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ENERGY AND QUADRATIC INVARIANTS PRESERVING METHODS FOR HAMILTONIAN SYSTEMS WITH HOLONOMIC CONSTRAINTS*

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Abstract

We introduce a new class of parametrized structure–preserving partitioned Runge-Kutta (α-PRK) methods for Hamiltonian systems with holonomic constraints. The methods are symplectic for any fixed scalar parameter α, and are reduced to the usual symplectic PRK methods like Shake-Rattle method or PRK schemes based on Lobatto IIIA-IIIB pairs when $\alpha = 0$. We provide a new variational formulation for symplectic PRK schemes and use it to prove that the α-PRK methods can preserve the quadratic invariants for Hamiltonian systems subject to holonomic constraints. Meanwhile, for any given consistent initial values (p_0, q_0) and small step size $h > 0$, it is proved that there exists $\alpha^* = \alpha(h, p_0, q_0)$ such that the Hamiltonian energy can also be exactly preserved at each step. Based on this, we propose some energy and quadratic invariants preserving α-PRK methods. These α-PRK methods are shown to have the same convergence rate as the usual PRK methods and perform very well in various numerical experiments.

Mathematics subject classification: 65P10, 65L05.
Key words: Hamiltonian systems, Holonomic constraints, symplecticity, Quadratic invariants, Partitioned Runge-Kutt methods.

1. Introduction

For a given differential equation, a numerical method is called a geometric numerical integrator if it can accurately preserve some of the geometric characteristics of the solution to the original equation [16]. The structure–preserving algorithms of differential equations have been enlarged by a lot of important developments. The idea of maintaining important structures of the original differential equation in numerical methods is widely accepted. For the Hamiltonian systems, the symplectic integrators preserving the symplectic geometry property of the solutions have been proved to own various excellent properties such as very good orbital tracking ability [12, 13, 16, 20]. Many effective methods for constructing symplectic integrators, such as the methods based on variational integrators [20], generating functions [13], Rung-Kutta (RK) methods [26,27] and composition method [32] have been developed and investigated. The

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theory of symplectic integrators for Hamiltonian systems has become more complete with the establishment of backward error analysis [4, 28] and discrete KAM theory [25]. Recently, some related numerical methods such as multi-symplectic methods for Hamiltonian partial differential equations [23] and stochastic symplectic methods for stochastic Hamiltonian systems [10] have been well developed. In addition to the symplectic property, another extremely important feature of the Hamiltonian system is the conservation of energy. Some important energy preserving methods include discrete gradient method [15, 21], average vector field method [24], HBVMs [7] and spectral methods [1].

When multiple important structures or physical quantities exist for a system, such as the symplectic structure and the energy for Hamiltonian system, a natural question arises: is it possible to construct a numerical method that preserves several of them? Regarding the symplectic structure and the energy for Hamiltonian system, one has unfortunately a negative answer in general with a constant step size. In fact, it is proved [14] that for non-integrable systems if a numerical method is symplectic and can conserve the Hamiltonian energy exactly, then it is the time advance map for the exact Hamiltonian systems up to a reparametrization of time. A similar negative result is proved in [9] for general Hamiltonian system by B-series method. However, the above negative results do not prevent people from constructing numerical methods to maintain both the energy and symplectic structure of the Hamilton system in some weaker sense.

A breakthrough work in this regard is the parameterized Gauss collocation method firstly developed by Brugnano et.al. [8]. Consider the canonical Hamiltonian systems in the form

$$\begin{cases} \dot{y} = J\nabla H(y), \\ y(t_0) = y_0 \in \mathbb{R}^{2d}, \end{cases} \qquad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \in \mathbb{R}^{2d\times 2d}, \tag{1.1}$$

where $y = (p^T, q^T)^T$ and I is the identity matrix and H is the Hamiltonian energy. Brugnano et.al. introduced a nice idea to develop a new family of Gauss type methods which share both the symplecticity-like and energy conservation features under suitable conditions. More precisely, they define a family of RK methods $y_1(\alpha) = \Phi_h(y_0, \alpha)$, where h is the step size of integration, α is a real parameter. This method satisfies the following three conditions simultaneously: (i) for $\alpha = 0$ one gets the Gauss collocation method of order $2s$, s is the number of stages of the RK method; (ii) for any fixed choice of $\alpha \neq 0$, the corresponding method is of order $2s-2$ and satisfies the conditions $b_i a_{i,j} + b_j a_{j,i} = b_i b_j$, thus being a quadratic invariant-preserving symplectic RK method; (iii) for any choice of y_0 and in a neighborhood of h, there exists a value of parameter $\alpha^* = \alpha^*(y_0, h)$ such that $H(y_1) = H(y_0)$(energy conservation). The resulting method $y_1 = \Phi_h(y_0, \alpha^*)$ has order $2s$, preserving the energy and quadratic invariants [1)] .

This method [8] has been rewritten in the framework of discrete linear integral methods [5], which leads to a more refined theoretical analysis and a nice practical implementation strategy for seeking the parameter α^*. Another extension from α-RK to α-PRK to make use of the additive structure of Hamiltonian system is given in [29]. This method is also used to construct

[1)] For standard RK method (c, A, b) with constant step size $h > 0$, the sufficient condition of symplecticity is given by $b_i a_{i,j} + b_j a_{j,i} = b_i b_j$ for all $i, j = 1, 2, ..., s$. For irreducible RK method, which can be intuitively understood to mean that this RK method is not equivalent to a RK method with a lower series, see more details in [17, pp.187], this condition is also necessary, and also sufficient and necessary for quadratic invariants-preserving. However, for the parametric α-RK methods $y_1(\alpha) = \Phi_h(y_0, \alpha^*)$ that preserve the energy, the parameter depends on the initial values, i.e., $\alpha^* = \alpha^*(y_0, h)$. Then, α-RK methods with condition $b_i a_{i,j} + b_j a_{j,i} = b_i b_j$ are in general not symplectic from the definition, but can preserve all the quadratic invariants.