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TWO NOVEL CLASSES OF ARBITRARY HIGH-ORDER STRUCTURE-PRESERVING ALGORITHMS FOR CANONICAL HAMILTONIAN SYSTEMS*

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Abstract

In this paper, we systematically construct two classes of structure-preserving schemes with arbitrary order of accuracy for canonical Hamiltonian systems. The one class is the symplectic scheme, which contains two new families of parameterized symplectic schemes that are derived by basing on the generating function method and the symmetric composition method, respectively. Each member in these schemes is symplectic for any fixed parameter. A more general form of generating functions is introduced, which generalizes the three classical generating functions that are widely used to construct symplectic algorithms. The other class is a novel family of energy and quadratic invariants preserving schemes, which is devised by adjusting the parameter in parameterized symplectic schemes to guarantee energy conservation at each time step. The existence of the solutions of these schemes is verified. Numerical experiments demonstrate the theoretical analysis and conservation of the proposed schemes.

Mathematics subject classification: 65L05, 65P10, 70H15, 70H20.
Key words: Hamiltonian systems, Symplectic schemes, Energy-preserving schemes, EQUIP schemes, Generating function methods, Symmetric composition methods.

1. Introduction

All real physical processes with negligible dissipation could be recast into the appropriate Hamiltonian form [13]. The canonical Hamiltonian system with d degrees of freedom has the following form

$$\dot{p} = -H_q(p,q), \quad \dot{q} = H_p(p,q), \quad p,q \in \mathcal{R}^d, \tag{1.1}$$

where H_p and H_q denote the column vectors of partial derivatives of the Hamiltonian. And the Hamiltonian mostly represents the physical meaning of the total energy. The system (1.1) serving as the basic mathematical formalism often appears in the relevant areas of analytical

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dynamics, geometrical optics, particle accelerators, plasma physics, control theory and hydrodynamics, etc. The most characteristic property of (1.1) is the symplecticity and energy conservation along any exact flows [5, 14, 17, 31]. These facts motivate to search for numerical methods that can preserve one or more conserved properties.

Numerical methods conserving the symplecticity are called symplectic integrators and generally have excellent behavior and stability in the long-term simulations [17,24,31]. Symplectic integrators were first introduced in the pioneering work [12] and developed in the early works [13, 22, 25, 27, 29, 30]. Feng [13] obtained symplectic schemes by verifying that the one-step mapping of a numerical method is symplectic. There are several approaches to construct symplectic methods, such as symplectic Runge-Kutta (RK) methods [11,30], symplectic partitioned RK methods [33,34], variational integrators [22] and the generating function method [15]. The generating function method as a general framework has significance in both the theory and the construction of symplectic algorithms.

Using the generating function method and symmetric composition methods [27], we first develop two types of arbitrary high-order parameterized symplectic schemes. The free parameter in these schemes will be adjusted later to derive energy and quadratic invariants preserving (EQUIP) schemes [6]. The complete theory of the generating function method has been established in [15] as well as a series of applications [3, 18, 32, 37]. The generating function is a solution of the Hamilton-Jacobi equation that can generate arbitrary symplectic mappings. It is possible to find such a function to generate a given symplectic transformation. Actually, for symplectic RK and partitioned RK methods, Hairer et al. [17] have defined the expression of their generating functions. However, the construction of generating functions is dependent on the different choices of coordinates. In this paper, we introduce a generating function with new coordinates and discuss the associated Hamilton-Jacobi equation. The new coordinates unify and generalize the traditional three generating functions. Following the research route [15, 17], we obtain the power series of the new generating function. Then, the first type of parameterized symplectic schemes is reported by truncating this series. In particular, a simple symplectic scheme with a free parameter λ is obtained as

$$\begin{cases} p_{n+1} = p_n - hH_q\big(\lambda p_{n+1} + (1-\lambda)p_n, \lambda q_n + (1-\lambda)q_{n+1}\big), \\ q_{n+1} = q_n + hH_p\big(\lambda p_{n+1} + (1-\lambda)p_n, \lambda q_n + (1-\lambda)q_{n+1}\big), \end{cases} \tag{1.2}$$

where h is the time step. We call the above scheme Scheme I. For the case where $\lambda = 0$, 1, 1/2, respectively, the symplectic Euler methods and the implicit midpoint rule are recognized. Noting that the correct pairing of variables of the Hamiltonian plays a key role in the symplecticity of Scheme I. Substituting $1-\lambda$ for λ yields its adjoint method, and the resulting method is still symplectic. By fixing the parameter to specific values, we can obtain more symplectic schemes with simple forms that can be widely applied in practical computations. The second type of parameterized symplectic schemes is derived by the composition of Scheme I and its adjoint method.

At present, the research on energy-preserving schemes of (1.1) is also a prominent project. For more details, please refer to the discrete gradient methods [23], the averaged vector field (AVF) method [8, 20, 28, 38], time finite element methods [1, 35] and the Hamiltonian boundary value methods [5, 7], etc. Although symplectic schemes are superior in long-time behavior, they fail to conserve non-quadratic invariants. It is natural to think about whether such a discretization scheme can be found to share both the symplecticity and energy conservation. It is verified that the constant time stepping scheme cannot inherit both features for gener-