Symplectic integration with Jacobi polynomials

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Abstract
In this paper, we study symplectic integration of canonical Hamiltonian systems with Jacobi polynomials. The relevant theoretical results of continuous-stage Runge-Kutta methods are revisited firstly and then symplectic methods with Jacobi polynomials will be established. A few numerical experiments are well performed to verify the efficiency of our new methods.

Keywords: Hamiltonian systems; Symplectic methods; Continuous-stage Runge-Kutta methods; Jacobi polynomials.

1. Introduction
We are interested in the numerical integration of canonical Hamiltonian systems [2]

$$\dot{z} = J^{-1} \nabla H(z), \quad z(t_0) = z_0 \in \mathbb{R}^{2d}, \quad z = \begin{pmatrix} p \\ q \end{pmatrix}, \quad J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix},$$

(1.1)

where $q = (q_1, \ldots, q_d)^T$ stands for the generalized position coordinates, $p = (p_1, \ldots, p_d)^T$ is the vector of conjugate momenta, and $H$ as a scalar function of $p$ and $q$ is the so-called Hamiltonian (namely the total energy). Such problems are rather important and frequently encountered in many scientific fields ranging from molecular dynamics to celestial mechanics with different scales [2] [15] [17] [20], and they have been actively investigated for nearly forty years [13] [17] [20] [22]. More precisely speaking, they are closely linked with the terminology “geometric numerical integration”—a significant research direction in numerical treatment of differential equations [12] [13] [17] [20] [21] [22]. It was firstly discovered by Poincaré (1899) [2] that symplecticity is a characteristic property of Hamiltonian systems in phase space (see also [17], page 185), and afterwards it was strongly suggested by three early numerical scientists namely de Vogelaere (1956) [13], Ruth (1983) [21] and Feng Kang (1984) [11] that numerical

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methods for Hamiltonian systems should reflect such geometric property — it is particularly worth mentioning that Feng Kang has a much more broader idea in this respect, which then gives birth to a large family of special-purpose methods entitled “structure-preserving methods” for solving various dynamic systems. As for Hamiltonian systems, these special methods are naturally granted the name “symplectic methods”, requiring the corresponding discrete numerical flow $\phi_h$ to be a symplectic transformation, i.e.,

$$
\phi'_h(z)^T J \phi'_h(z) = J,
$$

where $\phi'_t$ is the Jacobian matrix of $\phi_t$. Symplectic methods have been highly-developed for these years and now it is convinced that they can reproduce correct qualitative behaviors of the given systems, and usually exhibit linear error growth, long-time near-conservation of first integrals, and existence of invariant tori, especially for those (near-)integrable systems. Moreover, the backward error analysis tells us that they can exactly preserve a modified Hamiltonian (close to the original Hamiltonian in the scale of algorithms’ order accuracy).

As is well known, symplectic Runge-Kutta (RK) methods were discovered independently by three authors in 1988, which have been drawn much attentions during the last decades. Since then, such type of methods are fully explored in the context of classic RK methods by many authors (see, for example, and a widely-used technique in literatures is the $W$-transformation. In contrast to this, a new technique based on orthogonal polynomial expansion have been developed recently, and various orthogonal polynomials including Legendre polynomials and Chebyshev polynomials can be used in the construction of symplectic, energy-preserving and symmetric RK-type methods. In the current paper, we are going to investigate symplectic integration with Jacobi polynomials within the context of continuous-stage RK methods. The similar techniques previously presented in will be further extended in detail to the case of using general Jacobi polynomials.

This paper can be outlined as follows: We firstly give a brief revisit of relevant theoretical results linked with continuous-stage RK methods in the next section. After that, we turn directly to our approach for constructing symplectic methods with Jacobi polynomials. Some numerical tests will be performed in Section 4. Finally, conclusions will be placed in Section 5.

2. Continuous-stage Runge-Kutta methods

The origin of continuous-stage RK methods can be led back to the early work of Butcher in 1972, stating that the “Butcher group” consisting of RK schemes can be extended by allowing “continuous” RK schemes with “infinitely many stages”. Following this idea, Hairer created a specific mathematical formalism for such methods in 2010, which will be introduced below for formally treating the following initial value problem

$$
\dot{z} = f(t, z), \quad z(t_0) = z_0 \in \mathbb{R}^d,
$$

(2.1)
where $f$ is assumed to be sufficiently differentiable.

**Definition 2.1.** [18] Let $A_{\tau,\sigma}$ be a function of two variables $\tau, \sigma \in [0, 1]$, and $B_{\tau}, C_{\tau}$ be functions of $\tau \in [0, 1]$. The one-step method $\Phi_h: z_0 \mapsto z_1$ given by

$$
\begin{align*}
Z_\tau &= z_0 + h \int_0^1 A_{\tau,\sigma}f(t_0 + C_{\sigma}h, Z_{\sigma}) \, d\sigma, \quad \tau \in [0, 1], \\
z_1 &= z_0 + h \int_0^1 B_{\tau}f(t_0 + C_{\tau}h, Z_{\tau}) \, d\tau,
\end{align*}
$$

(2.2)
is called a *continuous-stage Runge-Kutta* (csRK) method, where $Z_\tau \approx z(t_0 + C_{\tau}h)$.

For convenience, we often use a triple $(A_{\tau,\sigma}, B_{\tau}, C_{\tau})$ to represent such a method. Moreover, the following assumption [18, 34, 39, 40] will be held on almost everywhere in this paper

$$
C_{\tau} \equiv \tau, \quad \tau \in [0, 1].
$$

(2.3)

Analogously to the classic case, we have the following *simplifying assumptions* [18]

$$
\begin{align*}
\check{B}(\xi) : \quad &\int_0^1 B_{\tau}C_{\tau}^{\kappa-1} \, d\tau = \frac{1}{\kappa}, \quad \kappa = 1, \ldots, \xi, \\
\check{C}(\eta) : \quad &\int_0^1 A_{\tau,\sigma}C_{\sigma}^{\kappa-1} \, d\sigma = \frac{1}{\kappa}C_{\tau}^{\kappa}, \quad \kappa = 1, \ldots, \eta, \\
\check{D}(\zeta) : \quad &\int_0^1 B_{\tau}C_{\tau}^{\kappa-1}A_{\tau,\sigma} \, d\tau = \frac{1}{\kappa}B_{\tau}(1 - C_{\sigma}^{\kappa}), \quad \kappa = 1, \ldots, \zeta,
\end{align*}
$$

(2.4)

and a counterpart of the well-known result by Butcher [6] can be stated below, which is useful for analyzing the order accuracy of a csRK method.

**Theorem 2.1.** [18, 34] If the coefficients $(A_{\tau,\sigma}, B_{\tau}, C_{\tau})$ of method (2.2) satisfy $\check{B}(\xi), \check{C}(\eta)$ and $\check{D}(\zeta)$, then the method is of order at least $\min(\xi, 2\eta + 2, \eta + \zeta + 1)$.

**Lemma 2.1.** [40] Under the assumption (2.3), the simplifying assumptions $\check{B}(\xi), \check{C}(\eta)$ and $\check{D}(\zeta)$ are equivalent to

$$
\begin{align*}
\check{B}(\xi) : \quad &\int_0^1 B_{\tau}\phi(\tau) \, d\tau = \int_0^1 \phi(x) \, dx, \quad \text{for all } \phi \text{ with } \deg(\phi) \leq \xi - 1, \\
\check{C}(\eta) : \quad &\int_0^1 A_{\tau,\sigma}\phi(\sigma) \, d\sigma = \int_0^\tau \phi(x) \, dx, \quad \text{for all } \phi \text{ with } \deg(\phi) \leq \eta - 1, \\
\check{D}(\zeta) : \quad &\int_0^1 B_{\tau}A_{\tau,\sigma}\phi(\tau) \, d\tau = B_{\sigma}\int_0^1 \phi(x) \, dx, \quad \text{for all } \phi \text{ with } \deg(\phi) \leq \zeta - 1,
\end{align*}
$$

(2.5) \hspace{1cm} (2.6) \hspace{1cm} (2.7)

where $\deg(\phi)$ stands for the degree of polynomial function $\phi$. 

3
To proceed with our discussions, we introduce the following weighted function space (Hilbert space) \[30\]

\[ L^2_w[a, b] = \{ u \text{ is measurable on } [a, b] : \int_a^b |u(x)|^2 w(x) \, dx < +\infty \} \]

which is equipped with a weighted inner product

\[(u, v)_w = \int_a^b u(x)v(x)w(x) \, dx,\]

where \( w \) is a non-negative and measurable weight function such that \( \int_a^b w(x) \, dx > 0 \) and the \( k \)-th moment \( \int_a^b x^k w(x) \, dx \) exists for \( \forall k \in \mathbb{N} \). It is known that there exists a sequence of orthogonal polynomials \( \{P_n(x)\}_{n=0}^\infty \) which makes up a complete orthogonal set in \( L^2_w[a, b] \).

Remark that \( P_n(x) \) is of degree \( n \) and it has exactly \( n \) real simple zeros in the open interval \((a, b)\). For simplicity and convenience, we assume they are normalized in \([a, b]\), i.e.,

\[(P_i, P_j)_w = \delta_{ij}, \quad i, j = 0, 1, 2, \ldots,\]

and sometimes we need to shift these polynomials from \([a, b]\) to \([0, 1]\) by using a transformation \( x = a + (b - a)\tau, \tau \in [0, 1] \). In what follows, we mainly consider using the shifted normalized orthogonal polynomials defined on the standard interval \([0, 1]\).

Suppose that \( A_{\tau, \sigma} = \hat{A}_{\tau, \sigma} w(\sigma), \ B_{\tau} = \hat{B}_{\tau} w(\tau) \),

where \( w \) is a weight function defined on \([0, 1]\), and then it gives the following weighted csRK method \[40\]

\[ Z_{\tau} = z_0 + h \int_0^1 \hat{A}_{\tau, \sigma} w(\sigma) f(t_0 + \sigma h, Z_{\sigma}) \, d\sigma, \quad \tau \in [0, 1], \]

\[ z_1 = z_0 + h \int_0^1 \hat{B}_{\tau} w(\tau) f(t_0 + \tau h, Z_{\tau}) \, d\tau. \] (2.8)

**Theorem 2.2.** \[40\] Suppose \( \hat{B}_{\tau}, \hat{A}_{\tau, \sigma}, (\hat{B}_{\tau} A_{\tau, \sigma}) \in L^2_w[0, 1] \), then, under the assumption \[2.3\] we have

(a) \( \hat{B}(\xi) \) holds \( \iff \) \( B_{\tau} \) has the following form in terms of the normalized orthogonal polynomials in \( L^2_w[0, 1] \):

\[ B_{\tau} = \left( \sum_{j=0}^{\xi-1} \int_0^1 P_j(x) \, dx P_j(\tau) + \sum_{j=\xi}^\infty \lambda_j P_j(\tau) \right) w(\tau), \] (2.9)

where \( \lambda_j \) are any real parameters;

\[\text{1} \text{We use the notation } A_{\tau, \sigma} \text{ to stand for the one-variable function in terms of } \sigma, \text{ and } A_{\tau, \star}, \hat{A}_{\tau, \sigma} \text{ can be understood likewise.}\]
(b) $\tilde{C}(\eta)$ holds $\iff$ $A_{\tau,\sigma}$ has the following form in terms of the normalized orthogonal polynomials in $L^2_w[0,1]$

$$A_{\tau,\sigma} = \left( \sum_{j=0}^{\eta-1} \int_0^\tau P_j(x) \, dx P_j(\sigma) + \sum_{j \geq \eta} \varphi_j(\tau) P_j(\sigma) \right) w(\sigma), \quad \text{(2.10)}$$

where $\varphi_j(\tau)$ are any real functions;

(c) $\tilde{D}(\zeta)$ holds $\iff$ $B_{\tau} A_{\tau,\sigma}$ has the following form in terms of the normalized orthogonal polynomials in $L^2_w[0,1]$

$$B_{\tau} A_{\tau,\sigma} = \left( \sum_{j=0}^{\zeta-1} B_j \int_0^\zeta P_j(x) \, dx P_j(\tau) + \sum_{j \geq \zeta} \psi_j(\sigma) P_j(\tau) \right) w(\tau), \quad \text{(2.11)}$$

where $\psi_j(\sigma)$ are any real functions.

Generally, we must truncate the series (2.9) and (2.10) suitably for practical use, and approximate the integrals of (2.8) with a weighted interpolatory quadrature formula

$$\int_0^1 \Phi(x) w(x) \, dx \approx \sum_{i=1}^s b_i \Phi(c_i), \quad c_i \in [0,1], \quad \text{(2.12)}$$

where

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

If $c_1, c_2, \ldots, c_s$ are chosen as the $s$ distinct zeros of the orthogonal polynomial $P_s(x)$ in $L^2_w[0,1]$, then the interpolatory quadrature formula (2.12) is exact for polynomials of degree $2s-1$, which makes it optimal with the highest order $p = 2s$. Such quadrature rule is known as “Gauss-Christoffel type”, whereas other suboptimal quadrature rules with some fixed nodes are also useful in practical applications [1, 26].

Applying the quadrature rule (2.12) to the weighted csRK method (2.8), it leads to a traditional $s$-stage RK method

$$\hat{Z}_i = z_0 + h \sum_{j=1}^s b_j \hat{A}_{c_i,j} f(t_0 + c_jh, \hat{Z}_j), \quad i = 1, \ldots, s, \quad \text{(2.13)}$$

$$z_1 = z_0 + h \sum_{i=1}^s b_i \hat{B}_{c_i} f(t_0 + c_ih, \hat{Z}_i),$$

where $\hat{Z}_i \approx Z_{c_i}$. After that, we can determine the order of the resulting RK methods by using the result below.

**Theorem 2.3.** [40] Assume the underlying quadrature formula (2.12) is of order $p$, and $\hat{A}_{\tau,\sigma}$ is of degree $\pi^\tau_A$ with respect to $\tau$ and of degree $\pi^\sigma_A$ with respect to $\sigma$, and $\hat{B}_\tau$ is of degree
If all the simplifying assumptions $\tilde{B}(\xi)$, $\tilde{C}(\eta)$ and $\tilde{D}(\zeta)$ in (2.4) are fulfilled, then the standard RK method (2.13) is at least of order

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

where $\rho = \min(\xi, p - \pi_B^r)$, $\alpha = \min(\eta, p - \pi_A^r)$ and $\beta = \min(\zeta, p - \pi_A^r - \pi_B^r)$.

Proof. Please refer to [40] for the details of proof.

3. Construction of symplectic methods with Jacobi polynomials

More recently, the present author has developed two new techniques for constructing symplectic RK-type methods in [40]. However, they are rather different in the ideas of constructing algorithms: The first technique is to let the algorithms satisfy order conditions prior to symplectic conditions, while the second technique is quite the opposite. It turns out that the second technique is better for practical use, and we strongly suggest that symplectic conditions should be considered in the first place. On account of this, in what follows we are going to develop new symplectic methods based on the second technique. Our construction of symplectic methods is heavily dependent on the following results (please refer to [39, 40] for more information).

Theorem 3.1. [39] If the coefficients of a csRK method (2.2) satisfy

$$B_A \tau, \sigma + B_B A_{\tau, \sigma} \equiv B, \tau, \sigma \in [0, 1],$$

then it is symplectic. In addition, the RK scheme with coefficients $\left(b_j A_{c_i, c_j}, b_i B_{c_i, c_j}\right)_{i=1}^s$ (derived by using quadrature formula, c.f., (2.13)) based on the underlying symplectic csRK method with coefficients satisfying (3.1) is always symplectic.

Theorem 3.2. [40] Under the assumption (2.3), for a symplectic csRK method with coefficients satisfying (3.1), we have the following statements:

(a) $\tilde{B}(\xi)$ and $\tilde{C}(\eta) \Rightarrow \tilde{D}(\zeta)$, where $\zeta = \min\{\xi, \eta\}$;

(b) $\tilde{B}(\xi)$ and $\tilde{D}(\zeta) \Rightarrow \tilde{C}(\eta)$, where $\eta = \min\{\xi, \zeta\}$.

Theorem 3.3. [40] Suppose that $A_{\tau, \sigma}/B_\sigma \in L^2_w([0, 1] \times [0, 1])$, then symplectic condition (3.1) is equivalent to the fact that $A_{\tau, \sigma}$ has the following form in terms of the orthogonal polynomials $P_n(x)$ in $L^2_w[0, 1]$

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

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

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On the basis of these preliminaries, we could introduce an operational procedure for establishing symplectic csRK methods. Actually, the following description was firstly presented in [40] but further refined and improved in [41]. Now we give a new version of it with a tiny modification in “Step 2”, which makes it more clearly and essentially. The new procedure is as follows:

**Step 1.** Make an ansatz for \(B_\tau\) which satisfies \(\hat{B}(\xi)\) with \(\xi \geq 1\) according to (2.9), and a finite number of \(\lambda_i\) could be kept as parameters;

**Step 2.** Suppose \(A_{\tau,\sigma}\) is in the form (by Theorem 3.3)

\[
A_{\tau,\sigma} = B_\sigma \left( \frac{1}{2} + \sum_{0 < i + j \in \mathbb{Z}} \alpha_{(i,j)} P_i(\tau)P_j(\sigma) \right), \quad \alpha_{(i,j)} = -\alpha_{(j,i)}, \tag{3.3}
\]

where \(\alpha_{(i,j)}\) are kept as parameters with a finite number, and then substitute \(A_{\tau,\sigma}\) into \(\hat{C}(\eta)\) (see (2.6), usually we let \(\eta < \xi\) for determining \(\alpha_{(i,j)}\):

\[
\int_0^1 A_{\tau,\sigma} \phi_k(\sigma) \, d\sigma = \int_0^\tau \phi_k(x) \, dx, \quad k = 0, 1, \ldots, \eta - 1,
\]

Here, \(\phi_k(x)\) stands for any polynomial of degree \(k\), which performs very similarly as the “test function” used in general finite element analysis;

**Step 3.** Write down \(B_\tau\) and \(A_{\tau,\sigma}\) (satisfy \(\hat{B}(\xi)\) and \(\hat{C}(\eta)\) automatically), which results in a symplectic csRK method of order at least \(\min\{\xi, 2\eta + 2, \eta + \zeta + 1\}\) with \(\zeta = \min\{\xi, \eta\}\) by Theorem 2.1 and 3.2. If needed, we then get symplectic RK methods by using quadrature rules (see the second statement of Theorem 3.1).

In fact, the procedure above only provides a general framework for deriving symplectic methods. For practical use, it needs to be more refined or particularized. In view of Theorem 2.3 and 3.2, it is suggested to design Butcher coefficients with low-degree \(\hat{A}_{\tau,\sigma}\) and \(\hat{B}_\tau\), and \(\eta\) is better to take as \(\eta \approx \frac{1}{2} \xi\). Besides, for the sake of conveniently computing those integrals of \(\hat{C}(\eta)\) in the second step, the following ansatz may be advisable (with \(C_\tau\) given by (2.3) and let \(\rho \geq \eta\) and \(\xi \geq 2\eta\))

\[
B_\tau = \sum_{j=0}^{\xi-1} \int_0^1 P_j(x) \, dx P_j(\tau) w(\tau), \quad A_{\tau,\sigma} = B_\sigma \left( \frac{1}{2} + \sum_{0 < i + j \in \mathbb{Z}} \alpha_{(i,j)} P_i(\tau)P_j(\sigma) \right), \tag{3.4}
\]

where \(\alpha_{(i,j)} = -\alpha_{(j,i)}\). Because of the index \(j\) restricted by \(j \leq \xi - \eta\) in the second formula of (3.4), we can use \(\hat{B}(\xi)\) to arrive at (please c.f. (2.5))

\[
\int_0^1 A_{\tau,\sigma} \phi_k(\sigma) \, d\sigma = \int_0^1 B_\sigma \left( \frac{1}{2} + \sum_{0 < i + j \in \mathbb{Z}} \alpha_{(i,j)} P_i(\tau)P_j(\sigma) \right) \phi_k(\sigma) \, d\sigma = \frac{1}{2} \int_0^1 \phi_k(x) \, dx + \sum_{0 < i + j \in \mathbb{Z}} \alpha_{(i,j)} P_i(\tau) \int_0^1 P_j(\sigma) \phi_k(\sigma) \, d\sigma, \quad 0 \leq k \leq \eta - 1.
\]
Therefore, $\tilde{C}(\eta)$ implies that
\[
\frac{1}{2} \int_0^1 \phi_k(x) \, dx + \sum_{\substack{0<i+j\leq \eta \\ i\leq \rho,j\leq \xi-\eta}} \alpha(i,j) P_i(\tau) \int_0^1 P_j(\sigma) \phi_k(\sigma) \, d\sigma = \int_0^\tau \phi_k(x) \, dx, \quad 0 \leq k \leq \eta - 1. \tag{3.5}
\]

Finally, it needs to settle $\alpha(i,j)$ by transposing, comparing or merging similar items of (3.5) after the polynomial on right-hand side being represented by the basis $\{P_j(x)\}_{j=0}^\infty$. In view of the skew-symmetry of $\alpha(i,j)$, if we let $r = \min\{\rho, \xi - \eta\}$, then actually the degrees of freedom of these parameters is $r(r + 1)/2$, by noticing that
\[
\alpha(i,i) = 0, \quad i \geq 1 \quad \text{and} \quad \alpha(i,j) = 0, \quad \text{for } i > r \text{ or } j > r.
\]

When $r(r+1)/2 \gg (r+1)\eta$ (number of equations), i.e., $r \gg 2\eta$, we can appropriately reduce the degrees of freedom of these parameters by imposing some of them to be zero in pairs, if needed.

**Remark 3.1.** By taking $\phi_k$ and $P_j$ as the same type of orthogonal polynomials in (3.5), e.g., Chebyshev polynomials of the first and second kind respectively as shown in [41], Chebyshev symplectic methods can be constructed (please see [41] for more details). However, such approach may not be convenient to use when general weighted orthogonal polynomials are considered.

Next, let us consider how to construct symplectic methods with Jacobi polynomials. We introduce the following normalized shifted Jacobi polynomial by Rodrigue’s formula [3, 30, 40]
\[
J_0^{(\alpha,\beta)}(x) = \frac{1}{\sqrt{\epsilon_0/2}} , \quad J_n^{(\alpha,\beta)}(x) = \frac{(-1)^n}{n! \sqrt{\epsilon_n/2}} \frac{d^n}{dx^n} (1 - x)^{\alpha} x^\beta d\tau^n (1 - x)^{\alpha+n} x^{\beta+n}, \quad n \geq 1, \tag{3.6}
\]
where
\[
\epsilon_0 = \frac{2^{\alpha+\beta+1} \Gamma(\alpha + 1) \Gamma(\beta + 1)}{\Gamma(\alpha + \beta + 2)}, \quad \epsilon_n = \frac{2^{\alpha+\beta+1} \Gamma(n + \alpha + 1) \Gamma(n + \beta + 1)}{(2n + \alpha + \beta + 1) \Gamma(n + \alpha + \beta + 1)n!}, \quad n \geq 1,
\]
and here
\[
\Gamma(s) = \int_0^{+\infty} x^{s-1} e^{-x} \, dx, \quad s \in \mathbb{R}^+,
\]
is the well-known Gamma function. It is known that these Jacobi polynomials satisfy the orthogonality on $[0, 1]$
\[
\int_0^1 w^{(\alpha,\beta)}(x) J_{m}^{(\alpha,\beta)}(x) J_{n}^{(\alpha,\beta)}(x) \, dx = \delta_{nm}, \quad n, m = 0, 1, 2, \ldots ,
\]

\footnote{Many literatures conducted a minor error by unifying $\epsilon_0$ into the formula of $\epsilon_n (n \geq 1)$. In fact, in the case of $n = 0$, when we take $\alpha + \beta = -1$, it will make no sense with the denominator of $\epsilon_n$ becoming zero.}
and the corresponding weight function is given by
\[ w^{(\alpha,\beta)}(x) = 2^{\alpha+\beta}(1-x)^\alpha x^\beta, \quad \alpha > -1, \beta > -1. \]

We mention some properties of Jacobi polynomials for use, as shown below.

**Theorem 3.4.** The shifted normalized Jacobi polynomials have the following properties:

(a) Derivatives’ recurrence relation:
\[ \frac{d}{dx^m} J^{(\alpha,\beta)}_k(x) = 2^m \sqrt{\frac{k!\Gamma(k+m+\alpha+\beta+1)}{(k-m)!\Gamma(k+\alpha+\beta+1)}} J^{(\alpha+m,\beta+m)}_{k-m}(x), \quad k \geq m. \tag{3.7} \]

Particularly, we have
\[ \frac{d}{dx} J^{(\alpha,\beta)}_k(x) = 2 \sqrt{k(k+\alpha+\beta+1)} J^{(\alpha+1,\beta+1)}_{k-1}(x), \quad k \geq 1. \tag{3.8} \]

(b) Symmetry relation:
\[ J^{(\alpha,\beta)}_k(1-x) = (-1)^k J^{(\beta,\alpha)}_k(x), \quad k \geq 0. \tag{3.9} \]

Particularly, we have
\[ J^{(\alpha,\beta)}_k(1) = \frac{\Gamma(k+\alpha+1)}{k!\Gamma(\alpha+1)\sqrt{\epsilon_k/2}}, \quad J^{(\alpha,\beta)}_k(0) = (-1)^k \frac{\Gamma(k+\beta+1)}{k!\Gamma(\beta+1)\sqrt{\epsilon_k/2}}. \tag{3.10} \]

**Proof.** We can use the available properties of standard Jacobi polynomials defined on \([-1,1]\) (see, for example, [3]) to get our results by changing of variables. \(\square\)

By virtue of \eqref{3.8}, it yields
\[
\begin{align*}
\int_0^1 J^{(\alpha+1,\beta+1)}_k(x) \, dx &= \frac{1}{\mu_k} \left( J^{(\alpha,\beta)}_{k+1}(1) - J^{(\alpha,\beta)}_{k+1}(0) \right), \quad k \geq 0, \\
\int_0^\tau J^{(\alpha+1,\beta+1)}_k(x) \, dx &= \frac{1}{\mu_k} \left( J^{(\alpha,\beta)}_{k+1}(\tau) - J^{(\alpha,\beta)}_{k+1}(0) \right), \quad k \geq 0,
\end{align*}
\]}

with \(\mu_k = 2 \sqrt{(k+1)(k+\alpha+\beta+2)}\).

Thanks to these beautiful properties, now we can construct symplectic methods conveniently according to the following guideline: Replace all the orthogonal polynomials \(P_j(x)\) appeared in \eqref{3.4} and \eqref{3.5} with \(J^{(\alpha,\beta)}_j(x)\) and take the “test function” \(\phi_k(x)\) as \(J^{(\alpha+1,\beta+1)}_k(x)\), and then \eqref{3.11} can be used. Besides, the integral placed in the middle of \eqref{3.5}, i.e.,
\[
\int_0^1 P_j(\sigma) \phi_k(\sigma) \, d\sigma = \int_0^1 J^{(\alpha,\beta)}_j(\sigma) J^{(\alpha+1,\beta+1)}_k(\sigma) \, d\sigma = \frac{1}{\mu_k} \int_0^1 J^{(\alpha,\beta)}_j(\sigma) \frac{d}{d\sigma} J^{(\alpha,\beta)}_k(\sigma) \, d\sigma, \quad k \geq 0
\]}

can be computed by any available symbolic computing softwares or tools (e.g., Maple, Mathematica, Matlab etc) and the factor \(\mu_k\) will be removed finally from both sides of the resulting
computing the middle integral of (3.5). Additionally, observe that the Jacobi sequence \( \{J_j^{(\alpha,\beta)}(x)\}_{j=0}^{\infty} \) is linearly independent, hence the final task to settle \( \alpha_{(i,j)} \) can be easily realized by comparing similar items and solving a system of linear algebraic equations in terms of \( \alpha_{(i,j)} \).

In the following, we show some specific examples and in view of the skew-symmetry of \( \alpha_{(i,j)} \), we only provide the values of \( \alpha_{(i,j)} \) with \( i < j \) in these examples.

**Example 3.1.** Take \( P_j(x) \) as \( J_j^{(0,0)}(x) = L_j(x) \) (shifted Legendre polynomials \([10]\)), and let \( \phi_k(x) = J_k^{(1,1)}(x) \) (shifted Jacobi type III polynomials \([9]\)) in (3.5), then we can retrieve all the symplectic csRK methods presented in \([31, 33, 34, 36]\) and by using Gauss, Radau, Lobatto quadrature rules it reproduces almost all the high-order symplectic RK methods appeared in classic literatures \([7, 12, 27, 28]\).

Actually, in such a case, it is more convenient to take the “test function” \( \phi_k(x) \) as Legendre polynomial \( J_k^{(0,0)}(x) \) itself, on the grounds that Legendre polynomials are orthogonal on \([0,1]\) associated with weight function \( w(x) = 1 \), which gives a larger reduction when computing the middle integral of (3.5). An alternative technique for constructing symplectic methods with Legendre polynomials has been developed by Tang et al \([31, 33, 34, 36]\).

| \( \frac{2-\sqrt{3}}{4} \) | \( \frac{1}{9} \) | \( \frac{10-5\sqrt{3}}{36} \) | \( + 5\gamma \) | \( \frac{1-\sqrt{3}}{9} \) | \( - 5\gamma \) |
| \( \frac{1}{2} \) | \( \frac{2+\sqrt{3}}{18} \) | \( - 2\gamma \) | \( \frac{5}{18} \) | \( \frac{2-\sqrt{3}}{18} \) | \( + 2\gamma \) |
| \( \frac{2+\sqrt{3}}{4} \) | \( \frac{1+\sqrt{3}}{9} \) | \( + 5\gamma \) | \( \frac{10+5\sqrt{3}}{36} \) | \( - 5\gamma \) | \( \frac{1}{9} \) |

Table 3.1: A family of one-parameter 3-stage 4-order symplectic RK methods, based on Chebyshev polynomials of the first kind.

Example 3.2. Take \( P_j(x) \) as \( J_j^{(-\frac{1}{2},-\frac{1}{2})}(x) = T_j(x) \) (shifted Chebyshev polynomials of the first kind \([13]\)), and let \( \phi_k(x) = J_k^{(\frac{1}{2},1)}(x) = U_k(x) \) (shifted Chebyshev polynomials of the second kind) in (3.5), then we can regain all the Chebyshev symplectic methods presented in Tab. 3.1-3.2 of \([41]\). A family of 4-order symplectic and symmetric methods is quoted from that paper which is shown in Tab. 3.1.

Example 3.3. Take \( P_j(x) \) as \( J_j^{(\frac{1}{2},-\frac{1}{2})}(x) = U_j(x) \) (shifted Chebyshev polynomials of the second kind \([13]\)), and let \( \phi_k(x) = J_k^{(\frac{1}{2},1)}(x) = U_k(x) \) (shifted Chebyshev polynomials of the second kind) in (3.5), then we can regain all the Chebyshev symplectic methods presented in Tab. 3.3-3.4 of \([41]\). A family of 4-order symplectic and symmetric methods is quoted from that paper which is shown in Tab. 3.2.

Example 3.4. Take \( P_j(x) \) as \( J_j^{(-\frac{1}{2},\frac{1}{2})}(x) = V_j(x) \) (shifted Chebyshev polynomials of the third kind \([13]\)), let \( \phi_k(x) = J_k^{(\frac{1}{2},-\frac{1}{2})}(x) \) in (3.5), and the following Gauss-Christoffel quadrature rule will be used \([1]\)

\[
\int_{0}^{1} \Phi(x) w(x) \, dx \approx \sum_{i=1}^{s} b_i \Phi(c_i), \quad c_i \in [0,1],
\]

(3.13)
Table 3.2: A family of one-parameter 3-stage 4-order symplectic RK methods, based on Chebyshev polynomials of the second kind.

| $2^{-\sqrt{2}/4}$ | $\frac{1}{6}$ | $\frac{2-\sqrt{2}}{12} + \gamma$ | $\frac{1-\sqrt{2}}{6} - \gamma$ |
| --- | --- | --- | --- |
| $\frac{1}{2}$ | $\frac{2+\sqrt{2}}{12} - \gamma$ | $\frac{1}{6}$ | $\frac{2-\sqrt{2}}{12} + \gamma$ |
| $2^{+\sqrt{2}/4}$ | $\frac{1+\sqrt{2}}{6} + \gamma$ | $\frac{2+\sqrt{2}}{12} - \gamma$ | $\frac{1}{6}$ |

where

$$w(x) = (1 - x)^{-\frac{1}{2}}x^\frac{1}{2}, \quad c_i = \cos^2 \left( \frac{2i - 1}{2s + 1} \pi \right), \quad b_i = \frac{2\pi}{2s + 1}c_i, \quad i = 1, \ldots, s.$$  

Now we consider the following three cases separately,

(i) Let $\xi = 2$, $\eta = 1$, $\rho = 1$, we have only one degree of freedom. After some elementary calculations, it gives a unique solution

$$\alpha_{(0,1)} = -\frac{\pi}{8},$$

which results in a symplectic csRK method of order 2. By using the 1-point quadrature rule it gives the same RK coefficients of implicit midpoint rule except that $c_1 = \frac{3}{4}$;

(ii) Let $\xi = 3$, $\eta = 1$, $\rho = 2$, after some elementary calculations, it gives

$$\alpha_{(0,1)} = \frac{1}{3}\alpha_{(1,2)} - \frac{\pi}{8}, \quad \alpha_{(0,2)} = \alpha_{(1,2)}.$$  

If we regard $\mu = \alpha_{(1,2)}$ as a free parameter (note that $\alpha_{(i,j)} = -\alpha_{(j,i)}$), then we get a family of $\mu$-parameter symplectic csRK methods of order 3. By using the 3-point quadrature rule we get a family of 3-stage 3-order symplectic RK methods. Amongst them, the method with $\mu = 0$ is shown in Tab. 3.3.

(iii) Alternatively, if we take $\xi = 5$, $\eta = 2$, $\rho = 2$, then it gives a unique solution

$$\alpha_{(0,1)} = -\frac{9\pi}{64}, \quad \alpha_{(1,2)} = \alpha_{(0,2)} = -\frac{3\pi}{64}, \quad \alpha_{(0,3)} = 0.$$  

The resulting symplectic csRK method is of order 5. By using the 5-point quadrature rule we get a 5-stage 5-order symplectic RK method numerically (the exact Butcher tableau is too complicated to be exhibited) which is shown in Tab. 3.4.

Example 3.5. Take $P_j(x)$ as $J_{j/2}^{(1/2,-1/2)}(x) = W_j(x)$ (shifted Chebyshev polynomials of the fourth kind [14]), let $\phi_k(x) = J_{k/2}^{(1/2,1/2)}(x)$ in (3.5), and the following Gauss-Christoffel quadrature rule will be used [1]

$$\int_0^1 \Phi(x)w(x)\,dx \approx \sum_{i=1}^s b_i\Phi(c_i), \quad c_i \in [0, 1], \quad (3.14)$$
Now we consider the following three cases separately.

(i) Let $\xi = 3$, $\eta = 1$, $\rho = 2$, after some elementary calculations, it gives a unique solution

$$\alpha_{(0,1)} = \frac{\pi}{8},$$

which results in a symplectic csRK method of order 2. By using the 1-point quadrature rule it gives the same RK coefficients of implicit midpoint rule except that $c_1 = \frac{1}{4}$.

(ii) Let $\xi = 3$, $\eta = 1$, $\rho = 2$, after some elementary calculations, it gives

$$\alpha_{(0,1)} = \frac{1}{3}\alpha_{(1,2)} = \frac{\pi}{8}, \quad \alpha_{(0,2)} = -\alpha_{(1,2)}.$$ 

If we regard $\mu = \alpha_{(1,2)}$ as a free parameter (note that $\alpha_{(i,j)} = -\alpha_{(j,i)}$), then we get a family of $\mu$-parameter symplectic csRK methods of order 3. By using the 3-point quadrature rule we get a family of 3-stage 3-order symplectic RK methods. Amongst them, the method with $\mu = 0$ is shown in Tab. 3.5.

(iii) Alternatively, if we take $\xi = 5$, $\eta = 2$, $\rho = 2$, then it gives a unique solution

$$\alpha_{(0,1)} = -\frac{9\pi}{64}, \quad \alpha_{(1,2)} = -\alpha_{(0,2)} = -\frac{3\pi}{64}, \quad \alpha_{(0,3)} = 0.$$ 

The resulting symplectic csRK method is of order 5. By using the 5-point quadrature rule we get a 5-stage 5-order symplectic RK method numerically (the exact Butcher tableau is too complicated to be exhibited) which is shown in Tab. 3.6.

Table 3.3: A 3-stage 3-order symplectic RK method, based on Chebyshev polynomials of the third kind.

| $\cos^2 \frac{\pi}{14}$ | $-2 \cos \frac{3\pi}{14} + \cos \frac{5\pi}{14} + 3$ | $-5 \cos \frac{3\pi}{14} + 10 \cos \frac{5\pi}{14} - 3 \cos \frac{7\pi}{14} + 8$ | $7 \cos \frac{3\pi}{14} + 3 \cos \frac{5\pi}{14} + 11 \cos \frac{7\pi}{14} + 7$ |
|-------------------------|--------------------------------|--------------------------------|--------------------------------|
| $\cos \frac{\pi}{14}$  | $-7 \cos \frac{3\pi}{14} - 3 \cos \frac{7\pi}{14} + 11 \cos \frac{9\pi}{14} + 7$ | $2 \cos \frac{5\pi}{14} - \cos \frac{7\pi}{14} + 3$ | $5 \cos \frac{3\pi}{14} + 10 \cos \frac{5\pi}{14} + 3 \cos \frac{7\pi}{14} + 8$ |
| $\cos \frac{5\pi}{14}$ | $-5 \cos \frac{3\pi}{14} - 10 \cos \frac{5\pi}{14} + 3 \cos \frac{7\pi}{14} + 8$ | $-7 \cos \frac{3\pi}{14} + 3 \cos \frac{5\pi}{14} - 11 \cos \frac{7\pi}{14} + 7$ | $2 \cos \frac{3\pi}{14} + \cos \frac{5\pi}{14} + 3$ |
| $\cos \frac{2\pi}{14}$ | $-4 \cos \frac{3\pi}{14} + 2 \cos \frac{5\pi}{14} + 6$ | $4 \cos \frac{5\pi}{14} - 2 \cos \frac{7\pi}{14} + 6$ | $4 \cos \frac{3\pi}{14} + 2 \cos \frac{5\pi}{14} + 6$ |

Table 3.4: A 5-stage 5-order symplectic RK method, based on Chebyshev polynomials of the third kind.

$w(x) = (1 - x)^{1/2}x^{1/2}$, $c_i = 1 - \cos^2 \left( \frac{2i - 1}{2s + 1/2} \right)$, $b_i = \frac{2\pi}{2s + 1}(1 - c_i)$, $i = 1, \cdots, s$. 

where
\[ \sin^2 \frac{\pi}{14} \cdot \frac{\cos \frac{2\pi}{7} - 2 \cos \frac{2\pi}{7} + 3}{21} = \frac{7 \cos \frac{2\pi}{7} - 5 \cos \frac{2\pi}{7} - 7 \cos \frac{2\pi}{7} + 5}{42} - \frac{5 \cos \frac{2\pi}{7} + 2 \cos \frac{2\pi}{7} + \cos \frac{2\pi}{7} + 4}{21} - \frac{7 \cos \frac{2\pi}{7} + 5 \cos \frac{2\pi}{7} + 7 \cos \frac{2\pi}{7} + 5}{42} - \frac{4 \cos \frac{2\pi}{7} + 2 \cos \frac{2\pi}{7} + 6}{21} \]

Table 3.5: A 3-stage 3-order symplectic RK method, based on Chebyshev polynomials of the fourth kind.

| \( \sin \frac{3\pi}{14} \) | \( \frac{\cos \frac{2\pi}{7} - 2 \cos \frac{2\pi}{7} + 3}{21} \) | \( \frac{7 \cos \frac{2\pi}{7} - 5 \cos \frac{2\pi}{7} - 7 \cos \frac{2\pi}{7} + 5}{42} \) | \( \frac{5 \cos \frac{2\pi}{7} + 2 \cos \frac{2\pi}{7} + \cos \frac{2\pi}{7} + 4}{21} \) | \( \frac{7 \cos \frac{2\pi}{7} + 5 \cos \frac{2\pi}{7} + 7 \cos \frac{2\pi}{7} + 5}{42} \) |
| \( \sin \frac{5\pi}{14} \) | \( \frac{4 \cos \frac{2\pi}{7} + 2 \cos \frac{2\pi}{7} + 6}{21} \) | \( \frac{4 \cos \frac{2\pi}{7} + 2 \cos \frac{2\pi}{7} + 6}{21} \) | \( \frac{4 \cos \frac{2\pi}{7} + 2 \cos \frac{2\pi}{7} + 6}{21} \) | \( \frac{4 \cos \frac{2\pi}{7} + 2 \cos \frac{2\pi}{7} + 6}{21} \) |

Table 3.6: A 5-stage 5-order symplectic RK method, based on Chebyshev polynomials of the fourth kind.

4. Numerical tests

In this section, we present some numerical comparisons between the newly-derived symplectic methods (given in Ex. 3.4 and 3.5) and a family of well-known symplectic methods named “Radau IIB methods” [27] of order 3 and 5, respectively. What will be used to test in our numerical experiments is the well-known Kepler’s problem determined by the Hamiltonian function \( H(p, q) = \frac{p_1^2 + p_2^2}{2} - \frac{1}{\sqrt{q_1^2 + q_2^2}} \)

with initial value conditions \( (p_1(0), p_2(0), q_1(0), q_2(0)) = (0, 1, 1, 0) \). The exact solution is

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

For convenience, we call the symplectic methods presented in Ex. 3.4 and 3.5 “Chebyshev III” and “Chebyshev IV” methods respectively. It is observed from Fig. 4.1 and Fig. 4.2 that our 3-order symplectic methods share very similar numerical behaviors with the Radau IIB method with the same order 3, and our methods exhibit a little bit better results in the aspects of growth of solution error and conservation of energy. As for the 5-order methods (see Fig. 4.3 and 4.4), our methods also show a little bit better results in comparison with the Radau IIB method of order 5. These numerical tests have verified our theoretical results very well.

5. Conclusions

This paper intensively discuss the symplectic integration with Jacobi polynomials. The construction of symplectic methods is based on the theory of continuous-stage RK methods and the crucial technique associated with orthogonal polynomial expansion (firstly developed
Figure 4.1: Comparison of solution errors by three symplectic methods of order 3, step size $h = 0.1$.

Figure 4.2: Comparison of energy errors by three symplectic methods of order 3, step size $h = 0.1$. 
Figure 4.3: Comparison of solution errors by three symplectic methods of order 5, step size $h = 0.1$.

Figure 4.4: Comparison of energy errors by three symplectic methods of order 5, step size $h = 0.1$. 
in [31]) is utilized. Although we only exhibit five examples to derive symplectic integrators in use of Jacobi polynomials, essentially the same technique can be extended to any other weighted orthogonal polynomials in a straightforward manner.

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