Energy-preserving continuous-stage partitioned Runge-Kutta methods

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Abstract

In this paper, we present continuous-stage partitioned Runge-Kutta (csPRK) methods for energy-preserving integration of Hamiltonian systems. A sufficient condition for the energy preservation of the csPRK methods is derived. It is shown that the presented condition contains the existing condition for energy-preserving continuous-stage Runge-Kutta methods as a special case. A noticeable and interesting result is that when we use the simplifying assumptions of order conditions and the normalized shifted Legendre polynomials for constructing high-order energy-preserving csPRK methods, both the Butcher “weight” coefficients $B_\tau$ and $\hat{B}_\tau$ must be equal to 1. As illustrative examples, new energy-preserving integrators are acquired by virtue of the presented condition, and for the sake of verifying our theoretical results, some numerical experiments are reported.

Keywords: Continuous-stage partitioned Runge-Kutta methods; Hamiltonian systems; Energy preservation; Symplecticity.

1. Introduction

In modern scientific computing, it is strongly suggested to properly simulate the long-time evolution of a dynamical system by means of a numerical integration. Geometric integrators are beneficial for this aspect as they possess an overwhelming superiority in reproducing the significant qualitative properties of the original systems especially when compared to conventional integrators without any geometric-feature preservations \cite{16,20,31}. By definition, if a numerical method can preserve at least one of geometric properties of the given system, then we call it a geometric integrator. Some typical geometric integrators can be listed as follows: symplectic methods, symmetric methods, volume-preserving methods, energy-preserving methods, Lie-group methods, multi-symplectic methods, etc. For more details, we refer the interested readers to \cite{3,16,20,24,31} and references therein.

In this paper, we are concerned with the well-known Hamiltonian systems. To be specific, a system consisting of $2d$-dimensional, elegant, first-order ordinary differential equations

\begin{equation}
\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,
\end{equation}

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is called a Hamiltonian system with $d$ degree-of-freedom. Here $H$ is referred to as the Hamiltonian function (the total energy), and $p, q$ represent the conjugate momenta and generalized coordinates respectively. We mention the following two significant properties of such system [2]:

a. Symplecticity (Poincaré 1899): $dp(t) \wedge dq(t) = dp(t_0) \wedge dq(t_0)$ for $\forall t$;

b. Energy preservation: $H(p(t), q(t)) = H(p(t_0), q(t_0))$ for $\forall t$.

Remark that symplecticity is a characteristic property for Hamiltonian systems and many interesting qualitative properties of the exact flow can be derived from it [2][20]. On the other hand, since energy (as well as other invariants) play a central role in mechanics, it is of fundamental importance to be able to preserve it in the numerical discretization. Hence, in early times people strongly hoped to have a numerical method that can preserve the symplecticity and energy simultaneously for solving general Hamiltonian systems. But unfortunately, this turns out to be impossible from a negative result given by Ge & Marsden [17], which states that for a Hamiltonian system without extra invariants such a method has to be a time re-parametrization of the exact flow (see also [12] for the case of B-series integrators). Therefore, people are constrained to consider methods satisfying one of these properties and to investigate how well the other would be fulfilled. As is well known, symplectic integrators have been intensively and extensively investigated by many researchers since 1980s [3][11][13][14][15][16][20][24][30][31][50], whereas energy-preserving integrators seemed to attract less attention in the past decades. However, in more recent years, there has been a rising interest in the study of energy-preserving integrators [11][5][6][10][13][21][25][26][27][28][29][34][37]. Between the two types of integrators, most people tend to hold the view that [11][20][23][31][33]: generally speaking, symplectic integrators can reproduce the main qualitative properties of Hamiltonian systems due to their global restriction [11][31][33] of the numerical solutions in all directions by the symplectic structure in phase space which gives rise to a near-preservation of first integrals (containing the energy as a special case) at the same time [20], while energy-preserving integrators may be applied principally for numerical integration of low-dimensional Hamiltonian systems [20][23][31], by noticing that they force the numerical solutions to be on the $(2d - 1)$-dimensional manifold of constant Hamiltonian but generally pose no other restrictions to the dynamics — this is clearly a rather weak restriction when $d$ is large [31]. Nonetheless, in contrast 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 [1][6][18][20][32]. Therefore, both types of integrators are of interest in practice and they are worth investigating.

In this paper, we are interested in the continuous-stage approaches for numerical discretization of ordinary differential equations, the seminal idea of which were introduced by Butcher in 1972 [7] (see also [8][9]) and subsequently developed by Hairer in 2010 [21]. We mention some typical applications of such approaches in the study of geometric integration as follows: there are several existing energy-preserving integrators that can be connected to Runge-Kutta (RK) methods with continuous stage [5][10][13][21][25][26][27][28][34][47]; the conjugate-symplecticity of energy-preserving methods can be discussed in the context of continuous-stage Runge-Kutta (csRK) methods [21][22][36]; both symplectic and symmetric integrators can be devised in use of the notions of Runge-Kutta (RK), partitioned Runge-Kutta (PRK) and Runge-Kutta-Nyström (RKN) methods with continuous stage [35][36][37][38][40][41][42][43][44][45][48]; it is known that some symplectic integrators derived from
Galerkin variational problems can be interpreted and analyzed in the framework of continuous-stage partitioned Runge-Kutta (csPRK) methods \cite{34,39,46}. Particularly, it is worth mentioning that energy-preserving integrators can be easily constructed by using csRK approaches \cite{26,27,35,36}, which result in energy-preserving RK methods by using quadrature formulas. In this paper, we are going to extend the study of energy-preserving csRK methods to the case of energy-preserving csPRK methods. For this sake, we will explore the sufficient condition for energy preservation in the first place, and then by means of the derived sufficient condition we investigate the construction of new energy-preserving integrators.

The outline of this paper is as follows. In Section 2, we present a sufficient condition for a csPRK method to be energy-preserving and some rephrasing versions of the condition are presented. Section 3 is devoted to discuss the construction of energy-preserving integrators with the help of the presented sufficient condition and the associated order conditions. We exhibit our numerical results in Section 4 and give some concluding remarks in Section 5 for ending this paper.

2. Energy-preserving condition for csPRK methods

Consider the following initial value problem of ordinary differential equations in a partitioned form

\[
\begin{align*}
\dot{y} &= f(t, y, z), \quad y(t_0) = y_0 \in \mathbb{R}^m, \\
\dot{z} &= g(t, y, z), \quad z(t_0) = z_0 \in \mathbb{R}^n,
\end{align*}
\]

where \(f, g\) are regular vector-valued functions and here \(m, n\) are not necessarily identical. The so-called csPRK methods have been previously proposed and developed in \cite{36,38} for constructing symplectic integrators, where the \(y\)-variable and \(z\)-variable are treated in different ways by following the idea of classical partitioned Runge-Kutta methods.

**Definition 2.1.** \cite{36,38} Let \(A_{\tau,\sigma}, \hat{A}_{\tau,\sigma}\) be functions of variables \(\tau, \sigma \in [0, 1]\) and \(B_{\tau}, \hat{B}_{\tau}, C_{\tau}, \hat{C}_{\tau}\) be functions of \(\tau \in [0, 1]\). The following one-step method for solving (2.1)

\[
\begin{align*}
\bar{y}_\tau &= y_0 + h \int_0^1 A_{\tau,\sigma} f(t_0 + C_{\sigma} h, Y_{\sigma}, Z_{\sigma}) \, d\sigma, \quad \tau \in [0, 1], \\
\bar{z}_\tau &= z_0 + h \int_0^1 \hat{A}_{\tau,\sigma} g(t_0 + \hat{C}_{\sigma} h, Y_{\sigma}, Z_{\sigma}) \, d\sigma, \quad \tau \in [0, 1], \\
y_1 &= y_0 + h \int_0^1 B_{\tau} f(t_0 + C_{\tau} h, Y_{\tau}, Z_{\tau}) \, d\tau, \\
z_1 &= z_0 + h \int_0^1 \hat{B}_{\tau} g(t_0 + \hat{C}_{\tau} h, Y_{\tau}, Z_{\tau}) \, d\tau.
\end{align*}
\]

is called a continuous-stage partitioned Runge-Kutta (csPRK) method.

The csPRK method (2.2) is said to have order \(p\), if for all sufficiently regular problems (2.1), as \(h \to 0\), its local error satisfies

\[
y_1 - y(t_0 + h) = O(h^{p+1}), \quad z_1 - z(t_0 + h) = O(h^{p+1}).
\]

**Remark 2.2.** Particularly, if we let \(\hat{A}_{\tau,\sigma} = A_{\tau,\sigma}, \hat{B}_{\tau} = B_{\tau}\) and \(\hat{C}_{\tau} = C_{\tau}\), then the corresponding method is reduced to a continuous-stage Rung-Kutta (csRK) method \cite{21,36,78}.
Now we apply the csPRK method (2.2) to the Hamiltonian system (1.1), then it yields

$$
P_\tau = p_0 - h \int_0^1 A_{\tau, \sigma} \nabla_q H(P_{\sigma}, Q_{\sigma}) \, d\sigma, \quad Q_\tau = q_0 + h \int_0^1 \tilde{A}_{\tau, \sigma} \nabla_p H(P_{\sigma}, Q_{\sigma}) \, d\sigma,
$$

\[ \quad p_1 = p_0 - h \int_0^1 B_{\tau} \nabla_q H(P_{\tau}, Q_{\tau}) \, d\tau, \quad q_1 = q_0 + h \int_0^1 \tilde{B}_{\tau} \nabla_p H(P_{\tau}, Q_{\tau}) \, d\tau, \]  \hspace{1cm} \text{(2.3)}

for \( \forall \tau \in [0, 1] \). For convenience, we also assume \( A_{\tau, \sigma}, \tilde{A}_{\tau, \sigma} \) are sufficiently differentiable. Obviously, to construct an energy-preserving csPRK method is to devise suitable Butcher coefficients so as to guarantee the energy preservation, i.e., \( H(p_{n+1}, q_{n+1}) = H(p_n, q_n), \ n = 0, 1, 2, \ldots \). For a one-step method, it suffices to consider the case after one step computation, i.e., verifying the following condition

$$
H(p_1, q_1) = H(p_0, q_0). \quad \text{(2.4)}
$$

In the following, we present a sufficient condition for the one-step method (2.3) to be an energy-preserving integrator.

**Theorem 2.3.** If the coefficients of the csPRK method (2.3) satisfy

$$
A_{0, \sigma} = 0, \ A_{1, \sigma} = B_{\sigma}, \ \forall \sigma \in [0, 1],
$$

$$
\tilde{A}_{0, \sigma} = 0, \ \tilde{A}_{1, \sigma} = \tilde{B}_{\sigma}, \ \forall \sigma \in [0, 1],
$$

\[ \frac{\partial}{\partial \tau} A_{\tau, \sigma} = \frac{\partial}{\partial \sigma} \tilde{A}_{\sigma, \tau}, \ \forall \tau, \sigma \in [0, 1], \]  \hspace{1cm} \text{(2.5)}

then the method is energy-preserving for solving Hamiltonian system (1.1).

**Proof.** It is seen that (2.5) implies

$$
P_0 = p_0, \ P_1 = p_1, \ Q_0 = q_0, \ Q_1 = q_1,
$$

and then, by the fundamental theorem of calculus it gives

$$
H(p_1, q_1) - H(p_0, q_0) = \int_0^1 \frac{d}{d\tau} H(P_{\tau}, Q_{\tau}) \, d\tau
$$

\[ = \int_0^1 \left[ (P_{\tau}')^T \nabla_p H(P_{\tau}, Q_{\tau}) + (Q_{\tau}')^T \nabla_q H(P_{\tau}, Q_{\tau}) \right] d\tau. \]  \hspace{1cm} \text{(2.6)}

By using (2.3), we compute

$$
\int_0^1 (P_{\tau}')^T \nabla_p H(P_{\tau}, Q_{\tau}) \, d\tau
$$

\[ = \int_0^1 \left[ \left( -h \int_0^1 \frac{\partial}{\partial \tau} A_{\tau, \sigma} (\nabla_q H(P_{\sigma}, Q_{\sigma}))^T \, d\sigma \right) \nabla_p H(P_{\tau}, Q_{\tau}) \right] d\tau
$$

\[ = -h \int_0^1 \left[ \frac{\partial}{\partial \tau} A_{\tau, \sigma} (\nabla_q H(P_{\sigma}, Q_{\sigma}))^T \nabla_p H(P_{\tau}, Q_{\tau}) \right] d\tau.\]
Similarly, we have
\[
\int_0^1 (Q')^T \nabla_q H(P, Q) \, d\tau
= \int_0^1 (Q')^T \nabla_q H(P, Q) \, d\sigma
= \int_0^1 \left[ (h \int_0^1 \frac{\partial}{\partial \sigma} \tilde{A}_{\sigma, \tau}(\nabla_q H(P, Q))^T \, d\tau) \nabla_q H(P, Q) \right] \, d\sigma
= h \int_0^1 \int_0^1 \left[ \frac{\partial}{\partial \sigma} \tilde{A}_{\sigma, \tau}(\nabla_q H(P, Q))^T \nabla_q H(P, Q) \right] \, d\tau \, d\sigma.
\]
Substituting the two formulas above into (2.6) and using the last formula of (2.5) yields (2.4), which completes the proof.

Remark 2.4. If we let \( \tilde{A}_{\tau, \sigma} = A_{\tau, \sigma} \) and \( \tilde{B}_\tau = B_\tau \) in (2.3) and (2.5), then we regain the corresponding energy-preserving sufficient condition given in [26] for the case of continuous-stage Runge-Kutta methods (which has been proved to be necessary under some assumptions in [27]). By the way, from the proof of the theorem, we observe that \( H \) can be arbitrarily chosen, thus the term \((\nabla_q H(P, Q))^T \nabla_q H(P, Q)\) of the integrand can also be changed freely within some extent. From this viewpoint, the derived condition \( \frac{\partial}{\partial \sigma} A_{\tau, \sigma} = \frac{\partial}{\partial \sigma} \tilde{A}_{\sigma, \tau} \) may be essentially “necessary” in some sense. For instance, if we additionally assume \( \varphi(\tau, \sigma) = \frac{\partial}{\partial \sigma} A_{\tau, \sigma} - \frac{\partial}{\partial \sigma} \tilde{A}_{\sigma, \tau} \) is a sign-invariant, continuous, binary function, then it must vanish because we can always take a special \( H(p, q) \), e.g., \( H(p, q) = p + q \), such that \((\nabla_q H(P, Q))^T \nabla_q H(P, Q) > 0\).

It is interesting to observe that (2.5) forms a simple linear system of partial differential equations, which may be solved. For this sake, we introduce the normalized shifted Legendre polynomial \( L_j(x) \) of degree \( j \), which can be defined by the Rodrigues’ formula
\[
L_0(x) = 1, \quad L_j(x) = \frac{\sqrt{2j + 1}}{j!} \frac{d^j}{dx^j} \left( x^j (x - 1)^j \right), \quad j = 1, 2, 3, \ldots.
\]
A well-known property of such polynomials is that they are orthogonal to each other with respect to the \( L^2 \) inner product
\[
\int_0^1 L_j(x) L_k(x) \, dx = \delta_{jk}, \quad j, k = 0, 1, 2, \ldots,
\]
and satisfy the following integration formulas
\[
\begin{align*}
\int_0^\tau L_j(x) \, dx &= \xi_{j+1} L_{j+1}(\tau) - \xi_j L_{j-1+\delta_{j0}}(\tau), \quad j = 0, 1, 2, \ldots, \\
\int_\tau^1 L_j(x) \, dx &= \delta_{j0} - \xi_{j+1} L_{j+1}(\tau) + \xi_j L_{j-1+\delta_{j0}}(\tau), \quad j = 0, 1, 2, \ldots,
\end{align*}
\]
where \( \delta_{jk} \) is the Kronecker delta and
\[
\xi_j = \begin{cases} \frac{1}{2\sqrt{4j^2 - 1}}, & j \geq 1; \\ \frac{1}{2}, & j = 0. \end{cases}
\]
Since \( \{L_i(\tau)L_j(\sigma) : i, j \geq 0\} \) constitutes a complete orthogonal set in \( L^2([0, 1] \times [0, 1]) \) (Hilbert space), we suppose that the following expansion for the last formula of (2.5) is allowed

\[
\frac{\partial}{\partial \tau} A_{\tau,\sigma} = \frac{\partial}{\partial \sigma} \hat{A}_{\sigma,\tau} = \sum_{i, j \geq 0} \alpha_{(i,j)} L_i(\tau)L_j(\sigma),
\]

where \( \alpha_{(i,j)} \) are real parameters. By taking integrals, it gives

\[
A_{\tau,\sigma} = \sum_{i, j \geq 0} \alpha_{(i,j)} \int_0^\tau L_i(x) \, dx L_j(\sigma) + \psi(\sigma), \quad \hat{A}_{\sigma,\tau} = \sum_{i, j \geq 0} \alpha_{(i,j)} L_i(\tau) \int_0^\sigma L_j(x) \, dx + \phi(\tau),
\]

where \( \psi, \phi \) are arbitrary functions. Noticing \( A_{0,\sigma} = 0, \hat{A}_{0,\tau} = 0 \) by (2.5), we have \( \psi \equiv 0, \phi \equiv 0 \), which then gives rise to

\[
A_{\tau,\sigma} = \sum_{i, j \geq 0} \alpha_{(i,j)} \int_0^\tau L_i(x) \, dx L_j(\sigma), \quad \hat{A}_{\sigma,\tau} = \sum_{i, j \geq 0} \alpha_{(i,j)} L_i(\tau) \int_0^\sigma L_j(x) \, dx.
\]

From the second formula above, it follows

\[
\hat{A}_{\tau,\sigma} = \sum_{i, j \geq 0} \alpha_{(j,i)} \int_0^\tau L_i(x) \, dx L_j(\sigma).
\]

By using a new notation \( \hat{\alpha}_{(i,j)} := \alpha_{(j,i)} \), then it gives

\[
\hat{A}_{\tau,\sigma} = \sum_{i, j \geq 0} \hat{\alpha}_{(i,j)} \int_0^\tau L_i(x) \, dx L_j(\sigma).
\]

Note that

\[
\int_0^1 L_i(x) \, dx = \delta_{i0}, \quad i = 0, 1, \ldots,
\]

then by using (2.5), we have

\[
B_\tau = A_{1,\tau} = \sum_{j \geq 0} \alpha_{(0,j)} L_j(\tau), \quad \hat{B}_\tau = \hat{A}_{1,\tau} = \sum_{j \geq 0} \hat{\alpha}_{(0,j)} L_j(\tau).
\]

**Theorem 2.5.** Suppose that \( A_{\tau,\sigma}, \hat{A}_{\tau,\sigma} \in L^2([0, 1] \times [0, 1]) \), then the energy-preserving condition given in (2.5) is equivalent to

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

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

where \( \hat{\alpha}_{(i,j)} = \alpha_{(j,i)} \) are real numbers.

For the sake of practical use, \( A_{\tau,\sigma} \) and \( \hat{A}_{\tau,\sigma} \) are usually assumed to be polynomial functions, then it is advisable to use the following finite expansion taking the place of (2.8)

\[
\frac{\partial}{\partial \tau} A_{\tau,\sigma} = \frac{\partial}{\partial \sigma} \hat{A}_{\sigma,\tau} = \sum_{i=0}^{s-1} \sum_{j=0}^{r-1} \alpha_{(i,j)} L_i(\tau)L_j(\sigma), \quad \text{with } s, r \geq 1.
\]

By using similar arguments, we then derive the following result which essentially corresponds to the modified version of Theorem 2.5 by truncating all the infinite series in (2.10).

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Theorem 2.6. If the coefficients of the csPRK method (2.3) are of the following forms

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

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

where \(\tilde{\alpha}_{(i,j)} = \alpha_{(j,i)}\), then the method is energy-preserving for solving Hamiltonian system (1.1).

Remark 2.7. Remark that we can use any other polynomial or non-polynomial basis for the formal expansion as shown in (2.11), which may result in a little more complicated form for rephrasing the energy-preserving condition (2.5). Particularly, functionally-fitted energy-preserving csPRK methods could be devised by using the similar techniques given in [25, 26].

In the practical implementation, generally we have to approximate the integrals of (2.3) by using quadrature formulas. Let \(b_i\) and \(c_i\) be the weights and abscissae of the following \(k\)-point interpolatory quadrature formula

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

(2.13)

where

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

Assume the Butcher coefficients of the method (2.3) are given by (2.12), then by using (2.13), it gives

\[
P_{\tau} = p_0 - h \sum_{j=1}^k b_j A_{\tau,c_j} \nabla_q H(P_{c_j}, Q_{c_j}), \quad \tau \in [0, 1],
\]

\[
Q_{\tau} = q_0 + h \sum_{j=1}^k b_j \tilde{A}_{\tau,c_j} \nabla_p H(P_{c_j}, Q_{c_j}), \quad \tau \in [0, 1],
\]

\[
p_1 = p_0 - h \sum_{i=1}^k b_i B_{c_i} \nabla_q H(P_{c_i}, Q_{c_i}),
\]

\[
q_1 = q_0 + h \sum_{i=1}^k b_i \tilde{B}_{c_i} \nabla_p H(P_{c_i}, Q_{c_i}).
\]

(2.14)

There are two ways to compute the numerical approximation solutions \(p_1\) and \(q_1\) to the exact solutions \(p(t_0 + h)\) and \(q(t_0 + h)\). One way is to resort to the standard form of PRK schemes, i.e., substituting \(\tau = c_i\) into the first two formulas of (2.14) and then regarding \(P_{c_i}\) and \(Q_{c_i}\) as the internal stages. However, when the number of abscissae \(c_i\) is too many, it may lead to too much computational work. In such a case, we realize that there are many redundant internal stages which can be expressed as linear combinations of a group of fundamental stages. In other words, all the
internal stages are not linear independent. Concerning this situation, an alternative way can be adopted on the basis of the polynomial expansions

\[ P_\tau = \sum_{j=1}^{s+1} \lambda_j \phi_j(\tau), \quad Q_\tau = \sum_{j=1}^{r+1} \mu_j \psi_j(\tau), \]  

(2.15)

where \( \{\phi_j(\tau)\} \) (resp. \( \{\psi_j(\tau)\} \)) is a suitable basis in the polynomial function space of degree \( s \) (resp. \( r \)) at most. As a consequence, all \( P_{c_i} \) and \( Q_{c_i} \) in (2.14) (with \( \tau = c_i \) being inserted) can be expressed in terms of the unknown expansion coefficients \( \lambda_j \) and \( \mu_j \), which constitutes an nonlinear algebraic system that can be solved by iteration. This implies that the computational cost for the solution of the associated nonlinear system is essentially independent of the number of quadrature abscissae, but only depends on the degrees of \( P_\tau \) and \( Q_\tau \) — the similar observation has been presented for Hamiltonian boundary value methods in [4, 5, 6].

If we are concerned with the polynomial Hamiltonian systems, then the integrands in (2.3) are also polynomials which can be exactly computed by means of a suitable quadrature formula. In such a case, it gives rise to an exact energy preservation by the quadrature-based PRK scheme (2.14) (with \( \tau = c_i \) being inserted) which can be precisely stated in the following result.

**Theorem 2.8.** If the coefficients of the underlying csPRK method are given by (2.12), then the PRK scheme (2.14) is exactly energy-preserving for the polynomial Hamiltonian system (1.1) with a \( \nu \)-degree Hamiltonian function \( H(p,q) \), provided that the quadrature formula (2.13) is of Gaussian type\(^1\) and the number of nodes, say \( k \), satisfies

\[ k \geq \frac{\mu \nu}{2}, \]

where \( \mu = \max(s, r) \).

*Proof.* The proof is on the basis of the fact that the Gaussian-type quadrature formula (2.13) with \( k \) nodes can exactly calculate the integrals of (2.3), if the degree of the integrands is no higher than the degree of precision of the quadrature. Particularly, one should notice that the degree of both \( \nabla_q H(P_\sigma, Q_\sigma) \) and \( \nabla_p H(P_\sigma, Q_\sigma) \) is \( (\nu - 1) \times \max(s, r) \).

We must stress that in most instances the PRK method (2.14) is able to preserve (exactly or up to round-off error) the nonlinear Hamiltonian \( H(p,q) \) (not necessarily polynomial) along the numerical solution, by taking the number of abscissae \( c_i \) large enough, since for the case of non-polynomial Hamiltonian systems, the Hamiltonian \( H(p,q) \) can be commonly approximated by polynomials locally in each step of the numerical computation (see [5] for the similar discussions in terms of Hamiltonian boundary value methods). In addition, the quadrature-based PRK method (2.14) possess the same order of the associated csPRK method since we have to use a quadrature formula with a high-enough degree of precision for the sake of energy preservation. For the connection between a csPRK method and its quadrature-based PRK method in terms of the order accuracy, we refer the readers to Theorem 2.5 of [38].

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\(^1\)It is seen from (2.14) that \( P_\tau \) (resp. \( Q_\tau \)) has the same degree as \( A_{\tau,c_i} \) (resp. \( \hat{A}_{\tau,c_i} \)) with respect to \( \tau \).

\(^2\)This means the quadrature formula is exact for all polynomial functions with degree \( \leq 2k - 1 \).
3. Construction of energy-preserving csPRK methods

Now we are in the position to discuss the construction of energy-preserving integrators by means of the derived sufficient condition (2.10).

3.1. Construction of energy-preserving integrators

As shown in the preceding section, we have acquired the characterizations for energy preservation of csPRK methods in use of Legendre polynomial expansions (see Theorem 2.5). However, we are facing infinitely many choices for taking the values of $\alpha(i,j)$. Concerning such problem, we may ask the following two questions:

a. How to determine the order of the method for a given group of $\alpha(i,j)$?

b. How to choose suitable $\alpha(i,j)$ to make the method possess a prescribed order?

The first question can be solved without difficulties by using the standard P-series theory in a similar manner as the classical case for PRK methods [19, 20], that is, one can determine the order of the method by verifying a set of order conditions related to bi-colored trees.

The second question, which is relatively more important than the first one, will be our central topic in the following discussions. Actually, it can be addressed by using the orthogonal polynomial expansion technique in conjunction with the order conditions. One possible way is that we can use the same approach as presented in [40, 41] for constructing methods of arbitrary order, i.e., substituting (2.10) into the order conditions one by one and determining the corresponding parameters $\alpha(i,j)$ (see Theorem 3.1 below as a simple example). However, such a approach may lead to increasing-complicated computations when the order goes much higher, hence it may be not suitable for devising high-order methods and for this reason we do not plan to pursue it here.

**Theorem 3.1.** The energy-preserving csPRK method with coefficients (2.10) has order at least 1 if and only if $\hat{\alpha}(0,0) = \alpha(0,0) = 1$.

**Proof.** By P-series theory [20], the order condition for 1-order csPRK methods should be

$$
\int_0^1 B_\tau d\tau = 1, \quad \int_0^1 \hat{B}_\tau d\tau = 1,
$$

(3.1)

which corresponds to the first two bi-colored bushy trees with only one vertex (see Table 2.1 of [20], page 67). Substituting (2.10) into (3.1) and using the orthogonality of Legendre polynomials, yields

$$
1 = \int_0^1 B_\tau d\tau = \alpha(0,0), \quad 1 = \int_0^1 \hat{B}_\tau d\tau = \hat{\alpha}(0,0),
$$

which completes the proof. \qed

\footnote{Note that the corresponding order conditions can be easily obtained by using P-series theory [19, 20].}
An alternative way is to use the following simplifying assumptions \[13, 38\]:

\[
\begin{align*}
\mathcal{B}(\xi) & : \int_0^1 B_\tau C_\tau^{\kappa-1} \hat{C}_\tau^\iota \, d\tau = \frac{1}{\kappa + \iota}, \quad 1 \leq \kappa + \iota \leq \xi, \\
\mathcal{C}(\eta) & : \int_0^1 A_{\tau, \sigma} C_\sigma^{\kappa-1} \hat{C}_\sigma^\iota \, d\sigma = \frac{C_\tau^{\kappa+\iota}}{\kappa + \iota}, \quad 1 \leq \kappa + \iota \leq \eta, \quad \tau \in [0, 1], \\
\hat{\mathcal{C}}(\eta) & : \int_0^1 \hat{A}_{\tau, \sigma} C_\sigma^{\kappa-1} \hat{C}_\sigma^\iota \, d\sigma = \frac{\hat{C}_\tau^{\kappa+\iota}}{\kappa + \iota}, \quad 1 \leq \kappa + \iota \leq \eta, \quad \tau \in [0, 1], \\
\mathcal{D}(\zeta) & : \int_0^1 B_\tau C_\tau^{\kappa-1} \hat{C}_\tau^\iota A_{\tau, \sigma} \, d\tau = \frac{B_\sigma (1 - \hat{C}_\sigma^{\kappa+\iota})}{\kappa + \iota}, \quad 1 \leq \kappa + \iota \leq \zeta, \quad \sigma \in [0, 1], \\
\hat{\mathcal{D}}(\zeta) & : \int_0^1 \hat{B}_\tau C_\tau^{\kappa-1} \hat{C}_\tau^\iota \hat{A}_{\tau, \sigma} \, d\tau = \frac{\hat{B}_\sigma (1 - \hat{C}_\sigma^{\kappa+\iota})}{\kappa + \iota}, \quad 1 \leq \kappa + \iota \leq \zeta, \quad \sigma \in [0, 1].
\end{align*}
\]

**Theorem 3.2.** [38] If the coefficients of a csPRK method \[2.2\] satisfy \(\hat{B}_\tau \equiv B_\tau\), \(C_\tau = \int_0^1 A_{\tau, \sigma} \, d\sigma\), \(\hat{C}_\tau = \int_0^1 \hat{A}_{\tau, \sigma} \, d\sigma\) for \(\forall \tau \in [0, 1]\), and moreover, all \(\mathcal{B}(\xi), \mathcal{C}(\eta), \hat{\mathcal{C}}(\eta), \mathcal{D}(\zeta), \hat{\mathcal{D}}(\zeta)\) hold, then the method is of order at least

\[
p = \min\{\xi, 2\eta + 2, \eta + \xi + 1\}.
\]

For ease of employing Theorem 3.2, hereafter we always assume \(C_\tau = \hat{C}_\tau = \tau\) which is a natural assumption used in the previous studies \[36, 41, 42\].

**Theorem 3.3.** If the coefficients of the csPRK method \[2.3\] are given by \[2.10\] and satisfy

\[
\tau = C_\tau = \int_0^1 A_{\tau, \sigma} \, d\sigma, \quad \text{and} \quad \tau = \hat{C}_\tau = \int_0^1 \hat{A}_{\tau, \sigma} \, d\sigma, \quad \forall \tau \in [0, 1],
\]

then we have \(B_\tau = \hat{B}_\tau = 1\) and moreover, the method is of order at least 2.

**Proof.** Firstly, since \(L_0(x) = 1\), we have

\[
C_\tau = \tau = \int_0^\tau L_0(x) \, dx, \quad (3.2)
\]

On the other hand, by noticing \[2.9\], it follows

\[
C_\tau = \int_0^1 A_{\tau, \sigma} \, d\sigma = \sum_{i \geq 0} \alpha_{i,(0)} \int_0^\tau L_i(x) \, dx. \quad (3.3)
\]

Note that the sequence of polynomials

\[
\int_0^\tau L_0(x) \, dx, \int_0^\tau L_1(x) \, dx, \int_0^\tau L_2(x) \, dx, \cdots
\]

constitutes a linearly independent set, thus by comparing \[3.2\] with \[3.3\] it yields

\[
\alpha_{i,(0)} = \delta_{i0}, \quad i = 0, 1, 2, \ldots.
\]

Similarly, by using \(\hat{C}_\tau = \tau\) and \(\hat{C}_\tau = \int_0^1 \hat{A}_{\tau, \sigma} \, d\sigma\) we have

\[
\hat{\alpha}_{i,(0)} = \delta_{i0}, \quad i = 0, 1, 2, \ldots.
\]

By combining the condition \(\hat{\alpha}_{i,(j)} = \alpha_{j,i}\) in \[2.10\], it gives \(B_\tau = \hat{B}_\tau = 1\). Besides, it is easy to verify that the method satisfies all the order conditions up to order 2 (see Table 2.1 of \[20\], page 67). \(\square\)
Remark 3.4. Remark that the elegant result $B_\tau = \hat{B}_\tau = 1$ may not be derived when other polynomial bases are used in the construction of high-order energy-preserving methods (see the 4-order integrator as examples presented in section 4.2 of [27]).

Under the same assumptions of Theorem 3.3, the associated simplifying assumptions become

$$B(\xi) : \int_0^1 \tau^{k-1} d\tau = \frac{1}{k}, \quad 1 \leq k \leq \xi,$$

$$C(\eta) : \int_0^1 A_{\tau, \sigma} \sigma^{k-1} d\sigma = \frac{\tau^k}{k}, \quad 1 \leq k \leq \eta, \quad \tau \in [0, 1],$$

$$D(\zeta) : \int_0^1 \tau^{k-1} A_{\tau, \sigma} d\tau = \frac{1 - \sigma^k}{k}, \quad 1 \leq k \leq \zeta, \quad \sigma \in [0, 1],$$

and we let $\hat{C}(\eta), \hat{D}(\zeta)$ be as $C(\eta), D(\zeta)$ with $A_{\tau, \sigma}$ replaced by $\hat{A}_{\tau, \sigma}$. Obviously, the first simplifying assumption $B(\xi)$ is always satisfied for any positive integer $\xi$. For convenience, we denote this fact by $B(\infty)$.

It is known that $C(\eta)$ can be recast in the equivalent form [42]

$$C(\eta) : \int_0^1 A_{\tau, \sigma} L_j(\sigma) d\sigma = \int_0^\tau L_j(x) dx, \quad j = 0, \cdots, \eta - 1. \quad (3.4)$$

By inserting the expression for $A_{\tau, \sigma}$ given in (2.10) into (3.4) and using the orthogonality of Legendre polynomials, it follows

$$\sum_{i \geq 0} \alpha_{(i,j)} \int_0^\tau L_i(x) dx = \int_0^\tau L_j(x) dx, \quad j = 0, \cdots, \eta - 1, \quad (3.5)$$

and clearly (3.5) holds true if and only if

$$\alpha_{(i,j)} = \delta_{ij}, \quad i \geq 0, \quad j = 0, \cdots, \eta - 1. \quad (3.6)$$

Consequently, it yields

$$A_{\tau, \sigma} = \sum_{j=0}^{\eta-1} \int_0^\tau L_j(x) dx L_j(\sigma) + \sum_{i \geq 0, j \geq \eta} \alpha_{(i,j)} \int_0^\tau L_i(x) dx L_j(\sigma), \quad B_\tau = 1, \quad (3.7)$$

which satisfies $C(\eta)$ automatically.

Analogously, we have

$$\hat{\alpha}_{(i,j)} = \delta_{ij}, \quad i \geq 0, \quad j = 0, \cdots, \eta - 1. \quad (3.8)$$

and

$$\hat{A}_{\tau, \sigma} = \sum_{j=0}^{\eta-1} \int_0^\tau L_j(x) dx L_j(\sigma) + \sum_{i \geq 0, j \geq \eta} \hat{\alpha}_{(i,j)} \int_0^\tau L_i(x) dx L_j(\sigma), \quad \hat{B}_\tau = 1, \quad (3.9)$$

which satisfies $\hat{C}(\eta)$.

Once again, by noticing $\hat{\alpha}_{(i,j)} = \alpha_{(j,i)}$, (3.8) implies

$$\alpha_{(j,i)} = \delta_{ij}, \quad i \geq 0, \quad j = 0, \cdots, \eta - 1,$$
or equivalently (by exchanging \( i \leftrightarrow j \)),

\[
\alpha_{(i,j)} = \delta_{ij}, \quad i = 0, \cdots, \eta - 1, \; j \geq 0,
\]

which is helpful for further simplifying (3.7), namely, it leads to

\[
A_{\tau,\sigma} = \sum_{j=0}^{\eta-1} \int_0^\tau L_j(x) \, dx L_j(\sigma) + \sum_{i \geq \eta, j \geq \eta} \alpha_{(i,j)} \int_0^\tau L_i(x) \, dx L_j(\sigma), \quad B_\tau = 1. \tag{3.10}
\]

Similarly, by using \( \hat{\alpha}_{(i,j)} = \alpha_{(j,i)} \) and (3.6), it yields

\[
\hat{A}_{\tau,\sigma} = \sum_{j=0}^{\eta-1} \int_0^\tau L_j(x) \, dx L_j(\sigma) + \sum_{i \geq \eta, j \geq \eta} \hat{\alpha}_{(i,j)} \int_0^\tau L_i(x) \, dx L_j(\sigma), \quad \hat{B}_\tau = 1. \tag{3.11}
\]

Next, let us investigate the fulfillment of \( D(\zeta) \) and \( \hat{D}(\zeta) \). For this sake, it is well to recognize that \( D(\zeta) \) can be equivalently transformed into (42)

\[
D(\zeta) : \int_0^1 L_k(\tau) A_{\tau,\sigma} \, d\tau = \int_0^1 L_k(x) \, dx, \quad k = 0, \cdots, \zeta - 1, \tag{3.12}
\]

and \( \hat{D}(\zeta) \) can be obtained by replacing \( A_{\tau,\sigma} \) with \( \hat{A}_{\tau,\sigma} \) in (3.12). By virtue of these preliminaries we get the following result.

**Theorem 3.5.** The csPRK method (2.3) with coefficients given by (3.10) and (3.11) (with \( \hat{\alpha}_{(i,j)} = \alpha_{(j,i)} \)) is energy-preserving and of order \( p = 2\eta \) (\( \eta \geq 1 \)) for solving the Hamiltonian system (1.1).

**Proof.** The energy-preserving property of the method is straightforward by Theorem 2.5. Let us analyze the order of the method in what follows.

First of all, we already have

\[
B_\tau = \hat{B}_\tau, \quad C_\tau = \int_0^1 A_{\tau,\sigma} \, d\sigma = \tau, \quad \hat{C}_\tau = \int_0^1 \hat{A}_{\tau,\sigma} \, d\sigma = \tau,
\]

which are conformed with the premise of Theorem 3.2. Besides, by the analysis from (3.4) to (3.9), it follows that \( C(\eta), \hat{C}(\eta) \) are satisfied by (3.10) and (3.11) respectively.

Next, let us consider the fulfillment of \( D(\zeta) \). By using (2.7), it follows from (3.10) that

\[
A_{\tau,\sigma} = \sum_{j=0}^{\eta-2} \int_0^\tau L_j(x) \, dx L_j(\tau) + \xi_{\eta-1} L_{\eta-2}(\sigma) L_{\eta-1}(\tau) + \xi_\eta L_{\eta-1}(\sigma) L_\eta(\tau) + \sum_{i \geq \eta, j \geq \eta} \alpha_{(i,j)} \int_0^\tau L_i(x) \, dx L_j(\sigma),
\]

where the term (a) can be recast as the form of (b) in view of (2.7) (here \( \gamma_j(\sigma) \) are functions depending only on \( \sigma \)). By substituting the formula above into (3.12), it follows that \( D(\zeta) \) holds

\[
\sum_{j=0}^{\eta-2} \int_0^\tau L_j(x) \, dx L_j(\tau) + \sum_{j \geq \eta-1} \gamma_j(\sigma) L_j(\tau), \quad \text{for } \forall \alpha_{(i,j)} \in \mathbb{R},
\]

\[
= \sum_{j=0}^{\eta-2} \int_0^\tau L_j(x) \, dx L_j(\tau) + \sum_{j \geq \eta-1} \gamma_j(\sigma) L_j(\tau), \quad \text{for } \forall \alpha_{(i,j)} \in \mathbb{R},
\]
with\(^4\) \(\zeta = \eta - 1\). Similarly, one can verify that \(\hat{D}(\zeta)\) holds true with \(\zeta = \eta - 1\). Recall that we already have \(B(\infty)\). As a consequence, the order is \(p = \min\{\xi, 2\eta + 2, \eta + \zeta + 1\} = 2\eta\) by Theorem 3.2.

**Remark 3.6.** Remark that for the sake of getting a finite form of the Butcher coefficients, we can always consider the suitable truncations of (3.10) and (3.11) in the same manner as shown in (2.12) of Theorem 2.6. For instance, we can restrict the summation indexes in terms of \(\alpha(i,j)\) in (3.10) by \(\eta \leq i \leq s - 1\) and \(\eta \leq j \leq r - 1\), while \(\hat{\alpha}(i,j)\) in (3.11) by \(\eta \leq i \leq r - 1\) and \(\eta \leq j \leq s - 1\).

### 3.2. Some energy-preserving integrators as examples

In the following, we give some energy-preserving integrators as illustrative examples.

**Example 3.1.** According to Theorem 2.6 and Theorem 3.1, if we let \(s = 2, r = 1, \alpha(0,0) = 1\) and denote \(\alpha(1,0) = \frac{\alpha}{\sqrt{3}}\), then it gives

\[
A_{r,\sigma} = \theta \tau^2 + (1 - \theta)\tau, \quad B_r = 1,
\]

\[
\hat{A}_{r,\sigma} = (2\theta + 1 - \theta)\tau, \quad \hat{B}_r = 2\theta + 1 - \theta,
\]

which results in a family of 1-order energy-preserving csPRK methods. By substituting these Butcher coefficients into the order conditions up to order 2, we find that it has order 2 if and only if \(\theta = 0\), which in turn leads to the average vector field (AVF) method [28]).

In what follows, we have to assume \(B_r = \hat{B}_r = 1\) for deriving higher order methods according to Theorem 3.3.

**Example 3.2.** According to Theorem 3.5 and Remark 3.6, if we let \(s = 3, r = 2, \eta = 1\) and denote \(\alpha(1,1) = \frac{\alpha_1}{3}, \alpha(2,1) = \frac{\alpha_2}{\sqrt{15}}\), then it gives

\[
A_{r,\sigma} = (4\theta - 2\theta_2)\tau^3 + (\theta_1 - 3\theta_2)(2\sigma - 1)\tau^2 + \left[1 + (\theta_2 - \theta_1)(2\sigma - 1)\right]\tau,
\]

\[
\hat{A}_{r,\sigma} = \left[(6\sigma^2 - 6\sigma + 1)\theta_2 + \theta_1(2\sigma - 1)\right] \tau^2 + \left[1 - \theta_1(2\sigma - 1) - \theta_2(6\sigma^2 - 6\sigma + 1)\right] \tau,
\]

which results in a family of 2-order energy-preserving integrators. Particularly, if we let \(\theta_1 = \theta_2 = 0\), then we once again retrieve the AVF method [28].

**Example 3.3.** According to Theorem 3.5 and Remark 3.6, if we let \(s = 4, r = 3, \eta = 2\) and denote \(\alpha(2,2) = \frac{\alpha_3}{5}, \alpha(3,2) = \frac{\alpha_4}{\sqrt{35}}\), then it gives

\[
A_{r,\sigma} = \theta_2(30\sigma^2 - 30\sigma + 5)\tau^4 + (2\theta_1 - 10\theta_2)(6\sigma^2 - 6\sigma + 1)\tau^3
\]

\[+ \left[(6\theta_2 - 3\theta_1)(6\sigma^2 - 6\sigma + 1) + 6\sigma - 3\right] \tau^2
\]

\[+ \left[(\theta_1 - 2\theta_2)(6\sigma^2 - 6\sigma + 1) - 6\sigma + 4\right] \tau,
\]

\[
\hat{A}_{r,\sigma} = 2\left[\theta_1(6\sigma^2 - 6\sigma + 1) + \theta_2(20\sigma^3 - 30\sigma^2 + 12\sigma - 1)\right] \tau^3
\]

\[+ 3\left[\theta_1(6\sigma^2 - 6\sigma + 1) + \theta_2(20\sigma^3 - 30\sigma^2 + 12\sigma - 1) - 2\sigma + 1\right] \tau^2
\]

\[+ \left[\theta_1(6\sigma^2 - 6\sigma + 1) + \theta_2(20\sigma^3 - 30\sigma^2 + 12\sigma - 1) - 6\sigma + 4\right] \tau,
\]

which results in a family of 4-order energy-preserving integrators.

\(^4\)Here if \(\eta = 1\), then it means \(D(\zeta)\) is not satisfied. In such a case, we can also use Theorem 3.2 to derive the order of the method by setting \(\zeta = 0\).
Example 3.4. By taking $\eta = \varsigma$ and $\alpha_{(i,j)} = 0$, $\alpha_{(i,j)} = 0$ for $i, j \geq \eta$ in Theorem 3.5, we regain the class of energy-preserving methods which are symmetric, conjugate-symplectic up to order $2s + 2$ and have a super-convergence order $2s \ [22, 36, 41]$. Such methods coincide with the limit form of Hamiltonian boundary value methods (denoted by HBVM($\infty$, $s$)) [3], the $s$-degree continuous time finite element methods [34] and the optimal order energy-preserving variant of collocation methods [21].

4. Numerical tests

In this section, we perform some numerical tests to verify our theoretical results.

Example 4.1. Consider the following 2-dimensional linear Hamiltonian system

$$\dot{z} = Lz, \quad L = \begin{pmatrix} b & -c \\ a & -b \end{pmatrix}, \quad z = \begin{pmatrix} p \\ q \end{pmatrix}$$

(4.1)

with the Hamiltonian function given by $H(p, q) = \frac{1}{2}ap^2 + \frac{1}{2}cq^2 - bpq$. When $b^2 - ac < 0$, such a system has periodic solutions. Concerning the initial value condition $(p(0), q(0)) = (p_0, q_0)$, the exact periodic solutions are known as

$$p(t) = \left( \cos(\omega t) + \frac{b}{\omega} \sin(\omega t) \right)p_0 - \frac{c}{\omega} \sin(\omega t)q_0, \quad q(t) = \frac{a}{\omega} \sin(\omega t)p_0 + \left( \cos(\omega t) - \frac{b}{\omega} \sin(\omega t) \right)q_0,$$

where $\omega = \sqrt{ac - b^2}$.
Figure 4.2: Energy (Hamiltonian) errors by six methods for linear Hamiltonian system (4.1), with step size $h = 0.1$.

Figure 4.3: Phase orbits by six methods for linear Hamiltonian system (4.1), with step size $h = 0.1$. 
We take \(a = 1, b = -1, c = 2\) and \(p(0) = 0.5, q(0) = 0\) in our numerical tests and six methods will be applied to this problem. Amongst these six methods, two energy-preserving methods shown in Example 3.1 with \(\theta = 1\) (denoted by EP-scheme I) and \(\theta = 2\) (denoted by EP-scheme II), and two symplectic schemes called symplectic Euler methods [50] (see also [20], page 189) will be used — for convenience, we denote the one with \(p\)-variable being explicit and \(q\)-variable being implicit by Sympl. Euler I, while the other one (in an opposite manner to the former one) by Sympl. Euler II. Besides, explicit Euler and implicit Euler methods are also used in the numerical comparison, noting that they are known to be neither symplectic nor energy-preserving.

Fig. 4.1 shows the order verification in a log-log plot, from which we see that all the methods are of the same order, say 1. The energy errors of all the six methods are presented in Fig. 4.2. It is observed that the energy is well preserved by our methods, while two symplectic methods have a bounded energy error. As is shown, explicit Euler and implicit Euler methods have the worst results in the preservation of the energy. The simulations of the phase orbits are exhibited in Fig. 4.3. As expected, the phase orbits computed by the two energy-preserving methods almost exactly coincide with the exact one, while the two symplectic methods show a little bit worse approximation to the exact orbit — this can be explained theoretically by backward error analysis [20], stating that symplectic methods can only preserve a modified Hamiltonian (hence a near preservation of the energy) in general. Therefore, for this low-dimensional Hamiltonian system, the solutions of the energy-preserving methods behave better than that of the two symplectic methods. We also observe that the numerical phase orbits of the explicit Euler and of the implicit Euler method spiral either outwards or inwards, which are completely incorrect.

**Example 4.2.** Consider the numerical integration of the well-known Hénon-Heiles model problem [20], which can be described by a second-order system

\[
\ddot{q}_1 = -q_1 - 2q_1q_2, \quad \ddot{q}_2 = -q_2 - q_1^2 + q_2^2.
\]

By introducing \(p_1 = \dot{q}_1\) and \(p_2 = \dot{q}_2\), such system can be transformed into a first-order Hamiltonian system with the Hamiltonian function

\[
H = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}(q_1^2 + q_2^2) + q_1q_2 - \frac{1}{3}q_2^3.
\]

In our experiment, the initial values are taken as

\[
p_1(0) = 0, \ p_2(0) = 0, \ q_1(0) = 0.1, \ q_2(0) = -0.5,
\]

which will lead to a chaotic behavior [20, 28]. Fig. 4.4 and 4.5 present the numerical results. In these figures, EP method I and EP method II represent the methods given in Example 3.2 with 3-point Gaussian quadrature being used for computing the integrals, and the corresponding parameters are taken as \(\theta_1 = 1, \theta_2 = 0\) and \(\theta_1 = 1, \theta_2 = 1\) respectively. For comparison, two symplectic methods of order 2 are also used which are referred to as the implicit midpoint rule and the Störmer-Verlet scheme [20]. From the numerical results, we see that our methods have a practical preservation for the energy, while the symplectic methods have a near-preservation of the energy (see Fig. 4.4). Moreover, all the methods numerically reproduce the correct behavior of the original system without points escaping from the equilateral triangle (see Fig. 4.5).
Figure 4.4: Energy (Hamiltonian) errors by four methods for Hénon-Heiles model problem, with step size $h = 0.1$.

Figure 4.5: Chaotic orbits by four methods for Hénon-Heiles model problem, with step size $h = 0.1$. 
Figure 4.6: Energy (Hamiltonian) errors by four methods for Kepler’s problem, with step size $h = 0.1$.

Figure 4.7: Angular momentum errors by four methods for Kepler’s problem, with step size $h = 0.1$. 
Figure 4.8: RLP invariant errors by four methods for Kepler’s problem, with step size $h = 0.1$.

Figure 4.9: Solution errors by four methods for Kepler’s problem, with step size $h = 0.1$. 
Example 4.3. Consider the numerical solution of the well-known Kepler’s problem [20] which can be described by

\[ \ddot{q}_1 = -\frac{q_1}{(q_1^2 + q_2^2)^{3/2}}, \quad \ddot{q}_2 = -\frac{q_2}{(q_1^2 + q_2^2)^{3/2}}. \] (4.2)

By introducing the momenta \( p_1 = \dot{q}_1, p_2 = \dot{q}_2 \), we can recast (4.2) as a nonlinear Hamiltonian system with the Hamiltonian

\[ H = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}}. \]

Besides the known invariant \( H \), such system possesses other two invariants \( I \) and \( L \): the quadratic angular momentum

\[ I = q_1p_2 - q_2p_1 = q^T \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \dot{q}, \quad q = \begin{pmatrix} q_1 \\ q_2 \end{pmatrix}, \]

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

\[ L = \begin{pmatrix} p_1 \\ p_2 \\ 0 \end{pmatrix} \times \begin{pmatrix} 0 & 1 \\ -1 & 0 \\ q_1p_2 - q_2p_1 \end{pmatrix} - \frac{1}{\sqrt{q_1^2 + q_2^2}} \begin{pmatrix} q_1 \\ q_2 \\ 0 \end{pmatrix}. \]

In the following, we take the initial values as

\[ p_1(0) = 0, \quad p_2(0) = 1, \quad q_1(0) = 1, \quad q_2(0) = 0. \]

and the corresponding exact solution is known as

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

We denote the 4-order methods with \( \theta_1 = 0, 1, 2 \) and \( \theta_2 = 0 \) shown in Example 4.3 by Method I, Method II and Method III respectively, and the 3-point Gaussian quadrature will be utilized.
For comparison, the well-known symplectic method named 2-stage 4-order Gauss-Legendre RK method is also applied for this system, and we use the simplified notation “GLRK-4” to represent it. Applying these four integrators to (4.2), we compute the global error of the numerical solutions as well as the invariant errors in terms of $H$, $I$ and $L$. These errors are shown in Fig. 4.6-4.9, where the errors at each time step are carried out in the maximum norm $||x||_{\infty} = \max(\left|x_1\right|, \ldots, \left|x_n\right|)$ for $x = (x_1, \cdots, x_n) \in \mathbb{R}^n$. It indicates that all the energy-preserving integrators show a practical preservation (up to the machine precision) of the Hamiltonian $H$ but fail to exactly preserve other two invariants. The GLRK-4 method (as a symplectic RK method) is shown to exactly preserve the quadratic angular momentum $I$. It is observed that our methods behave better than the symplectic method in the preservation of $H$, $L$ as well as in the error growth of the numerical solutions. Fig. 4.9 presents a linear error growth for all the energy-preserving methods and the symplectic method. Besides, all the numerical orbits computed by these methods (see Fig. 4.10) are in the shape of an ellipse, approximating to the exact one with a high degree of precision. From these observations, we find that the presented energy-preserving methods are comparable to the symplectic methods for solving Hamiltonian systems.

5. Concluding remarks

The constructive theory of energy-preserving continuous-stage partitioned Runge-Kutta (csPRK) methods for Hamiltonian systems is intensively examined in this paper. A sufficient condition for a csPRK method to be energy-preserving is presented and it can be rephrased in use of series expansions. With the derived condition, we can devise many new energy-preserving integrators and their effectiveness can be numerically verified.

We think that further studies in the subject of energy-preserving continuous-stage methods are possible, for instance, we have already discovered that the similar approach presented in this paper can be directly extended to the case of energy-preserving continuous-stage Runge-Kutta-Nyström methods, which will be presented elsewhere. Last but not least, as mentioned at the beginning of the paper, it is impossible for us to gain a method being symplectic and energy-preserving at the same time for general Hamiltonian systems. Nevertheless, the existence of conjugate-symplectic (a symplectic-like conception in a weak sense) energy-preserving B-series integrators is known — though it is still a task of great challenge to find a computational method of such type. Therefore, it is of interest to study the conjugate symplecticity of the energy-preserving methods presented in this paper. However, the derived methods are not B-series integrators in general (except for the degenerate situations when csPRK methods become csRK methods), but they fall into a bigger class of integrators, i.e., P-series integrators. Unfortunately, to our knowledge, there are very few relevant theories for investigating the conjugate symplecticity of P-series integrators. In a word, this is a challenging subject being worth further investigating.

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