

Original articles

Two high-order energy-preserving and symmetric Gauss collocation integrators for solving the hyperbolic Hamiltonian systems[☆]

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Abstract

In this paper, we first derive the energy-preserving collocation integrator for solving the hyperbolic Hamiltonian systems. Then, two concrete high-order energy-preserving and symmetric integrators are presented by choosing the collocation nodes as two and three Gauss–Legendre points, respectively. The convergence and the symmetry of the constructed energy-preserving integrators are rigorously analysed. Numerical results verify the energy conservation property and the accuracy of the proposed integrators.

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1. Introduction

In this paper, we focus our attention on constructing high-order, symmetric and energy-preserving integrators for the following hyperbolic Hamiltonian system

$$\begin{cases} \partial_t^2 u(t) = f(u(t)), & t \in [t_0, T], \\ u(t_0) = \phi, & \partial_t u(t_0) = \varphi, \end{cases} \quad (1.1)$$

where ϕ and φ are two given functions defined on a suitable Hilbert space \mathcal{X} , and $f : \mathcal{X} \rightarrow \mathcal{X}$ is the negative gradient of a real-valued function $V(\cdot)$, that is, $f(u) = -\nabla_u V(u)$. Introducing the new variable $v(t) = \partial_t u(t)$, the system (1.1) can be rewritten as the following initial value problem

$$\begin{cases} \partial_t u(t) = \nabla_v H(u, v), & u(t_0) = \phi, \\ \partial_t v(t) = -\nabla_u H(u, v), & v(t_0) = \varphi, \end{cases}$$

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with the Hamiltonian (or energy)

$$H(u(t), v(t)) = \frac{1}{2} \|v(t)\|^2 + V(u(t)). \quad (1.2)$$

Here, $\|\cdot\|$ is the norm defined on \mathcal{X} , which is induced by the inner product (\cdot, \cdot) in \mathcal{X} .

The Hamiltonian system (1.1) is widely used in many significant fields, including the biological chemistry, the celestial mechanics, the plasma physics, the molecular dynamics and so on. As is known to all, the energy conservation along the exact flow is one of the most characteristic properties of the Hamiltonian system (see, e.g. [1,7,17]). Therefore, the essential energy-preserving property should be better respected while constructing efficient numerical integrators for solving the system (1.1). A numerical method, which can exactly preserve the Hamiltonian, is called the energy-preserving integrator. In the literature (see, e.g. [4,5,16]), the energy-preserving integrators, such as the energy–momentum method, the discrete gradient method, the energy-preserving B-series method and the average vector field (AVF) method etc., have been considered for several decades. For instance, considering the first-order Hamiltonian system

$$\dot{q}(t) = J^{-1} \nabla H(q), \quad (1.3)$$

where J is antisymmetric matrix or skew-adjoint operator and H is an arbitrary smooth function. McLachlan et al. [13] introduced the AVF method

$$q^{n+1} = q^n + hJ^{-1} \int_0^1 \nabla H((1-\sigma)q^n + \sigma q^{n+1}) d\sigma \quad (1.4)$$

to exactly preserve the energy H . Applying the AVF method (1.4) to system (1.1), we obtain the following energy-preserving integrator

$$\begin{cases} u^{n+1} = u^n + h\dot{u}^n + \frac{h^2}{2} \int_0^1 f((1-\sigma)u^n + \sigma u^{n+1}) d\sigma, \\ \dot{u}^{n+1} = \dot{u}^n + h \int_0^1 f'((1-\sigma)u^n + \sigma u^{n+1}) d\sigma. \end{cases} \quad (1.5)$$

The integrator (1.5) is of order two. It is well known that the high-order and energy-preserving integrators usually have much excellent long-term behaviour (see, e.g. [7,18]). Therefore, we are motivated to explore high-order and energy-preserving integrators for the Hamiltonian system (1.1).

Many investigations on the energy-preserving methods with high precision for Hamiltonian systems have been achieved. For instance, E. Hairer has proposed a kind of energy-preserving collocation integrators with high accuracy for the first-order Hamiltonian systems [6]. For the purpose of practical computation, the proposed collocation integrators in [6] were further expressed as the continuous-stage Runge–Kutta (RK) method. After that, Miyatake et al. [15] investigated the necessary and sufficient condition for the continuous-stage RK methods to exactly preserve the energy. L. Brugnano (see, e.g. [2,3]) developed the energy-preserving Hamiltonian Boundary Value methods (HBVM). Moreover, the energy-preserving function-fitting method [8] and energy-preserving exponential-fitting method [14] are also investigated. However, these integrators are specially designed for the first-order Hamiltonian system. Applying these integrators directly to the system (1.1) will increase the computational storage and reduce the efficiency, especially for multi-dimensional problems. To our best of knowledge, there are few investigations on developing high-order and energy-preserving integrators for solving the hyperbolic Hamiltonian system (1.1). Tang [19] investigated the sufficient conditions of the energy-preserving continuous-stage Runge–Kutta–Nyström methods for the second-order Hamiltonian ODEs' system. However, it still suffers from solving huge amounts of algebraic equations to construct high-order and energy-preserving integrators for the hyperbolic Hamiltonian system (1.1).

Inspired by the above-mentioned research works, we pay our attention to constructing high-order and energy-preserving Gauss collocation integrators for solving the hyperbolic Hamiltonian system (1.1). The rest of the paper is organized as follows: In Section 2, we present the energy-preserving collocation integrator, which is equivalent to the collocation Runge–Kutta–Nyström method with a continuous stage $\tau \in [0, 1]$. By choosing the two and three Gauss–Legendre points as the collocation nodes, two concrete high-order energy-preserving integrators are derived. The convergence and symmetry of the two integrators are rigorously analysed. Numerical experiments are carried out to verify the energy conservation and accuracy of the proposed integrators in Section 3. The last section is devoted to a brief conclusion.

2. Energy-preserving Gauss collocation integrators

In this section, two high-order and energy-preserving Gauss collocation integrators will be constructed and analysed for solving the hyperbolic Hamiltonian system (1.1).

2.1. Construction of the energy-preserving integrators

For any positive integer N , set $h = (T - t_0)/N$ be the step size and denote the steps as

$$t_n = t_0 + nh, \quad n = 0, 1, \dots, N.$$

Let $0 \leq c_1 < \dots < c_s \leq 1$ be distinct collocation nodes and

$$l_i(x) = \prod_{j=1, j \neq i}^s \frac{x - c_j}{c_i - c_j}, \quad b_i = \int_0^1 l_i(x) dx, \quad i = 1, 2, \dots, s$$

be the Lagrange basis polynomials in interpolation and the weights of the corresponding interpolatory quadrature formula, respectively. Introducing the approximations

$$u^n \approx u(t_n), \quad \dot{u}^n \approx \partial_t u(t_n), \quad U_\tau^n \approx u(t_n + \tau h), \quad \forall \tau \in [0, 1],$$

the collocation integrator for system (1.1) is defined as follows.

Definition 2.1. Let $0 \leq c_1 < \dots < c_s \leq 1$ be distinct collocation nodes. For each time step, the collocation integrator is to find the polynomial $y(t)$ of degree s such that

$$\begin{cases} \ddot{y}(t_n + c_i h) = \frac{1}{b_i} \int_0^1 l_i(\tau) f(y(t_n + \tau h)) d\tau, & i = 1, 2, \dots, s, \\ y(t_n) = u^n, \quad \dot{y}(t_n) = \dot{u}^n. \end{cases} \quad (2.1)$$

Then, defining the numerical solution of the system (1.1) as $u^{n+1} = y(t_n + h)$ and $\dot{u}^{n+1} = \dot{y}(t_n + h)$.

Remark 2.1. Approximating the integral appeared in the first equations of (2.1) with the interpolatory quadrature formula corresponding to the collocation nodes c_i and weights b_i for $i = 1, 2, \dots, s$, Eqs. (2.1) can be replaced by

$$\begin{cases} \ddot{u}(t_n + c_i h) = f(u(t_n + c_i h)), & i = 1, 2, \dots, s, \\ u(t_n) = u^n, \quad \dot{u}(t_n) = \dot{u}^n. \end{cases}$$

That means the collocation integrator defined in Definition 2.1 would reduce to the classical collocation method.

The defined collocation integrator could be interpreted as the continuous-stage collocation Runge–Kutta–Nyström method.

Theorem 2.1. The collocation integrator defined in Definition 2.1 can be expressed as

$$\begin{cases} U_\tau^n = u^n + \tau h \dot{u}^n + h^2 \int_0^1 \bar{A}_{\tau, \sigma} f(U_\sigma^n) d\sigma, \\ u^{n+1} = u^n + h \dot{u}^n + h^2 \int_0^1 (1 - \sigma) f(U_\sigma^n) d\sigma, \\ \dot{u}^{n+1} = \dot{u}^n + h \int_0^1 f(U_\sigma^n) d\sigma, \end{cases} \quad (2.2)$$

where the weight is given by

$$\bar{A}_{\tau,\sigma} = \int_0^1 A_{\tau,\alpha} \cdot A_{\alpha,\sigma} d\alpha \quad \text{with} \quad A_{\tau,\sigma} = \sum_{i=1}^s \frac{l_i(\sigma)}{b_i} \int_0^\tau l_i(\alpha) d\alpha. \quad (2.3)$$

Proof. By denoting $k_i^n = \ddot{y}(t_n + c_i h)$ and $U_\tau^n = y(t_n + \tau h)$, then the derivative $\ddot{y}(t_n + \tau h)$ can be expressed as

$$\ddot{y}(t_n + \tau h) = \sum_{i=1}^s l_i(\tau) k_i^n. \quad (2.4)$$

Inserting (2.1) into (2.4) yields

$$\ddot{y}(t_n + \tau h) = \sum_{i=1}^s \frac{l_i(\tau)}{b_i} \int_0^1 l_i(\sigma) f(y(t_n + \sigma h)) d\sigma. \quad (2.5)$$

The conclusion of the theorem can be obtained by using the variation-of-constant formula to (2.5) directly. Here, we skip the detailed process of the proof. \square

Remark 2.2. Obviously, the weight $\bar{A}_{\tau,\sigma}$ is a binary polynomial of degree s and $s - 1$ with respect to τ and σ , respectively. Therefore, $\bar{A}_{\tau,\sigma}$ is bounded over the region $[0, 1] \times [0, 1]$, that is, there exists a positive number $M > 0$ such that

$$\max_{(\tau,\sigma) \in [0,1] \times [0,1]} |\bar{A}_{\tau,\sigma}| \leq M.$$

In what follows, we will pay our attention to verify the energy conservation of the collocation integrators (2.2) with the weight (2.3).

Theorem 2.2. The collocation integrator (2.2) with the weight (2.3) can exactly preserve the energy (1.2) of the Hamiltonian system (1.1).

Proof. Substituting Eq. (2.2) into the Hamiltonian (1.2) leads to

$$\begin{aligned} H(u^{n+1}, \dot{u}^{n+1}) &= \frac{1}{2} \left(\dot{u}_n + h \int_0^1 f(U_\sigma^n) d\sigma, \dot{u}_n + h \int_0^1 f(U_\sigma^n) d\sigma \right) + V(u^{n+1}) \\ &= H(u^n, \dot{u}^n) + h \left(\dot{u}^n, \int_0^1 f(U_\sigma^n) d\sigma \right) + \frac{h^2}{2} \left(\int_0^1 f(U_\sigma^n) d\sigma, \int_0^1 f(U_\sigma^n) d\sigma \right) \\ &\quad + V(u^{n+1}) - V(u^n). \end{aligned} \quad (2.6)$$

By using the fundamental theorem of calculus, we have

$$\begin{aligned} V(u^{n+1}) - V(u^n) &= \int_0^1 dV(U_\tau^n) = - \int_0^1 \left(\frac{dU_\tau^n}{d\tau}, f(U_\tau^n) \right) d\tau \\ &= - \int_0^1 \left(h\dot{u}^n + h^2 \int_0^1 \frac{d}{d\tau} \bar{A}_{\tau,\sigma} \cdot f(U_\sigma^n) d\sigma, f(U_\tau^n) \right) d\tau \\ &= - h \left(\dot{u}^n, \int_0^1 f(U_\tau^n) d\tau \right) - h^2 \int_0^1 \left(\int_0^1 \frac{d}{d\tau} \bar{A}_{\tau,\sigma} \cdot f(U_\sigma^n) d\sigma, f(U_\tau^n) \right) d\tau. \end{aligned} \quad (2.7)$$

According to the definition of the weight $\bar{A}_{\tau,\sigma}$, we obtain

$$\begin{aligned}
 \frac{d}{d\tau} \bar{A}_{\tau,\sigma} &= \int_0^1 \frac{d}{d\tau} A_{\tau,\alpha} \cdot A_{\alpha,\sigma} d\alpha = \int_0^1 \sum_{i=1}^s \frac{1}{b_i} l_i(\tau) l_i(\alpha) \sum_{j=1}^s \frac{1}{b_j} \int_0^\alpha l_j(x) dx l_j(\sigma) d\alpha \\
 &= \sum_{i,j=1}^s \frac{l_i(\tau) l_j(\sigma)}{b_i b_j} \int_0^1 \left(l_i(\alpha) \int_0^\alpha l_j(x) dx \right) d\alpha \\
 &= \sum_{i,j=1}^s \frac{l_i(\tau) l_j(\sigma)}{b_i b_j} \left(\int_0^\alpha l_i(x) dx \int_0^\alpha l_j(x) dx \Big|_0^1 - \int_0^1 \left(l_j(\alpha) \int_0^\alpha l_i(x) dx \right) d\alpha \right) \\
 &= \sum_{i,j=1}^s \frac{l_i(\tau) l_j(\sigma)}{b_i b_j} \left(b_i b_j - \int_0^1 \left(l_j(\alpha) \int_0^\alpha l_i(x) dx \right) d\alpha \right) \\
 &= \sum_{i,j=1}^s l_i(\tau) l_j(\sigma) - \sum_{i,j=1}^s \frac{l_i(\tau) l_j(\sigma)}{b_i b_j} \int_0^1 \left(l_j(\alpha) \int_0^\alpha l_i(x) dx \right) d\alpha \\
 &= 1 - \sum_{i,j=1}^s \frac{l_i(\tau) l_j(\sigma)}{b_i b_j} \int_0^1 \left(l_j(\alpha) \int_0^\alpha l_i(x) dx \right) d\alpha \\
 &= 1 - \sum_{i,j=1}^s \frac{l_j(\tau) l_i(\sigma)}{b_i b_j} \int_0^1 \left(l_i(\alpha) \int_0^\alpha l_j(x) dx \right) d\alpha \\
 &= 1 - \sum_{i,j=1}^s \frac{l_j(\tau) l_i(\sigma) - l_i(\tau) l_j(\sigma)}{b_i b_j} \int_0^1 \left(l_i(\alpha) \int_0^\alpha l_j(x) dx \right) d\alpha \\
 &\quad - \sum_{i,j=1}^s \frac{l_i(\tau) l_j(\sigma)}{b_i b_j} \int_0^1 \left(l_i(\alpha) \int_0^\alpha l_j(x) dx \right) d\alpha \\
 &= 1 - \sum_{i,j=1}^s \frac{l_j(\tau) l_i(\sigma) - l_i(\tau) l_j(\sigma)}{b_i b_j} \int_0^1 \left(l_i(\alpha) \int_0^\alpha l_j(x) dx \right) d\alpha - \frac{d}{d\tau} \bar{A}_{\tau,\sigma}.
 \end{aligned}$$

Therefore,

$$\frac{d}{d\tau} \bar{A}_{\tau,\sigma} = \frac{1}{2} - \frac{1}{2} \sum_{i,j=1}^s \frac{l_j(\tau) l_i(\sigma) - l_i(\tau) l_j(\sigma)}{b_i b_j} \int_0^1 \left(l_i(\alpha) \int_0^\alpha l_j(x) dx \right) d\alpha. \quad (2.8)$$

Combining the results in (2.7) with (2.8), we yield

$$\begin{aligned}
 V(u^{n+1}) - V(u^n) &= -h \left(\dot{u}^n, \int_0^1 f(U_\tau^n) d\tau \right) - \frac{1}{2} h^2 \left(\int_0^1 f(U_\sigma^n) d\sigma, \int_0^1 f(U_\tau^n) d\tau \right) \\
 &\quad - \frac{1}{2} h^2 \sum_{i,j=1}^s \frac{\int_0^1 \left(l_i(\alpha) \int_0^\alpha l_j(x) dx \right) d\alpha}{b_i b_j} \int_0^1 \int_0^1 (l_j(\tau) l_i(\sigma) - l_i(\tau) l_j(\sigma)) (f(U_\sigma^n), f(U_\tau^n)) d\sigma d\tau.
 \end{aligned}$$

Notice that

$$\int_0^1 \int_0^1 (l_j(\tau) l_i(\sigma) - l_i(\tau) l_j(\sigma)) (f(U_\sigma^n), f(U_\tau^n)) d\sigma d\tau = 0.$$

Therefore, we have

$$V(u^{n+1}) - V(u^n) = -h \left(\dot{u}^n, \int_0^1 f(U_\tau^n) d\tau \right) - \frac{1}{2} h^2 \left(\int_0^1 f(U_\sigma^n) d\sigma, \int_0^1 f(U_\tau^n) d\tau \right). \quad (2.9)$$

By comparing the results in (2.6) and (2.9), we obtain

$$H(u^{n+1}, \dot{u}^{n+1}) = H(u^n, \dot{u}^n), \quad n = 0, 1, \dots, N.$$

The conclusion of the theorem is confirmed. \square

According to Theorem 2.1 and Theorem 2.2, a class of energy-preserving integrators will be formulated by choosing suitable nodes. In this paper, the zeros of the *shifted Gauss–Legendre polynomial*

$$\frac{d^s}{dx^s} (x^s(1-x)^s)$$

are chosen as the collocation nodes $\{c_i\}_{i=1}^s$ to construct concrete energy-preserving integrators.

EPI2: Choosing two Gauss–Legendre quadrature points

$$c_1 = \frac{3 - \sqrt{3}}{6}, \quad c_2 = \frac{3 + \sqrt{3}}{6}$$

as the collocation nodes give the following energy-preserving integrator

$$\begin{cases} U_\tau^n = u^n + \tau h \dot{u}^n + h^2 \int_0^1 \bar{A}_2(\tau, \sigma) f(U_\sigma^n) d\sigma, \\ u^{n+1} = u^n + h \dot{u}^n + h^2 \int_0^1 (1 - \sigma) f(U_\sigma^n) d\sigma, \\ \dot{u}^{n+1} = \dot{u}^n + h \int_0^1 f(U_\sigma^n) d\sigma. \end{cases} \quad (2.10)$$

Here, the weight $\bar{A}_2(\tau, \sigma)$ is given by

$$\bar{A}_2(\tau, \sigma) = \frac{\tau}{2} (1 + \tau - 2\sigma).$$

EPI3: Choosing three Gauss–Legendre quadrature points

$$c_1 = \frac{5 - \sqrt{15}}{10}, \quad c_2 = \frac{1}{2}, \quad c_3 = \frac{5 + \sqrt{15}}{10},$$

as the collocation nodes give the following energy-preserving integrator

$$\begin{cases} U_\tau^n = u^n + \tau h \dot{u}^n + h^2 \int_0^1 \bar{A}_3(\tau, \sigma) f(U_\sigma^n) d\sigma, \\ u^{n+1} = u^n + h \dot{u}^n + h^2 \int_0^1 (1 - \sigma) f(U_\sigma^n) d\sigma, \\ \dot{u}^{n+1} = \dot{u}^n + h \int_0^1 f(U_\sigma^n) d\sigma. \end{cases} \quad (2.11)$$

Here, the weight $\bar{A}_3(\tau, \sigma)$ is given by

$$\bar{A}_3(\tau, \sigma) = \frac{\tau}{2} (1 + 3\tau - 2\tau^2 + 2(-3 + 2\tau^2)\sigma - 6(-1 + \tau)\sigma^2).$$

Remark 2.3. In practice, the integrals in **EPI2** and **EPI3** usually cannot be evaluated exactly. In our numerical experiments, the eighth-order Gauss quadrature formula with nodes

$$\tilde{c}_1 = \frac{1 - \sqrt{\frac{15+2\sqrt{30}}{35}}}{2}, \quad \tilde{c}_2 = \frac{1 - \sqrt{\frac{15-2\sqrt{30}}{35}}}{2}, \quad \tilde{c}_3 = \frac{1 + \sqrt{\frac{15-2\sqrt{30}}{35}}}{2}, \quad \tilde{c}_4 = \frac{1 + \sqrt{\frac{15+2\sqrt{30}}{35}}}{2}$$

and weights

$$\tilde{b}_1 = \frac{18 - \sqrt{30}}{72}, \quad \tilde{b}_2 = \frac{18 + \sqrt{30}}{72}, \quad \tilde{b}_3 = \frac{18 + \sqrt{30}}{72}, \quad \tilde{b}_4 = \frac{18 - \sqrt{30}}{72},$$

is used to approximate the integrals in (2.10) and (2.11).

2.2. Convergence and symmetry of the energy-preserving integrators

Inserting the exact solution $u(t)$ into the energy-preserving integrator (2.2), we obtain

$$\begin{cases} u(t_n + \tau h) = u(t_n) + \tau \dot{u}(t_n) + h^2 \int_0^1 \bar{A}_{\tau, \sigma} f(u(t_n + \sigma h)) d\sigma + \Delta_\tau^n, \\ u(t_n + h) = u(t_n) + h \dot{u}(t_n) + h^2 \int_0^1 (1 - \sigma) f(u(t_n + \sigma h)) d\sigma, \\ \dot{u}(t_n + h) = \dot{u}(t_n) + h \int_0^1 f(u(t_n + \sigma h)) d\sigma. \end{cases} \quad (2.12)$$

Here, Δ_τ^n is the residual of internal stage. Defining

$$e_\tau^n = u(t_n + \tau h) - U_\tau^n, \quad e^n = u(t_n) - u^n, \quad \dot{e}^n = \dot{u}(t_n) - \dot{u}^n,$$

and subtracting (2.2) from (2.12) yields the following error system

$$\begin{cases} e_\tau^n = e^n + \tau h \dot{e}^n + h^2 \int_0^1 \bar{A}_{\tau, \sigma} (f(u(t_n + \sigma h)) - f(U_\sigma^n)) d\sigma + \Delta_\tau^n, \quad \tau \in [0, 1], \\ e^{n+1} = e^n + h \dot{e}^n + h^2 \int_0^1 (1 - \sigma) (f(u(t_n + \sigma h)) - f(U_\sigma^n)) d\sigma, \\ \dot{e}^{n+1} = \dot{e}^n + h \int_0^1 (f(u(t_n + \sigma h)) - f(U_\sigma^n)) d\sigma. \end{cases} \quad (2.13)$$

In order to clarify the remainder of the energy-preserving integrators EPI2 and EPI3, we represent the exact solution of the system (1.1) as the following variation-of-constants formula

$$\begin{cases} u(t_n + \tau h) = u(t_n) + h \dot{u}(t_n) + h^2 \int_0^\tau (\tau - \sigma) f(u(t_n + \sigma h)) d\sigma, \\ \dot{u}(t_n + \tau h) = \dot{u}(t_n) + h \int_0^\tau f(u(t_n + \sigma h)) d\sigma. \end{cases} \quad (2.14)$$

Comparing (2.14) with (2.12), we can find that the error mainly comes from the approximation of the internal stage. We also assume that the nonlinear function f satisfies the Lipschitz condition

$$\|f(x) - f(y)\| \leq L \|x - y\| \quad \text{for } \forall x, y \in \mathcal{X},$$

which will be used for the convergence and stability analysis of the integrators.

Theorem 2.3. Suppose that the exact solution $u(t)$ is sufficiently smooth and the step size h satisfies $h \leq \sqrt{\frac{1}{2ML}}$. Then, we have the following error estimation

$$\|e^n\| + h \|\dot{e}^n\| \leq Ch \sum_{k=0}^{n-1} \int_0^1 \|\Delta_\tau^k\| d\tau,$$

where the constant C depends on L and T but is independent of h and n .

Proof. Taking norms on both sides of (2.13) and using the Lipschitz condition, we have

$$\begin{cases} \|e_\tau^n\| \leq \|e^n\| + \tau h \|\dot{e}^n\| + h^2 LM \int_0^1 \|e_\sigma^n\| d\sigma + \|\Delta_\tau^n\|, \quad \tau \in [0, 1], \\ \|e^{n+1}\| \leq \|e^n\| + h \|\dot{e}^n\| + h^2 L \int_0^1 \|e_\sigma^n\| d\sigma, \\ \|\dot{e}^{n+1}\| \leq \|\dot{e}^n\| + h L \int_0^1 \|e_\sigma^n\| d\sigma. \end{cases} \quad (2.15)$$

Integrating both sides of the first inequality in (2.15) from 0 to 1 with respect to τ leads to

$$\int_0^1 \|e_\tau^n\| d\tau \leq \|e^n\| + \frac{h}{2} \|\dot{e}^n\| + h^2 LM \int_0^1 \|e_\sigma^n\| d\sigma + \int_0^1 \|\Delta_\tau^n\| d\tau.$$

Under the condition $h \leq \sqrt{\frac{1}{2ML}}$, the above inequality can be simplified as

$$\int_0^1 \|e_\tau^n\| d\tau \leq 2\|e^n\| + h\|\dot{e}^n\| + 2 \int_0^1 \|\Delta_\tau^n\| d\tau. \quad (2.16)$$

Furthermore, the last two inequalities of (2.15) give

$$\|e^{n+1}\| + h\|\dot{e}^{n+1}\| \leq \|e^n\| + 2h\|\dot{e}^n\| + 2h^2 L \int_0^1 \|e_\sigma^n\| d\sigma \quad (2.17)$$

and

$$\|\dot{e}^n\| \leq hL \sum_{k=0}^{n-1} \int_0^1 \|e_\sigma^k\| d\sigma. \quad (2.18)$$

Inserting (2.18) into (2.17) yields that

$$\|e^{n+1}\| + h\|\dot{e}^{n+1}\| \leq \|e^n\| + h\|\dot{e}^n\| + 2h^2 L \sum_{k=0}^n \int_0^1 \|e_\sigma^k\| d\sigma. \quad (2.19)$$

Substituting the estimation (2.16) into (2.19), after a careful calculation, we obtain

$$\|e^{n+1}\| + h\|\dot{e}^{n+1}\| \leq \|e^n\| + h\|\dot{e}^n\| + 4h^2 L \sum_{k=0}^n \left(\|e^k\| + h\|\dot{e}^k\| \right) + 4h^2 L \sum_{k=0}^n \int_0^1 \|\Delta_\tau^k\| d\tau. \quad (2.20)$$

Applying the mathematical induction to (2.20) and using the discrete Gronwall's inequality yield

$$\begin{aligned} \|e^n\| + h\|\dot{e}^n\| &\leq 4h^2 L \sum_{m=0}^{n-1} \sum_{k=0}^m \left(\|e^k\| + h\|\dot{e}^k\| \right) + 4h^2 L \sum_{m=0}^{n-1} \sum_{k=0}^m \int_0^1 \|\Delta_\tau^k\| d\tau \\ &\leq 4h(T - t_0)L \sum_{k=0}^{n-1} \left(\|e^k\| + h\|\dot{e}^k\| \right) + 4h(T - t_0)L \sum_{k=0}^{n-1} \int_0^1 \|\Delta_\tau^k\| d\tau \\ &\leq Ch \sum_{k=0}^{n-1} \int_0^1 \|\Delta_\tau^k\| d\tau. \end{aligned} \quad (2.21)$$

Obviously, C is a constant, which depends on L and T but is independent of h and n . The conclusion of the theorem is verified. \square

In order to analyse the stability of the proposed EP integrator (2.2), we suppose the perturbed system of (1.1) is

$$\begin{cases} \partial_t^2 v(t) = f(v(t)), & t \in [t_0, T], \\ v(t_0) = \phi + \tilde{\phi}, & \partial_t v(t_0) = \varphi + \tilde{\varphi}, \end{cases} \quad (2.22)$$

where $\tilde{\phi}$ and $\tilde{\varphi}$ are perturbation. Letting $\eta(t) = v(t) - u(t)$ and subtracting (1.1) from (2.22) yield

$$\begin{cases} \partial_t^2 \eta(t) = f(v(t)) - f(u(t)), & t \in [t_0, T], \\ \eta(t_0) = \tilde{\phi}, & \partial_t \eta(t_0) = \tilde{\varphi}. \end{cases} \quad (2.23)$$

Applying the EP integrator (2.2) to (2.23), we obtain

$$\begin{cases} \eta_\tau^n = \eta^n + \tau h \dot{\eta}^n + h^2 \int_0^1 \bar{A}_{\tau,\sigma} \left(f(v(t_n + \sigma h)) - f(u(t_n + \sigma h)) \right) d\sigma, & \tau \in [0, 1], \\ \eta^{n+1} = \eta^n + h \dot{\eta}^n + h^2 \int_0^1 (1 - \sigma) \left(f(v(t_n + \sigma h)) - f(u(t_n + \sigma h)) \right) d\sigma, \\ \dot{\eta}^{n+1} = \dot{\eta}^n + h \int_0^1 \left(f(v(t_n + \sigma h)) - f(u(t_n + \sigma h)) \right) d\sigma. \end{cases} \quad (2.24)$$

Theorem 2.4. Suppose that $\eta(t)$ is sufficiently smooth and h satisfies $h \leq \sqrt{\frac{1}{2ML}}$. Then, we have the following stability result

$$\|\eta^n\| + h\|\dot{\eta}^n\| \leq \tilde{C}(\|\tilde{\phi}\| + \|\tilde{\varphi}\|),$$

where the constant \tilde{C} is independent of h and n .

Proof. Taking norms on both sides of (2.24) and using the Lipschitz condition, we yield

$$\begin{cases} \|\eta_\tau^n\| \leq \|\eta^n\| + \tau h\|\dot{\eta}^n\| + h^2 M L \int_0^1 \|\eta_\sigma^n\| d\sigma, & \tau \in [0, 1], \\ \|\eta^{n+1}\| \leq \|\eta^n\| + h\|\dot{\eta}^n\| + h^2 L \int_0^1 \|\eta_\sigma^n\| d\sigma, \\ \|\dot{\eta}^{n+1}\| \leq \|\dot{\eta}^n\| + h L \int_0^1 \|\eta_\sigma^n\| d\sigma. \end{cases} \quad (2.25)$$

Similar as the prove process of Theorem 2.3, we obtain the following recursive relationship

$$\|\eta^{n+1}\| + h\|\dot{\eta}^{n+1}\| \leq \|\eta^n\| + h\|\dot{\eta}^n\| + 4h^2 L \sum_{k=0}^n \left(\|\eta^k\| + h\|\dot{\eta}^k\| \right) + h\|\dot{\eta}^0\|. \quad (2.26)$$

The mathematical induction and the discrete Gronwall's inequality yield the approximation

$$\|\eta^n\| + h\|\dot{\eta}^n\| \leq \tilde{C}(\|\tilde{\phi}\| + \|\tilde{\varphi}\|). \quad (2.27)$$

Here, \tilde{C} is a constant and also independent of h and n . \square

Now, we turn our attention to investigate the convergence of the concrete energy-preserving integrators EPI2 and EPI3. For simplicity, we set $g(t) = f(u(t))$ and expand it as the following Taylor expansion with integral remainder

$$g(t_n + \sigma h) = \sum_{k=0}^{q-1} \frac{\sigma^k h^k}{k!} g^{(k)}(t_n) + \frac{h^q}{(q-1)!} \int_0^\sigma (\sigma - z)^q g^{(q)}(t_n + zh) dz. \quad (2.28)$$

By using the Taylor expansion, the first equation of the exact solution (2.14) can be expressed as

$$u(t_n + \tau h) = u(t_n) + h \dot{u}(t_n) + \sum_{k=0}^{q-1} \frac{h^{k+2} \tau^{k+2}}{(k+2)!} g^{(k)}(t_n) + \frac{h^{q+2}}{(q-1)!} \int_0^\tau \int_0^\sigma (\tau - \sigma)(\sigma - z)^q g^{(q)}(t_n + zh) dz d\sigma. \quad (2.29)$$

Applying the Taylor expansion to the first equation of (2.12) gives

$$\begin{aligned} u(t_n + \tau h) = & u(t_n) + \tau h \dot{u}(t_n) + \sum_{k=0}^{q-1} \frac{h^{k+2}}{k!} \int_0^1 \bar{A}(\tau, \sigma) \sigma^k d\sigma g^{(k)}(t_n) \\ & + \frac{h^{q+2}}{(q-1)!} \int_0^1 \int_0^\sigma \bar{A}(\tau, \sigma)(\sigma - z)^q g^{(q)}(t_n + zh) dz d\sigma + \Delta_\tau^n. \end{aligned} \quad (2.30)$$

It follows from (2.29) and (2.30) that

$$\begin{aligned} \Delta_\tau^n = & \sum_{k=0}^{q-1} h^{k+2} \left(\frac{\tau^{k+2}}{(k+2)!} - \frac{1}{k!} \int_0^1 \bar{A}(\tau, \sigma) \sigma^k d\sigma \right) g^{(k)}(t_n) \\ & + \frac{h^{q+2}}{(q-1)!} \left(\int_0^\tau \int_0^\sigma (\tau - \sigma)(\sigma - z)^q g^{(q)}(t_n + zh) dz d\sigma \right. \\ & \left. - \int_0^1 \int_0^\sigma \bar{A}(\tau, \sigma)(\sigma - z)^q g^{(q)}(t_n + zh) dz d\sigma \right). \end{aligned} \quad (2.31)$$

Therefore, in light of Theorem 2.3, the convergence of the energy-preserving integrators **EPI2** and **EPI3** can be easily verified.

Theorem 2.5. Suppose that $f(u(t)) \in C^1([t_0, T]; \mathcal{X})$ and the step h satisfies $h \leq \sqrt{\frac{1}{2ML}}$. Then we have

$$\|u(t_n) - u^n\| \leq C_1 h^3,$$

where the constant C_1 is independent of h and n . Therefore, the order of convergence of the energy-preserving integrator **EPI2** is at least three.

Proof. Inserting the exact solution $u(t)$ into **EPI1**, we have

$$\begin{cases} u(t_n + \tau h) = u(t_n) + \tau h \dot{u}(t_n) + h^2 \int_0^1 \bar{A}_2(\tau, \sigma) f(u(t_n + \sigma h)) d\sigma + \delta_\tau^n, \\ u(t_n + h) = u(t_n) + h \dot{u}(t_n) + h^2 \int_0^1 (1 - \sigma) f(u(t_n + \sigma h)) d\sigma, \\ \dot{u}(t_n + h) = \dot{u}(t_n) + h \int_0^1 f(u(t_n + \sigma h)) d\sigma, \end{cases} \quad (2.32)$$

In light of the form $\bar{A}_2(\tau, \sigma) = \frac{\tau}{2}(1 + \tau - 2\sigma)$ and comparing (2.29) with (2.30), it can be checked that

$$\delta_\tau^n = h^3 \left(\int_0^\tau \int_0^\sigma (\tau - \sigma)(\sigma - z) g'(t_n + zh) dz d\sigma - \int_0^1 \int_0^\sigma \bar{A}_2(\tau, \sigma)(\sigma - z) g'(t_n + zh) dz d\sigma \right).$$

According to Theorem 2.3, there exists a constant C_1 such that

$$\|e^n\| + h \|\dot{e}^n\| \leq C_1 h^3.$$

The conclusion of the theorem is proved. \square

Similarly, the convergence of the energy-preserving integrator **EPI3** (2.11) is analysed in the following theorem.

Theorem 2.6. Suppose that $f(u(t)) \in C^2([t_0, T]; \mathcal{X})$ and the step h satisfies $h \leq \sqrt{\frac{1}{2ML}}$. Then, we have

$$\|u(t_n) - u^n\| \leq C_2 h^4,$$

where the constant C_2 is independent of h and n . Therefore, the order of convergence of the energy-preserving integrator **EPI3** is at least four.

Proof. Substituting the exact solution $u(t)$ into the energy-preserving integrator **EPI3**, we have

$$\begin{cases} u(t_n + \tau h) = u(t_n) + \tau h \dot{u}(t_n) + h^2 \int_0^1 \bar{A}_3(\tau, \sigma) f(u(t_n + \sigma h)) d\sigma + \tilde{\delta}_\tau^n, \\ u(t_n + h) = u(t_n) + h \dot{u}(t_n) + h^2 \int_0^1 (1 - \sigma) f(u(t_n + \sigma h)) d\sigma, \\ \dot{u}(t_n + h) = \dot{u}(t_n) + h \int_0^1 f(u(t_n + \sigma h)) d\sigma. \end{cases} \quad (2.33)$$

Similar to the proof of [Theorem 2.5](#), the residual $\tilde{\delta}_\tau^n$ can be expressed as

$$\tilde{\delta}_\tau^n = h^4 \left(\int_0^\tau \int_0^\sigma (\tau - \sigma)(\sigma - z)^2 g''(t_n + zh) dz d\sigma - \int_0^1 \int_0^\sigma \bar{A}_3(\tau, \sigma)(\sigma - z)^2 g''(t_n + zh) dz d\sigma \right).$$

Hence, there exists a constant C_2 such that

$$\|e^n\| + h\|\dot{e}^n\| \leq C_2 h^4.$$

The conclusion of the theorem is proved. \square

The symmetric methods have excellent long-time behaviour for solving the reversible systems (See Hairer et al. [7]). Therefore, we turn our attention to discuss the symmetry of the designed energy-preserving integrators **EPI2** and **EPI3**.

Theorem 2.7. *The energy-preserving integrators **EPI2** and **EPI3** are symmetric.*

Proof. We verify the symmetry of the energy-preserving integrator **EPI2**. The symmetry of **EPI3** can be obtained in a similar way.

Exchanging $u^{n+1} \leftrightarrow u^n$, $\dot{u}^{n+1} \leftrightarrow \dot{u}^n$ and replacing $h \leftrightarrow -h$, $\tau \leftrightarrow 1 - \tau$ in (2.10), we yield

$$\begin{cases} U_{1-\tau}^n = u^{n+1} - (1 - \tau)h\dot{u}^{n+1} + \frac{1 - \tau}{2}h^2 \int_0^1 (2 - \tau - 2\sigma)f(U_\sigma^n)d\sigma, \\ u^n = u^{n+1} - h\dot{u}^{n+1} + h^2 \int_0^1 (1 - \sigma)f(U_\sigma^n)d\sigma, \\ \dot{u}^n = \dot{u}^{n+1} - h \int_0^1 f(U_\sigma^n)d\sigma. \end{cases} \quad (2.34)$$

It follows from the last two formulae in (2.34) that

$$\begin{cases} u^{n+1} = u^n + h\dot{u}^n + h^2 \int_0^1 \sigma f(U_\sigma^n)d\sigma, \\ \dot{u}^{n+1} = \dot{u}^n + h \int_0^1 f(U_\sigma^n)d\sigma. \end{cases} \quad (2.35)$$

Inserting (2.35) into the first formula in (2.34) leads to

$$U_{1-\tau}^n = u^n + \tau h\dot{u}^{n+1} + \frac{\tau}{2}h^2 \int_0^1 (-1 + \tau + 2\sigma)f(U_\sigma^n)d\sigma. \quad (2.36)$$

Applying the transformation $\sigma = 1 - \xi$ to integrals in the formulae (2.35) and (2.36), we obtain

$$\begin{cases} U_{1-\tau}^n = u^n + \tau h\dot{u}^{n+1} + \frac{\tau}{2}h^2 \int_0^1 (1 + \tau - 2\xi)f(U_{1-\xi}^n)d\xi, \\ u^{n+1} = u^n + h\dot{u}^n + h^2 \int_0^1 (1 - \xi)f(U_{1-\xi}^n)d\xi, \\ \dot{u}^{n+1} = \dot{u}^n + h \int_0^1 f(U_{1-\xi}^n)d\xi, \end{cases} \quad (2.37)$$

which shows that (2.37) is same as (2.10). Therefore, the integrator (2.10) is symmetric. \square

Remark 2.4. Due to the symmetry of the integrators, the numerical experiments in next section show that the proposed energy-preserving integrators **EPI2** and **EPI3** could convergent to fourth-order and sixth-order, respectively.

3. Numerical results

In this section, the energy preservation and accuracy of the integrators **EPI2** and **EPI3** are verified by computing two model problems. For practical computation, the fixed-point iteration is used to solve the nonlinear algebraic

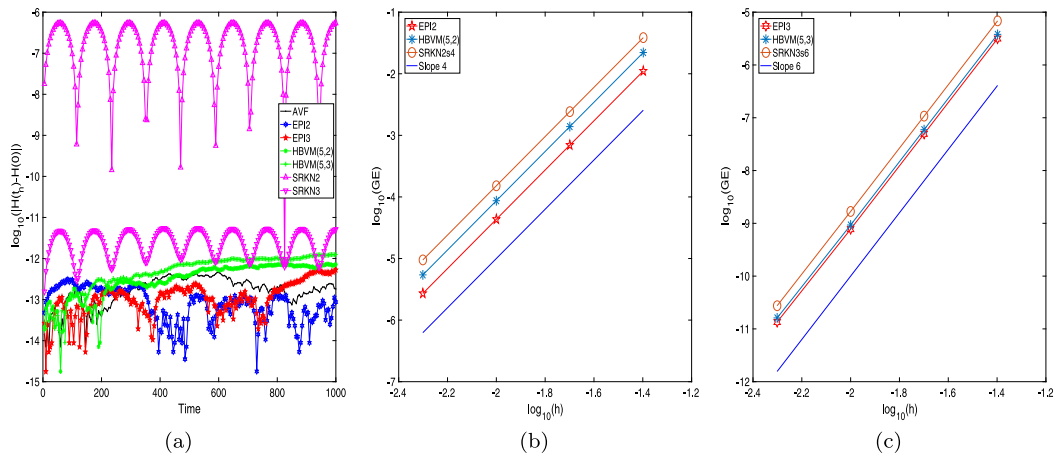


Fig. 1. Results for Problem 1. (a) the logarithm of the energy error against time with $h = 0.01$. (b) and (c) the log-log plot of global error against different time steps h for **EPI2** and **EPI3**, respectively.

equations in every step. The maximum iterative number and the error tolerance are set as 100 and 10^{-15} , respectively. The convergent rate is computed by

$$\text{Rate} = \log_2 \frac{\text{Error}(h)}{\text{Error}(h/2)} \quad \text{with} \quad \text{Error}(h) = \|u(T; h) - u(T; h/2)\|_{\infty},$$

where $u(T; h)$ represents the numerical solution at time T with step size h . In order to demonstrate the superiority of the proposed integrators, the following integrators are chosen for comparison:

- **AVF**: the energy-preserving second-order averaged vector field method (see, e.g. [6,7]);
- **HBVM(5,2)**: the fourth-order Hamiltonian Boundary Value Method (see, e.g. [2,3]);
- **HBVM(5,3)**: the sixth-order Hamiltonian Boundary Value Method (see, e.g. [2,3]);
- **SRKN2s4**: the continuous-stage symplectic RKN method of order four (see, e.g. [19,20]);
- **SRKN3s6**: the continuous-stage symplectic RKN method of order six (see, e.g. [19,20]).

Problem 1. Consider the Duffing equation (see, e.g. [11,12])

$$\begin{cases} \ddot{q} = -(\omega^2 + k^2)q + 2k^2q^3, & 0 \leq k < \omega, \\ q(0) = 0, \quad \dot{q}(0) = \omega, \end{cases} \quad (3.1)$$

with the Hamiltonian

$$H(q, \dot{q}) = \frac{1}{2}\dot{q}^2 + \frac{\omega^2 + k^2}{2}q^2 - \frac{k^2}{2}q^4.$$

The analytic solution can be expressed by the Jacobian elliptic function

$$q(t) = \text{sn}(\omega t, k/\omega).$$

We integrate the problem over $[0, 1000]$ with $k = 0.03$, $\omega = 5$. In Fig. 1(a), the numerical result indicates that the proposed integrators **EPI2** and **EPI3** are energy-preserving as well as the classical AVF method and the Hamiltonian Boundary Value method. Fig. 1(b) and (c) demonstrate that the proposed integrators **EPI2** and **EPI3** are much more accuracy than the chosen integrators. The results in Table 1 verify that the integrators **EPI2** and **EPI3** have fourth-order and sixth-order convergence, respectively.

Problem 2. Consider the two-dimensional periodic sine-Gordon equation (see, e.g. [9,10,12]):

$$\begin{cases} u_{tt} - \kappa^2(u_{xx} + u_{yy}) = -\sin(u), & (x, y) \in (0, 1) \times (0, 1), \quad 0 < t \leq 100, \\ u(x, y, 0) = 4 \arctan\left(\exp\left(3 - \frac{1}{\kappa^2}\sqrt{x^2 + y^2}\right)\right), & u_t(x, y, 0) = 0, \end{cases} \quad (3.2)$$

Table 1

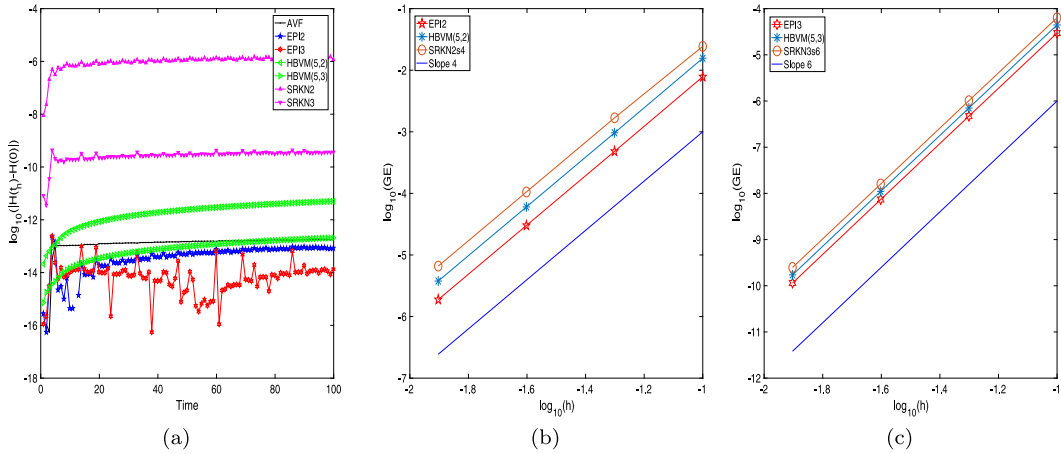
Convergence order of “EPI2” and “EPI3” for Problem 1.

$h = 0.04$	EPI2		EPI3	
	Error	Order	Error	Order
h	1.1071E-02	—	3.1651E-06	—
$h/2$	6.9357E-04	3.9966	4.9547E-08	5.9973
$h/2^2$	4.3368E-05	3.9993	7.7509E-10	5.9983
$h/2^3$	2.7112E-06	3.9996	1.3490E-11	5.8444

Table 2

Convergence order of “EPI2” and “EPI3” for solving Problem 2.

$h = 0.2$	EPI2		EPI3	
	Error	Order	Error	Order
h	7.8299E-03	—	2.9562E-05	—
$h/2$	4.8164E-04	4.0230	4.7003E-07	5.9748
$h/2^2$	3.0145E-05	3.9980	7.3791E-09	5.9932
$h/2^3$	1.8864E-06	3.9982	1.1469E-10	6.0076

**Fig. 2.** Results for Problem 2. (a) the logarithm of the energy error against time with $h = 0.1$. (b) and (c) the log-log plot of global error against different time steps h for EPI2 and EPI3, respectively.

where the dimensionless parameter κ is chosen as $\kappa = 20$. We first approximate the spatial derivatives by the two-dimensional Fourier pseudo-spectral method. Then, Eq. (3.2) is converted into the following Hamiltonian ordinary differential equations:

$$U''(t) = -D_2^x U(t) - U(t) D_2^y - \sin(U(t)),$$

where $D_2^x = \mathcal{F}_{M_x}^{-1} \Lambda_2^x \mathcal{F}_{M_x}$ and $D_2^y = \mathcal{F}_{M_y}^{-1} \Lambda_2^y \mathcal{F}_{M_y}$ are the second-order Fourier spectral matrices in x direction and y direction, respectively. The discrete energy is given by

$$H(U(t), \dot{U}(t)) = \frac{1}{2} \|\dot{U}(t)\|_2^2 + \frac{1}{2} |U(t)|_1^2 + \Delta x \Delta y \sum_{l=1}^{M_x} \sum_{j=1}^{M_y} (1 - \cos(U_{lj}(t))), \quad (3.3)$$

where $\Delta x = 2/M_x$ and $\Delta y = 2/M_y$ are the spatial step sizes. We set the mesh sizes $M_x = M_y = 512$. In addition, as the solution of the 2D sine-Gordon equation cannot be represented explicitly, the posterior error (PE) is used to compute the convergent rate. The numerical results in Fig. 2 and Table 2 again show that the proposed integrators EPI2 and EPI3 are energy-preserving and could achieve fourth-order and sixth-order, respectively.

4. Conclusion

In this paper, a novel class of high-order and energy-preserving numerical integrators are proposed for the hyperbolic Hamiltonian system (1.1). The basic idea of constructing the energy-preserving integrators is the strategy of collocation. The proposed energy-preserving integrators could also be interpreted as the continuous-stage collocation Runge–Kutta–Nyström methods. For practical computation, the energy-preserving integrators with order four and order six are obtained by choosing two and three Gauss–Legendre points as the collocation nodes, respectively. Numerical experiments are conducted to illustrate the accuracy and energy preservation of the integrators.

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