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HIGH-ORDER SYMPLECTIC AND SYMMETRIC COMPOSITION METHODS FOR MULTI-FREQUENCY AND MULTI-DIMENSIONAL OSCILLATORY HAMILTONIAN SYSTEMS*

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Abstract

The multi-frequency and multi-dimensional adapted Runge-Kutta-Nyström (ARKN) integrators, and multi-frequency and multi-dimensional extended Runge-Kutta-Nyström (ERKN) integrators have been developed to efficiently solve multi-frequency oscillatory Hamiltonian systems. The aim of this paper is to analyze and derive high-order symplectic and symmetric composition methods based on the ARKN integrators and ERKN integrators. We first consider the symplecticity conditions for the multi-frequency and multi-dimensional ARKN integrators. We then analyze the symplecticity of the adjoint integrators of the multi-frequency and multi-dimensional symplectic ARKN integrators and ERKN integrators, respectively. On the basis of the theoretical analysis and by using the idea of composition methods, we derive and propose four new high-order symplectic and symmetric methods for the multi-frequency oscillatory Hamiltonian systems. The numerical results accompanied in this paper quantitatively show the advantage and efficiency of the proposed high-order symplectic and symmetric methods.

Mathematics subject classification: 65L05, 65L06, 65M20, 65P10
Key words: Symplectic and symmetric composition methods, Multi-frequency and multi-dimensional ERKN integrators, ARKN integrators, Multi-frequency oscillatory Hamiltonian systems.

1. Introduction

Geometric numerical integration is designed specially for the numerical solution of differential equations which possess some geometric/physical properties (Hamiltonian, divergence-free, symmetry, symplecticity, etc.) that should be preserved by numerical methods as much as possible. We refer the reader to [3, 4, 10, 13, 15, 18, 30] for this topic. Oscillation is also an important physical property. In fact, differential equations having oscillatory solutions are usually encountered in many fields of the applied sciences and engineering, such as celestial mechanics, theoretical physics, quantum chemistry and molecular dynamics. The modeling and simulation of oscillations is of particular interest in applications. A lot of theoretical and numerical analysis has been made on this research [10, 30]. A variety of methods and analytical tools arise in this area such as stroboscopic averaging methods, heterogeneous multiscale methods, the technique of modified Fourier expansions. For these mehtods, we refer the reader to [5–7, 9, 17] and the references therein.

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Among typical topics is the numerical integration of an oscillatory system of the form

$$\begin{cases} q''(t) + Kq(t) = f(q(t)), & t \in [t_0, T], \\ q(t_0) = q_0, \quad q'(t_0) = q'_0, \end{cases} \tag{1.1}$$

where K is a $d \times d$ positive semi-definite matrix that implicitly contains the frequencies of the oscillatory problem and $f : \mathbb{R}^d \to \mathbb{R}^d$, $q \in \mathbb{R}^d, q' \in \mathbb{R}^d$. It should be noted that (1.1) is a *multi-frequency and multi-dimensional nonlinear oscillatory problem*. The design and analysis of numerical method for nonlinear oscillators is an important problem that has received a great deal of attention in the last few years.

It has now become a common practice in geometric numerical integration that, numerical algorithms should take advantage of the special structure of the underlying problem. In [28], the authors took account of the special structure of system (1.1) brought by the linear term Kq and proposed the so-called multi-frequency and multi-dimensional ARKN (Adapted Runge-Kutta-Nyström) integrators. An outstanding advantage of multi-frequency and multi-dimensional ARKN integrators for (1.1) is that their updates are incorporated with the special structure of the system (1.1) so that they naturally integrate exactly the multi-frequency oscillatory homogeneous system $y'' + Ky = 0$. Very recently, Wu *et al.* [29] formulated a standard form of the multi-frequency and multi-dimensional ERKN (extended Runge-Kutta-Nyström) methods in which both the internal stages and updates are incorporated with the special structure of the system (1.1). The ERKN methods exactly integrate the multi-frequency oscillatory homogeneous system $y''+Ky = 0$ as well. The ERKN integrators exhibit the correct qualitative behaviour much better than the classical RKN methods. For references on this topic, we refer the reader to [19, 21, 23, 25–28, 31].

On the other hand, the idea of composition methods is quite useful to improve the order of a basic method while preserving some desirable properties. It is well-known that numerical integrators of arbitrarily high order can be achieved by composition of an integrator with low order. Let φ_h be a basic method and $\gamma_1, \dots, \gamma_s$ real numbers. Then we call its composition

$$\psi_h = \varphi_{\gamma_s h} \circ \cdots \circ \varphi_{\gamma_1 h} \tag{1.2}$$

the corresponding *composition method*.

A more general case is that consider the composition of both the basic integrators and its adjoint integrators with different stepsizes, i.e., replace composition (1.2) by the more general formula

$$\psi_h = \varphi_{\alpha_s h} \circ \varphi^*_{\beta_s h} \circ \cdots \circ \varphi^*_{\beta_2 h} \circ \varphi_{\alpha_1 h} \circ \varphi^*_{\beta_1 h}. \tag{1.3}$$

The adjoint method of a method is defined as follows [11].

Definition 1.1. *The adjoint method Φ^*_h of a method Φ_h is defined as the inverse map of the original method with reversed time step $-h$, i.e., $\Phi^*_h := \Phi^{-1}_{-h}$. A method with $\Phi^*_h = \Phi_h$ is called symmetric.*

With regard to composition methods, we refer the reader to [1, 2, 14, 16, 22, 32]. For a systematic introduction of the idea of composition methods, including the order conditions for composition methods, we refer to [10].

In this paper, we focus ourselves on the compositions of multi-frequency and multi-dimensional symplectic ARKN and ERKN integrators. The remainder of this paper is organized as follows. In Section 2 and Section 3, we derive some properties for ARKN and ERKN integrators. Based on these properties, we derive four novel high-order symplectic and symmetric methods by using the composition of multi-frequency and multi-dimensional symplectic ARKN and ERKN