Energy-preserving continuous-stage Runge-Kutta-Nyström methods

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Abstract

Many practical problems can be described by second-order system $\ddot{q} = -M \nabla U(q)$, in which people give special emphasis to some invariants with explicit physical meaning, such as energy, momentum, angular momentum, etc. However, conventional numerical integrators for such systems will fail to preserve any of these quantities which may lead to qualitatively incorrect numerical solutions. This paper is concerned with the development of energy-preserving continuous-stage Runge-Kutta-Nyström (csRKN) methods for solving second-order systems. Sufficient conditions for csRKN methods to be energy-preserving are presented and it is proved that all the energy-preserving csRKN methods satisfying these sufficient conditions can be essentially induced by energy-preserving continuous-stage partitioned Runge-Kutta methods. Some illustrative examples are given and relevant numerical results are reported.

Keywords: Continuous-stage Runge-Kutta-Nyström methods; Hamiltonian systems; Symplectic; Energy preservation.

1. Introduction

In science and engineering fields, there are many problems that can be modelled by ordinary, or partial, differential equations, amongst which those special ones possessing geometric features have drawn much attention in numerical differential equations \cite{3,15,19,22,29}. In this paper, we are concerned with the following Hamiltonian system of ordinary differential equations \cite{2}

$$
\dot{p} = -\nabla_q H(p, q), \quad \dot{q} = \nabla_p H(p, q), \quad p(t_0) = p_0 \in \mathbb{R}^d, \quad q(t_0) = q_0 \in \mathbb{R}^d, \quad (1.1)
$$

where $H(p, q)$ is called the Hamiltonian function (the total energy) of the system. This system has two important geometric properties in phase space: symplecticity and energy conservation \cite{2}. As is well known, for such system, a famous geometric integration approach called “symplectic integration” has been placed on a central position in modern scientific computing since 1980s (see \cite{3,10,13,14,15,19,22,28,29,47} and references therein), while in more recent years there has been a rising interest in the subject of energy-preserving integration \cite{4,5,9,12,20,23,24,25,26,27,31,46}. Symplectic integrators are important and rather popular due to their global restriction of the numerical solutions in all directions by the symplectic structure in the phase space. In contrast, as

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pointed out in [29], energy-preserving integrators may be more beneficial for numerical integration of low-dimensional Hamiltonian systems, by noticing the fact that the preservation of energy is a rather weak restriction for the numerical solutions when the dimension of the system is large. However, compared to symplectic integrators, energy-preserving integrators can be more adaptable for variable time step computation and usually excellent for the integration of chaotic systems, molecular systems and stiff systems [11, 15, 17, 19, 30]. Unfortunately, in general it is impossible for us to construct a method preserving the symplecticity and energy at the same time for a general nonlinear Hamiltonian system [11, 16], hence we can not have the benefits of preserving both properties. Nevertheless, symplectic methods are known to preserve a modified Hamiltonian [19] which implies a near-preservation of the energy, and there is another interesting result shown in [11] stating that a symplectic method is formally conjugate to a method that preserves the Hamiltonian (the total energy) exactly. Conversely, the existence of conjugate-symplectic (a symplectic-like conception in a weak sense) energy-preserving B-series integrators is affirmative — though it is still a great challenge to find a computational method of such type [21].

Recently, continuous-stage approaches are introduced and developed for solving initial value problems of ordinary differential equations (ODEs), following the pioneering work of Butcher [6, 7, 8] and Hairer [20]. Such approaches have led to many interesting applications in geometric integration. Some typical applications can be found in literature, such as: symplectic integrators can be derived from Galerkin variational problems, and these integrators can be interpreted and analyzed by virtue of continuous-stage methods [31, 36, 43]; a number of newly-developed energy-preserving methods can be closely connected to continuous-stage methods [4, 9, 12, 20, 23, 24, 25, 26, 31, 46]; a wide variety of novel symplectic and symmetric methods can be constructed in use of continuous-stage approaches [32, 33, 34, 35, 37, 38, 39, 40, 41, 42, 44]; the conjugate-symplecticity of energy-preserving methods can be investigated in the context of continuous-stage methods [20, 21, 33]. Hopefully, other new applications of continuous-stage methods in geometric integration can be explored in the forthcoming future.

As is well known, second-order ordinary differential equations (ODEs) in the form \( \ddot{q} = -M \nabla U(q) \) (with a constant symmetric matrix \( M \)) are frequently encountered in various fields such as celestial mechanics, molecular dynamics, plasma physics, biological chemistry and so on [15, 19, 20]. More recently, for solving such second-order ODEs, the present author et al. [34, 37, 44, 45] have developed many new families of symplectic and symmetric integrators by using various weighted orthogonal polynomials in the context of continuous-stage Runge-Kutta-Nyström (csRKN) methods. A highlighted advantage for adopting RKN-type methods in the numerical integration is that they can save about half of the storage and reduce the computational cost accordingly when compared to Runge-Kutta methods [18]. In this paper, we focus on the development of energy-preserving continuous-stage Runge-Kutta-Nyström (csRKN) methods. For this sake, we shall first explore the sufficient conditions for csRKN methods to be energy-preserving, and then by virtue of the derived conditions we discuss the construction of new RKN-type energy-preserving integrators.

This paper will be organized as follows. In Section 2, we first present the sufficient conditions for csRKN methods to be energy-preserving, and then it is shown that they can be closely related to continuous-stage partitioned Runge-Kutta (csPRK) methods. This is followed by Section 3, where some illustrative examples for the construction of energy-preserving integrators will be included and some discussions on their numerical implementations will be given. Section 4 is devoted to exhibit some numerical results. At last, we end our paper in Section 5.
2. Energy-preserving conditions

Consider the following initial value problem governed by a second-order system

\[ \ddot{q} = -M \nabla U(q), \quad q(t_0) = q_0 \in \mathbb{R}^d, \quad \dot{q}(t_0) = \dot{q}_0 \in \mathbb{R}^d, \quad (2.1) \]

where \( M \in \mathbb{R}^{d \times d} \) is a constant, symmetric and invertible matrix, and \( U(q) \) (the potential energy) is a differentiable scalar function. Such system can be transformed into a special separable Hamiltonian system with the Hamiltonian \( H(p, q) = \frac{1}{2} p^T M p + U(q) = \frac{1}{2} \dot{q}^T M^{-1} \dot{q} + U(q), \) which reads

\[ \dot{p} = -\nabla U(q), \quad \dot{q} = M \ddot{p}, \quad (2.2) \]

and the corresponding initial value condition is given by \( p(t_0) = M^{-1} \dot{q}_0, \) \( q(t_0) = q_0. \) It is known that \( H(p, q) \) (the total energy) is an invariant or a first integral of the system, say \( H(p(t), q(t)) = \text{Const} \) along the solution curves of \( (2.2), \) which will to be considered in the energy-preserving time-discretization of the system later.

By using the notation \( p_0 = M^{-1} \dot{q}_0, \) we introduce the following continuous-stage Runge-Kutta-Nyström (csRKN) method for solving \( (2.1) \) \[34, 37\]

\begin{align}
Q_\tau &= q_0 + h C_\tau M p_0 - h^2 M \int_0^1 \bar{A}_{\tau, \sigma} \nabla U(Q_\sigma) d\sigma, \quad \tau \in [0, 1], \quad (2.3a) \\
q_1 &= q_0 + h M p_0 - h^2 M \int_0^1 \bar{B}_\tau \nabla U(Q_\tau) d\tau, \quad (2.3b) \\
p_1 &= p_0 - h \int_0^1 \bar{B}_\tau \nabla U(Q_\tau) d\tau. \quad (2.3c)
\end{align}

where \( \bar{A}_{\tau, \sigma} \) is a smooth function of variables \( \tau, \sigma \in [0, 1] \) and \( \bar{B}_\tau, \bar{B}_\tau, C_\tau \) are smooth functions of \( \tau \in [0, 1] \). The method \( (2.3) \) is said to have order \( p \), if for all sufficiently regular problem \( (2.1) \), as \( h \to 0 \), its local error satisfies \[18\]

\[ q_1 - q(t_0 + h) = \mathcal{O}(h^{p+1}), \quad p_1 - p(t_0 + h) = \mathcal{O}(h^{p+1}). \]

By definition, to construct a energy-preserving csRKN method is to design suitable Butcher coefficient functions \( \bar{A}_{\tau, \sigma}, \bar{B}_\tau, B_\tau, C_\tau \) so as to guarantee the preservation of energy, i.e.,

\[ H(p_{n+1}, q_{n+1}) = H(p_n, q_n), \quad n = 0, 1, 2, \cdots. \]

Without loss of generality, for a one-step method, it suffices to consider the case after one step computation. In our case, we need to impose the following requirement

\[ H(p_1, q_1) = H(p_0, q_0), \quad (2.4) \]

on the one-step scheme \( (2.3) \).

**Theorem 2.1.** If there exists a smooth binary function \( A_{\tau, \sigma} \), such that the coefficients of the csRKN method \( (2.3) \) satisfy

\begin{align}
C_0 &= 0 \quad \text{and} \quad C_1 = 1, \quad (2.5a) \\
\bar{A}_{0, \sigma} &= 0, \quad \bar{A}_{1, \sigma} = \bar{B}_\sigma, \quad \forall \sigma \in [0, 1], \quad (2.5b) \\
A_{0, \sigma} &= 0, \quad A_{1, \sigma} = B_\sigma = C_\sigma', \quad \forall \sigma \in [0, 1], \quad (2.5c) \\
\int_0^1 A'_{\tau, \eta} A_{\tau, \zeta} d\tau &= \bar{A}'_{\eta, \zeta}, \quad \forall \eta, \zeta \in [0, 1], \quad (2.5d)
\end{align}
where

\[ A'_{\tau,\sigma} = \frac{\partial}{\partial \tau} A_{\tau,\sigma}, \quad \bar{A}'_{\tau,\sigma} = \frac{\partial}{\partial \tau} \bar{A}_{\tau,\sigma}, \]

then the method is energy-preserving for solving system (2.1).

Proof. Firstly, we define \( P_{\tau} \) as

\[ p(t_0 + \tau h) \approx P_{\tau} = p_0 - h \int_{0}^{1} A_{\tau,\sigma} \nabla U(Q_{\sigma}) d\sigma, \quad \tau \in [0, 1], \] (2.6)

and here \( A_{\tau,\sigma} \) is assumed to satisfy (2.5c). From (2.5a)-(2.5c), it follows

\[ P_0 = p_0, \quad P_1 = p_1, \quad Q_0 = q_0, \quad Q_1 = q_1, \]

which means \( P_{\tau} \) and \( Q_{\tau} \) as continuous functions join the numerical solutions at the two ends of integration interval \([t_0, t_0 + h]\) and they can be regarded as the approximations to the exact solutions \( p(t) = p(t_0 + \tau h) \) and \( q(t) = q(t_0 + \tau h) \), \( \tau \in [0, 1] \). Hence, by means of the fundamental theorem of calculus and using \( M^T = M \), we have

\[ H(p_1, q_1) - H(p_0, q_0) = \int_{0}^{1} \frac{d}{d\tau} H(P_{\tau}, Q_{\tau}) d\tau \]

(2.7)

By using (2.6), it gives

\[ \int_{0}^{1} P_{\tau}^T M P'_{\tau} d\tau = \int_{0}^{1} \left( p_0^T - h \int_{0}^{1} A_{\tau,\zeta} (\nabla U(Q_{\zeta}))^T d\zeta \right) M \left( - h \int_{0}^{1} A'_{\tau,\eta} \nabla U(Q_{\eta}) d\eta \right) d\tau \]

\[ = -h \int_{0}^{1} \left[ \int_{0}^{1} A_{\tau,\eta} d\tau \left( p_0^T M \nabla U(Q_{\eta}) \right) \right] d\eta + h^2 \int_{0}^{1} \left[ \left( \int_{0}^{1} A_{\tau,\zeta} A'_{\tau,\eta} d\tau \right) (\nabla U(Q_{\zeta}))^T M \nabla U(Q_{\eta}) \right] d\eta d\zeta \]

\[ = -h \int_{0}^{1} B_{\eta} p_0^T M \nabla U(Q_{\eta}) d\eta + h^2 \int_{0}^{1} \int_{0}^{1} \left[ \left( \int_{0}^{1} A'_{\tau,\eta} A_{\tau,\zeta} d\tau \right) (\nabla U(Q_{\zeta}))^T M \nabla U(Q_{\eta}) \right] d\eta d\zeta, \]

where we have used the following identity

\[ \int_{0}^{1} A'_{\tau,\eta} d\tau = A_{\tau,\eta}\bigg|_{0}^{1} = B_{\eta}. \]

\(^1\)Hereafter we always use primes for denoting the partial derivatives with respect to the first variable (subscript) of binary functions. Moreover, the notation \( A_{\tau,\eta}\big|_{0}^{1} = A_{1,\eta} - A_{0,\eta} \) as well as other similar notations is also associated with the first variable.
Similarly, by using (2.3a) we have

\[
\int_{0}^{1} (Q')^{T} \nabla U(Q) \, d\tau = \int_{0}^{1} (Q')^{T} \nabla U(Q) \, d\eta = \int_{0}^{1} \left[ \left( hC'_{0}p_{0}^{T} M - h^{2} \int_{0}^{1} \hat{A}'_{\eta,\zeta} (\nabla U(Q_{\zeta}))^{T} M \, d\zeta \right) \nabla U(Q) \right] \, d\eta \\
= h \int_{0}^{1} C'_{0}p_{0}^{T} M \nabla U(Q_{\eta}) \, d\eta - h^{2} \int_{0}^{1} \int_{0}^{1} \left[ \hat{A}'_{\eta,\zeta} (\nabla U(Q_{\zeta}))^{T} M \nabla U(Q_{\eta}) \right] \, d\eta \, d\zeta.
\]

Substituting the two formulas above into (2.7) yields (2.4) which completes the proof.

Theorem 2.2. The conditions (2.5c) and (2.5d) imply

\[
\bar{A}'_{\tau,\sigma} + \hat{A}'_{\sigma,\tau} \equiv B_{\tau}B_{\sigma}, \quad \forall \tau, \sigma \in [0, 1].
\]

If we assume \( B_{\tau} \equiv 1 \), then (2.8) becomes

\[
\bar{A}'_{\tau,\sigma} + \hat{A}'_{\sigma,\tau} \equiv 1, \quad \forall \tau, \sigma \in [0, 1].
\]

Proof. By exchanging the variables \( \eta \) and \( \zeta \) in (2.5d), it yields

\[
\int_{0}^{1} A'_{\tau,\zeta} A_{\tau,\eta} \, d\tau = \hat{A}'_{\zeta,\eta}, \quad \forall \eta, \zeta \in [0, 1].
\]

Adding (2.10) with (2.5d) and using (2.5c) gives

\[
\bar{A}'_{\eta,\zeta} + \hat{A}'_{\zeta,\eta} = \int_{0}^{1} \left( A'_{\tau,\eta} A_{\tau,\zeta} + A'_{\tau,\zeta} A_{\tau,\eta} \right) \, d\tau = A_{\tau,\eta} A_{\tau,\zeta} \bigg|_{0}^{1} = B_{\eta}B_{\zeta}, \quad \forall \eta, \zeta \in [0, 1],
\]

which leads to (2.8). The formulae (2.9) is straightforward from (2.8) when \( B_{\tau} \equiv 1 \).

Theorem 2.3. If we define

\[
\hat{A}_{\tau,\sigma} = \int_{0}^{\tau} A'_{\sigma,\zeta} \, d\zeta, \quad \forall \tau, \sigma \in [0, 1],
\]

then it gives

\[
\hat{A}_{0,\sigma} = 0, \quad \bar{A}'_{\tau,\sigma} = \hat{A}'_{\sigma,\tau}, \quad \forall \tau, \sigma \in [0, 1],
\]

and vice versa. Moreover, under the condition \( \hat{A}_{0,\sigma} = 0 \) (see also (2.5a)), the formula (2.5d) implies

\[
\hat{A}_{\tau,\sigma} = \int_{0}^{1} \hat{A}_{\tau,\rho} A'_{\rho,\sigma} \, d\rho, \quad \forall \tau, \sigma \in [0, 1].
\]

Proof. The equivalence between (2.11) and (2.12) is easy to verify by conducting some elementary calculations. By taking integral of (2.5d) with respect to \( \tau \) and using \( \hat{A}_{0,\sigma} = 0 \), it follows

\[
\int_{0}^{1} \hat{A}_{\alpha,\rho} A'_{\rho,\sigma} \, d\rho = \int_{0}^{1} \left( \int_{0}^{\alpha} A'_{\rho,\tau} \, d\tau \right) A'_{\rho,\sigma} \, d\rho = \int_{0}^{\alpha} \hat{A}'_{\tau,\rho} \, d\tau = \hat{A}_{\tau,\rho} \bigg|_{0}^{\alpha} = \hat{A}_{\alpha,\sigma}, \quad \forall \alpha, \sigma \in [0, 1],
\]

which gives (2.13) by replacing the notation \( \alpha \) with \( \tau \).
By virtue of Theorem 2.3, we derive a modified version of Theorem 2.1.

**Theorem 2.4.** If there exists a smooth binary function \( A_{\tau,\sigma} \), such that the coefficients of the csRKN method (2.3) satisfy

\[
C_0 = 0 \quad \text{and} \quad C_1 = 1, \quad (2.14a)
\]
\[
\bar{A}_{0,\sigma} = 0, \quad \bar{A}_{1,\sigma} = B_\sigma, \quad \forall \sigma \in [0,1], \quad (2.14b)
\]
\[
A_{0,\sigma} = 0, \quad A_{1,\sigma} = B_\sigma = C'_\sigma, \quad \forall \sigma \in [0,1], \quad (2.14c)
\]
\[
\tilde{A}_{\tau,\sigma} = \int_0^1 \tilde{A}_{\tau,\rho} A_{\rho,\sigma} d\rho, \quad \forall \tau, \sigma \in [0,1], \quad (2.14d)
\]

where \( \tilde{A}_{\tau,\rho} \) is defined via (2.11), then the method is energy-preserving for solving system (2.1).

Particularly, if \( B_\tau = 1 \), \( C_\tau = \tau \), then the first condition (2.14a) can be removed and accordingly (2.14c) should be replaced by

\[
A_{0,\sigma} = 0, \quad A_{1,\sigma} = 1, \quad \forall \sigma \in [0,1]. \quad (2.15)
\]

**Proof.** This is a direct result of Theorem 2.1 and Theorem 2.3. \( \square \)

In what follows, we show that all the energy-preserving csRKN methods determined by Theorem 2.4 can be derived from energy-preserving continuous-stage partitioned Runge-Kutta (csPRK) methods. To show this, we need the following two theorems.

**Theorem 2.5.** Suppose that \( B_\sigma \) satisfy (2.5a) and (2.5c), and by means of (2.11) we define \( \hat{B}_\sigma \) as

\[
\hat{B}_\sigma = \hat{A}_{1,\sigma} = \int_0^1 A'_{\sigma,\zeta} d\zeta, \quad \forall \sigma \in [0,1],
\]

where \( A_{\sigma,\zeta} \) is assumed to satisfy (2.5c), then we have

\[
\int_0^1 B_\sigma d\sigma = 1, \quad \int_0^1 \hat{B}_\sigma d\sigma = 1. \quad (2.16)
\]

**Proof.** By using (2.5a) and (2.5c), we have

\[
\int_0^1 B_\sigma d\sigma = \int_0^1 C'_\sigma d\sigma = C_\sigma \bigg|_0^1 = 1.
\]

Besides, by exchanging the order of integration and using (2.5c), it follows

\[
\int_0^1 \hat{B}_\sigma d\sigma = \int_0^1 ( \int_0^1 A'_{\sigma,\zeta} d\zeta ) d\sigma = \int_0^1 ( \int_0^1 A'_{\sigma,\zeta} d\sigma ) d\zeta = \int_0^1 A_{\sigma,\zeta} \bigg|_0^1 d\zeta = \int_0^1 B_\zeta d\zeta = 1.
\]

**Theorem 2.6.** The conditions (2.5a) and (2.5c) implies that

\[
C_\tau = \int_0^1 \tilde{A}_{\tau,\sigma} d\sigma, \quad \forall \tau \in [0,1], \quad (2.17)
\]

where \( \tilde{A}_{\tau,\rho} \) is defined via (2.11).
Proof. By using (2.5a) and (2.5c) we get
\[ C_\tau = C_\tau - C_0 = \int_0^\tau C'_\sigma d\sigma = \int_0^\tau A_{1,\sigma} d\sigma. \]

On the other hand, for each fixed \( \tau \), by exchanging the order of integration and using (2.5c) it follows
\[ \int_0^1 \hat{A}_{\tau,\sigma} d\sigma = \int_0^\tau \left( \int_0^1 A'_{\sigma,\zeta} d\zeta \right) d\sigma = \int_0^\tau A_{\sigma,\zeta} \bigg|_0^1 d\zeta = \int_0^\tau A_{1,\zeta} d\zeta, \]
which gives rise to (2.17) by comparing the two formulae above.

In addition, let us review some existing results presented in [46]. For the numerical integration of a general Hamiltonian system (1.1), the so-called csPRK method (a kind of P-series integrators [19]) can be formulated as [46]
\[
\begin{align*}
P_\tau &= p_0 - h \int_0^1 A_{\tau,\sigma} \nabla q H(P_\sigma, Q_\sigma) d\sigma, \quad \tau \in [0, 1], \\
Q_\tau &= q_0 + h \int_0^1 \hat{A}_{\tau,\sigma} \nabla p H(P_\sigma, Q_\sigma) d\sigma, \quad \tau \in [0, 1], \\
p_1 &= p_0 - h \int_0^1 B_{\tau} \nabla q H(P_\tau, Q_\tau) d\tau, \\
q_1 &= q_0 + h \int_0^1 \hat{B}_{\tau} \nabla p H(P_\tau, Q_\tau) d\tau,
\end{align*}
\] (2.18)

and the corresponding energy-preserving condition can be stated as follows.

**Theorem 2.7.** [46] If the coefficients of the csPRK method (2.18) satisfy
\[
\begin{align*}
A_{0,\sigma} &= 0, \quad A_{1,\sigma} = B_{\sigma}, \quad \forall \sigma \in [0, 1], \\
\hat{A}_{0,\sigma} &= 0, \quad \hat{A}_{1,\sigma} = \hat{B}_{\sigma}, \quad \forall \sigma \in [0, 1], \\
A'_{\tau,\sigma} &= A'_{\sigma,\tau}, \quad \forall \tau, \sigma \in [0, 1],
\end{align*}
\] (2.19)
then the method is energy-preserving for solving Hamiltonian system (1.1).

Particularly, if we apply the csPRK method (2.18) with coefficients satisfying (2.19) to the Hamiltonian system (2.2), then it gives
\[
\begin{align*}
P_\tau &= p_0 - h \int_0^1 A_{\tau,\sigma} \nabla U(Q_\sigma) d\sigma, \quad \tau \in [0, 1], \\
Q_\tau &= q_0 + h \int_0^1 \hat{A}_{\tau,\sigma} M P_\sigma d\sigma, \quad \tau \in [0, 1], \\
p_1 &= p_0 - h \int_0^1 B_{\tau} \nabla U(Q_\tau) d\tau, \\
q_1 &= q_0 + h \int_0^1 \hat{B}_{\tau} M P_\tau d\tau,
\end{align*}
\] (2.20)
and here we assume\textsuperscript{\textsuperscript{2}}
\[ \int_0^1 B_\tau d\tau = 1, \quad \int_0^1 \hat{B}_\tau d\tau = 1. \] (2.21)

It is observed that (2.20a) is superfluous for obtaining the numerical solutions \( p_1 \) and \( q_1 \), because we can substitute it into other formulae to get a simplified scheme and then it can be removed. To be specific, by inserting (2.20a) into (2.20b), it yields
\[ Q_\tau = q_0 + hC_\tau M p_0 - h^2 M \int_0^1 \hat{A}_{\tau,\sigma} \nabla U(Q_\sigma) d\sigma, \] (2.22)
where
\[ C_\tau = \int_0^1 \hat{A}_{\tau,\sigma} d\sigma, \quad \hat{A}_{\tau,\rho} = \int_0^1 \hat{A}_{\tau,\rho} A_{\rho,\sigma} d\rho. \] (2.23)

Similarly, by inserting (2.20a) into (2.20d) and using (2.21), we have
\[ q_1 = q_0 + hM p_0 - h^2 M \int_0^1 \hat{B}_\tau \nabla U(Q_\tau) d\tau, \] (2.24)
where
\[ \hat{B}_\tau = \int_0^1 \hat{B}_\rho A_{\rho,\tau} d\rho. \] (2.25)

Moreover, by using (2.19), we get
\[ \hat{A}_{0,\sigma} = \int_0^1 \hat{A}_{0,\rho} A_{\rho,\sigma} d\rho = 0, \quad \hat{A}_{1,\sigma} = \int_0^1 \hat{A}_{1,\rho} A_{\rho,\sigma} d\rho = \int_0^1 \hat{B}_\rho A_{\rho,\sigma} d\rho = \bar{B}_\sigma. \] (2.26)

Consequently, (2.20c), (2.22) and (2.24) constitute a csRKN method in the form (2.3), and the csRKN coefficients satisfy (2.23), (2.25) and (2.26). On the basis of these analyses above, the following result is derived.

**Theorem 2.8.** An energy-preserving csRKN method acquired by Theorem 2.1 is equivalent to an energy-preserving csPRK method originated from Theorem 2.7 (with the condition (2.21) being satisfied). Moreover, the csRKN method is at least of the same order of the associated csPRK method.

**Proof.** On account of the process from (2.20) to (2.26), the statement can be easily obtained by combining Theorem 2.3 Theorem 2.4 Theorem 2.5 Theorem 2.6 and Theorem 2.7. The only fact needs to be proved is the converse of Theorem 2.6. From the first formula of (2.23) (see also (2.17)), it is clear that
\[ C_0 = \int_0^1 \hat{A}_{0,\sigma} d\sigma = 0, \quad C_1 = \int_0^1 \hat{A}_{1,\sigma} d\sigma = \int_0^1 \hat{B}_\sigma d\sigma = 1, \]
where we have used (2.19) and (2.21). Besides, we have
\[ C'_\tau = \int_0^1 \hat{A}'_{\tau,\sigma} d\sigma. \] (2.27)
By Theorem 2.3, (2.19) implies (2.11). Therefore, inserting (2.11) into (2.27) and using (2.19) yields

\[ C'_r = \int_0^1 A'_{\sigma, r} \, d\sigma = A_{\sigma, r}\big|_0^1 = A_{1, r} = B_r. \]  

(2.28)

Consequently, we get (2.5a) and (2.5c) from (2.23) and (2.19).

\[ \text{Remark 2.9.} \text{ We must stress that, in general, a csRKN method (excluding the class of energy-preserving methods presented in this paper) is not necessarily equivalent to the method induced by a csPRK method. The reason lies in the fact that the coefficients of a csRKN method do not necessarily satisfy (2.23) and (2.25). This fact is similar to the classical case (see [18], P.284).} \]

From Theorem 2.8, it is suggested that one might as well construct an energy-preserving csRKN method by virtue of an energy-preserving csPRK method, while the derivation of energy-preserving csPRK methods has been discussed in the previous study by the present author [46]. For convenience, in the following we mention two useful results which are based on the normalized shifted Legendre polynomial \( L_j(x) \):

\[ L_0(x) = 1, \quad L_j(x) = \frac{\sqrt{2j + 1}}{j!} \frac{d^j}{dx^j} \left( x^j(x-1)^j \right), \quad j = 1, 2, 3, \ldots. \]

**Theorem 2.10.** [46] If the coefficients of the csPRK method (2.18) are of the following forms

\[ A_{\tau, \sigma} = \sum_{i=0}^{s-1} \sum_{j=0}^{r-1} \alpha_{(i,j)} \int_0^\tau L_i(x) \, dx L_j(\sigma), \quad B_\tau = \sum_{j=0}^{r-1} \alpha_{(0,j)} L_j(\tau), \]

\[ \hat{A}_{\tau, \sigma} = \sum_{i=0}^{r-1} \sum_{j=0}^{s-1} \hat{\alpha}_{(i,j)} \int_0^\tau L_i(x) \, dx L_j(\sigma), \quad \hat{B}_\tau = \sum_{j=0}^{s-1} \hat{\alpha}_{(0,j)} L_j(\tau), \]

where the real coefficients \( \hat{\alpha}_{(i,j)} \) and \( \alpha_{(j,i)} \) satisfy \( \hat{\alpha}_{(i,j)} = \alpha_{(j,i)} \), then the method is energy-preserving for solving a general Hamiltonian system (1.1). Moreover, the method has order at least 1 if and only if \( \hat{\alpha}_{(0,0)} = \alpha_{(0,0)} = 1 \).

**Theorem 2.11.** [46] The csPRK method (2.18) with coefficients given by \((s, r \geq \eta + 1)\)

\[ A_{\tau, \sigma} = \sum_{j=0}^{\eta-1} \int_0^\tau L_j(x) \, dx L_j(\sigma) + \sum_{i=\eta}^{r-1} \sum_{j=\eta}^{r-1} \alpha_{(i,j)} \int_0^\tau L_i(x) \, dx L_j(\sigma), \quad B_\tau = 1, \]

\[ \hat{A}_{\tau, \sigma} = \sum_{j=0}^{\eta-1} \int_0^\tau L_j(x) \, dx L_j(\sigma) + \sum_{i=\eta}^{r-1} \sum_{j=\eta}^{r-1} \hat{\alpha}_{(i,j)} \int_0^\tau L_i(x) \, dx L_j(\sigma), \quad \hat{B}_\tau = 1, \]

is energy-preserving and at least of order \( p = 2\eta \) (\( \eta \geq 1 \)) for solving a general Hamiltonian system (1.1), where the real coefficients \( \hat{\alpha}_{(i,j)} \) and \( \alpha_{(j,i)} \) satisfy \( \hat{\alpha}_{(i,j)} = \alpha_{(j,i)} \).

### 3. Examples of energy-preserving methods and numerical implementations

In this section, we present some examples for illustrating the construction of energy-preserving RKN-type methods and give some comments about their numerical implementations. We introduce two approaches to devise such methods. The first one is a direct way by considering using the method of undetermined coefficients on the basis of Theorem 2.1 and Theorem 2.2 As an illustration, we present the following example.
Example 3.1. Assume $B_\tau = 1$, $C_\tau = \tau$ and let
\[ \tilde{A}_{\tau,\sigma} = a\tau^2 + b\tau\sigma + c\tau + d, \quad A_{\tau,\sigma} = \hat{a}\tau^2\sigma + \hat{b}\tau\sigma + \hat{c}\tau + \hat{d}, \]
where $a, b, c, d$ are coefficients to be determined, noting that by Theorem 2.1 it needs to verify the existence of $A_{\tau,\sigma}$ by finding out the undetermined coefficients $\hat{a}, \hat{b}, \hat{c}, \hat{d}$. By using (2.9), we get $b = -2a, c = \frac{1}{2}$. Besides, from (2.5b) and (2.5c), it gives $d = 0, \hat{d} = 0, \hat{c} = 1, b = -\hat{a}$ and $\tilde{B}_{\sigma} = \tilde{A}_{1,\sigma} = a - 2a\sigma + \frac{1}{2}$. Finally, by inserting (3.1) into (2.5d), it follows that $\hat{a} = 12a, \hat{b} = -12a$, which verifies the existence of $A_{\tau,\sigma}$. As a consequence, we get a family of energy-preserving csRKN methods with coefficients given by
\[ \tilde{A}_{\tau,\sigma} = a\tau^2 - 2a\tau\sigma + \frac{\tau}{2}, \quad \tilde{B}_{\tau} = a - 2a\tau + \frac{1}{2}, \quad B_\tau = 1, \quad C_\tau = \tau, \]
which is at least of order $2$. Particularly, when $a = \frac{1}{2}$, the corresponding method is symmetric and of order 4.

The second approach is not direct but very effective, the idea of which is based on Theorem 2.8. To illustrate this approach, in what follows we make use of some available energy-preserving csPRK methods (derived by Theorem 2.10 or Theorem 2.11, see [46] for more details) to get new energy-preserving csRKN methods.

Example 3.2. The $\theta$-parameter family of energy-preserving csPRK methods with coefficients given by [46]
\[ A_{\tau,\sigma} = \theta\tau^2 + (1 - \theta)\tau, \quad B_\tau = 1; \quad \tilde{A}_{\tau,\sigma} = (2\theta\sigma + 1 - \theta)\tau, \quad \tilde{B}_{\tau} = 2\theta\tau + 1 - \theta, \]
has order at least 1 (if and only if $\theta = 0$ the order becomes higher, say, 2). Substituting (3.3) into (2.23) and (2.25), it gives
\[ \tilde{A}_{\tau,\sigma} = \frac{\tau}{2}, \quad \tilde{B}_{\tau} = \frac{1}{2}, \quad B_\tau = 1, \quad C_\tau = \tau, \]
which corresponds to a special case of (3.2) when $a = 0$ and the method is of order 2. Moreover, if we interchange the role of $(A_{\tau,\sigma}, B_\tau)$ and $(\tilde{A}_{\tau,\sigma}, \tilde{B}_\tau)$ in (3.3), then it leads to
\[ A_{\tau,\sigma} = \frac{(\theta\tau^2 + \tau - \theta\tau)(2\theta\sigma + 1 - \theta)}{2}, \quad B_\tau = \theta\tau + \frac{1 - \theta}{2}, \quad B_\tau = 2\tilde{B}_\tau, \quad C_\tau = \theta\tau^2 + (1 - \theta)\tau, \]
which produces a family of 1-order energy-preserving csRKN methods. Particularly, if we let $\theta = 0$ in (3.5), then we retrieve (3.4).

Example 3.3. A family of 4-order energy-preserving csPRK integrators is given by [46]
\[
A_{\tau,\sigma} = \theta_2(30\sigma^2 - 30\sigma + 5)\tau^4 + (2\theta_1 - 10\theta_2)(6\sigma^2 - 6\sigma + 1)\tau^3 \\
+ [6\theta_2 - 3\theta_1](6\sigma^2 - 6\sigma + 1) + 6\sigma - 3]\tau^2 \\
+ [(\theta_1 - \theta_2)(6\sigma^2 - 6\sigma + 1) - 6\sigma + 4]\tau, \quad B_\tau = 1, \\
\tilde{A}_{\tau,\sigma} = 2[\theta_1(6\sigma^2 - 6\sigma + 1) + \theta_2(20\sigma^3 - 30\sigma^2 + 12\sigma - 1)]\tau^3 \\
- 3[\theta_1(6\sigma^2 - 6\sigma + 1) + \theta_2(20\sigma^3 - 30\sigma^2 + 12\sigma - 1) - 2\sigma + 1]\tau^2 \\
+ [\theta_1(6\sigma^2 - 6\sigma + 1) + \theta_2(20\sigma^3 - 30\sigma^2 + 12\sigma - 1) - 6\sigma + 4]\tau, \quad \tilde{B}_\tau = 1.
\]
Substituting (3.6) into (2.23) and (2.25), it gives a family of 4-order energy-preserving csRKN methods with coefficients

\[ A_{\tau,\sigma} = \frac{1}{10} \left[ (4\theta_1\sigma - 2\theta_1)^3 + (-6\theta_1\sigma^2 + 2\theta_1 + 5)\tau^2 
+ (6\theta_1\sigma^2 - 4\theta_1\sigma - 10\sigma + 5)\tau \right], \]

(3.7)

\[ \tilde{B}_\tau = 1 - \tau, \quad B_\tau = 1, \quad C_\tau = \tau. \]

By exchanging the role of \((A_{\tau,\sigma}, B_\tau)\) and \((\tilde{A}_{\tau,\sigma}, \tilde{B}_\tau)\) in (3.6), it gives another family of 4-order energy-preserving csRKN methods with coefficients

\[ \tilde{A}_{\tau,\sigma} = \frac{1}{10} \left[ (10\theta_2\sigma - 5\theta_2)^4 + (-20\theta_2\sigma + 4\theta_1\sigma - 2\theta_1 + 10\theta_2)\tau^3 
+ (-20\theta_2\sigma^3 - 6\theta_1\sigma^2 + 30\theta_2\sigma^2 + 2\theta_1 - 5\theta_2 + 5)\tau^2 
+ (20\theta_2\sigma^3 + 6\theta_1\sigma^2 - 30\theta_2\sigma^2 - 4\theta_1\sigma + 10\theta_2\sigma - 10\sigma + 5)\tau \right], \]

(3.8)

\[ \tilde{B}_\tau = 1 - \tau, \quad B_\tau = 1, \quad C_\tau = \tau. \]

It is observed that (3.8) contains (3.7) as a special case by considering taking \(\theta_2 = 0\). Besides, if we let \(\theta_1 = \theta_2 = 0\) in (3.8), then we retrieve the 4-order method given by (3.2) with \(a = \frac{1}{2}\). It is clear that the coefficients of csRKN methods are much simpler than those of the original csPRK methods.

As for the practical implementation, usually we have to approximate the integrals of (2.3) by numerical quadrature. Let \(b_i\) and \(c_i\) be the weights and abscissae of the following \(k\)-point interpolatory quadrature rule

\[ \int_0^1 \phi(x) \, dx \approx \sum_{i=1}^{k} b_i \phi(c_i), \quad c_i \in [0, 1], \]

(3.9)

where

\[ b_i = \int_0^1 \ell_i(x) \, dx, \quad \ell_i(x) = \prod_{j=1, j \neq i}^{k} \frac{x - c_j}{c_i - c_j}, \quad i = 1, \cdots, k. \]

By applying the quadrature formula (3.9) of order \(p\) to (2.3), we derive a \(k\)-stage classical RKN method

\[ Q_i = q_0 + hC_iMp_0 - h^2M \sum_{j=1}^{k} b_{ij} \tilde{A}_{ij} \nabla U(Q_j), \quad i = 1, \cdots, k, \]

\[ q_1 = q_0 + hMp_0 - h^2M \sum_{i=1}^{k} b_i \tilde{B}_i \nabla U(Q_i), \]

(3.10)

\[ p_1 = p_0 - h \sum_{i=1}^{k} b_i \tilde{B}_i \nabla U(Q_i), \]

where \(\tilde{A}_{ij} = \tilde{A}_{c_i,c_j}, \tilde{B}_i = \tilde{B}_{c_i}, B_i = B_{c_i}, C_i = C_{c_i} \) for \(i, j = 1, \cdots, k\).

**Remark 3.1.** Remark that usually the quadrature-based RKN scheme (3.10) possess the same order of the associated csRKN method when we use a quadrature formula with a high-enough degree of precision. For the connection between the underlying csRKN method and its quadrature-based RKN method in terms of the order accuracy, we refer the readers to Theorem 3.7 of [33].

11
If the potential energy function $U(q)$ is a polynomial, then the integrands in (2.3) can be precisely computed by means of a suitable quadrature formula. In such a case, the quadrature-based RKN scheme (3.10) produces an exact energy-preserving integration of (2.1) — as for the non-polynomial case, usually the RKN method (3.10) can also be able to preserve the nonlinear Hamiltonian $H(p,q)$ up to round-off error, given that we adopt a quadrature rule with high enough algebraic precision (some similar observations have been presented in [4, 5] for Hamiltonian boundary value methods).

**Theorem 3.2.** If the coefficients of the underlying energy-preserving csRKN method (2.3) acquired by Theorem 2.4 are polynomial functions, then the RKN scheme (3.10) is exactly energy-preserving for the polynomial system (2.1) with a $\nu$-degree potential energy function $U(q)$, provided that the quadrature formula (3.9) is of Gaussian type\(^5\) and the number of nodes, say $k$, satisfies

$$k \geq \max \left\{ \frac{(\nu - 1)\alpha + \beta + 1 + (\nu - 1)\alpha + \gamma + 1}{2}, \right\},$$

where $\bar{A}_{\tau,\sigma}$ is assumed to be of degree $\alpha$ in $\tau$ and of degree $\beta$ in $\sigma$, and $B_\tau$ is assumed to be of degree $\gamma$.

**Proof.** The key of the proof lies in the fact that $k$-point Gaussian-type quadrature formula can precisely compute the integrals of (2.3), if the degrees of the integrands are no higher than the algebraic precision of the quadrature. It is well to notice that the degree of $B_\tau$ is $\beta$ (since $\bar{B}_\alpha = \bar{A}_{1,\sigma}$ by Theorem 2.4), the degree of $Q_\tau$ is the same as that of $\bar{A}_{\tau,\sigma}$ in $\tau$, say $\alpha$, and then the degree of $\nabla U(Q_\tau)$ is $(\nu - 1)\alpha$.

4. **Numerical tests**

In this section, we report some numerical tests to verify our theoretical results. The following eight methods are selected for comparisons in our experiments:

1. Method I: the 2-order energy-preserving csRKN method shown in (3.2) with $a = 0.1$;
2. Method II: the 2-order energy-preserving csRKN method shown in (3.2) with $a = 0.2$;
3. Method III: the 1-order energy-preserving csRKN method shown in (3.5) with $\theta = 0.1$;
4. Method IV: the 1-order energy-preserving csRKN method shown in (3.5) with $\theta = 0.2$;
5. Method V: the 4-order energy-preserving csRKN method shown in (3.7) with $\theta_1 = 0.1$;
6. Method VI: the 4-order energy-preserving csRKN method shown in (3.7) with $\theta_1 = 0.2$;
7. GLRK 2: the Gauss-Legendre Runge-Kutta method which is symplectic and of order 2 [18];
8. GLRK 4: the Gauss-Legendre Runge-Kutta method which is symplectic and of order 4 [18].

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\(^5\)This means the quadrature formula is exact for all polynomial functions with degree $\leq 2k - 1$. 

12
Figure 4.1: Energy (Hamiltonian) errors by eight methods for polynomial system (4.1), with step size $h = 0.1$.

Figure 4.2: Energy (Hamiltonian) errors by eight methods for mathematical pendulum problem (4.2), with step size $h = 0.1$. 
4.1. Test problem I

Consider the second-order system
\[ \ddot{q} = \frac{1}{2} q^2 - q, \quad (4.1) \]
which can be transformed into a polynomial Hamiltonian system and the associated Hamiltonian function is
\[ H = \frac{1}{2} (p^2 + q^2) - \frac{1}{6} q^3, \quad \text{with } p = \dot{q}. \]

We take the initial value condition as \( p_0 = 1, q_0 = 0 \) and use the time step size \( h = 0.1 \) for numerical integration with 10,000 steps. Since the potential energy function \( U(q) = -\frac{1}{6} q^3 \) is a cubic polynomial, by Theorem 3.2 we can precisely compute the integrals of the associated csRKN methods. For this problem, we use 3-point Gaussian quadrature for approximating the integrals of method I, II, III and IV, but 4-point Gaussian quadrature for method V and VI. The numerical result is presented in Fig. 4.1, which clearly shows the energy-preserving property of our new methods, while two symplectic methods only give a near-preservation of the energy.

4.2. Test problem II

Consider the mathematical pendulum equation
\[ \ddot{q} = -\sin q, \quad (4.2) \]
which corresponds to a non-polynomial Hamiltonian system and the corresponding Hamiltonian function is
\[ H = \frac{1}{2} p^2 - \cos q, \quad \text{with } p = \dot{q}. \]

In our experiments, we take \( p_0 = 0.5, q_0 = 0, h = 0.1 \) for the numerical integration with 10,000 steps and 4-point Gaussian quadrature is used for calculating the integrals of method I, II, V and VI, but for the method III and IV which possess the lowest order (order 1), the 6-point Gaussian quadrature is used. Fig. 4.2 exhibits a very similar result as that shown in test problem I.

4.3. Test problem III

Consider the well-known Kepler’s problem described by the following second-order system [19]
\[ \begin{align*}
\ddot{q}_1 &= -\frac{q_1}{(q_1^2 + q_2^2)^{3/2}}, \\
\ddot{q}_2 &= -\frac{q_2}{(q_1^2 + q_2^2)^{3/2}}.
\end{align*} \quad (4.3) \]

By introducing \( p_1 = \dot{q}_1, p_2 = \dot{q}_2 \), (4.3) can be recast as a nonlinear Hamiltonian system with the Hamiltonian (the total energy)
\[ H = \frac{1}{2} (p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}}. \]

It is known that such system possesses other two invariants: the quadratic angular momentum
\[ I = q_1 p_2 - q_2 p_1 = q^T \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \dot{q}, \quad q = \begin{pmatrix} q_1 \\ q_2 \end{pmatrix}, \]
Figure 4.3: Energy (Hamiltonian) errors by eight methods for Kepler's problem (4.3), with step size $h = 0.1$.

Figure 4.4: Angular momentum errors by eight methods for Kepler's problem (4.3), with step size $h = 0.1$. 
Figure 4.5: RLP invariant errors by eight methods for Kepler's problem (4.3), with step size $h = 0.1$.

Figure 4.6: Solution errors by eight methods for Kepler’s problem (4.3), with step size $h = 0.1$. 
Figure 4.7: Numerical orbits by eight methods for Kepler’s problem (4.3), with step size $h = 0.1$.

and the Runge–Lenz–Pauli-vector (RLP) invariant

$$L = \begin{pmatrix} p_1 \\ p_2 \\ 0 \end{pmatrix} \times \begin{pmatrix} 0 \\ 0 \\ q_1 p_2 - q_2 p_1 \end{pmatrix} - \frac{1}{\sqrt{q_1^2 + q_2^2}} \begin{pmatrix} q_1 \\ q_2 \\ 0 \end{pmatrix}.$$

We will take the initial values as

$q_1(0) = 1, \quad q_2(0) = 0, \quad p_1(0) = 0, \quad p_2(0) = 1,$

and the corresponding exact solution is known as

$q_1(t) = \cos(t), \quad q_2(t) = \sin(t), \quad p_1(t) = -\sin(t), \quad p_2(t) = \cos(t).$

For such a non-polynomial system, we use 4-point Gaussian quadrature for approximating the integrals of method V and VI, and 5-point Gaussian quadrature for method I and II, while for method III and IV, 8-point Gaussian quadrature is applied. In our numerical experiments, we compute and compare the accumulative errors of three invariants $H, I$ and $L$ with 10,000-step integration. These results are shown in Fig. 4.3-4.5, where the errors at each time step are carried out in the maximum norm $||x||_\infty = \max(|x_1|, \ldots, |x_n|)$ for $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$. It indicates that our methods show a practical preservation of the energy but a near-preservation of other invariants, while two symplectic methods exhibit a practical preservation of the quadratic angular momentum$^{6}$ but show a near-preservation of other invariants. The global errors of numerical solutions are shown

$^{6}$It is known that Gauss-Legendre Runge-Kutta methods can preserve all quadratic invariants of a general first-order system $\dot{y} = f(y)$ $^{19}$.
in Fig. 4.6 and from which linear error growths for all the methods are observed. Moreover, the numerical solutions are plotted on the phase plane (see Fig. 4.7), showing that all the methods can mimic the phase orbits very well. These numerical observations have well conformed with our theoretical results.

5. Concluding remarks

The constructive theory of energy-preserving continuous-stage Runge-Kutta-Nyström methods is developed for solving a special class of second-order differential equations. Sufficient conditions for a continuous-stage Runge-Kutta-Nyström method to be energy-preserving are presented. With the presented conditions and relevant results, we can derive many new effective energy-preserving integrators. Besides, the relationship between energy-preserving continuous-stage Runge-Kutta-Nyström methods and partitioned Runge-Kutta methods is examined. Numerical experiments have verified our theoretical results very well.

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