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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

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

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