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Energy-Preserving Parareal-RKN Algorithms for Hamiltonian Systems

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Abstract. In this paper, we formulate and analyse a kind of parareal-RKN algorithms with energy conservation for Hamiltonian systems. The proposed algorithms are constructed by using the ideas of parareal methods, Runge-Kutta-Nyström (RKN) methods and projection methods. It is shown that the algorithms can exactly preserve the energy of Hamiltonian systems. Moreover, the convergence of the integrators is rigorously analysed. Three numerical experiments are carried out to support the theoretical results presented in this paper and show the numerical behaviour of the derived algorithms.

AMS subject classifications: 65L05, 65L20, 65P10

Key words: Parareal methods, Runge-Kutta-Nyström methods, Hamiltonian systems, energy conservation.

1. Introduction

In computer science and engineering, the effective numerical solution of time-dependent ordinary and partial differential equations has traditionally been a key area of study. By discovering new parallelization techniques, we can use the many-core high-performance computing architectures to achieve faster simulations. After spatial parallelization, the idea of the time-related problem of parallelization in the time direction has received increasing attention, such as parareal (parallel in real time), PFASST (parallel full approximation scheme in space and time), MGRIT (multigrid reduction in time) [7, 22, 24], etc.

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Hamiltonian systems are widely recognized to occur often in many fields of research and engineering, including applied mathematics, molecular biology, electronics, chemistry, astronomy, mechanics, and quantum physics [9, 17]. There is potential to parallelize the Hamiltion equation based on the time-consuming problem solved in long times. About the parallelization methods, we are interested in a kind of multiple shooting methods focusing entirely on the time direction, i.e., the parareal method proposed by Lions *et al.* [22] (see also [13, 18, 30]). The parareal method adopts two types of calculation strategies: coarse propagator and fine propagator. They are combined for the prediction and correction to bring updates to the values at the coarse time points. The iteration sequence will converge to the solution of the fine propagator in the whole time interval. Here, the fine propagator in time subintervals is only performed sequentially, which can be implemented in parallel. Further studies based on the parareal method include the parallel implicit time-integrator (PITA) [8], ParaExp [10], adaptive parareal method [19, 23], etc. Parareal can also be constructed by combining with other techniques, such as the strategies of domain decomposition and waveform relaxation [3,12,20], the diagonalization technique [14], and the application of probabilistic methods to time-parallelization [25].

Although the common parareal method is efficient in theory, direct application of parareal has some problems in some specific cases, such as the Hamiltonian systems. Some related studies on Hamiltonian systems provide several ideas. Among them, [5] has pointed that even when the coarse and fine propagators in parareal use symplectic and symmetric integrators which are known to be suitable integrators for Hamiltonian systems, the whole algorithm does not enjoy adequate geometrical properties. So they put forward a symmetric version of the parareal algorithm, which contains a projection in each iteration, to guarantee the long-time properties of the numerical flow. After that, [11] presents the long-time error estimates for the parareal iterates for Hamiltonian systems and present a variant of the parareal algorithm for high accuracy computations. The parareal based on the projection of each iterative solution onto the manifold can also be used to solve hyperbolic type problems [6].

As an important class of structure-preserving algorithm, the energy-preserving algorithm has been widely studied in many problems in recent years [1, 2, 4, 21, 26–29]. However, for the standard parareal algorithms, the energy conservation does not hold. Motivated by the above projection approach, we intend to provide a class of specific energy-preserving parareal algorithms for Hamiltonian systems but in another approach. This work focuses on the structure-preserving algorithms of Hamiltonian systems which can be expressed by a system of differential equations of the form

$$\begin{aligned} \dot{q} &= \nabla_p H(q,p), \qquad q(0) = q_0, \\ \dot{p} &= -\nabla_q H(q,p), \quad p(0) = p_0, \end{aligned} \tag{1.1}$$

where $H : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is the Hamiltonian function, the dimension d is the number of degrees of freedom, $q(t) : \mathbb{R} \to \mathbb{R}^d$ represents generalized positions, and $p(t) : \mathbb{R} \to \mathbb{R}^d$ represents generalized momenta. The Hamiltonian function often has the special separable structure $H(q,p) = \mathcal{T}(p) + U(q)$. In this paper, we are interested in a Hamiltonian system of the form (1.1) with the following Hamiltonian:

$$H(q,p) = \frac{1}{2}p^{\intercal}p + U(q), \tag{1.2}$$

where $U(q)$ is a real-valued function with continuous second derivatives. In this paper, $\|\cdot\|_2$ presents the Euclidean norm of a vector or spectral norm of a matrix. This Hamiltonian system is in fact identical to the following second-order differential equations:

$$\ddot{q}(t) = F\big(q(t)\big), \quad q(0) = q_0, \quad \dot{q}(0) = \dot{q}_0, \quad t \in [0,T], \quad T > 0, \tag{1.3}$$

where $F(q) = -\nabla_q U(q)$.

In the existing literatures of the parareal algorithms, we found that the algorithm construction for second-order differential equations or hyperbolic problems are often achieved by transforming into a first-order differential systems. The coarse and fine propagators are not constructed based on direct integrators. To be precise, the construction of a coarse propagator of parareal directly for second-order differential equations means that the approximation of both the solution and its first-order derivative at the coarse points should be calculated in each iteration. Based on this idea, we adopt the Runge-Kutta-Nyström (RKN) integrator [17] to approximate and analyze a class of parareal-RKN algorithms which are energy-preserving.

The paper is organized as follows. We will construct the energy-preserving parareal-RKN algorithms in Section 2 by introducing the RKN-type coarse and fine propagators and providing some practical schemes. In Section 3, the main results of the energy conservation and convergence are first given, and then the proofs. We also show that the projection does not deteriorate the convergence result of the underlying method. Finally, the energy errors of three numerical experiments with respect to the time t and the iterations are illustrated in Section 4 to verify the convergence orders of these parareal-RKN algorithms.

2. Energy-preserving parareal-RKN algorithms

In this section, we present the formulation of the algorithms, which starts by the restatement of parareal algorithms.

Consider a system of first-order initial value problem

$$\dot{u}(t) = f\big(u(t)\big), \quad u(0) = u_0, \quad t \in [0,T] \tag{2.1}$$

and let $u_0^j = u_0$ for the iteration index $j = 0,1,2,\ldots$. The parareal algorithm (see [22]) for solving this system is defined by

$$u_{n+1}^{j+1} = \mathcal{G}_{\Delta t}\big(T_n, u_n^{j+1}\big) + \mathcal{F}_{\delta t}\big(T_n, u_n^j\big) - \mathcal{G}_{\Delta t}\big(T_n, u_n^j\big), \quad n = 0,1,\ldots,T/\Delta T - 1,$$

where $\{u_n^0\}_{n\geq 1}$ is the initial guess, $\mathcal{F}$ is the fine propagator using a small time stepsize δt, $\mathcal{G}$ is the coarse propagator with a large time stepsize Δt, and ΔT is an even larger time interval which partitions the time interval $[0, T]$ with $T_n = n\Delta T$. We note here that the notations $\mathcal{F}_{\delta t}(T_n, u_n^j)$ and $\mathcal{G}_{\Delta t}(T_n, u_n^j)$ are referred to the numerical solutions of (2.1) at $t = T_{n+1}$ with the initial value u_n^j at $t = T_n$. In this paper we generate the initial guess $\{u_n^0\}_{n\geq 1}$ by the $\mathcal{G}$-propagator.

2.1. RKN-type coarse and fine propagators

We firstly formulate the numerical methods for coarse and fine propagators. Applying the well-known variation-of-constants formula to (1.3) gives the following integral equations (see [17]):

$$q(t) = q_0 + t\dot{q}_0 + \int_0^t (t-\xi)\hat{F}(\xi)d\xi, \quad \dot{q}(t) = \dot{q}_0 + \int_0^t \hat{F}(\xi)d\xi \tag{2.2}$$

for any real number $t \in [0, T]$, where $\hat{F}(\xi) = F(q(\xi))$.

Partition the time interval $[0, T]$ of (1.3) by ΔT and then consider

$$\ddot{q}(t) = F\big(q(t)\big), \quad q(T_n) = q_n, \quad \dot{q}(T_n) = \dot{q}_n, \quad t \in [T_n, T_n + \Delta T]. \tag{2.3}$$

With the help of (2.2), the following RKN-type coarse propagator is chosen for solving (2.3):

$$\begin{aligned}
&q_{n,0} = q_n, \quad \dot{q}_{n,0} = \dot{q}_n,\\
&F_{n,(m-1)\Delta t} = F\big(q_{n,(m-1)\Delta t} + \Delta t c_1 \dot{q}_{n,(m-1)\Delta t}\big),\\
&q_{n,m\Delta t} = q_{n,(m-1)\Delta t} + \Delta t \dot{q}_{n,(m-1)\Delta t} + \Delta t^2 \bar{b}_1 F_{n,(m-1)\Delta t},\\
&\dot{q}_{n,m\Delta t} = \dot{q}_{n,(m-1)\Delta t} + \Delta t b_1 F_{n,(m-1)\Delta t},\\
&q_{n+1} = q_{n,\Delta T}, \quad \dot{q}_{n+1} = \dot{q}_{n,\Delta T},
\end{aligned} \tag{2.4}$$

where $m = 1, 2, \ldots, \Delta T/\Delta t$, $c_1 \in [0, 1]$ is a real constant, and b_1 and $\bar{b}_1$ are coefficients of a one-stage RKN method. This coarse propagator over one coarse stepsize Δt is denoted by

$$[q_{n,m\Delta t}; \dot{q}_{n,m\Delta t}] = \mathcal{G}_{T_n+(m-1)\Delta t}^{T_n+m\Delta t}\big([q_{n,(m-1)\Delta t}; \dot{q}_{n,(m-1)\Delta t}]\big). \tag{2.5}$$

In this propagator, replacing the coarse stepsize Δt by the fine one δt leads to a choice of fine propagator, which reads for $m = 1, 2, \ldots, \Delta T/\delta t$

$$\begin{aligned}
&q_{n,0} = q_n, \quad \dot{q}_{n,0} = \dot{q}_n,\\
&F_{n,(m-1)\delta t} = F\big(q_{n,(m-1)\delta t} + \delta t c_1 \dot{q}_{n,(m-1)\delta t}\big),\\
&q_{n,m\delta t} = q_{n,(m-1)\delta t} + \delta t \dot{q}_{n,(m-1)\delta t} + \delta t^2 \bar{b}_1 F_{n,(m-1)\delta t},\\
&\dot{q}_{n,m\delta t} = \dot{q}_{n,(m-1)\delta t} + \delta t b_1 F_{n,(m-1)\delta t},\\
&q_{n+1} = q_{n,\Delta T}, \quad \dot{q}_{n+1} = \dot{q}_{n,\Delta T}.
\end{aligned} \tag{2.6}$$

Denote the fine propagator as

$$[q_{n,m\delta t}; \dot{q}_{n,m\delta t}] = \mathcal{F}_{T_n+(m-1)\delta t}^{T_n+m\delta t}\big([q_{n,(m-1)\delta t}; \dot{q}_{n,(m-1)\delta t}]\big). \tag{2.7}$$

As an example, choosing

$$c_1 = \frac{1}{2}, \quad b_1 = 1, \quad \bar{b}_1 = \frac{1}{2} \tag{2.8}$$

gives a second-order RKN integrator.

It is remarked that high-order RKN method can be taken into account for the fine propagator. For example, we can consider a three-stage explicit RKN integrator of order three

$$\begin{aligned}
&q_{n,0} = q_n, \quad \dot{q}_{n,0} = \dot{q}_n, \\
&F_{n,(m-1)\delta t,j} = F\bigg(q_{n,(m-1)\delta t} + \delta t c_j \dot{q}_{n,(m-1)\delta t} + \delta t^2 \sum_{k=1}^{j-1} \bar{a}_{jk} F_{n,(m-1)\delta t,k}\bigg), \quad j = 1,2,3, \\
&q_{n,m\delta t} = q_{n,(m-1)\delta t} + \delta t \dot{q}_{n,(m-1)\delta t} + \delta t^2 \sum_{j=1}^{3} \bar{b}_j F_{n,(m-1)\delta t,j}, \\
&\dot{q}_{n,m\delta t} = \dot{q}_{n,(m-1)\delta t} + \delta t \sum_{j=1}^{3} b_j F_{n,(m-1)\delta t,j}, \\
&q_{n+1} = q_{n,\Delta T}, \quad \dot{q}_{n+1} = \dot{q}_{n,\Delta T}
\end{aligned} \tag{2.9}$$

with

$$\begin{aligned}
&c_1 = 0, \quad c_2 = \frac{6-\sqrt{6}}{10}, \quad c_3 = \frac{6+\sqrt{6}}{10}, \\
&b_1 = \frac{c_2c_3\phi_1 - (c_2+c_3)\phi_2 + 2\phi_3}{c_2c_3}, \quad b_2 = \frac{c_3\phi_2 - 2\phi_3}{c_2c_3 - c_2^2}, \quad b_3 = \frac{c_2\phi_2 - 2\phi_3}{c_2c_3 - c_3^2}, \\
&\bar{b}_1 = \frac{c_2c_3\phi_2 - (c_2+c_3)\phi_3 + 2\phi_4}{c_2c_3}, \quad \bar{b}_2 = \frac{c_3\phi_3 - 2\phi_4}{c_2c_3 - c_2^2}, \quad \bar{b}_3 = \frac{c_2\phi_3 - 2\phi_4}{c_2c_3 - c_3^2}, \\
&\bar{a}_{21} = c_2^2\phi_2, \quad \bar{a}_{31} = c_3^2\phi_2 - \bar{a}_{32}, \quad \bar{a}_{32} = 0,
\end{aligned} \tag{2.10}$$

and $\phi_k = 1/k!$ for $k = 1,2,3,4$.

With these preparations, we are in the position to present the parareal-RKN algorithms for (1.3).

Definition 2.1. *Let $q_0^j = q_0$, $\dot{q}_0^j = \dot{q}_0$ for the iteration index $j = 0,1,2,\ldots$. Given a time interval ΔT. Choose a small time stepsize $0 < \delta t < 1$, and a large time stepsize $0 < \Delta t < 1$. The parareal-RKN algorithm for solving* (1.3) *is defined by*

$$\begin{aligned}
\big[q_{n+1}^{j+1}; \dot{q}_{n+1}^{j+1}\big] = {} & \mathcal{G}_{T_n+(\frac{\Delta T}{\Delta t}-1)\Delta t}^{T_n+\frac{\Delta T}{\Delta t}\Delta t} \circ \cdots \circ \mathcal{G}_{T_n+\Delta t}^{T_n+2\Delta t} \circ \mathcal{G}_{T_n}^{T_n+\Delta t}\big(\big[q_n^{j+1}; \dot{q}_n^{j+1}\big]\big) \\
& + \mathcal{F}_{T_n+(\frac{\Delta T}{\delta t}-1)\delta t}^{T_n+\frac{\Delta T}{\delta t}\delta t} \circ \cdots \circ \mathcal{F}_{T_n+\delta t}^{T_n+2\delta t} \circ \mathcal{F}_{T_n}^{T_n+\delta t}\big(\big[q_n^j; \dot{q}_n^j\big]\big) \\
& - \mathcal{G}_{T_n+(\frac{\Delta T}{\Delta t}-1)\Delta t}^{T_n+\frac{\Delta T}{\Delta t}\Delta t} \circ \cdots \circ \mathcal{G}_{T_n+\Delta t}^{T_n+2\Delta t} \circ \mathcal{G}_{T_n}^{T_n+\Delta t}\big(\big[q_n^j; \dot{q}_n^j\big]\big)
\end{aligned} \tag{2.11}$$

for $n = 0,1,\ldots,T/\Delta T$, where the coarse and fine propagators are given by (2.5) *and* (2.7)*, respectively. The initial guess $\{q_n^0\}_{n\geq 1}$ and $\{\dot{q}_n^0\}_{n\geq 1}$ are generated by the $\mathcal{G}$-propagator* (2.5).

2.2. Energy-preserving parareal-RKN algorithm

From the point of Hamiltonian system, it is well known that the energy (1.2) is exactly preserved by the solution of (1.3). This important property can also be kept by the numerical methods named as energy-preserving (EP) algorithms. However, it is a pity that the parareal-RKN algorithm (2.11) is not energy-preserving even EP algorithms are used for the coarse and fine propagators. To make the parareal-RKN algorithm (2.11) be energy-preserving, the technique of standard projection method [17, Chapter IV] is used in this paper and the procedure is stated blew.

Denote the energy-preserving manifold by

$$\mathcal{M} := \big\{[q;p] | g(q,p) := H(q,p) - H(q_0,p_0) = 0\big\}$$

and we project the results obtained from parareal-RKN algorithm (2.11) onto $\mathcal{M}$. More precisely, first assume that $[\tilde{q}_n^j; \dot{\tilde{q}}_n^j]$ and $[\tilde{q}_n^{j+1}; \dot{\tilde{q}}_n^{j+1}] \in \mathcal{M}$. Then using the parareal-RKN algorithm (2.11), one gets the result $[q_{n+1}^{j+1}; \dot{q}_{n+1}^{j+1}]$ from $[\tilde{q}_n^j; \dot{\tilde{q}}_n^j]$ and $[\tilde{q}_n^{j+1}; \dot{\tilde{q}}_n^{j+1}]$. Finally project the result $[q_{n+1}^{j+1}; \dot{q}_{n+1}^{j+1}]$ onto the manifold $\mathcal{M}$ to obtain $[\tilde{q}_{n+1}^{j+1}; \dot{\tilde{q}}_{n+1}^{j+1}] \in \mathcal{M}$, which is denoted by

$$\left[\tilde{q}_{n+1}^{j+1}; \dot{\tilde{q}}_{n+1}^{j+1}\right] = \pi_{\mathcal{M}} \left[q_{n+1}^{j+1}; \dot{q}_{n+1}^{j+1}\right]. \tag{2.12}$$

This procedure can be done in the whole parareal-RKN algorithm (2.11).

For the computation of $[\tilde{q}_{n+1}^{j+1}; \dot{\tilde{q}}_{n+1}^{j+1}]$ in (2.12), we have to solve the following constrained minimization problem:

$$\begin{aligned} &\left\| \left[\tilde{q}_{n+1}^{j+1}; \dot{\tilde{q}}_{n+1}^{j+1}\right] - \left[q_{n+1}^{j+1}; \dot{q}_{n+1}^{j+1}\right] \right\|_2 \to \min \\ &\text{s.t.} \quad g\left(\tilde{q}_{n+1}^{j+1}, \dot{\tilde{q}}_{n+1}^{j+1}\right) = 0. \end{aligned}$$

To this end, introduce the Lagrange multiplier λ and consider the Lagrange function

$$L\left(\left[\tilde{q}_{n+1}^{j+1}; \dot{\tilde{q}}_{n+1}^{j+1}\right], \lambda\right) = \frac{1}{2} \left\| \left[\tilde{q}_{n+1}^{j+1}; \dot{\tilde{q}}_{n+1}^{j+1}\right] - \left[q_{n+1}^{j+1}; \dot{q}_{n+1}^{j+1}\right] \right\|_2^2 - \lambda g\left(\tilde{q}_{n+1}^{j+1}, \dot{\tilde{q}}_{n+1}^{j+1}\right).$$

From the necessary condition $\partial L / \partial [\tilde{q}_{n+1}^{j+1}; \dot{\tilde{q}}_{n+1}^{j+1}] = 0$, it follows that

$$\tilde{q}_{n+1}^{j+1} = q_{n+1}^{j+1} - \lambda F\left(q_{n+1}^{j+1}\right), \tag{2.13a}$$

$$\dot{\tilde{q}}_{n+1}^{j+1} = \dot{q}_{n+1}^{j+1} + \lambda \dot{q}_{n+1}^{j+1}, \tag{2.13b}$$

$$g\left(\tilde{q}_{n+1}^{j+1}, \dot{\tilde{q}}_{n+1}^{j+1}\right) = 0. \tag{2.13c}$$

To save some evaluations, it is noted that in the above derivations $\tilde{q}_{n+1}^{j+1}$ and $\dot{\tilde{q}}_{n+1}^{j+1}$ are replaced by q_{n+1}^{j+1} and $\dot{q}_{n+1}^{j+1}$, respectively. By inserting Egs. (2.13a) and (2.13b) into (2.13c), a nonlinear system for λ is obtained and the following simplified Newton iteration is considered here:

$$
\begin{aligned}
\lambda_{k+1} &= \lambda_k + \triangle\lambda_k g\left(q_{n+1}^{j+1} - \lambda_k F(q_{n+1}^{j+1}), \dot{q}_{n+1}^{j+1} + \lambda_k \dot{q}_{n+1}^{j+1}\right),\\
\triangle\lambda_k &= -\left(\frac{d}{d\lambda} g\left(q_{n+1}^{j+1} - \lambda F\left(q_{n+1}^{j+1}\right), \dot{q}_{n+1}^{j+1} + \lambda \dot{q}_{n+1}^{j+1}\right)|_{\lambda=0}\right)^{-1}\\
&= -\left(\left(\dot{q}_{n+1}^{j+1}\right)^{\intercal}\left(\dot{q}_{n+1}^{j+1}\right) + \left(F\left(q_{n+1}^{j+1}\right)\right)^{\intercal}\left(F\left(q_{n+1}^{j+1}\right)\right)\right)^{-1}.
\end{aligned}
$$

The details of the projection method $\pi_{\mathcal{M}}$ are given in Algorithm 2.1.

Algorithm 2.1 Projection Method $[\tilde{q}_{n+1}^{j+1}; \dot{\tilde{q}}_{n+1}^{j+1}] = \pi_{\mathcal{M}}[q_{n+1}^{j+1}; \dot{q}_{n+1}^{j+1}]$.

Set $\lambda := 0$.
Set $A := -F(q_{n+1}^{j+1}),\ B := -(A^{\intercal}A + (\dot{q}_{n+1}^{j+1})^{\intercal}(\dot{q}_{n+1}^{j+1}))^{-1}$.
Set $\Delta\lambda := Bg(q_{n+1}^{j+1}, \dot{q}_{n+1}^{j+1})$.
while $|\Delta\lambda| \geq$ Tol **do**
    Set $\lambda := \lambda + \Delta\lambda$.
    Set $\Delta\lambda := Bg(q_{n+1}^{j+1} + \lambda A, \dot{q}_{n+1}^{j+1} + \lambda\dot{q}_{n+1}^{j+1})$.
end while
Set $\tilde{q}_{n+1}^{j+1} := q_{n+1}^{j+1} + \lambda A$.
Set $\dot{\tilde{q}}_{n+1}^{j+1} := \dot{q}_{n+1}^{j+1} + \lambda\dot{q}_{n+1}^{j+1}$.

On the basis of the above derivations, we are in a position to present the energy-preserving parareal-RKN (EPPRKN) algorithm whose details are given in the following definition.

Definition 2.2. *Generate the initial guess* $\{q_n^0\}_{n\geq 1}$ *and* $\{\dot{q}_n^0\}_{n\geq 1}$ *by the* $\mathcal{G}$*-propagator* (2.5) *and then with Algorithm* 2.1*, we get* $[\tilde{q}_n^0; \dot{\tilde{q}}_n^0] = \pi_{\mathcal{M}}[q_n^0; \dot{q}_n^0]$*. Denote* $\tilde{q}_0^j = q_0,\ \dot{\tilde{q}}_0^j = \dot{q}_0$ *for the iteration index* $j = 0, 1, 2, \ldots$*. The energy-preserving parareal-RKN (EPPRKN) algorithm for* (1.3) *is defined by*

$$
\begin{aligned}
\left[q_{n+1}^{j+1}; \dot{q}_{n+1}^{j+1}\right] &= \mathcal{G}_{T_n+(\frac{\Delta T}{\Delta t}-1)\Delta t}^{T_n+\frac{\Delta T}{\Delta t}\Delta t} \circ \cdots \circ \mathcal{G}_{T_n+\Delta t}^{T_n+2\Delta t} \circ \mathcal{G}_{T_n}^{T_n+\Delta t}\left([\tilde{q}_n^{j+1}; \dot{\tilde{q}}_n^{j+1}]\right)\\
&\quad + \mathcal{F}_{T_n+(\frac{\Delta T}{\delta t}-1)\delta t}^{T_n+\frac{\Delta T}{\delta t}\delta t} \circ \cdots \circ \mathcal{F}_{T_n+\delta t}^{T_n+2\delta t} \circ \mathcal{F}_{T_n}^{T_n+\delta t}\left([\tilde{q}_n^{j}; \dot{\tilde{q}}_n^{j}]\right)\\
&\quad - \mathcal{G}_{T_n+(\frac{\Delta T}{\Delta t}-1)\Delta t}^{T_n+\frac{\Delta T}{\Delta t}\Delta t} \circ \cdots \circ \mathcal{G}_{T_n+\Delta t}^{T_n+2\Delta t} \circ \mathcal{G}_{T_n}^{T_n+\Delta t}\left([\tilde{q}_n^{j}; \dot{\tilde{q}}_n^{j}]\right),\\
\left[\tilde{q}_{n+1}^{j+1}; \dot{\tilde{q}}_{n+1}^{j+1}\right] &= \pi_{\mathcal{M}}\left[q_{n+1}^{j+1}; \dot{q}_{n+1}^{j+1}\right]
\end{aligned}
\tag{2.14}
$$

for $n = 0, 1, \ldots, T/\Delta T$*, where the coarse and fine propagators are given by* (2.5) *with* Δt *and* (2.7) *with* δt*, respectively.*

The parareal algorithm using the integrator (2.8) as the fine and coarse propagators is denoted by EPPRKN2. Replacing the propagator of EPPRKN2 by the third order RKN integrator (2.10) yields another parareal which is referred to EPPRKN3. If (2.10) is considered as the coarse propagator and (2.8) is for the fine one, the third parareal is obtained which is denoted by EPPRKN2-3.

3. Energy conservation and error bounds

3.1. The main results

In the light of the projection process, we get the following energy preservation immediately.

Theorem 3.1 (Energy Preservation). *For the numerical result* $[\tilde{q}_n^j, \dot{\tilde{q}}_n^j]$ *produced by* (2.14)*, it exactly preserves the energy* (1.2) *of the Hamiltonian system* (1.1)*, i.e.,*

$$H\big(\tilde{q}_n^j, \dot{\tilde{q}}_n^j\big) \equiv H(q_0, \dot{q}_0) \quad \textit{for any} \quad j = 0, 1, \ldots, \quad \textit{and any} \quad n = 0, 1, \ldots, T/\Delta T.$$

The next theorem is devoted to the convergence of the EPPRKN algorithms given in Definition 2.2.

Theorem 3.2 (Convergence Result). *Denote the solution of* (1.3) *by the propagator* $\mathcal{E}$*, i.e.,*

$$[q(t), \dot{q}(t)] = \mathcal{E}_0^t[q(0), \dot{q}(0)].$$

It is assumed that there exists a constant $C_1 > 0$ *such that*

$$\big\|\mathcal{E}_0^t[q(0), \dot{q}(0)]\big\|_2 \le C_1 \big\|[q(0), \dot{q}(0)]\big\|_2, \quad t \in [0, T]. \tag{3.1}$$

Moreover, let F *be locally Lipschitz-continuous. Choose* $\Delta T = \Delta t$ *in the EPPRKN algorithms, and then the global errors of the proposed methods are given by*

$$\begin{aligned} &\textit{EPPRKN2}: && \|\tilde{q}_n^j - q(t_n)\|_2 + \|\dot{\tilde{q}}_n^j - \dot{q}(t_n)\|_2 \le C\big(\Delta t^{2j+2} + \delta t^2\big)\big(1 + \|[q_0; \dot{q}_0]\|_2\big), \\ &\textit{EPPRKN3}: && \|\tilde{q}_n^j - q(t_n)\|_2 + \|\dot{\tilde{q}}_n^j - \dot{q}(t_n)\|_2 \le C\big(\Delta t^{3j+3} + \delta t^3\big)\big(1 + \|[q_0; \dot{q}_0]\|_2\big), \\ &\textit{EPPRKN2-3}: && \|\tilde{q}_n^j - q(t_n)\|_2 + \|\dot{\tilde{q}}_n^j - \dot{q}(t_n)\|_2 \le C\big(\Delta t^{2j+2} + \delta t^3\big)\big(1 + \|[q_0; \dot{q}_0]\|_2\big), \end{aligned} \tag{3.2}$$

where $0 < t_n := n\Delta t \le T$ *and* $j = 0, 1, \ldots$. *Here* C *is a generic constant independent of* $\Delta t, \delta t$ *or* n, j *but depends on* T, C_1 *and the bounds of the first- and second-order partial derivative of* F *with respect to* q.

Remark 3.1. From these two theorems, it can be seen that the EPPRKN algorithms not only exactly preserve the energy of the considered Hamiltonian system but also have good convergence. Meanwhile, it can also be observed from the proof that the convergence presented above also holds for the algorithms without projection.

3.2. The proof of Theorem 3.2

The proof is presented for the algorithm EPPRKN2 and it can be easily modified for the other two algorithms which is skipped for brevity. To prove the convergence, we firstly need to study the stability and boundedness of the propagators. Then based on the results, the global errors will be derived.

3.2.1. Stability of the propagators

We firstly pay attention to the coarse propagator (2.4). From the scheme (2.4), it follows that

$$
\begin{aligned}
&\mathcal{G}_{T_n}^{T_n+\Delta t}([q;\dot q]) - \mathcal{G}_{T_n}^{T_n+\Delta t}\big([\tilde q;\dot{\tilde q}]\big)\\
&= \begin{pmatrix} 1 & \Delta t \\ 0 & 1 \end{pmatrix}\big([q;\dot q]-[\tilde q;\dot{\tilde q}]\big)\\
&\quad + \Delta t \begin{pmatrix} \Delta t\bar b_1\big(F(q+\Delta t c_1\dot q)-F(\tilde q+\Delta t c_1\dot{\tilde q})\big) \\ b_1\big(F(q+\Delta t c_1\dot q)-F(\tilde q+\Delta t c_1\dot{\tilde q})\big) \end{pmatrix}\\
&= \big([q;\dot q]-[\tilde q;\dot{\tilde q}]\big) + \Delta t \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\big([q;\dot q]-[\tilde q;\dot{\tilde q}]\big)\\
&\quad + \Delta t \begin{pmatrix} \Delta t\bar b_1\big(F(q+\Delta t c_1\dot q)-F(\tilde q+\Delta t c_1\dot{\tilde q})\big) \\ b_1\big(F(q+\Delta t c_1\dot q)-F(\tilde q+\Delta t c_1\dot{\tilde q})\big) \end{pmatrix}.
\end{aligned}
$$

Considering the Lipschitz condition of F, we get

$$
\big\|F\big(q+\Delta t c_1\dot q\big)-F\big(\tilde q+\Delta t c_1\dot{\tilde q}\big)\big\|_2 \le L\big(\|q-\tilde q\|_2+\Delta t\|\dot q-\dot{\tilde q}\|_2\big),
$$

and further have

$$
\begin{aligned}
&\Big\|\mathcal{G}_{T_n}^{T_n+\Delta t}([q;\dot q]) - \mathcal{G}_{T_n}^{T_n+\Delta t}([\tilde q;\dot{\tilde q}])\Big\|_2\\
&\le (1+C\Delta t)\,\big\|[q;\dot q]-[\tilde q;\dot{\tilde q}]\big\|_2 + (\Delta t^2+\Delta t)L\big(\,\|q-\tilde q\|_2+\Delta t\|\dot q-\dot{\tilde q}\|_2\big)\\
&\le (1+C\Delta t)\,\big\|[q;\dot q]-[\tilde q;\dot{\tilde q}]\big\|_2 + 2(\Delta t^2+\Delta t)L\,\big\|[q;\dot q]-[\tilde q;\dot{\tilde q}]\big\|_2 .
\end{aligned}
$$

This immediately shows that for all $0<n\Delta t\le T$

$$
\Big\|\mathcal{G}_{T_n}^{T_n+\Delta t}([q;\dot q]) - \mathcal{G}_{T_n}^{T_n+\Delta t}([\tilde q;\dot{\tilde q}])\Big\|_2 \le \big(1+C\Delta t+C\Delta t^2\big)\,\big\|[q;\dot q]-[\tilde q;\dot{\tilde q}]\big\|_2, \tag{3.3}
$$

and similarly

$$
\Big\|\mathcal{F}_{T_n}^{T_n+\delta t}([q;\dot q]) - \mathcal{F}_{T_n}^{T_n+\delta t}([\tilde q;\dot{\tilde q}])\Big\|_2 \le \big(1+C\delta t+C\delta t^2\big)\,\big\|[q;\dot q]-[\tilde q;\dot{\tilde q}]\big\|_2 .
$$

The propagator $\mathcal{G}$ after many integrations are deduced as

$$
\begin{aligned}
&\Big\|\mathcal{G}_{T_n+(l-1)\Delta t}^{T_n+m\Delta t}\circ\cdots\circ\mathcal{G}_{T_n}^{T_n+\Delta t}([q;\dot q]) - \mathcal{G}_{T_n+(l-1)\Delta t}^{T_n+m\Delta t}\circ\cdots\circ\mathcal{G}_{T_n}^{T_n+\Delta t}([\tilde q;\dot{\tilde q}])\Big\|_2\\
&\le \big(1+C\Delta t+C\Delta t^2\big)^m\,\big\|[q;\dot q]-[\tilde q;\dot{\tilde q}]\big\|_2\\
&\le \bigg(1+\big(C\Delta t+C\Delta t^2\big)\frac{\Delta T}{\Delta t}+\mathcal{O}(\Delta t)\bigg)\,\big\|[q;\dot q]-[\tilde q;\dot{\tilde q}]\big\|_2\\
&\le C\,\big\|[q;\dot q]-[\tilde q;\dot{\tilde q}]\big\|_2, \quad m=\frac{\Delta T}{\Delta t}>1.
\end{aligned}
$$

In a same way, one gets

$$
\begin{aligned}
&\Big\|\mathcal{F}_{T_n+(m-1)\delta t}^{T_n+m\delta t}\circ\cdots\circ\mathcal{F}_{T_n}^{T_n+\delta t}([q;\dot q]) - \mathcal{F}_{T_n+(m-1)\delta t}^{T_n+m\delta t}\circ\cdots\circ\mathcal{F}_{T_n}^{T_n+\delta t}([\tilde q;\dot{\tilde q}])\Big\|_2\\
&\le C\,\big\|[q;\dot q]-[\tilde q;\dot{\tilde q}]\big\|_2, \quad m=\frac{\Delta T}{\delta t}>1.
\end{aligned} \tag{3.4}
$$

3.2.2. Local errors and boundedness of the propagators

Define the local errors of propagators

$$\begin{aligned} e^{\mathcal{G}}_{n,m}([q;\dot q]) &= \mathcal{G}^{T_n+m\Delta t}_{T_n+(m-1)\Delta t}\circ\cdots\circ\mathcal{G}^{T_n+2\Delta t}_{T_n+\Delta t}\circ\mathcal{G}^{T_n+\Delta t}_{T_n}([q;\dot q]) - \mathcal{E}^{T_n+m\Delta t}_{T_n}([q;\dot q]),\\ e^{\mathcal{F}}_{n,m}([q;\dot q]) &= \mathcal{F}^{T_n+m\delta t}_{T_n+(m-1)\delta t}\circ\cdots\circ\mathcal{F}^{T_n+2\delta t}_{T_n+\delta t}\circ\mathcal{F}^{T_n+\delta t}_{T_n}([q;\dot q]) - \mathcal{E}^{T_n+m\delta t}_{T_n}([q;\dot q]), \end{aligned}$$

and in what follows we study the stability of these errors.

We start with $e^{\mathcal{G}}_{n,1}([q;\dot q])$ and it can be expressed as

$$e^{\mathcal{G}}_{n,1}([q;\dot q]) = \begin{pmatrix} \Delta t^2\bar b_1\hat F_{n,c_1} - \Delta t^2\displaystyle\int_0^1(1-z)\hat F(T_n+\Delta tz)dz \\ \Delta t b_1\hat F_{n,c_1} - \Delta t\displaystyle\int_0^1\hat F(T_n+\Delta tz)dz \end{pmatrix},$$

where

$$\begin{aligned} \hat F_{n,c_1} &= F\big(q(T_n)+\Delta tc_1\dot q(T_n)\big),\\ \hat F(T_n+\Delta tz) &= F\big(q(T_n+\Delta tz)\big). \end{aligned}$$

By the variation-of-constants formula (2.2), we have

$$q(T_n+c_1\Delta t) = q(T_n)+\Delta tc_1\dot q(T_n)+\Delta t^2\int_0^1(1-z)\hat F(T_n+c_1\Delta tz)dz.$$

Then it is deduced that $e^{\mathcal{G}}_{n,1}([q;\dot q]) = [q_1^\intercal, q_2^\intercal]^\intercal$ with

$$\begin{aligned} q_1 &= \Delta t^2\bar b_1\hat F(T_n+c_1\Delta t) - \Delta t^2\int_0^1(1-z)\hat F(T_n+\Delta tz)dz + \Delta t^4\bar b_1\Lambda,\\ q_2 &= \Delta tb_1\hat F(T_n+c_1\Delta t) - \Delta t\int_0^1\hat F(T_n+\Delta tz)dz + \Delta t^3 b_1\Lambda,\\ \Lambda &= \partial_2F\big(q(T_n)+\Delta tc_1\dot q(T_n)+\theta(T_n+c_1\Delta t)\big)\int_0^1(1-z)\hat F(T_n+c_1\Delta tz)dz, \quad 0\le\theta\le 1. \end{aligned}$$

By some computations, it is obtained that

$$\begin{aligned} X_1 &= \Delta t^2\left(\bar b_1-\frac12\right)\hat F(T_n) + c_1\Delta t^3\varepsilon^2\bar b_1\hat F'\big(T_n+\theta_1^{X_1}c_1\Delta t\big)\\ &\quad - \Delta t^3\int_0^1 z(1-z)\hat F'\big(T_n+\theta_2^{X_1}\Delta tz\big)dz + \Delta t^4\bar b_1\Lambda,\\ X_2 &= \Delta t(b_1-1)\hat F(T_n) + \Delta t^2\left(c_1b_1-\frac12\right)\hat F'(T_n)\\ &\quad + c_1\Delta t^3 b_1\hat F''\big(T_n+\theta_1^{X_2}c_1\Delta t\big)\\ &\quad - \Delta t^3\int_0^1 z\hat F''\big(T_n+\theta_2^{X_2}\Delta tz\big)dz + \Delta t^3 b_1\Lambda, \end{aligned}$$

where $\theta_1^{X_1}, \theta_2^{X_1}, \theta_1^{X_2}, \theta_2^{X_2} \in [0,1]$. With the above results and on noticing the fact that

$$\frac{1}{2} - \bar{b}_1 = 0, \quad 1 - b_1 = 0, \quad \frac{1}{2} - c_1 b_1 = 0,$$

we obtain that

$$\left\| e_{n,1}^{\mathcal{G}}([q;\dot{q}]) \right\|_2 \le C\Delta t^3 \left\| [q;\dot{q}] \right\|_2.$$

Using the same arguments leads to

$$\left\| e_{n,1}^{\mathcal{G}}([q;\dot{q}]) - e_{n,1}^{\mathcal{G}}([\tilde{q};\dot{\tilde{q}}]) \right\|_2 \le C\Delta t^3 \left\| [q;\dot{q}] - [\tilde{q};\dot{\tilde{q}}] \right\|_2. \tag{3.5}$$

Similarly, we derive

$$\left\| e_{n,1}^{\mathcal{F}}([q;\dot{q}]) - e_{n,1}^{\mathcal{F}}([\tilde{q};\dot{\tilde{q}}]) \right\|_2 \le C\delta t^3 \left\| [q;\dot{q}] - [\tilde{q};\dot{\tilde{q}}] \right\|_2.$$

Now we concentrate on the $e_{n,m}^{\mathcal{G}}$ which has the decomposition

$$\begin{aligned} e_{n,m}^{\mathcal{G}} &= \mathcal{G}_{T_n+(m-1)\Delta t}^{T_n+m\Delta t} \circ \cdots \circ \mathcal{G}_{T_n+\Delta t}^{T_n+2\Delta t} \circ \mathcal{G}_{T_n}^{T_n+\Delta t} - \mathcal{E}_{T_n}^{T_n+m\Delta t} \\ &= \sum_{l=1}^{m} \left[\mathcal{E}_{T_n}^{T_n+(m-l)\Delta t} \circ \left(\mathcal{G}_{T_n}^{T_n+\Delta t} - \mathcal{E}_{T_n}^{T_n+\Delta t} \right) \circ \left(\mathcal{G}_{T_n+(l-1)\Delta t}^{T_n+m\Delta t} \circ \cdots \circ \mathcal{G}_{T_n}^{T_n+\Delta t} \right) \right] \\ &= \sum_{l=1}^{m} \left[\mathcal{E}_{T_n}^{T_n+(m-l)\Delta t} \circ e_{n,1}^{\mathcal{G}} \circ \left(\mathcal{G}_{T_n+(l-1)\Delta t}^{T_n+m\Delta t} \circ \cdots \circ \mathcal{G}_{T_n}^{T_n+\Delta t} \right) \right]. \end{aligned}$$

With this result, we obtain

$$\begin{aligned} &\left\| e_{n,m}^{\mathcal{G}}([q;\dot{q}]) - e_{n,m}^{\mathcal{G}}([\tilde{q};\dot{\tilde{q}}]) \right\|_2 \\ \le\, & C\Delta t^3 \sum_{l=1}^{m} \left\| \mathcal{G}_{T_n+(l-1)\Delta t}^{T_n+m\Delta t} \circ \cdots \circ \mathcal{G}_{T_n}^{T_n+\Delta t}([q;\dot{q}]) - \mathcal{G}_{T_n+(l-1)\Delta t}^{T_n+m\Delta t} \circ \cdots \circ \mathcal{G}_{T_n}^{T_n+\Delta t})([\tilde{q};\dot{\tilde{q}}]) \right\|_2 \\ \le\, & C\Delta t^3 m \left\| [q;\dot{q}] - [\tilde{q};\dot{\tilde{q}}] \right\|_2 \le C\Delta T \Delta t^2 \left\| [q;\dot{q}] - [\tilde{q};\dot{\tilde{q}}] \right\|_2, \quad m = \frac{\Delta T}{\Delta t}. \end{aligned} \tag{3.6}$$

Similar result holds for the propagator $\mathcal{F}$

$$\left\| e_{n,m}^{\mathcal{F}}([q;\dot{q}]) - e_{n,m}^{\mathcal{F}}([\tilde{q};\dot{\tilde{q}}]) \right\|_2 \le C\Delta T \delta t^2 \left\| [q;\dot{q}] - [\tilde{q};\dot{\tilde{q}}] \right\|_2, \quad m = \frac{\Delta T}{\delta t}. \tag{3.7}$$

Based on these results, we can find the boundedness of the coarse and fine propagators which is shown below. Letting $[\tilde{q};\dot{\tilde{q}}] = [0;0]$ and $[q;\dot{q}] = [q_{n,0};\dot{q}_{n,0}]$ gives

$$\begin{aligned} &\left\| \mathcal{G}_{T_n+(m-1)\Delta t}^{T_n+m\Delta t} \circ \cdots \circ \mathcal{G}_{T_n+\Delta t}^{T_n+2\Delta t} \circ \mathcal{G}_{T_n}^{T_n+\Delta t}([q_{n,0};\dot{q}_{n,0}]) - \mathcal{E}_{T_n}^{T_n+m\Delta t}([q_{n,0};\dot{q}_{n,0}]) \right\|_2 \\ \le\, & C\Delta T \Delta t^2 \left\| [q_{n,0};\dot{q}_{n,0}] \right\|_2. \end{aligned}$$

Combing the above result and the boundedness of $\mathcal{E}$ presented in (3.1), one gets the following estimate:

$$\begin{aligned}&\Big\|\mathcal{G}_{T_n+(m-1)\Delta t}^{T_n+m\Delta t}\circ\cdots\circ\mathcal{G}_{T_n+\Delta t}^{T_n+2\Delta t}\circ\mathcal{G}_{T_n}^{T_n+\Delta t}([q_{n,0},\dot{q}_{n,0}])\Big\|_2\\ &\leq C\|[q_{n,0},\dot{q}_{n,0}]\|_2,\quad m=\frac{\Delta T}{\Delta t}.\end{aligned}\tag{3.8}$$

In a similar way, the propagator $\mathcal{F}$ is bounded by

$$\begin{aligned}&\Big\|\mathcal{F}_{T_n+(m-1)\delta t}^{T_n+m\delta t}\circ\cdots\circ\mathcal{F}_{T_n+\delta t}^{T_n+2\delta t}\circ\mathcal{F}_{T_n}^{T_n+\delta t}([q_{n,0},\dot{q}_{n,0}])\Big\|_2\\ &\leq C\left\|[q_{n,0},\dot{q}_{n,0}]\right\|_2,\quad m=\frac{\Delta T}{\delta t}.\end{aligned}\tag{3.9}$$

3.2.3. Global errors

This part is devoted to the parareal-RKN algorithm (2.11) without using the projection method Algorithm 2.1. It is noted that the stepsize of the coarse propagator is chosen as $\Delta t=\Delta T$ and we show by induction over $j\geq 0$ that

$$\big\|[q_n^j;\dot{q}_n^j]-[q(T_n);\dot{q}(T_n)]\big\|_2\leq C\big(\Delta t^{2j+2}+\delta t^2\big)\big(1+\|[q_0;\dot{q}_0]\|_2\big).\tag{3.10}$$

We first consider $j=0$ and in this case, one needs to derive the global errors for the $\mathcal{G}$-propagator which generates the values $\{[q_n^0;\dot{q}_n^0]\}_{n\geq 1}$. Denote errors of the $\mathcal{G}$-propagator by

$$e_n=q(T_n)-q_n^0,\quad \dot{e}_n=\dot{q}(T_n)-\dot{q}_n^0,\quad E_n=q\big(t_n+c_1\Delta t\big)-\big(q_n^0+\Delta t c_1\dot{q}_n^0\big).$$

According to the scheme (2.4) of the $\mathcal{G}$-propagator and the variation-of-constants formula (2.2), it is easy to have the error equations

$$\begin{aligned}E_n&=e_n+c_1\Delta t\dot{e}_n^q+\hat{\Delta}_{n1},\\ e_{n+1}&=e_n+\Delta t\dot{e}_n^q+\Delta t^2\bar{b}_1\left(F\big(q(t_n+c_1\Delta t)\big)-F_{n,\Delta t}^0\right)+\hat{\delta}_{n+1},\\ \dot{e}_{n+1}&=\dot{e}_n+\Delta t b_1\left(F\big(q(t_n+c_1\Delta t)\big)-F_{n,\Delta t}^0\right)+\hat{\delta}'_{n+1}\end{aligned}\tag{3.11}$$

with $t_n=n\Delta t$, $F_{n,\Delta t}^0=F(q_n^0+\Delta t c_1\dot{q}_n^0)$, the initial values $e_0=0,\dot{e}_0=0$ and the local errors

$$\|\hat{\Delta}_{n1}\|_2\leq C\Delta t^2,\quad \|\hat{\delta}_{n+1}\|_2\leq C\Delta t^3,\quad \|\hat{\delta}'_{n+1}\|_2\leq C\Delta t^3,\tag{3.12}$$

which are derived in the same way as (3.5).

The last two formulae of (3.11) immediately imply

$$\begin{aligned}&\|e_{n+1}\|_2\leq\|e_n\|_2+\Delta t\|\dot{e}_n\|_2+\Delta t^2\big\|F\big(q(t_n+c_1\Delta t)\big)-F_{n,\Delta t}^0\big\|_2+\|\hat{\delta}_{n+1}\|_2,\\ &\|\dot{e}_{n+1}\|_2\leq\|\dot{e}_n\|_2+\Delta t\big\|F\big(q(t_n+c_1\Delta t)\big)-F_{n,\Delta t}^0\big\|_2+\|\hat{\delta}'_{n+1}\|_2.\end{aligned}$$

Combining these two results, it is arrived that

$$\begin{aligned}\|e_{n+1}\|_2+\|\dot{e}_{n+1}\|_2\le\ &\|e_n\|_2+\|\dot{e}_n\|_2+\Delta t\|\dot{e}_n\|_2+\Delta t(1+\Delta t)C\|E_n\|_2\\ &+\|\hat{\delta}_{n+1}\|_2+\|\hat{\delta}'_{n+1}\|_2.\end{aligned}\tag{3.13}$$

Meanwhile, from the first formula of (3.11) it follows that

$$\|E_n\|_2\le\|e_n\|_2+c_1\Delta t\|\dot{e}_n\|_2+\|\hat{\Delta}_{n1}\|_2.\tag{3.14}$$

Inserting (3.14) into (3.13) gives

$$\begin{aligned}\|e_{n+1}\|_2+\|\dot{e}_{n+1}\|_2\le\ &\|e_n\|_2+\|\dot{e}_n\|_2+\Delta t\|\dot{e}_n\|_2\\ &+\Delta t(1+\Delta t)C\big(\|e_n\|_2+c_1\Delta t\|\dot{e}_n\|_2+\|\hat{\Delta}_{n1}\|_2\big)\\ &+\|\hat{\delta}_{n+1}\|_2+\|\hat{\delta}'_{n+1}\|_2,\end{aligned}$$

which can be simplified as

$$\begin{aligned}\|e_{n+1}\|_2+\|\dot{e}_{n+1}\|_2\le\ &\big(1+\Delta t(1+(1+\Delta t)C)\big)\big(\|e_n\|_2+\|\dot{e}_n\|_2\big)\\ &+\|\hat{\delta}_{n+1}\|_2+\|\hat{\delta}'_{n+1}\|_2+\Delta t(1+\Delta t)C\|\hat{\Delta}_{n1}\|_2.\end{aligned}\tag{3.15}$$

By the local error bounds (3.12), there holds

$$\|\hat{\delta}_{n+1}\|_2+\|\hat{\delta}_{n+1}\|_2+\Delta t(1+\Delta t)C\|\hat{\Delta}_{n1}\|_2\le C\Delta t^3.$$

Using the Gronwall inequality, we find that

$$\|e_{n+1}\|_2+\|\dot{e}_{n+1}\|_2\le\exp\big(n\Delta t(1+(1+\Delta t)C)\big)Cn\Delta t^3,$$

which proves (3.10) for $j=0$.

In what follows, we prove the result (3.10) for $j+1$ under the assumption that (3.10) is true for j. With the previous preparations, the errors can be expressed as

$$\begin{aligned}&\big[q_{n+1}^{j+1};\dot{q}_{n+1}^{j+1}\big]-\big[q(T_{n+1});\dot{q}(T_{n+1})\big]\\ &=\mathcal{G}_{T_n}^{T_{n+1}}\big(\big[q_n^{j+1};\dot{q}_n^{j+1}\big]\big)+\mathcal{F}_{T_n}^{T_{n+1}}\big(\big[q_n^j;\dot{q}_n^j\big]\big)\\ &\quad-\mathcal{G}_{T_n}^{T_{n+1}}\big(\big[q_n^j;\dot{q}_n^j\big]\big)-\mathcal{E}_{T_n}^{T_{n+1}}\big(\,[q(T_n);\dot{q}(T_n)]\,\big)\end{aligned}$$

with the notations

$$\begin{aligned}\mathcal{G}_{T_n}^{T_{n+1}}&:=\mathcal{G}_{T_n+(m-1)\Delta t}^{T_n+m\Delta t}\circ\cdots\circ\mathcal{G}_{T_n+\Delta t}^{T_n+2\Delta t}\circ\mathcal{G}_{T_n}^{T_n+\Delta t},\quad m=\frac{\Delta T}{\Delta t},\\ \mathcal{F}_{T_n}^{T_{n+1}}&:=\mathcal{F}_{T_n+(m-1)\delta t}^{T_n+m\delta t}\circ\cdots\circ\mathcal{F}_{T_n+\delta t}^{T_n+2\delta t}\circ\mathcal{F}_{T_n}^{T_n+\delta t},\quad m=\frac{\Delta T}{\delta t}.\end{aligned}$$

The above expression can be further split as

$$\begin{aligned}&\big[q_{n+1}^{j+1};\dot{q}_{n+1}^{j+1}\big]-\big[q(T_{n+1});\dot{q}(T_{n+1})\big]\\ &=\mathcal{G}_{T_n}^{T_{n+1}}\big(\big[q_n^{j+1};\dot{q}_n^{j+1}\big]\big)-\mathcal{G}_{T_n}^{T_{n+1}}\big(\,[q(T_n);\dot{q}(T_n)]\,\big)\end{aligned}$$

$$
\begin{aligned}
&+\left(\mathcal{E}_{T_n}^{T_{n+1}}-\mathcal{G}_{T_n}^{T_{n+1}}\right)\left(\left[q_n^j;\dot{q}_n^j\right]\right)-\left(\mathcal{E}_{T_n}^{T_{n+1}}-\mathcal{G}_{T_n}^{T_{n+1}}\right)\left(\left[q(T_n);\dot{q}(T_n)\right]\right)\\
&-\left(\mathcal{E}_{T_n}^{T_{n+1}}-\mathcal{F}_{T_n}^{T_{n+1}}\right)\left(\left[q_n^j;\dot{q}_n^j\right]\right)+\left(\mathcal{E}_{T_n}^{T_{n+1}}-\mathcal{F}_{T_n}^{T_{n+1}}\right)\left(\left[q(T_n);\dot{q}(T_n)\right]\right)\\
&-\left(\mathcal{E}_{T_n}^{T_{n+1}}-\mathcal{F}_{T_n}^{T_{n+1}}\right)\left(\left[q(T_n);\dot{q}(T_n)\right]\right)\\
=\;&\mathcal{G}_{T_n}^{T_{n+1}}\left(\left[q_n^{j+1};\dot{q}_n^{j+1}\right]\right)-\mathcal{G}_{T_n}^{T_{n+1}}\left(\left[q(T_n);\dot{q}(T_n)\right]\right)-e^{\mathcal{G}}_{n,\frac{\Delta T}{\Delta t}}\left(\left[q_n^j;\dot{q}_n^j\right]\right)\\
&+e^{\mathcal{G}}_{n,\frac{\Delta T}{\Delta t}}\left(\left[q(T_n);\dot{q}(T_n)\right]\right)+e^{\mathcal{F}}_{n,\frac{\Delta T}{\delta t}}\left(\left[q_n^j;\dot{q}_n^j\right]\right)\\
&-e^{\mathcal{F}}_{n,\frac{\Delta T}{\delta t}}\left(\left[q(T_n);\dot{q}(T_n)\right]\right)+e^{\mathcal{F}}_{n,\frac{\Delta T}{\delta t}}\left(\left[q(T_n);\dot{q}(T_n)\right]\right).
\end{aligned}
$$

With the stability and boundedness derived above, we could obtain

$$
\begin{aligned}
&\left\|\left[q_{n+1}^{j+1};\dot{q}_{n+1}^{j+1}\right]-\left[q(T_{n+1});\dot{q}(T_{n+1})\right]\right\|_2\\
\leq\;&\left\|\mathcal{G}_{T_n}^{T_{n+1}}\left(\left[q_n^{j+1};\dot{q}_n^{j+1}\right]\right)-\mathcal{G}_{T_n}^{T_{n+1}}\left(\left[q(T_n);\dot{q}(T_n)\right]\right)\right\|_2\\
&+\left\|e^{\mathcal{G}}_{n,\frac{\Delta T}{\Delta t}}\left(\left[q_n^j;\dot{q}_n^j\right]\right)-e^{\mathcal{G}}_{n,\frac{\Delta T}{\Delta t}}\left(\left[q(T_n);\dot{q}(T_n)\right]\right)\right\|_2\\
&+\left\|e^{\mathcal{F}}_{n,\frac{\Delta T}{\delta t}}\left(\left[q_n^j;\dot{q}_n^j\right]\right)-e^{\mathcal{F}}_{n,\frac{\Delta T}{\delta t}}\left(\left[q(T_n);\dot{q}(T_n)\right]\right)\right\|_2\\
&+\left\|e^{\mathcal{F}}_{n,\frac{\Delta T}{\delta t}}\left(\left[q(T_n);\dot{q}(T_n)\right]\right)\right\|_2\\
\leq\;&(1+C\Delta t)\left\|\left[q_n^{j+1};\dot{q}_n^{j+1}\right]-\left[q(T_n);\dot{q}(T_n)\right]\right\|_2\\
&+C\Delta t^3\left\|\left[q_n^j;\dot{q}_n^j\right]-\left[q(T_n);\dot{q}(T_n)\right]\right\|_2\\
&+C\Delta t\delta t^2\left\|\left[q_n^j;\dot{q}_n^j\right]-\left[q(T_n);\dot{q}(T_n)\right]\right\|_2\\
&+C\Delta t\delta t^2\left\|\left[q(T_n);\dot{q}(T_n)\right]\right\|_2.
\end{aligned}
\tag{3.16}
$$

The induction hypothesis

$$
\left\|\left[q_n^j;\dot{q}_n^j\right]-\left[q(T_n);\dot{q}(T_n)\right]\right\|_2\leq C\left(\Delta t^{2j+2}+\delta t^2\right)\left(1+\|[q_0;\dot{q}_0]\|_2\right)
$$

and the boundedness of $[q(T_n);\dot{q}(T_n)]$ further imply

$$
\begin{aligned}
&\left\|\left[q_{n+1}^{j+1};\dot{q}_{n+1}^{j+1}\right]-\left[q(T_{n+1});\dot{q}(T_{n+1})\right]\right\|_2\\
\leq\;&(1+C\Delta t)\left\|\left[q_n^{j+1};\dot{q}_n^{j+1}\right]-\left[q(T_n);\dot{q}(T_n)\right]\right\|_2\\
&+C\Delta t\left(\Delta t^2+\delta t^2\right)\left(\Delta t^{2j+2}+\delta t^2\right)\left(1+\|[q_0;\dot{q}_0]\|_2\right)\\
&+C\Delta t\delta t^2\|[q_0;\dot{q}_0]\|_2.
\end{aligned}
$$

If we require

$$
\left(\Delta t^2+\Delta t^{2j+2}+\delta t^2\right)\left(1+\|[q_0;\dot{q}_0]\|_2\right)\leq 1,
$$

it is obtained that

$$\begin{aligned}&\left\|\left[q_{n+1}^{j+1};\dot{q}_{n+1}^{j+1}\right]-\left[q(T_{n+1});\dot{q}(T_{n+1})\right]\right\|_2\\ \le{}&(1+C\Delta t)\left\|\left[q_n^{j+1};\dot{q}_n^{j+1}\right]-\left[q(T_n);\dot{q}(T_n)\right]\right\|_2\\ &+C\Delta t\big(\Delta t^{2j+4}+\delta t^2\big)\big(1+\|[q_0;\dot{q}_0]\|_2\big),\end{aligned}$$

which shows (3.10) for $j+1$ in the light of the discrete Gronwall lemma.

Remark 3.2. We can also show the convergence in the sense of iterations. For convenience, denote by

$$\begin{aligned}&\varepsilon_n^j:=\left\|\left[q_n^j;\dot{q}_n^j\right]-\left[q(T_n);\dot{q}(T_n)\right]\right\|_2,\\ &\alpha:=1+C\Delta t,\quad \beta:=C\left(\Delta t^3+\Delta t\delta t^2\right),\\ &\gamma:=C\Delta t\delta t^2,\qquad \eta:=C\Delta t^3.\end{aligned}$$

We have the recurrence inequality according to (3.16) and (3.15)

$$\varepsilon_{n+1}^{j+1}\le\alpha\varepsilon_n^{j+1}+\beta\varepsilon_n^j+\gamma,\quad \varepsilon_{n+1}^0\le\alpha\varepsilon_n^0+\eta,\quad j=0,1,\dots,\quad n=0,1,\dots,T/\Delta T-1.$$

The above relation can be solved by introducing a sequence of generating functions $\rho_j(\xi)=\sum_{n=1}^{\infty}\varepsilon_n^j\zeta^n$ $(0<\xi<1)$, which is induced as the following bound [15]:

$$\varepsilon_n^j\le C_n^{j+1}\alpha^{n-j-1}\beta^j\eta+C_n^{n-1}(\alpha+\beta)^{n-1}\gamma,\quad j=0,1,\dots.$$

Thus it yields for $j\le n$ that

$$\begin{aligned}&\left\|\left[q_n^j;\dot{q}_n^j\right]-\left[q(T_n);\dot{q}(T_n)\right]\right\|_2\\ \le{}&C_n^{j+1}(1+C\Delta t)^{n-j-1}\big(C(\Delta t^3+\Delta t\delta t^2)\big)^j\left(C\Delta t^3\right)\\ &+C_n^{n-1}\big(1+C(\Delta t+\Delta t^3+\Delta t\delta t^2)\big)^{n-1}\left(C\Delta t\delta t^2\right)\\ \le{}&\frac{C(n\Delta t^3)^{j+1}\mathrm{e}^{C(n-j-1)\Delta t}}{(j+1)!}+Cn\Delta t\delta t^2\mathrm{e}^{Cn\Delta t}.\end{aligned}$$

Furthermore, if $j\ge n$, it shows

$$\left\|\left[q_n^j;\dot{q}_n^j\right]-\left[q(T_n);\dot{q}(T_n)\right]\right\|_2\le Cn\Delta t\delta t^2\mathrm{e}^{Cn\Delta t}$$

since the fact that $[q_0^j;\dot{q}_0^j]\equiv[q(0);\dot{q}(0)]$.

3.2.4. Convergence for the algorithm with projection

In this part, it is shown that the projection $\pi_{\mathcal{M}}$ (2.12) does not deteriorate the convergent order. To this end, we first assume that the parareal-RKN algorithm introduced in the first formula of (2.14) has the following accuracy:

$$\left[q_{n+1}^j;\dot{q}_{n+1}^j\right]=\left[\tilde{q}_n^j;\dot{\tilde{q}}_n^j\right]+\mathcal{O}(\Delta t^r).\tag{3.17}$$

Then we show that after the projection $\pi_{\mathcal{M}}$, the accuracy is not deteriorated, i.e.,

$$\big[\tilde{q}^j_{n+1};\dot{\tilde{q}}^j_{n+1}\big] := \pi_{\mathcal{M}}\big[q^j_{n+1};\dot{q}^j_{n+1}\big] = \big[q^j_{n+1};\dot{q}^j_{n+1}\big] + \mathcal{O}(\Delta t^r). \tag{3.18}$$

Here and in the rest of this subsection, the constant in the $\mathcal{O}$-notation is independent of n. Inserting (3.17) into the energy function leads to

$$H\big(q^j_{n+1},\dot{q}^j_{n+1}\big) = H\big(\tilde{q}^j_n,\dot{\tilde{q}}^j_n\big) + \mathcal{O}(\Delta t^r). \tag{3.19}$$

Meanwhile, if we consider (2.13) for the energy function, the following result is obtained:

$$H\big(q^j_{n+1},\dot{q}^j_{n+1}\big) = H\big([\tilde{q}^j_{n+1};\dot{\tilde{q}}^j_{n+1}] - \lambda\nabla H\big) = H\big(\tilde{q}^j_{n+1},\dot{\tilde{q}}^j_{n+1}\big) + \mathcal{O}(\lambda). \tag{3.20}$$

Noticing $H(\tilde{q}^j_n,\dot{\tilde{q}}^j_n) = H(\tilde{q}^j_{n+1},\dot{\tilde{q}}^j_{n+1})$ and comparing (3.19) and (3.20), we have

$$\lambda = \mathcal{O}(\Delta t^r),$$

which implies (3.18) by combining (2.13). The proof for EPPRKN2 is complete. $\square$

4. Numerical experiments

In this section, to demonstrate the performance of the derived methods, we present three numerical experiments. For our schemes, we consider the following settings:

- EPPRKN2: choose $j=1, \Delta T = \Delta t$ and $\delta t = \Delta t^2$ and then its accuracy is $\mathcal{O}(\Delta t^4)$.
- EPPRKN3: consider $j=1, \Delta T = \Delta t$ and $\delta t = \Delta t^2$ and then its accuracy is $\mathcal{O}(\Delta t^6)$.
- EPPRKN2-3: consider $j=2, \Delta T = \Delta t$ and $\delta t = \Delta t^2$ and then its accuracy is $\mathcal{O}(\Delta t^6)$.

In the following experiments, we uniformly denote $h := \Delta t$.

Problem 1. For computing the motion of two bodies which attract each other, we consider the system

$$\begin{aligned}
\ddot{q}_1(t) &= -\frac{q_1(t)}{(q_1^2(t)+q_2^2(t))^{3/2}}, \quad q_1(0) = 1-e, \quad q_1'(0) = 0,\\
\ddot{q}_2(t) &= -\frac{q_2(t)}{(q_1^2(t)+q_2^2(t))^{3/2}}, \quad q_2(0) = 0, \qquad q_2'(0) = \sqrt{\frac{1+e}{1-e}}, \quad t\in[0,T]
\end{aligned}$$

with $e = 0.6$. The Hamiltonian function of the system is given by

$$H(p,q) = \frac{1}{2}\left(p_1^2+p_2^2\right) - \frac{1}{\sqrt{q_1^2(t)+q_2^2(t)}}.$$

We first solve this problem with different step sizes $h = 1/(2^i)$, $i = 2,3,\ldots,6$, and present the global error

$$err := \|\tilde{q}^j_n - q(t_n)\|_2/\|q(t_n)\|_2 + \|\dot{\tilde{q}}^j_n - \dot{q}(t_n)\|_2/\|\dot{q}(t_n)\|_2$$

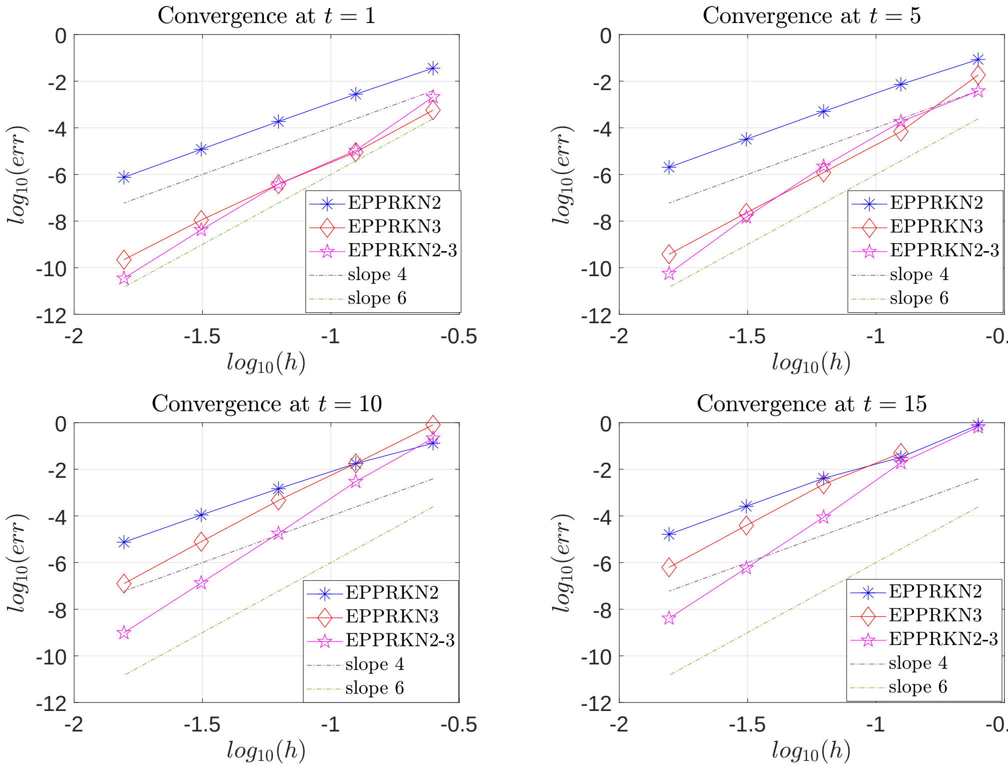

Figure 1: Problem 1: The logarithm of the relative errors err against the logarithm of h for different ε.

at different $t = t_n$ in Fig. 1. Then this problem is integrated with the step size $h = 0.01$ and Fig. 2 presents the energy error

$$errH := H\big(\tilde{q}_n^j, \dot{\tilde{q}}_n^j\big) - H\big(q(0), \dot{q}(0)\big)$$

for different methods. For comparison, here we consider the method EPPRKN2 without using the projection method and denote it by EPPRKN2-W. Finally, to show the convergence for different iterations j, we consider a very small step size for the fine propagator used in EPPRKN2-3 such that the error brought by the fine propagator can be ignored. The errors for this EPPRKN2-3 with $\Delta t = 0.1$ and different j are displayed in Fig. 3.

Problem 2. We consider a Fermi-Pasta-Ulam problem discussed by Hairer *et al.* in [16]. The motion is described by a Hamiltonian system with total energy

$$\begin{aligned} H(y,x) = & \frac{1}{2}\sum_{i=1}^{2m} y_i^2 + \frac{\omega^2}{2}\sum_{i=1}^{m} x_{m+i}^2 \\ & + \frac{1}{4}\left[(x_1 - x_{m+1})^4 + \sum_{i=1}^{m-1}(x_{i+1} - x_{m+i-1} - x_i - x_{m+i})^4 + (x_m - x_{2m})^4\right], \end{aligned}$$

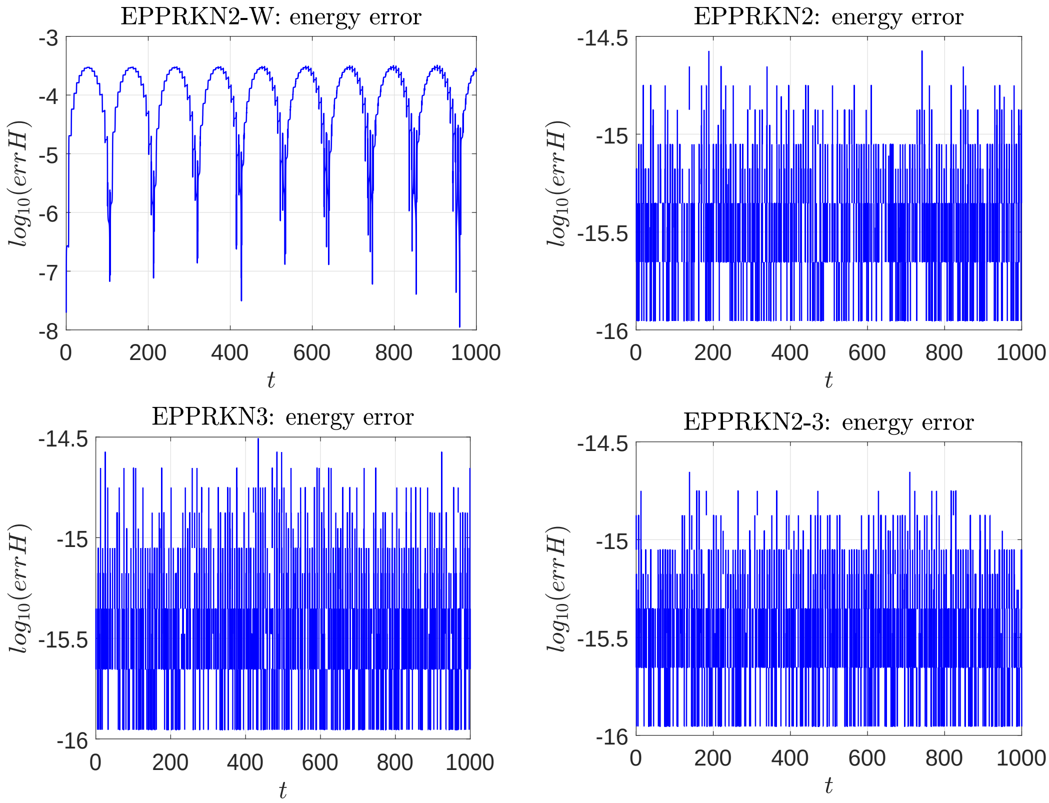

Figure 2: Problem 1: The energy errors $errH$ against t.

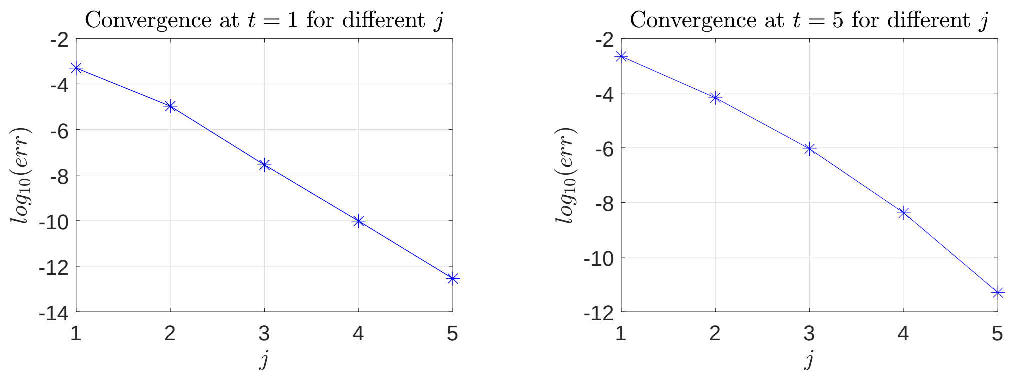

Figure 3: Problem 1: The logarithm of the relative errors err against different iterations j.

where x_i represents a scaled displacement of the i-th stiff spring, x_{m+i} is a scaled expansion (or compression) of the i-th stiff spring, and y_i, y_{m+i} are their velocities (or momenta). The corresponding Hamiltonian system is

$$\begin{cases} x' = H_y(y, x), \\ y' = -H_x(y, x), \end{cases}$$

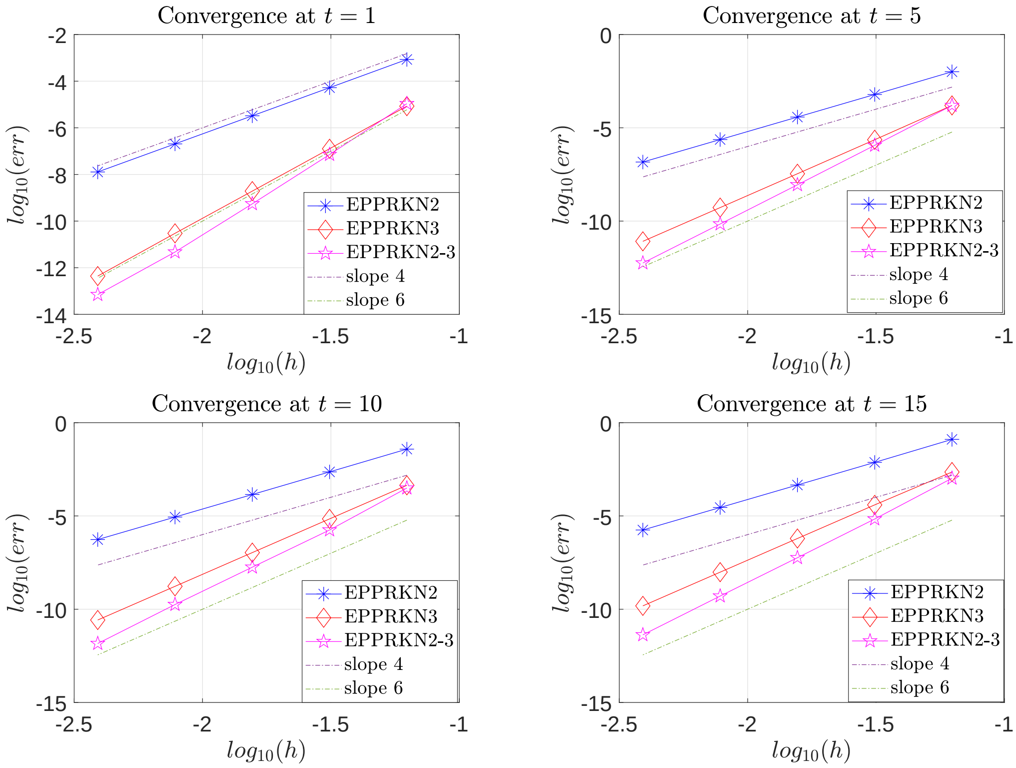

Figure 4: Problem 2: The logarithm of the relative errors err against the logarithm of h for different ε.

which is equivalent to $x'' = -H_x(y, x)$. This leads to

$$x''(t) + Mx(t) = -\nabla U(x), \quad t \in [0, T],$$

where

$$M = \begin{pmatrix} \mathbf{0}_{m\times m} & \mathbf{0}_{m\times m} \\ \mathbf{0}_{m\times m} & \omega^2 I_{m\times m} \end{pmatrix},$$

and

$$U(x) = \frac{1}{4}\left[(x_1 - x_{m+1})^4 + \sum_{i=1}^{m-1}(x_{i+1} - x_{m+i-1} - x_i - x_{m+i})^4 + (x_m - x_{2m})^4\right].$$

For this test, we consider $m = 3, \omega = 5$ and the initial values $x(0) = [1, 0, 0, 0.2, 0, 0]$, $y(0) = [1, 0, 0, 1, 0, 0]$. This problem is firstly solved with different step sizes $h = 1/(2^i)$, $i = 4, 5, \ldots, 8$, and the global errors are shown in Fig. 4. Then we display the energy conservation of different methods in Fig. 5 with the step size $h = 0.01$.

Problem 3. Consider a nonlinear wave equation

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} - \dfrac{\partial^2 u}{\partial x^2} = -\dfrac{1}{5}u^3 - \dfrac{1}{10}u^2, \quad 0 < x < 1, \quad t > 0, \\ u(0, t) = u(1, t) = 0, \quad u(x, 0) = \dfrac{\sin(\pi x)}{2}, \quad u_t(x, 0) = 0. \end{cases}$$

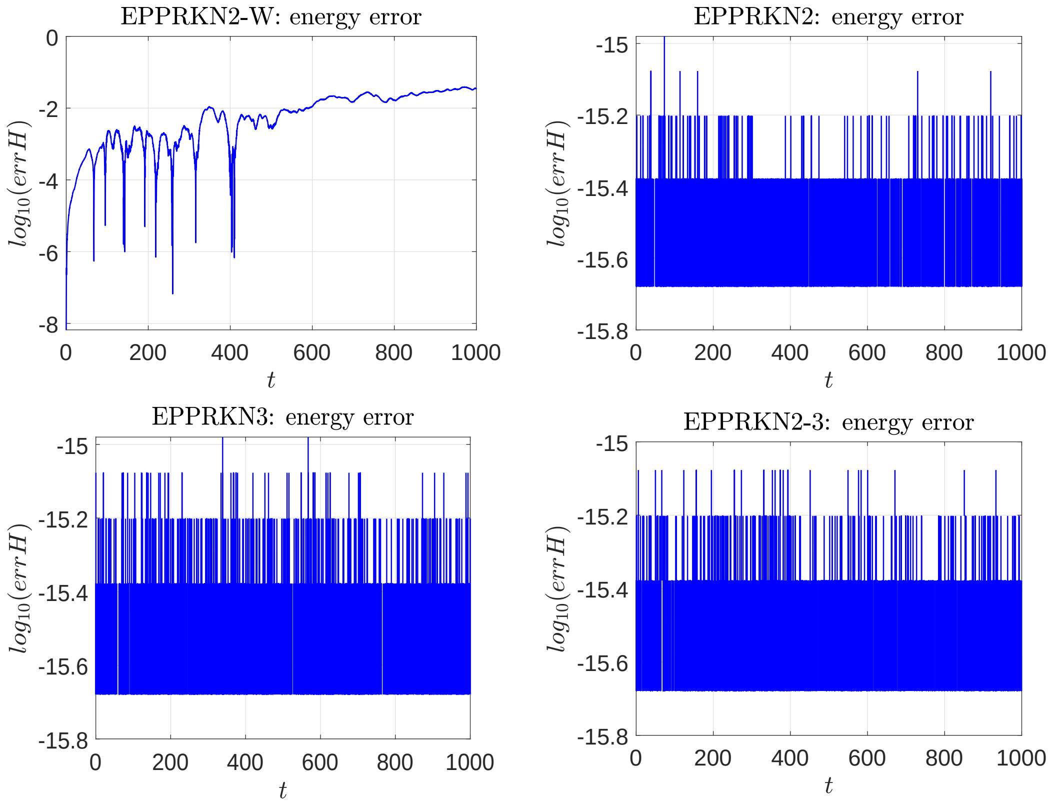

Figure 5: Problem 2: The energy errors $errH$ against t.

By using second-order symmetric differences, this problem is converted into a system in time

$$\begin{cases} \dfrac{\partial^2 u_i}{\partial t^2} - \dfrac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} = -\dfrac{1}{5}u_i^3 - \dfrac{1}{10}u_i^2, \quad 0 < t \leq T, \\ u_i(0) = \dfrac{\sin(\pi x_i)}{2}, \quad u_i'(0) = 0, \quad i = 1, \ldots, N-1, \end{cases}$$

where $\Delta x = 1/N$ is the spatial mesh step and $x_i = i\Delta x$. This semi-discrete oscillatory system has the form

$$\begin{cases} \dfrac{\partial^2 U}{\partial t^2} + MU = F(t, U), \quad 0 < t \leq T, \\ U(0) = \left(\dfrac{\sin(\pi x_1)}{2}, \ldots, \dfrac{\sin(\pi x_{N-1})}{2} \right)^T, \quad U'(0) = \mathbf{0}, \end{cases} \tag{4.1}$$

where $U(t) = (u_1(t), \ldots, u_{N-1}(t))^T$ with $u_i(t) \approx u(x_i, t), i = 1, \ldots, N-1$, and

$$F(t, U) = F(t, U) = \left(-\frac{1}{5}u_1^3 - \frac{1}{10}u_1^2, \ldots, -\frac{1}{5}u_{N-1}^3 - \frac{1}{10}u_{N-1}^2 \right)^T,$$

$$M = \frac{1}{\Delta x^2}\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}. \tag{4.2}$$

The Hamiltonian of (4.1) is given by

$$H(U', U) = \frac{1}{2}U'^T U' + \frac{1}{2}U^T M U + G(U),$$

where

$$G(U) = \left(\frac{1}{20}u_1^4 + \frac{1}{30}u_1^3, \ldots, \frac{1}{20}u_{N-1}^4 + \frac{1}{30}u_{N-1}^3\right)^T.$$

In this test we take $N = 16$ and present the errors in Fig. 6 with $h = 1/(2^i)$, $i = 3, 4, \ldots, 6$. The energy conservation is demonstrated in Fig. 7 with $h = 0.01$.

From the results presented in these problems, we have the following observations:

a) In terms of accuracy, it can be observed that the global error lines of our methods EPPRKN2 and EPPRKN3, EPPRKN2-3 are respectively nearly parallel to the lines

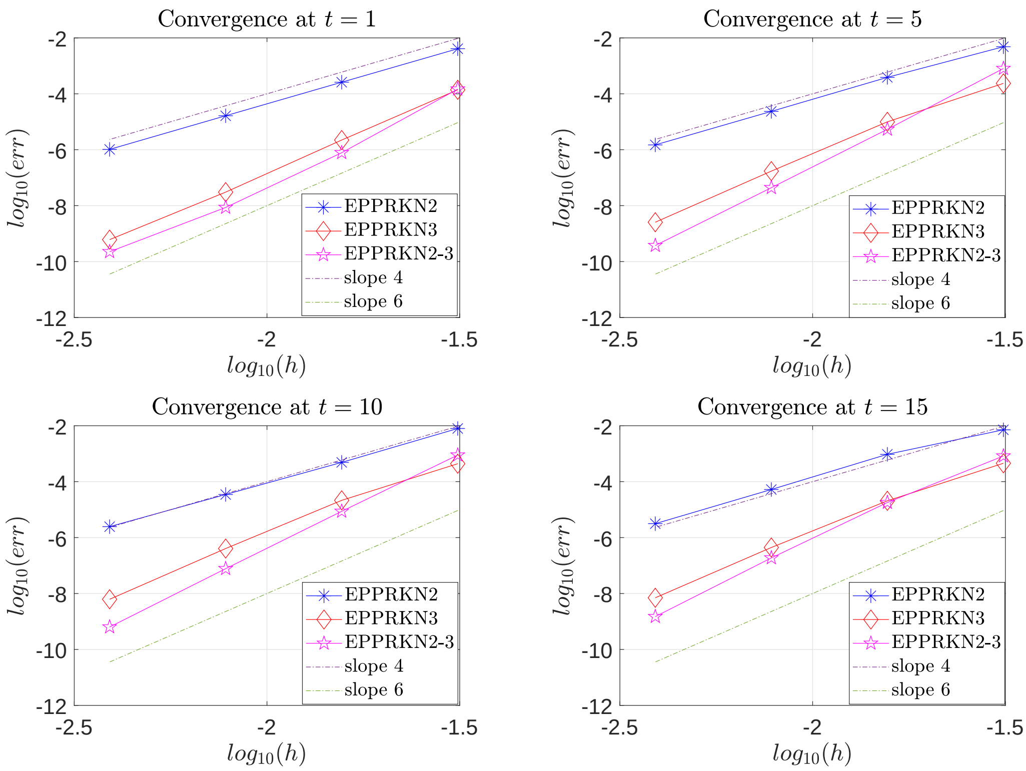

Figure 6: Problem 3: The logarithm of the relative errors err against the logarithm of h for different ε.

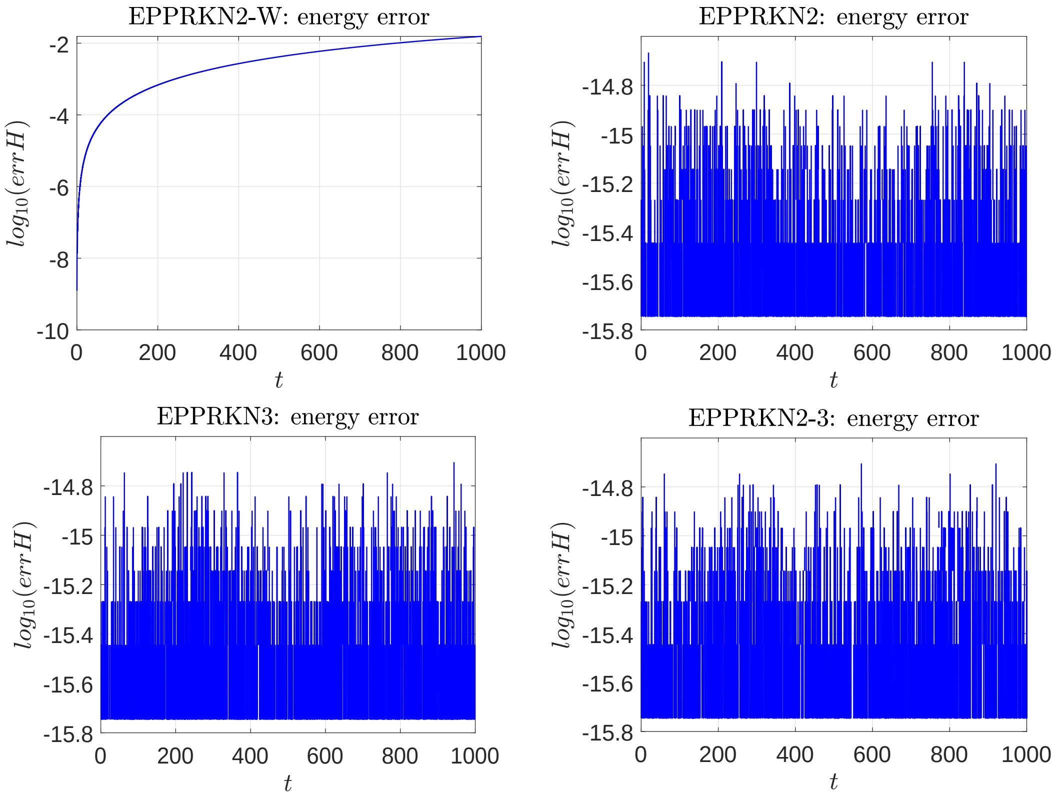

Figure 7: Problem 3: The energy errors $errH$ against t.

of slope four and six. This indicates that they have the convergence as stated in Theorem 3.2.

b) From the energy conservation, it is clear that our methods can preserve the energy exactly while the method EPPRKN2-W without using the projection method does not have such nice property.

5. Conclusions

Hamiltonian systems quite frequently arise in many applications and the design and analysis of numerical schemes for such systems has received a great deal of attention in the last few decades. In this paper we paid our attention to the analysis and construction of the energy-preserving parareal-RKN algorithms for solving the Hamiltonian system (1.2). We formulated a kind of parareal algorithms by using Runge-Kutta-Nyström (RKN) methods and projection methods. The energy conservation and convergence were analyzed in detail. Three of the algorithms were presented as examples to show the efficiency and robustness by three numerical experiments.

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