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A SIXTH ORDER AVERAGED VECTOR FIELD METHOD*

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Abstract

In this paper, based on the theory of rooted trees and B-series, we propose the concrete formulas of the substitution law for the trees of order = 5. With the help of the new substitution law, we derive a B-series integrator extending the averaged vector field (AVF) methods for general Hamiltonian system to higher order. The new integrator turns out to be order of six and exactly preserves energy for Hamiltonian systems. Numerical experiments are presented to demonstrate the accuracy and the energy-preserving property of the sixth order AVF method.

Mathematics subject classification: 65D15, 65L05, 65L70, 65P10.
Key words: Hamiltonian systems, B-series, Energy-preserving method, Sixth order AVF method, Substitution law.

1. Introduction

With the fast development of computer, geometric methods become more and more powerful in scientific research. A numerical method which can conserve the geometric properties of a system is called geometric method [2, 29]. Geometric methods, such as symplectic methods, symmetric methods, volume-preserving methods, energy-preserving methods and so on, have been successfully used in many application areas [4, 12, 14, 17, 18, 20, 24, 27, 30–33].

The conservation of the energy function is one of the most relevant features characterizing a Hamiltonian system. Methods that exactly preserve energy have been considered for several decades and many energy-preserving methods have been proposed [5–7, 11, 16]. Here we list some examples. The discrete gradient method is one of the most popular methods for designing integral preserving schemes for ordinary differential equations, which was perhaps first discussed by Gonzalez [15]. Matsuo proposed discrete variational method for nonlinear wave equation [25]. L. Brugnano and F. Iavernaro proposed Hamiltonian boundary value methods [1, 21]. More recently, the existence of energy-preserving B-series methods has been shown in [13], and a

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practical integrator which is the averaged vector field (AVF) method of order two has been proposed [5, 6, 26, 28]. This method exactly preserves the energy of Hamiltonian systems, and in contrast to projection-type integrators, only requires evaluations of the vector field. It is symmetric and its Taylor series has the structure of a B-series. For polynomial Hamiltonians, the integral can be evaluated exactly, and the implementation is comparable to that of the implicit mid-point rule [16].

In recent years, there has been growing interest in high-order AVF methods, and the second, third and fourth order AVF methods have been proposed in succession [28]. It is shown that the theory of B-series and the substitution law obtained by substituting a B-series into the vector field appearing in another B-series play an important role in constructing high order methods [13, 14]. The substitution law for the trees of order ≤ 4 has been shown in [8, 9, 14]. The fourth order AVF method is obtained by the concrete formulas of the substitution law for the trees of order ≤ 4. To construct a B-series method which not only has high order accuracy but also preserves the Hamiltonian is an important and interesting topic. However, the concrete formulas of the substitution law for the trees of order ≥ 5 have not been proposed, as the corresponding calculations are sufficiently complicated.

There are two aims in this paper. The first aim is to propose the concrete formulas of the substitution law for the trees of order $= 5$. As we know, a low order B-series integrator can be extend to high order by the substitution law. Using the new obtained concrete formulas of the substitution law for the trees of order $= 5$, one can extend a low order geometric B-series integrator to sixth order naturally, easily and automatically, such as the symplectic integrator, the energy-preserving integrator, the momentum-preserving integrator and so on. Using the new obtained substitution law, we also easily obtained the same sixth order symplectic integrator in [9]. The second aim is to derive a sixth order AVF method for Hamiltonian systems. By expanding the second order AVF method into a B-series and considering the substitution law for the trees of order $= 5$, a new method can be constructed. The new method is derived by the concrete formulas of the substitution law for the trees of order $= 5$. We prove that the new method is of order six and can also preserve the energy of Hamiltonian systems exactly.

The paper is organized as follows: In Sect. 2, we introduce the AVF method. In Sect. 3, we recall a few definitions and properties related to trees and B-series. The substitution law for the trees of order ≤ 4 is shown and we obtain that for the trees of order $= 5$. In Sect. 4, we derive the sixth order AVF method, and prove that the new method is of order six and it can preserve the Hamiltonian. A few numerical experiments are given in Sect. 5 to confirm the theoretical results. We finish the paper with conclusions in Sect. 6.

2. The AVF Method and Its Energy-Preserving Property

Here we briefly discuss the AVF method and its energy-preserving property. We consider a Hamiltonian differential equation, written in the form

$$\dot{z} = f(z) = S\nabla H(z), \quad z(0) = z_0, \quad z \in \mathbb{R}^n, \tag{2.1}$$

where $f(z) : \mathbb{R}^n \to \mathbb{R}$, S is a skew-symmetric constant matrix, n is an even number, and the Hamiltonian $H(z)$ is assumed to be sufficiently differentiable. From system (2.1), we can get

$$\frac{dH(z(t))}{dt} = \nabla H(z)^T f(z) = \nabla H(z)^T S\nabla H(z) = 0. \tag{2.2}$$