectic csRK methods

In this part, we will firstly study the condition for csRK methods to be symplectic, and then discuss the construction of symplectic methods.

Theorem 3.1. *If the coefficients of a csRK method (2.2) satisfy*

$$B_\tau A_{\tau,\sigma} + B_\sigma A_{\sigma,\tau} \equiv B_\tau B_\sigma, \quad \tau, \sigma \in [0, 1], \quad (3.2)$$

then it is symplectic.

Proof. Applying a csRK method to Hamiltonian system (3.1) it gives

$$\begin{aligned} \mathbf{Z}_\tau &= \mathbf{z}_0 + h \int_0^\tau A_{\tau,\sigma} \mathbf{f}(\mathbf{Z}_\sigma) d\sigma, \quad \tau \in [0, 1], \\ \mathbf{z}_1 &= \mathbf{z}_0 + h \int_0^1 B_\tau \mathbf{f}(\mathbf{Z}_\tau) d\tau, \end{aligned} \quad (3.3)$$

³For linear Hamiltonian systems, there exists numerical methods which exactly preserve energy and symplecticity simultaneously, e.g., symplectic RK methods can preserve all quadratic invariants including the quadratic Hamiltonian [17].

where $\mathbf{f}(\mathbf{z}) = J^{-1}\nabla H(\mathbf{z})$. Our aim is to verify the following identity

$$d\mathbf{z}_1 \wedge Jd\mathbf{z}_1 = d\mathbf{z}_0 \wedge Jd\mathbf{z}_0. \quad (3.4)$$

In the following, we denote the (k, l) -element of J by J_{kl} and the i th component of a vector \mathbf{v} by $\mathbf{v}^{(i)}$. From the first formula of (3.3), we conclude

$$d\mathbf{z}_0^{(i)} = d\mathbf{Z}_\tau^{(i)} - h \int_0^1 A_{\tau, \sigma} d\mathbf{f}^{(i)}(\mathbf{Z}_\sigma) d\sigma = d\mathbf{Z}_\sigma^{(i)} - h \int_0^1 A_{\sigma, \tau} d\mathbf{f}^{(i)}(\mathbf{Z}_\tau) d\tau, \quad 1 \leq i \leq 2d, \quad (3.5)$$

which will be used later. Making difference between left-hand side and right-hand side of (3.4), it yields

$$\begin{aligned} d\mathbf{z}_1 \wedge Jd\mathbf{z}_1 - d\mathbf{z}_0 \wedge Jd\mathbf{z}_0 &= \sum_{k,l} J_{kl} d\mathbf{z}_1^{(k)} \wedge d\mathbf{z}_1^{(l)} - \sum_{k,l} J_{kl} d\mathbf{z}_0^{(k)} \wedge d\mathbf{z}_0^{(l)} \\ &= \sum_{k,l} J_{kl} \left((d\mathbf{z}_0^{(k)} + h \int_0^1 B_\tau d\mathbf{f}^{(k)}(\mathbf{Z}_\tau) d\tau) \wedge (d\mathbf{z}_0^{(l)} + h \int_0^1 B_\sigma d\mathbf{f}^{(l)}(\mathbf{Z}_\sigma) d\sigma) - d\mathbf{z}_0^{(k)} \wedge d\mathbf{z}_0^{(l)} \right) \\ &= \sum_{k,l} J_{kl} \left(h \int_0^1 B_\sigma d\mathbf{z}_0^{(k)} \wedge d\mathbf{f}^{(l)}(\mathbf{Z}_\sigma) d\sigma + h \int_0^1 B_\tau d\mathbf{f}^{(k)}(\mathbf{Z}_\tau) \wedge d\mathbf{z}_0^{(l)} d\tau \right. \\ &\quad \left. + h^2 \int_0^1 \int_0^1 B_\tau B_\sigma d\mathbf{f}^{(k)}(\mathbf{Z}_\tau) \wedge d\mathbf{f}^{(l)}(\mathbf{Z}_\sigma) d\tau d\sigma \right) \\ &= \sum_{k,l} J_{kl} \left(h \int_0^1 B_\sigma \underbrace{(d\mathbf{Z}_\sigma^{(k)} - h \int_0^1 A_{\sigma, \tau} d\mathbf{f}^{(k)}(\mathbf{Z}_\tau) d\tau)}_{(a)} \wedge d\mathbf{f}^{(l)}(\mathbf{Z}_\sigma) d\sigma \right. \\ &\quad \left. + h \int_0^1 B_\tau d\mathbf{f}^{(k)}(\mathbf{Z}_\tau) \wedge \underbrace{(d\mathbf{Z}_\tau^{(l)} - h \int_0^1 A_{\tau, \sigma} d\mathbf{f}^{(l)}(\mathbf{Z}_\sigma) d\sigma)}_{(b)} d\tau \right. \\ &\quad \left. + h^2 \int_0^1 \int_0^1 B_\tau B_\sigma d\mathbf{f}^{(k)}(\mathbf{Z}_\tau) \wedge d\mathbf{f}^{(l)}(\mathbf{Z}_\sigma) d\tau d\sigma \right) \\ &= \sum_{k,l} J_{kl} \left(h \int_0^1 B_\sigma d\mathbf{Z}_\sigma^{(k)} \wedge d\mathbf{f}^{(l)}(\mathbf{Z}_\sigma) d\sigma + h \int_0^1 B_\tau d\mathbf{f}^{(k)}(\mathbf{Z}_\tau) \wedge d\mathbf{Z}_\tau^{(l)} d\tau \right. \\ &\quad \left. - h^2 \int_0^1 \int_0^1 \underbrace{M_{\tau, \sigma} d\mathbf{f}^{(k)}(\mathbf{Z}_\tau) \wedge d\mathbf{f}^{(l)}(\mathbf{Z}_\sigma) d\tau d\sigma}_{(c)} \right) \\ &= h \sum_{k,l} J_{kl} \left(\int_0^1 B_\sigma d\mathbf{Z}_\sigma^{(k)} \wedge d\mathbf{f}^{(l)}(\mathbf{Z}_\sigma) d\sigma + \int_0^1 B_\tau d\mathbf{f}^{(k)}(\mathbf{Z}_\tau) \wedge d\mathbf{Z}_\tau^{(l)} d\tau \right) \\ &= h \left(\int_0^1 B_\sigma d\mathbf{Z}_\sigma \wedge Jd\mathbf{f}(\mathbf{Z}_\sigma) d\sigma + \int_0^1 B_\tau d\mathbf{f}(\mathbf{Z}_\tau) \wedge Jd\mathbf{Z}_\tau d\tau \right) \\ &= 2h \int_0^1 B_\sigma d\mathbf{Z}_\sigma \wedge Jd\mathbf{f}(\mathbf{Z}_\sigma) d\sigma, \end{aligned}$$

where (a) and (b) are derived by using (3.5), and (c) vanishes by (3.2) since $M_{\tau,\sigma} := B_\tau A_{\tau,\sigma} + B_\sigma A_{\sigma,\tau} - B_\tau B_\sigma \equiv 0$. At last, the proof finishes by taking into account that

$$d\mathbf{Z}_\sigma \wedge Jd\mathbf{f}(\mathbf{Z}_\sigma) = d\mathbf{Z}_\sigma \wedge JJ^{-1}\nabla^2 H(\mathbf{Z}_\sigma)d\mathbf{Z}_\sigma = d\mathbf{Z}_\sigma \wedge \nabla^2 H(\mathbf{Z}_\sigma)d\mathbf{Z}_\sigma = 0.$$

□

Remark 3.1. *The symplectic condition (3.2) is very similar to the classic result for traditional RK methods (which has been proved to be necessary for irreducible methods [17]). Thus, we conjecture that the condition is also essentially necessary. We leave the proof of this conjecture to our future work.*

It is not an easy task to find out all the symplectic csRK methods from the condition given in Theorem 3.1. Tang et al [34, 36] have presented an alternative condition for symplecticity, which can be seen as a reduction of (3.2). Now we revisit the result given in [34, 36], and actually it suffices for us to get symplectic integrators of arbitrarily high order.

Theorem 3.2. *[34, 36] A csRK method with $B_\tau = 1$, $C_\tau = \tau$ is symplectic if $A_{\tau,\sigma}$ has the following form in terms of Legendre polynomials*

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

where $\alpha_{(i,j)}$ is skew-symmetric, i.e., $\alpha_{(i,j)} = -\alpha_{(j,i)}$, $i + j > 0$.

Proof. Under the assumption $B_\tau = 1$, $C_\tau = \tau$, symplectic condition (3.2) is reduced to

$$A_{\tau,\sigma} + A_{\sigma,\tau} \equiv 1, \quad \text{for } \tau, \sigma \in [0, 1], \quad (3.7)$$

By using the expansion (2.5) and exchanging $\tau \leftrightarrow \sigma$, we have

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

Substituting this formula into (3.7) and collecting the like terms gives

$$\alpha_{(0,0)} = \frac{1}{2}; \quad \alpha_{(i,j)} = -\alpha_{(j,i)}, \quad i + j > 0,$$

which completes the proof. □

Consequently, a simple way to design symplectic csRK methods of arbitrarily high order pops out by putting Theorem 3.2 and 2.5 together, due to that suitable RK coefficients can be easily tuned according to these theorems. Another way is to substitute (3.6) into order conditions (cf. subsection 2.1) one by one, which then produces symplectic methods order by order.

Here we give the following result to show that symplectic RK methods can be easily derived based on symplectic csRK methods. It was shown in [34, 36] that many classic high-order symplectic RK methods including Gauss-Legendre RK schemes, Radau IB, Radau IIB and Lobatto IIIE can be retrieved in this way.

Theorem 3.3. *The RK scheme (2.11) (with coefficients $(b_j A_{c_i, c_j}, b_i B_{c_i}, c_i)$) based on a symplectic csRK method with coefficients satisfying (3.2) is always symplectic.*

Proof. By taking into account that

$$B_{c_i} A_{c_i, c_j} + B_{c_j} A_{c_j, c_i} = B_{c_i} B_{c_j}, \quad i, j = 1, \dots, s,$$

we have

$$(b_i B_{c_i})(b_j A_{c_i, c_j}) + (b_j B_{c_j})(b_i A_{c_j, c_i}) = (b_i B_{c_i})(b_j B_{c_j}), \quad i, j = 1, \dots, s,$$

which get the final result by a classic theorem (cf., [17], page 192). \square

3.2. Symmetric csRK methods

As pointed out in [17], symmetric methods as well as symplectic methods play a central role in the geometric integration of differential equations. In this part, we will give the condition for a csRK method to be symmetric and then show a simple way to construct such geometric integrators.

Definition 3.1. [17] A one-step method ϕ_h is called symmetric (or time-reversible) if it satisfies

$$\phi_h^* = \phi_h,$$

where $\phi_h^* = \phi_{-h}^{-1}$ is referred to as the adjoint method of ϕ_h .

By the definition, a method $z_1 = \phi_h(z_0; t_0, t_1)$ is symmetric if exchanging $h \leftrightarrow -h$, $z_0 \leftrightarrow z_1$ and $t_0 \leftrightarrow t_1$ leaves the original method unaltered. From the definition above, we can prove the following theorem.

Theorem 3.4. *Under the assumption (2.3) and we suppose $\check{B}(\rho)$ holds with $\rho \geq 1$ (which means the method is of order at least 1), then a csRK method is symmetric if*

$$A_{\tau, \sigma} + A_{1-\tau, 1-\sigma} \equiv B_{\sigma}, \quad \tau, \sigma \in [0, 1]. \quad (3.8)$$

Proof. Obviously, (3.8) implies $B_{\sigma} \equiv B_{1-\sigma}$ in $[0, 1]$. Furthermore, by taking an integral on both sides of (3.8) with respect to σ , we get $C_{\tau} + C_{1-\tau} \equiv 1$, $\tau \in [0, 1]$.

Next, let us establish the adjoint method of a given csRK method. From (2.2), by interchanging t_0, z_0, h with $t_1, z_1, -h$ respectively, we have

$$\begin{aligned} \mathbf{Z}_{\tau} &= z_1 - h \int_0^1 A_{\tau, \sigma} \mathbf{f}(t_1 - C_{\sigma} h, \mathbf{Z}_{\sigma}) d\sigma, \quad \tau \in [0, 1], \\ z_0 &= z_1 - h \int_0^1 B_{\tau} \mathbf{f}(t_1 - C_{\tau} h, \mathbf{Z}_{\tau}) d\tau, \end{aligned}$$

Note that $t_1 - C_{\tau} h = t_0 + (1 - C_{\tau})h$, then the second formula can be recast as

$$z_1 = z_0 + h \int_0^1 B_{\tau} \mathbf{f}(t_0 + (1 - C_{\tau})h, \mathbf{Z}_{\tau}) d\tau.$$

By plugging it into the first formula, then it ends up with

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

By replacing τ and σ with $1 - \tau$ and $1 - \sigma$ respectively, and with the help of change of integral variables, we obtain an equivalent scheme

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

which is the adjoint method of the original method, where $\mathbf{Z}_\tau^* = \mathbf{Z}_{1-\tau}$ and

$$\begin{aligned}A_{\tau,\sigma}^* &= B_{1-\sigma} - A_{1-\tau,1-\sigma} \equiv B_\sigma - A_{1-\tau,1-\sigma}, \\ B_\tau^* &= B_{1-\tau} \equiv B_\tau, \quad C_\tau^* = 1 - C_{1-\tau} \equiv C_\tau.\end{aligned}$$

Note that a csRK method can be uniquely determined by its coefficients (cf. Theorem 2.1), hence if we require $A_{\tau,\sigma}^* = A_{\tau,\sigma}$, i.e., (3.8), then the original csRK method is symmetric. \square

Remark 3.2. *The symmetric condition (3.8) is very similar to the classic result for traditional RK methods (which has been proved to be necessary for irreducible methods [17]). Thus, we conjecture that the condition is also essentially necessary. We don't plan to pursue this conjecture here.*

Theorem 3.5. *If the underlying symmetric csRK method with coefficients $(A_{\tau,\sigma}, B_\tau, C_\tau)$ satisfying the condition of Theorem 3.4, then the associated RK method (2.11) is symmetric, provided that the quadrature weights and abscissae satisfy $b_{s+1-i} = b_i$ and $c_{s+1-i} = 1 - c_i$ for all i .*

Proof. An available classic result for an s -stage standard RK method (a_{ij}, b_i, c_i) to be symmetric has revealed the following sufficient condition (see, e.g., [17])

$$a_{ij} + a_{s+1-i, s+1-j} = b_j, \quad i, j = 1, \dots, s.$$

Observe that

$$A_{c_i, c_j} + A_{1-c_i, 1-c_j} = B_{c_j}, \quad i, j = 1, \dots, s, \quad (3.9)$$

and on account of $b_{s+1-i} = b_i$, $c_{s+1-i} = 1 - c_i$, it yields

$$(b_j A_{c_i, c_j}) + (b_{s+1-j} A_{c_{s+1-i}, c_{s+1-j}}) = b_j B_{c_j}, \quad i, j = 1, \dots, s, \quad (3.10)$$

which completes the proof by the classic result. \square

Theorem 3.6. [34] *The csRK method with $B_\tau = 1$ and $C_\tau = \tau$ is symmetric if $A_{\tau,\sigma}$ has the following form in terms of Legendre polynomials*

$$A_{\tau,\sigma} = \frac{1}{2} + \sum_{\substack{i+j \text{ is odd} \\ 0 \leq i,j \in \mathbb{Z}}} \omega_{ij} P_i(\tau) P_j(\sigma), \quad \omega_{ij} \in \mathbb{R}. \quad (3.11)$$

Proof. The result can be easily verified by using the same technique shown in Theorem 3.2 (or cf. [34]). \square

Theorem 3.6 is very useful for constructing symmetric csRK methods in conjunction with Theorem 2.5. It is easy to get a symmetric RK methods based on symmetric csRK methods by using a symmetric quadrature formula [34].

3.3. Energy-preserving csRK methods

Energy-preserving csRK methods were firstly studied in [20, 26, 3, 18, 32, 34], and it was shown that there exists energy-preserving csRK methods which are conjugate-symplectic up to a finite order [18, 19, 34]. Miyatake [24] provided a sufficient condition for energy conservation, and then he & Butcher provided a proof for the necessity of the condition in a “weak” sense [25].

Theorem 3.7. [25] *A csRK method is energy-preserving if $\frac{\partial}{\partial \tau} A_{\tau,\sigma}$ is symmetric, i.e.,*

$$\frac{\partial}{\partial \tau} A_{\tau,\sigma} \equiv \frac{\partial}{\partial \sigma} A_{\sigma,\tau}, \text{ for } \tau, \sigma \in [0, 1],$$

and $A_{0,\sigma} \equiv 0$, $A_{1,\sigma} \equiv B_\sigma$.

Theorem 3.8. [32, 34] *Consider the csRK method (2.2) with $B_\tau = 1$, $C_\tau = \tau$ and*

$$A_{\tau,\sigma} = \sum_{0 \leq l \in \mathbb{Z}} \omega_l \int_0^\tau g_l(x) dx g_l(\sigma), \quad \omega_l \in \mathbb{R}, \quad (3.12)$$

where $g_l(x) \in L^2([0, 1])$ with $g_l(x) = \sum_{0 \leq \kappa \in \mathbb{Z}} a_{l\kappa} P_\kappa(x)$ (Legendre expansion), $a_{l\kappa} \in \mathbb{R}$, then we have

(a) $\check{C}(\eta)$ holds if and only if the parameters ω_l and $a_{l\kappa}$ ($l, \kappa = 0, 1, 2, \dots$) satisfy

$$\sum_{0 \leq l \in \mathbb{Z}} \omega_l a_{li} a_{lj} = \begin{cases} \delta_{ij}, & 0 \leq i, j \leq \eta - 1, \\ 0, & 0 \leq i \leq \eta - 1, j \geq \eta; \end{cases}$$

(b) if $\check{C}(\eta)$ holds, then $\check{D}(\eta - 1)$ also holds;

(c) the method is of order $2\eta_M$, where $\eta_M = \max\{\eta \in \mathbb{Z} : \check{C}(\eta) \text{ holds}\}$, and exactly preserves the energy of system (3.1).

Actually, the condition shown in Theorem 3.7 is essentially equivalent to the formula⁴ (3.12), since we can recast it as a series in terms of Legendre polynomials. Some existing energy-preserving integrators (e.g., AVF methods [26], ∞ -HBVMs [3], EPCMs [18], Galerkin time finite element methods [33, 35] etc) can be transformed into the csRK methods described in Theorem 3.8, and all of them possess an even order. The following result says that there exists energy-preserving B-series integrators which are conjugate-symplectic up to a finite order (higher than their algorithm order).

Theorem 3.9. [34] *Apply the csRK method (2.2) with $B_\tau = 1$, $C_\tau = \tau$ and*

$$A_{\tau, \sigma} = \sum_{0 \leq \iota \in \mathbf{Z}} \omega_\iota \int_0^\tau P_\iota(x) dx P_\iota(\sigma), \quad \omega_0 \equiv 1, \quad \omega_\iota \in \mathbb{R} \quad (3.13)$$

to Hamiltonian system (3.1), where $P_\iota(x)$ is the ι -degree Legendre polynomial. Assume $\kappa := \min\{\iota \in \mathbf{Z} : \omega_\iota \neq 1\} < \infty$, then the method is of order 2κ , symmetric, energy-preserving and conjugate-symplectic up to order at least $2\kappa+2$. If we additionally require $\frac{\omega_\kappa}{2\kappa-1} - \frac{\omega_{\kappa+1}}{2\kappa+1} = \frac{2}{4\kappa^2-1}$, then the method is conjugate-symplectic up to order $2\kappa+4$.

Remark 3.3. *If $\kappa = \min\{\iota \in \mathbf{Z} : \omega_\iota \neq 1\} < \infty$ goes to ∞ , then the energy-preserving csRK method formally approximates to a conjugate-symplectic method (namely up to order ∞). We tend to conjecture that within the framework of csRK methods there exists no computational energy-preserving methods which are conjugate to a symplectic method, though it needs to be further investigated.*

4. Concluding remarks

This note investigates the construction theory of RK-type methods based on the recently-developed framework of RK methods with “infinitely many stages”. In the construction of RK-type algorithms, a crucial technique associated with orthogonal polynomial expansion is fully utilized. By using this approach, we do not need to study the tedious solution of multi-variable nonlinear algebraic equations stemming from order conditions. We develop two ways to construct RK-type methods of arbitrarily high order. As an important application for these theory, we study and discuss the geometric numerical integration of Hamiltonian systems by csRK methods. A sufficient algebraic condition for csRK methods to be symplectic (resp. symmetric) is presented which is very similar to the classic result. The necessity of these conditions will be investigated elsewhere.

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⁴Alternatively, please refer to our earlier work [32] which was presented as a report during the international conference “ICNAAM2012”.

true origin of continuous-stage Runge-Kutta methods is from his paper “An algebraic theory of integration methods” published in 1972. And we claim that the descriptions about the origin in our earlier paper [34] is not accurate.

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