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MULTISYMPLECTIC COMPOSITION INTEGRATORS OF HIGH ORDER *1)

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Abstract

A composition method for constructing high order multisymplectic integrators is presented in this paper. The basic idea is to apply composition method to both the time and the space directions. We also obtain a general formula for composition method.

Key words: Multisymplectic integrators, Composition method.

1. Introduction

Composition method originates from the construction of symplectic integrators for separable Hamiltonian systems. Yoshida applied symmetric composition method to obtaining high order decomposition of vector field and suggested the composition method for Hamiltonian systems [12]. Based on the theory of Lie series and formal vector field, Qin and Zhu systematically suggested the composition method for general ordinary differential equations [8]. Suzuki established the general theory of high order decomposition of exponential operators [10]. We will show in this paper that Suzuki's theory can be used to obtain a general formula for composition method.

Recently multisymplectic Hamiltonian systems and multisymplectic integrators are drawing a lot of attention [1, 2, 9, 3, 4]. Bridges first introduced the concept of multisymplectic Hamiltonian systems which possess a completely local multisymplectic conservation law [1]. Bridges and Reich suggested the concept of multisymplectic integrators which preserve a discrete version of multisymplectic conservation law [2]. Reich showed that Gauss-Legendre collocation in space and time leads to multisymplectic integrators [9]. However, in high order case, the multisymplectic integrators obtained by Reich are very difficult to implement. Therefore, we suggest a composition method for high order multisymplectic integrators. The resulting high order multisymplectic integrators are very easy to implement.

An outline of the paper is as follows. In §2, we present the composition method for ordinary differential equations. The basic formula for composition method is obtained. §3 is devoted to developing composition method for constructing high order multisymplectic integrators. We present numerical experiments in §4. Some conclusions are included in §5.

2. Composition Method for ODEs

We first present the composition method for ordinary differential equations (ODEs). We know that every one-step integrator for $y' = f(y)$ can be written

$$y_{n+1} = s(\tau)y_n,$$

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where $s(\tau)$ is the operator corresponding to the integrator, and τ is the step length.

Definition 1. *Suppose there are n integrators whose corresponding operators are $s_1(\tau)$, $s_2(\tau)$, $\ldots$, $s_n(\tau)$ respectively, and their corresponding order is $p_1, p_2, \ldots, p_n$ respectively. If there exist constants $c_1, c_2, \ldots, c_n$ such that the order of the integrator whose operator is the composition $s_1(c_1\tau)s_2(c_2\tau)\cdots s_n(c_n\tau)$ is $m, m > max(p_i), 1 \leq i \leq n$, then the new integrator is called composition integrator of the original n integrators. This method which is used to construct higher order integrators from the lower ones is called composition method.*

In the discussion as follows, we also need the concept of adjoint operator and self-adjoint operator.

Definition 2. *An operator $s^*(\tau)$ is called the adjoint operator of $s(\tau)$, if*

$$s^*(-\tau)s(\tau) = s(\tau)s^*(-\tau) = I, \tag{2.1}$$

where I is the identity operator.

Definition 3. *We call an operator $s(\tau)$ is self-adjoint, if $s^*(\tau) = s(\tau)$.*

The development of composition method relies on the theory of Lie series [5, 7, 11] and the following theorem [6].

Theorem 1. *Every operator $s(\tau)$ has a formal exponential representation*

$$s(\tau) = exp(\tau A + \tau^2 B + \tau^3 C + \tau^4 D + \cdots),$$

where $A, B, C, D, \ldots$ are first order differential operators.

According to the definition of composition method, constructing higher order integrator $s_1(c_1\tau)s_2(c_2\tau)\cdots s_n(c_n\tau)$ is to determine constants $c_1, c_2, \ldots, c_n$ such that the scheme $s_1(c_1\tau)$ s_2 $(c_2\tau)\cdots s_n(c_n\tau)$ has order m. Now we will deduce the basis formula for determining the constants $c_i (i = 1, \ldots, n)$. By theorem 1, we have

$$s_j(\tau) = \exp(\tau w_{j1} + \tau^2 w_{j2} + \tau^3 w_{j3} + \cdots + \tau^{p_j} w_{jp_j} + \tau^{p_j+1} w_{jp_{j+1}} + \cdots).$$

Since $s_j(\tau)$ has order p_j, $w_{j1} = L_f, w_{j2} = w_{j3} = \cdots = w_{jp_j} = 0, w_{jp_{j+1}} \neq 0$. Here L_f is the differential operator corresponding to $y' = f(y)$ [8]. As in [10], we introduce *symmetrization operator S*

$$S(x^p z^q) = \frac{p!q!}{(p+q)!} \sum_{P_m} P_m(x^p z^q),$$

where x, z are arbitrary noncommutable operators, P_m denotes the summation of all the operators obtained in all possible ways of permutation.

We also introduce *time-ordering operator P*

$$P(x_i x_j) = \begin{cases} x_i x_j, & \text{if } i < j; \\ x_j x_i & \text{if } j < i, \end{cases}$$

where x_i, x_j are noncommutable operators.