Journal of Computational Mathematics
Vol.34, No.5, 2016, 479–498.
http://www.global-sci.org/jcm
doi:10.4208/jcm.1601-m2015-0265

A SIXTH ORDER AVERAGED VECTOR FIELD METHOD*

Haochen Li
Jiangsu Key Laboratory for NSLSCS, School of Mathematical Sciences, Nanjing Normal University, Jiangsu, 210023, China
Email: lihaochen_bjut@sina.com
Yushun Wang [1)]
Jiangsu Key Laboratory for NSLSCS, School of Mathematical Sciences, Nanjing Normal University, Jiangsu, 210023, China
Email: wangyushun@njnu.edu.cn
Mengzhao Qin
Lsec, Academy of Mathematics and System Sciences, Chinese Academy of Science, PoBox 2719, Beijing, China
Email: qmz@lsec.cc.ac.cn

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

* Received April 21, 2015 / Revised version received October 13, 2015 / Accepted January 29, 2016 / Published online September 14, 2016 /
1) Corresponding author

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

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

Therefore, the flow of the system (2.1) preserves the Hamiltonian $H(z)$ exactly.

The so-called AVF method [5, 28] is defined by

$$\frac{z_1 - z_0}{h} = \int_0^1 f(\xi z_1 + (1-\xi)z_0) d\xi, \tag{2.3}$$

where h is the time step. The AVF method (2.3) can be rewritten as

$$\frac{z_1 - z_0}{h} = S \int_0^1 \nabla H(\xi z_1 + (1-\xi)z_0) d\xi.$$

We can obtain

$$\begin{aligned}
&\frac{1}{h}(H(z_1) - H(z_0)) = \frac{1}{h}\int_0^1 \frac{d}{d\xi} H(\xi z_1 + (1-\xi)z_0) d\xi \\
=& \left(\int_0^1 \nabla H(\xi z_1 + (1-\xi)z_0) d\xi\right)^T \left(\frac{z_1 - z_0}{h}\right) \\
=& \left(\int_0^1 \nabla H(\xi z_1 + (1-\xi)z_0) d\xi\right)^T S \int_0^1 \nabla H(\xi z_1 + (1-\xi)z_0) d\xi = 0.
\end{aligned}$$

It follows that the Hamiltonian H is conserved at every time step.

McLachlan and Quispel also proposed a higher order energy-preserving method [28]

$$\frac{z_1^i - z_0^i}{h} = \left(\delta_j^i + \alpha h^2 f_k^i(\hat{z}) f_j^k(\hat{z})\right) \int_0^1 f^j(\xi z_1 + (1-\xi)z_0) d\xi, \tag{2.4}$$

where α is an arbitrary constant, δ_i^j is the Kronecker delta, and we can take e.g. $\hat{z} = z_0$ or $\hat{z} = (z_0 + z_1)/2$. For $\alpha = 0$, we recover the second order method (2.3). For $\alpha = -\frac{1}{12}$ and $\hat{z} = z_0$, the method is of order three. For $\alpha = -\frac{1}{12}$ and $\hat{z} = (z_0 + z_1)/2$, the method is of order four.

Up to now, the highest order of existing AVF methods is four, and here we derive a AVF method of order six.

3. Preliminaries

In this section, we briefly recall a few definitions and properties related to rooted trees and B-series [3, 8–10, 13, 14, 17–19].

3.1. Trees and B-series

Let $\emptyset$ denote the empty tree.

Definition 3.1. (Unordered trees [14]) *The set $\mathcal{T}$ of (rooted) unordered trees is recursively defined by*

$$\bullet \in \mathcal{T}, \quad [\tau_1, \ldots, \tau_m] \in \mathcal{T}, \quad \forall\, \tau_1, \ldots, \tau_m \in \mathcal{T}, \tag{3.1}$$

where $\bullet$ is the tree with only one vertex, and $\tau = [\tau_1, \ldots, \tau_m]$ represents the rooted tree obtained by grafting the roots of $\tau_1, \ldots, \tau_m \in \mathcal{T}$ to a new vertex. Trees τ_i are called the branches of τ.

We note that τ does not depend on the ordering of $\tau_1, \ldots, \tau_m$. For instance, we do not distinguish between $[\bullet, [\bullet]]$ and $[[\bullet], \bullet]$.

Definition 3.2. (Coefficients [18]) *The following coefficients are defined recursively for all trees* $\tau = [\tau_1, \dots, \tau_m] \in \mathcal{T}$*:*

$$|\tau| = 1 + \sum_{i=1}^{m} |\tau_i| \qquad (\textit{the order, i.e. the number of vertices}),$$

$$\alpha(\tau) = \frac{(|\tau| - 1)!}{|\tau_1|! \cdot \ldots \cdot |\tau_m|!} \alpha(\tau_1) \cdot \ldots \cdot \alpha(\tau_m) \frac{1}{\mu_1! \mu_2! \ldots} \qquad (\textit{Connes} - \textit{Moscovici weights}),$$

$$\sigma(\tau) = \alpha(\tau_1) \cdot \ldots \cdot \alpha(\tau_m) \cdot \mu_1! \mu_2! \cdot \ldots \qquad (\textit{symmetry}),$$

$$\gamma(\tau) = |\tau| \gamma(\tau_1) \cdot \ldots \cdot \gamma(\tau_m) \qquad (\textit{density}),$$

where the integers $\mu_1, \mu_2, \dots$ *count equal trees among* $\tau_1, \dots, \tau_m$.

Definition 3.3. (Elementary differentials [17]) *For a vector field* $f : \mathbb{R}^d \to \mathbb{R}^d$*, and for an unordered tree* $\tau = [\tau_1, \dots, \tau_m] \in \mathcal{T}$*, the so-called elementary differential is a mapping* $F_f(\tau) : \mathbb{R}^d \to \mathbb{R}^d$*, recursively defined by*

$$F_f(\bullet)(z) = f(z), \quad F_f(\tau)(z) = f^m(z)(F_f(\tau_1)(z), \dots, F_f(\tau_m)(z)).$$

Definition 3.4. (B-series [17]) *For a mapping* $a : \mathcal{T} \bigcup \{\emptyset\} \to \mathbb{R}$*, a formal series of the form*

$$B_f(a, z) = a(\emptyset) z + \sum_{\tau \in \mathcal{T}} \frac{h^{|\tau|}}{\sigma(\tau)} a(\tau) F_f(\tau)(z)$$

is called a B-series.

Theorem 3.1. (Exact solution [18]) *If* $z(t)$ *denotes the exact solution of* (2.1)*, it holds for all* $j \geq 1$,

$$\frac{1}{j!} z^{(j)}(0) = \sum_{\tau \in \mathcal{T}, |\tau| = j} \frac{1}{\sigma(\tau)\gamma(\tau)} F_f(\tau)(z_0).$$

Therefore, letting $\gamma(\emptyset) = 1$*, the exact solution of* (2.1) *is (formally) given by*

$$z(h) = B_f(\frac{1}{\gamma}, z_0).$$

3.2. Basic tools for trees

3.2.1. Partitions and skeletons

In order to manipulate trees more conveniently, it is useful to consider the set $\mathcal{OT}$ of ordered trees defined below.

Definition 3.5. (Ordered trees [18]) *The set* $\mathcal{OT}$ *of ordered trees is recursively defined by*

$$\bullet \in \mathcal{OT}, \quad (\omega_1, \dots, \omega_m) \in \mathcal{OT}, \quad \forall\ \omega_1, \dots, \omega_m \in \mathcal{OT}.$$

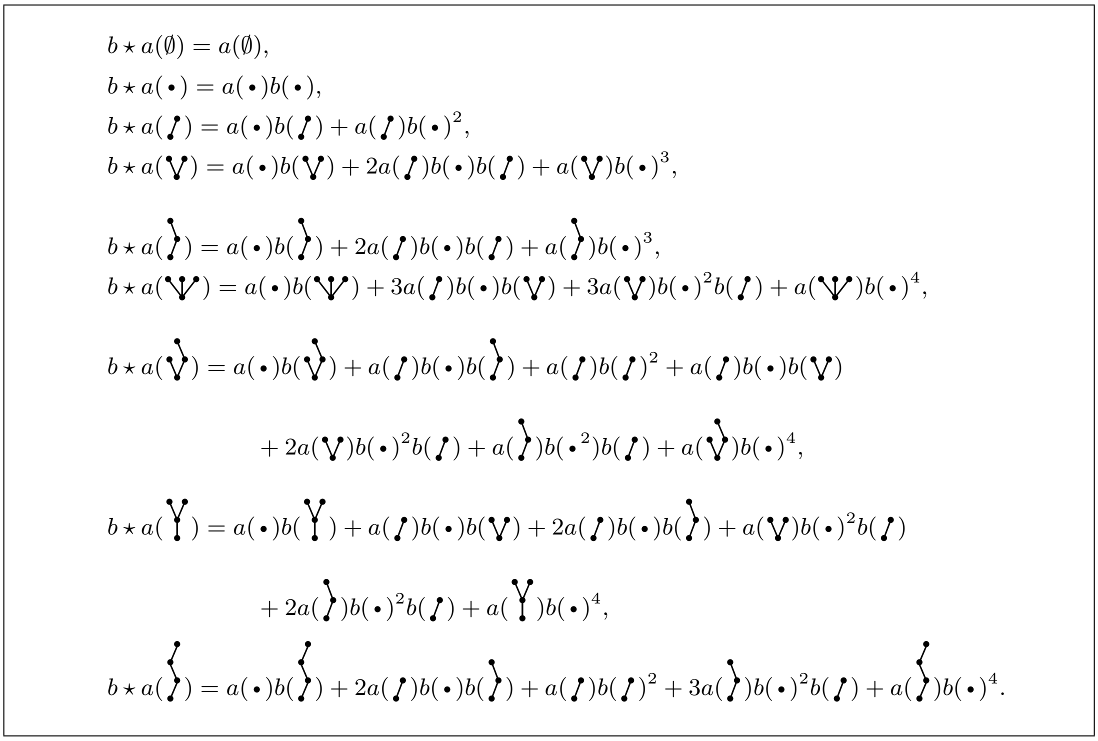
In contrast to $\mathcal{T}$*, the ordered tree* ω *depends on the ordering* $\omega_1, \dots, \omega_m$.

Neglecting the ordering, a tree $\tau \in \mathcal{T}$ can be considered as an equivalent class of ordered trees, denoted $\tau = \overline{\omega}$. Therefore, any function ψ defined on $\mathcal{T}$ (such as order, symmetry, density,...) can be extended to $\mathcal{OT}$ by putting $\psi(\omega) = \psi(\overline{\omega})$ for all $\omega \in \mathcal{OT}$. Moreover, for all $\tau \in \mathcal{T}$, we can choose a tree $\omega(\tau) \in \mathcal{OT}$ such as $\tau = \overline{\omega(\tau)}$ [8].

Definition 3.6. (Partitions of a tree [8]) *A partition p^θ of an ordered tree $\theta \in \mathcal{OT}$ is the (ordered) tree obtained from θ by replacing some of its edges by dashed ones. We denote $P(p^\theta) = \{s_1, \ldots, s_k\}$ the list of subtrees $s_i \in \mathcal{T}$ obtained from p^θ by removing dashed edges and by neglecting the ordering of each subtree. We denote $\#(p^\theta) = k$ the number of s_i's. We observe that precisely one of the s_i's contains the root of θ. We denote this distinguished tree by $R(p^\theta) \in \mathcal{T}$. We denote $P^*(p^\theta) = P(p^\theta)\backslash\{R(p^\theta)\}$ the list of s_i's that do not contain the root of θ. Eventually, the set of all partitions p^θ of θ is denoted $\mathcal{P}(\theta)$. Finally, for $\tau \in \mathcal{T}$, we put $\mathcal{P}(\tau) = \mathcal{P}(\omega(\tau))$ where $\omega(\tau) \in \mathcal{OT}$ is given in definition 3.5.*

Definition 3.7. (Skeleton of a partition [10]) *The skeleton $\chi(p^\tau) \in \mathcal{T}$ of a partition $p^\tau \in \mathcal{P}(\tau)$ of a tree $\tau \in \mathcal{T}$ is the tree obtained by replacing in p^τ each tree of $P(p^\tau)$ by a single vertex and then dashed edges by solid ones. We can notice that $|\chi(p^\tau)| = \#(p^\tau)$.*

Table 3.1: The concrete formulas of the substitution law $\star$ defined in (3.2) for trees of order ≤ 4 [8,14].



3.2.2. Substitution law

Theorem 3.2. (Substitution law [8,9,14]) *Let $a, b : \mathcal{T}\bigcup\{\emptyset\} \to \mathbb{R}$ be two mappings with $b(\emptyset) = 0$. Given a field $f : \mathbb{R}^d \to \mathbb{R}^d$, consider the (h-dependent) field $g : \mathbb{R}^d \to \mathbb{R}^d$ defined by*

$$hg(z) = B_f(b, z),$$

Then, there exists a mapping $b \star a : \mathcal{T}\bigcup\{\emptyset\} \to \mathbb{R}$ satisfying

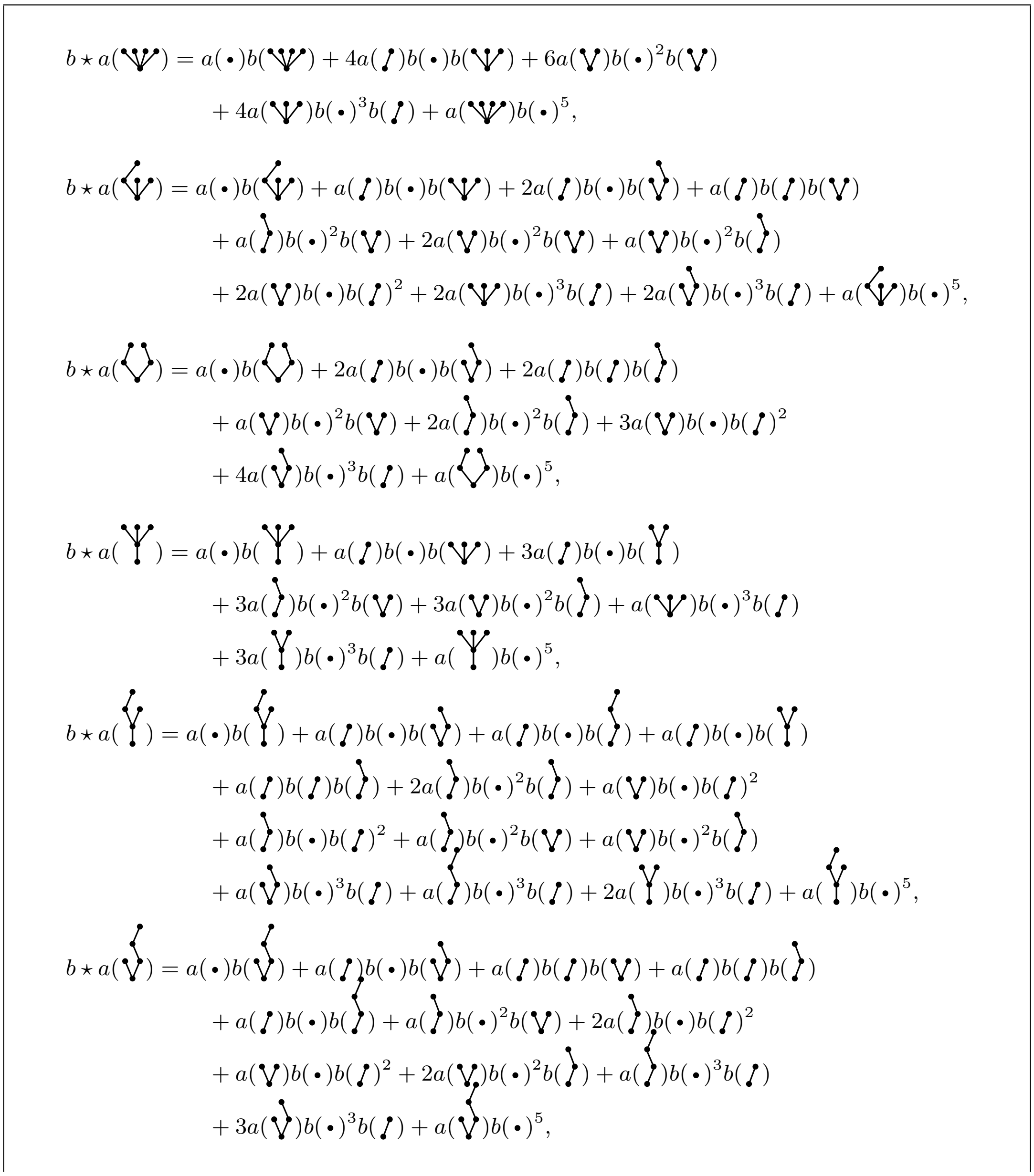
$$B_g(a, z) = B_f(b \star a, z),$$

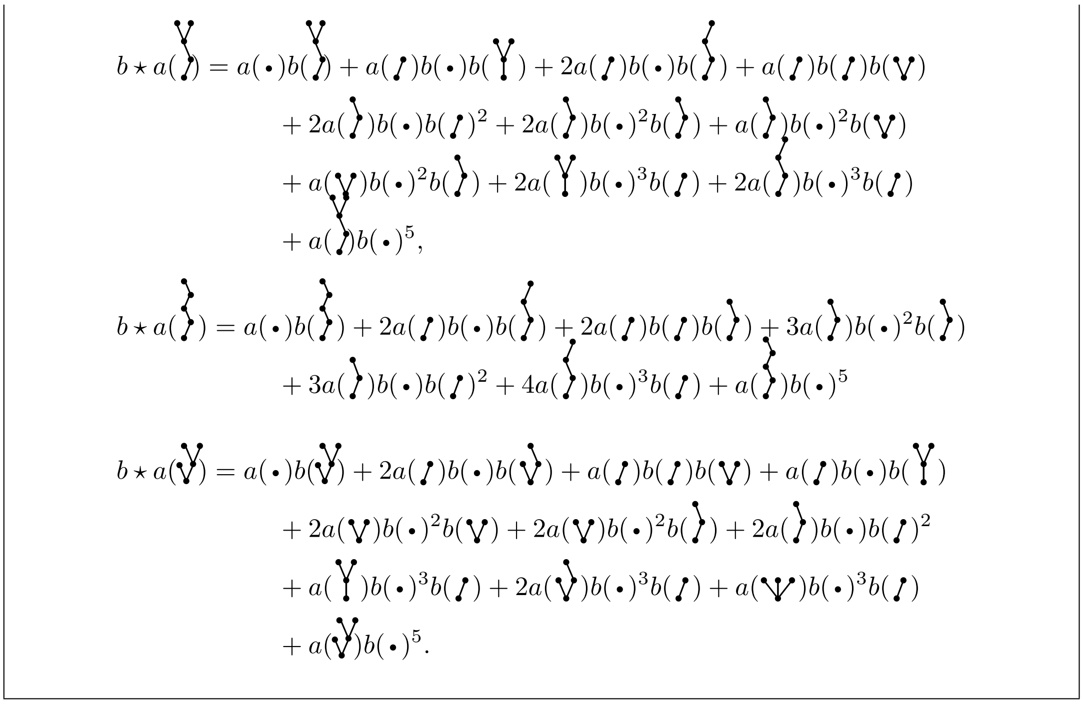
and $b\star a$ is defined by

$$b\star a(\emptyset)=a(\emptyset),\quad \forall\tau\in\mathcal{T}, b\star a(\tau)=\sum_{p^\tau\in\mathcal{P}(\tau)} a(\chi(p^\tau))\prod_{\delta\in P(p^\tau)} b(\delta). \tag{3.2}$$

In [8, 14], the concrete formulas of the substitution law for the trees of order ≤ 4 was proposed (see table 3.1). In this paper, we obtain the concrete formulas of the substitution law for the trees of order $= 5$ (see table 3.2).

Table 3.2: The concrete formulas of the substitution law $\star$ defined in (3.2) for trees of order $= 5$.





4. Sixth Order AVF Method

4.1. The second order AVF method and its B-series

Consider an ordinary differential equation

$$\dot{z} = f(z), \quad z \in \mathbb{R}^n, \quad z(t_0) = z_0, \tag{4.1}$$

and the second order AVF method [28]

$$\Phi_h^f(z_0) = z_1 = z_0 + h \int_0^1 f(\xi z_1 + (1-\xi) z_0) d\xi. \tag{4.2}$$

Theorem 4.1. *The AVF method* (4.2) *can be expanded into a B-series*

$$\Phi_h^f(z_0) = B_f(a, z_0) = a(\emptyset) z_0 + \sum_{\tau \in \mathcal{T}} \frac{h^{|\tau|}}{\sigma(\tau)} a(\tau) F_f(\tau)(z_0), \tag{4.3}$$

where $a(\emptyset) = a(\bullet) = 1$, *and for all* $\tau = [\tau_1, \ldots, \tau_m] \in \mathcal{T}$,

$$a(\tau) = \frac{1}{m+1} a(\tau_1) \cdots a(\tau_m).$$

Proof. We develop the derivatives of (4.2), by Leibniz's rule, and obtain

$$\begin{aligned} z_1^{(q)} &= \left[h \int_0^1 f(\xi z_1 + (1-\xi) z_0) d\xi \right]^{(q)} \\ &= h \left[\int_0^1 f(\xi z_1 + (1-\xi) z_0) d\xi \right]^{(q)} + q \left[\int_0^1 f(\xi z_1 + (1-\xi) z_0) d\xi \right]^{q-1}. \end{aligned}$$

This gives, for $h=0$, $z^{(q)} := z_1^{(q)}|_{h=0} = q[\int_0^1 f(\xi z_1 + (1-\xi)z_0)d\xi]^{q-1}|_{h=0}$, $q \geq 1$, and considering $z_1|_{h=0} = z_0$, we can obtain

$$\dot{z} = \int_0^1 f(\xi z_0 + (1-\xi)z_0)d\xi = 1 \cdot 1 \cdot 1 \cdot f(z_0), \tag{4.4a}$$

$$\ddot{z} = 2\int_0^1 \xi f'(\xi z_0 + (1-\xi)z_0)\dot{z}d\xi = f(z_0) = 2 \cdot 1 \cdot \frac{1}{2}f'(z_0)\dot{z}, \tag{4.4b}$$

$$z^{(3)} = 3 \cdot (1 \cdot \frac{1}{3}f''(z_0)(\dot{z},\dot{z}) + 1 \cdot \frac{1}{2}f'(z_0)\ddot{z}), \tag{4.4c}$$

and so on. We now insert in (4.4a) recursively the computed derivatives $\dot{z}, \ddot{z}, \ldots$ into the right side of the subsequent formulas. Letting $f^{(q)} := f^{(q)}(z_0)$ and $F(\tau) = F_f(\tau)(z_0)$, we can obtain

$$\begin{aligned} \dot{z} &= 1 \cdot 1 \cdot 1 \cdot f = \gamma(\bullet)\alpha(\bullet)a(\bullet)F(\bullet), \\ \ddot{z} &= 2 \cdot 1 \cdot \frac{1}{2}f'f = \gamma([\bullet])\alpha([\bullet])a([\bullet])F([\bullet]), \\ z^{(3)} &= 3 \cdot 1 \cdot \frac{1}{3}f''(f,f) + (2 \cdot 3) \cdot 1 \cdot (\frac{1}{2} \cdot \frac{1}{2})f'f'f \\ &= \gamma([\bullet,\bullet])\alpha([\bullet,\bullet])a([\bullet,\bullet])F([\bullet,\bullet]) + \gamma([[\bullet]])\alpha([[\bullet]])a([[\bullet]])F([[\bullet]]), \end{aligned} \tag{4.5}$$

and so on. For all $\tau = [\tau_1, \ldots, \tau_m] \in \mathcal{T}$, letting $\alpha = \frac{(|\tau|-1)!}{|\tau_1|! \cdot \ldots \cdot |\tau_m|!}\frac{1}{\mu_1!\mu_2!\ldots}$, where the integers $\mu_1, \mu_2, \ldots$ count equal trees among $\tau_1, \ldots, \tau_m$, we can obtain

$$\begin{aligned} & \gamma(\tau)\alpha(\tau)a(\tau)F(\tau) \\ = \ & |\tau|\int_0^1 \alpha\xi^m f^m(z_0)(\gamma(\tau_1)\alpha(\tau_1)a(\tau_1)F(\tau_1), \ldots, \gamma(\tau_m)\alpha(\tau_m)a(\tau_m)F(\tau_m))d\xi \\ = \ & [|\tau|\gamma(\tau_1) \cdot \ldots \cdot \gamma(\tau_m)] \cdot [\alpha\alpha(\tau_1) \cdot \ldots \cdot \alpha(\tau_m)] \\ & \cdot \left[\frac{1}{m+1}a(\tau_1)\cdots a(\tau_m)\right] \cdot f^m(z_0)(F(\tau_1), \ldots, F(\tau_m)) \\ = \ & \gamma(\tau)\alpha(\tau)\left[\frac{1}{m+1}a(\tau_1)\cdots a(\tau_m)\right]F(\tau). \end{aligned}$$

So we have

$$z^{(q)} = \sum_{\tau \in \mathcal{T}, |\tau| = q} \gamma(\tau)\alpha(\tau)a(\tau)F(\tau),$$

where $a(\bullet) = 1$, and

$$\text{for all } \tau = [\tau_1, \ldots, \tau_m] \in \mathcal{T}, \quad a(\tau) = \frac{1}{m+1}a(\tau_1)\cdots a(\tau_m).$$

Letting $a(\emptyset) = 1$, and considering $\sigma(\tau) = \frac{|\tau|!}{\alpha(\tau)\gamma(\tau)}$, we obtain

$$\Phi_h^f(z_0) = z_1 = a(\emptyset)z_0 + \sum_{\tau \in \mathcal{T}} \frac{h^{|\tau|}}{\sigma(\tau)}a(\tau)F_f(\tau) = B_f(a, z_0).$$

The proof is completed. □

The B-series (4.3) can be rewritten as

$$\begin{aligned}\Phi_h^f(z_0) =& z_0 + hF(\bullet) + \frac{1}{2}h^2F([\bullet]) + h^3(\frac{1}{2\cdot 3}F([\bullet,\bullet]) + \frac{1}{4}F([[\bullet]])) + h^4(\frac{1}{4\cdot 6}F([\bullet,\bullet,\bullet]) + \frac{1}{6}F([[\bullet],\bullet])\\ &+ \frac{1}{2\cdot 6}F([[\bullet,\bullet]]) + \frac{1}{8}F([[[\bullet]]])) + h^5(\frac{1}{5\cdot 24}F([\bullet,\bullet,\bullet,\bullet]) + \frac{1}{2\cdot 8}F([[\bullet],\bullet,\bullet]) + \frac{1}{2\cdot 12}F([[\bullet],[\bullet]])\\ &+ \frac{1}{6\cdot 8}F([[\bullet,\bullet,\bullet]]) + \frac{1}{12}F([[[\bullet],\bullet]]) + \frac{1}{12}F([[[\bullet]],\bullet]) + \frac{1}{2\cdot 12}F([[[\bullet,\bullet]]]) + \frac{1}{16}F([[[[\bullet]]]]) + \frac{1}{2\cdot 9}F([[\bullet,\bullet],\bullet])) + \dots\end{aligned}$$

4.2. Sixth order AVF method

Let $a : \mathcal{T}\bigcup\{\emptyset\} \to \mathbb{R}$ be a mapping satisfying $a(\emptyset) = 1$, $a(\bullet) \neq 0$, and let $f : \mathbb{R}^d \to \mathbb{R}^d$ be a field. We consider here the numerical flow Φ_h^g, where $g : \mathbb{R}^d \to \mathbb{R}^d$ denotes the modified field of f, whose B-series expansion is

$$\Phi_h^g(z) = B_g(a, z).$$

The fundamental idea of obtaining sixth order AVF method consists in interpreting the numerical solution $z_1 = \Phi_h^g$ of the initial value problem $z(0) = z_0$, $\dot{z} = g(z)$ as the exact solution of a modified differential equation $\dot{z} = f(z)$ [13, 14].

Theorem 4.2. *If $z_1 = \Phi_h^f(z_0)$, which is a numerical solution of (4.1), can be expanded into a B-series*

$$\Phi_h^f(z_0) = z_1 = B_f(a, z_0), \quad a(\emptyset) = 1,$$

and $b : \mathcal{T}\bigcup\{\emptyset\} \to \mathbb{R}$ be a mapping with $b(\emptyset) = 0$ satisfying

$$\forall\tau \in \mathcal{T}, \quad b \star a(\tau) = \frac{1}{\gamma(\tau)}, \tag{4.6}$$

then we can obtain a new numerical solution $\Phi_h^g(z_0) = B_g(a, z_0)$, satisfying

$$\Phi_h^g(z_0) = \varphi_h^f(z_0),$$

where $\varphi_h^f(z_0)$ denotes the exact solution of (4.1), and $g : \mathbb{R}^n \to \mathbb{R}^n$ is a (h-dependent) field defined by

$$hg(y) = B_f(b, y).$$

Proof. From Theorem 3.1, $\varphi_h^f(z_0) = B_f(\frac{1}{\gamma}, z_0)$. And from Theorem 3.2, we obtain

$$\Phi_h^g(z_0) = B_g(a, z_0) = B_f(b \star a, z_0) = B_f(\frac{1}{\gamma}, z_0) = \varphi_h^f(z_0).$$

The proof is completed. □

Letting $e(\tau) = \frac{1}{\gamma(\tau)}$, we calculate $b(\tau)$ defined in (4.6) for trees of order ≤ 2 as follows:

$$\begin{aligned}&|\tau| = 1, \quad a(\bullet)b(\bullet) = e(\bullet), \quad a(\bullet) = 1, e(\bullet) = 1, && b(\bullet) = 1,\\ &|\tau| = 2, \quad a(\bullet)b([\bullet]) + a([\bullet])b(\bullet)^2 = e([\bullet]), a([\bullet]) = \frac{1}{2}, e([\bullet]) = \frac{1}{2}, && b([\bullet]) = 0.\end{aligned}$$

In the same way, we can obtain $b(\tau)$ for trees of order ≤ 5 (see table 4.1) and $b(\tau) = 0$ for trees of order $= 6$.

Then we obtain the exact modified field $g(z_0) = \frac{1}{h}B_f(b, z_0)$ and the sixth order modified field

$$\breve{g}(z_0) = f(z_0) - \frac{h^2}{12}F(\ ) + \frac{h^4}{720}[6F(\ ) + 4F(\ ) + F(\ ) + 4F(\ ) + F(\ )$$

$$+ F(\ ) + 3F(\ ) + 8F(\ )],$$

satisfying $g(z_0) = \breve{g}(z_0) + \mathcal{O}(h^6)$ and $\Phi_h^g(z_0) = \varphi_h^f(z_0)$. And considering $\Phi_h^{\breve{g}}(z_0) = z_1 = z_0 + h\int_0^1 \breve{g}(\xi z_1 + (1-\xi)z_0)d\xi$, we have

$$z_1 - z_0 = h\int_0^1 f(\xi z_1 + (1-\xi)z_0)d\xi + \mathcal{O}(h^3).$$

Let $\hat{z} := \frac{z_1+z_0}{2}$, $f^{(q)} := f^{(q)}(\hat{z})$, $F := \int_0^1 f(\xi z_1 + (1-\xi)z_0)d\xi$ and $\eta = \xi - \frac{1}{2}$.

Considering $|\tau| = 1$, we have $\tau = \bullet$ and

$$\int_0^1 F_f(\tau)(\xi z_1 + (1-\xi)z_0)d\xi = \int_0^1 f(\xi z_1 + (1-\xi)z_0)d\xi = F.$$

We consider $\int_{-\frac{1}{2}}^{\frac{1}{2}} \eta d\eta = \int_{-\frac{1}{2}}^{\frac{1}{2}} \eta^3 d\eta = 0$, $\int_{-\frac{1}{2}}^{\frac{1}{2}} \eta^2 d\eta = \frac{1}{12}$. For $|\tau| = 3$, we have $\tau =$ and

$$z_1 - z_0 = h\int_{-\frac{1}{2}}^{\frac{1}{2}} f(\hat{z} + \eta(z_1 - z_0))d\eta + \mathcal{O}(h^3) = hF + \mathcal{O}(h^3) \tag{4.7}$$

$$or \quad z_1 - z_0 = h\int_{-\frac{1}{2}}^{\frac{1}{2}} [f(\hat{z}) + \eta f'(\hat{z})(z_1 - z_0) + \mathcal{O}(h^2)]d\eta + \mathcal{O}(h^3) \tag{4.8}$$

$$= hf(\hat{z}) + \mathcal{O}(h^3) = hf + \mathcal{O}(h^3)$$

$$or \quad z_1 - z_0 = \mathcal{O}(h). \tag{4.9}$$

So we can obtain

$$\begin{aligned}
&\int_{-\frac{1}{2}}^{\frac{1}{2}} F_f(\ )(\hat{z} + \eta(z_1 - z_0))d\eta \\
=&\int_{-\frac{1}{2}}^{\frac{1}{2}} f'(\hat{z} + \eta(z_1 - z_0))f'(\hat{z} + \eta(z_1 - z_0))f(\hat{z} + \eta(z_1 - z_0))d\eta \\
=&\int_{-\frac{1}{2}}^{\frac{1}{2}} [f'(\hat{z}) + \eta f''(\hat{z})(z_1 - z_0) + \frac{\eta^2}{2!}f'''(\hat{z})(z_1 - z_0, z_1 - z_0) \\
&+ \frac{\eta^3}{3!}f^{(4)}(\hat{z})(z_1 - z_0, z_1 - z_0, z_1 - z_0) + \mathcal{O}(h^4)] \cdot [f'(\hat{z}) + \eta f''(\hat{z})(z_1 - z_0) \\
&+ \frac{\eta^2}{2!}f'''(\hat{z})(z_1 - z_0, z_1 - z_0) + \frac{\eta^3}{3!}f^{(4)}(\hat{z})(z_1 - z_0, z_1 - z_0, z_1 - z_0) + \mathcal{O}(h^4)] \\
&\cdot f(\hat{z} + \eta(z_1 - z_0))d\eta
\end{aligned}$$

$$
\begin{aligned}
=&\int_{-\frac{1}{2}}^{\frac{1}{2}}\{f'(\hat z)f'(\hat z)f(\hat z+\eta(z_1-z_0))+f'(\hat z)[\eta f''(\hat z)(z_1-z_0)+\frac{\eta^2}{2!}f'''(\hat z)(z_1-z_0,z_1-z_0)\\
&+\frac{\eta^3}{3!}f^{(4)}(\hat z)(z_1-z_0,z_1-z_0,z_1-z_0)]\cdot[f(\hat z)+\eta f'(\hat z)(z_1-z_0)\\
&+\frac{\eta^2}{2!}f''(\hat z)(z_1-z_0,z_1-z_0)+\mathcal{O}(h^3)]+[\eta f''(\hat z)(z_1-z_0)+\frac{\eta^2}{2!}f'''(\hat z)(z_1-z_0,z_1-z_0)\\
&+\frac{\eta^3}{3!}f^{(4)}(\hat z)(z_1-z_0,z_1-z_0,z_1-z_0)]\cdot[f'(\hat z)+\eta f''(\hat z)(z_1-z_0)\\
&+\frac{\eta^2}{2!}f'''(\hat z)(z_1-z_0,z_1-z_0)+\frac{\eta^3}{3!}f^{(4)}(\hat z)(z_1-z_0,z_1-z_0,z_1-z_0)]\\
&\cdot[f(\hat z)+\eta f'(\hat z)(z_1-z_0)+\frac{\eta^2}{2!}f''(\hat z)(z_1-z_0,z_1-z_0)+\mathcal{O}(h^3)]\}d\eta+\mathcal{O}(h^4)\\
=&f'(\hat z)f'(\hat z)\int_{-\frac{1}{2}}^{\frac{1}{2}}f(\hat z+\eta(z_1-z_0))d\eta+\int_{-\frac{1}{2}}^{\frac{1}{2}}[\eta^2f'(\hat z)f''(\hat z)(z_1-z_0,f'(\hat z)(z_1-z_0))\\
&+\frac{\eta^2}{2!}f'(\hat z)f'''(\hat z)(z_1-z_0,z_1-z_0,f(\hat z))+\eta^2f''(\hat z)(z_1-z_0,f'(\hat z)f'(\hat z)(z_1-z_0))\\
&+\eta^2f''(\hat z)(z_1-z_0,f''(\hat z)(z_1-z_0,f(\hat z)))+\frac{\eta^2}{2!}f'''(\hat z)(z_1-z_0,z_1-z_0,f'(\hat z)f(\hat z))]d\eta+\mathcal{O}(h^4)\\
=&f'f'F+\frac{h^2}{12}[f'f''(f'f,F)+f''(f'f'f,F)+f''(f''(f,f),F)+\frac{1}{2}f'f'''(f,f,F)\\
&+\frac{1}{2}f'''(f'f,f,F)]+\mathcal{O}(h^4).
\end{aligned}
$$

Considering $|\tau|=5$, we have

$$
\begin{aligned}
&\int_{-\frac{1}{2}}^{\frac{1}{2}}F_f(\ )(\hat z+\eta(z_1-z_0))d\eta\\
=&\int_{-\frac{1}{2}}^{\frac{1}{2}}f'(\hat z+\eta(z_1-z_0))f'(\hat z+\eta(z_1-z_0))f'(\hat z+\eta(z_1-z_0))f'(\hat z+\eta(z_1-z_0))f(\hat z+\eta(z_1-z_0))d\eta\\
=&\int_{-\frac{1}{2}}^{\frac{1}{2}}[f'(\hat z)+\eta f''(\hat z)(z_1-z_0)+\mathcal{O}(h^2)]\cdot[f'(\hat z)+\eta f''(\hat z)(z_1-z_0)+\mathcal{O}(h^2)]\\
&\cdot[f'(\hat z)+\eta f''(\hat z)(z_1-z_0)+\mathcal{O}(h^2)]\cdot[f'(\hat z)+\eta f''(\hat z)(z_1-z_0)+\mathcal{O}(h^2)]\\
&\cdot[f(\hat z)+\eta f'(\hat z)(z_1-z_0)+\mathcal{O}(h^2)]d\eta\\
=&\int_{-\frac{1}{2}}^{\frac{1}{2}}f'(\hat z)f'(\hat z)f'(\hat z)f'(\hat z)f(\hat z+\eta(z_1-z_0))d\eta+\mathcal{O}(h^2)\\
=&f'f'f'f'F+\mathcal{O}(h^2):=A(\ )F+\mathcal{O}(h^2),
\end{aligned}
$$

where the coefficient matrix $A(\ )$ is defined by $f'f'f'f'F=A(\ )F$. In the same way, we can obtain

$$
\begin{aligned}
&\int_{-\frac{1}{2}}^{\frac{1}{2}}F_f(\ )(\hat z+\eta(z_1-z_0))d\eta=\ f''(f''(F,f),f)+\mathcal{O}(h^2):=A(\ )F+\mathcal{O}(h^2),\\
&\int_{-\frac{1}{2}}^{\frac{1}{2}}F_f(\ )(\hat z+\eta(z_1-z_0))d\eta=\ f'f'f''(F,f)+\mathcal{O}(h^2):=A(\ )F+\mathcal{O}(h^2),
\end{aligned}
$$

$$\int_{-\frac{1}{2}}^{\frac{1}{2}} F_f(\ )(\hat{z}+\eta(z_1-z_0))d\eta = f''(f'f'F,f)+\mathcal{O}(h^2) := A(\ )F+\mathcal{O}(h^2),$$
$$\int_{-\frac{1}{2}}^{\frac{1}{2}} F_f(\ )(\hat{z}+\eta(z_1-z_0))d\eta = f'f'''(F,f,f)+\mathcal{O}(h^2) := A(\ )F+\mathcal{O}(h^2),$$
$$\int_{-\frac{1}{2}}^{\frac{1}{2}} F_f(\ )(\hat{z}+\eta(z_1-z_0))d\eta = f'''(f'F,f,f)+\mathcal{O}(h^2) := A(\ )F+\mathcal{O}(h^2),$$
$$\int_{-\frac{1}{2}}^{\frac{1}{2}} F_f(\ )(\hat{z}+\eta(z_1-z_0))d\eta = f''(f'F,f'f)+\mathcal{O}(h^2) := A(\ )F+\mathcal{O}(h^2),$$
$$\int_{-\frac{1}{2}}^{\frac{1}{2}} F_f(\ )(\hat{z}+\eta(z_1-z_0))d\eta = f'f''(F,f'f)+\mathcal{O}(h^2) := A(\ )F+\mathcal{O}(h^2).$$

So we have

$$\begin{aligned}
&\int_0^1 \breve{g}(\xi z_1+(1-\xi)z_0)d\xi = \int_{-\frac{1}{2}}^{\frac{1}{2}} \breve{g}(\hat{z}+\eta(z_1-z_0))d\eta \\
=& \Big\{ I - \frac{h^2}{12}A(\ ) - \frac{h^4}{720}[5A(\ )+5A(\ )+5A(\ )+\frac{5}{2}A(\ )+\frac{5}{2}A(\ )] \\
&+ \frac{h^4}{720}[6A(\ )+4A(\ )+A(\ )+4A(\ )+A(\ )+A(\ )+3A(\ )+8A(\ )]\Big\}F+\mathcal{O}(h^6) \\
=& \Big\{ I - \frac{h^2}{12}A(\ ) + \frac{h^4}{720}[6A(\ )-A(\ )+A(\ )-A(\ )-\frac{3}{2}A(\ )-\frac{3}{2}A(\ ) \\
&+3A(\ )+3A(\ )]\Big\}F+\mathcal{O}(h^6).
\end{aligned}$$

We obtain the sixth order AVF method

$$\begin{aligned}
\Phi_h(z_0) = z_1 &= c(\emptyset)z_0 + \left(\sum_{\tau\in\mathcal{T}} h^{|\tau|}c(\tau)A(\tau)\right)\int_0^1 f(\xi z_1+(1-\xi)z_0)d\xi \\
&= z_0 + \Big\{ hI - \frac{h^3}{12}A(\ ) + \frac{h^5}{720}\Big[6A(\ )-A(\ )+A(\ )-A(\ )-\frac{3}{2}A(\ ) \\
&\quad -\frac{3}{2}A(\ )+3A(\ )+3A(\ )\Big]\Big\}\int_0^1 f(\xi z_1+(1-\xi)z_0)d\xi, \qquad (4.10)
\end{aligned}$$

where $A(\tau)=A(\tau)(\frac{z_1+z_0}{2})$ are coefficient matrices of $F=\int_0^1 f(\xi z_1+(1-\xi)z_0)d\xi$, and $c(\tau)=0$ for all $|\tau|\geq 6$.

Theorem 4.3. *The sixth order AVF method $\Phi_h(z_0)$ satisfies*

$$||\Phi_h(z_0)-\varphi_h^f(z_0)|| = \mathcal{O}(h^7).$$

Proof. Now we have

$$\Phi_h^{\breve{g}}(z_0)=\Phi_h(z_0)+\mathcal{O}(h^7), \ \textit{and} \quad \Phi_h^g(z_0)=\varphi_h^f(z_0),$$

so we can obtain

$$
\begin{aligned}
&||\Phi_h(z_0) - \varphi_h^f(z_0)|| = ||\Phi_h(z_0) - \Phi_h^g(z_0)|| = ||(\Phi_h^{\breve{g}}(z_0) + \mathcal{O}(h^7)) - \Phi_h^g(z_0)|| \\
&= ||(z_1 - z_0) + h\int_{-1}^{1} [\breve{g}(\xi z_1 + (1-\xi)z_0)) - g(\xi z_1 + (1-\xi)z_0))]d\xi + \mathcal{O}(h^7)|| \\
&= \mathcal{O}(h^7).
\end{aligned}
$$

The proof is complete. □

Theorem 4.4. *If* (4.1) *is a Hamiltonian system, the sixth order AVF method* $\Phi_h(z_0)$ *can preserve the discrete energy of it, i.e.*

$$\frac{1}{h}(H(z_1) - H(z_0)) = 0.$$

Proof. (4.1) can be rewritten as

$$\dot{z} = f(z) = S\nabla H(z),$$

where S denotes an arbitrary constant skew-symmetric matrix and H denotes the Hamiltonian. So the sixth order AVF method (4.10) can be rewritten as

$$\frac{z_1 - z_0}{h} = \tilde{S}\int_0^1 \nabla H(\xi z_1 + (1-\xi)z_0))d\xi, \tag{4.11}$$

where

$$
\begin{aligned}
\tilde{S} = \ &\{I - \frac{h^2}{12}A(\ ) + \frac{h^4}{720}[6A(\ ) - A(\ ) + A(\ ) - A(\ ) \\
&- \frac{3}{2}A(\ ) - \frac{3}{2}A(\ ) + 3A(\ ) + 3A(\ )]\}S,
\end{aligned}
$$

is a skew-symmetric matrix. It is given by

$$
\begin{aligned}
&IS = S, \quad A(\ )S = S\mathcal{H}S\mathcal{H}S, \quad A(\ )S = S\mathcal{H}S\mathcal{H}S\mathcal{H}S\mathcal{H}S, \quad A(\ )S = S\mathcal{T}S\mathcal{T}S, \\
&A(\ )S = S\mathcal{H}S\mathcal{H}S\mathcal{T}S, \quad A(\ )S = S\mathcal{T}S\mathcal{H}S\mathcal{H}S, \quad A(\ )S = S\mathcal{H}S\mathcal{L}S, \\
&A(\ )S = S\mathcal{L}S\mathcal{H}S, \quad A(\ )S = S\mathcal{R}S\mathcal{H}S, \quad A(\ )S = S\mathcal{H}S\mathcal{R}S,
\end{aligned}
$$

with the symmetric matrices $\mathcal{H}(z)$, $\mathcal{T}(z)$, $\mathcal{L}(z)$ and $\mathcal{R}(z)$ being given by

$$
\begin{aligned}
&\mathcal{H}_{ij} := \frac{\partial^2 H}{\partial z_i \partial z_j}, \quad \mathcal{T}_{ij} := \frac{\partial^3 H}{\partial z_i \partial z_j \partial z_k} S^{kl} \frac{\partial H}{\partial z_l}, \\
&\mathcal{L}_{ij} := \frac{\partial^4 H}{\partial z_i \partial z_j \partial z_k \partial z_l} S^{km} \frac{\partial H}{\partial z_m} S^{ln} \frac{\partial H}{\partial z_n}, \quad \mathcal{R}_{ij} := \frac{\partial^3 H}{\partial z_i \partial z_j \partial z_k} S^{kl} \frac{\partial^2 H}{\partial z_l \partial z_m} S^{mn} \frac{\partial H}{\partial z_n},
\end{aligned}
$$

and

$$(\mathcal{SHSHSTS} - \mathcal{STSHSHS})^T = \mathcal{STSHSHS} - \mathcal{SHSHSTS} = -(\mathcal{SHSHSTS} - \mathcal{STSHSHS}),$$
$$(\mathcal{SHSLS} + \mathcal{SLSHS})^T = -\mathcal{SLSHS} - \mathcal{SHSLS} = -(\mathcal{SHSLS} + \mathcal{SLSHS}),$$
$$(\mathcal{SRSHS} + \mathcal{SHSRS})^T = -\mathcal{SHSRS} - \mathcal{SRSHS} = -(\mathcal{SRSHS} + \mathcal{SHSRS}).$$

So $\tilde{S}$ is also a skew-symmetric matrix and the Hamiltonian H is conserved at every time step. The proof is complete. □

Table 4.1: Coefficients $\sigma(\tau)$, $\gamma(\tau)$, $a(\tau)$, $b(\tau)$ and $c(\tau)$ for trees of order ≤ 5.

τ	$\emptyset$	$\bullet$							
$\sigma(\tau)$		1	1	2	1	6	1	2	1
$\gamma(\tau)$		1	2	3	6	4	8	12	24
$a(\tau)$	1	1	1/2	1/3	1/4	1/4	1/6	1/6	1/8
$b(\tau)$	0	1	0	0	-1/12	0	0	0	0
$c(\tau)$	1	1	0	0	-1/12	0	0	0	0

τ									
$\sigma(\tau)$	24	2	2	6	1	1	2	1	2
$\gamma(\tau)$	5	10	20	20	40	30	60	120	15
$a(\tau)$	1/5	1/8	1/12	1/8	1/12	1/12	1/12	1/16	1/9
$b(\tau)$	0	1/360	1/120	1/120	1/90	1/180	1/360	1/120	1/90
$c(\tau)$	0	-1/480	1/240	-1/480	1/240	-1/720	1/720	1/120	-1/720

Remark 4.1. In the same way, we can also obtain a fifth order method

$$\tilde{\Phi}_h(z_0) = z_1 = \; z_0 + \{hI - \frac{h^3}{12}A(\;) - \frac{h^4}{24}[A(\;) + A(\;)] + \frac{h^5}{720}[6A(\;) - 16A(\;) + A(\;) - 16A(\;) - 9A(\;) - 9A(\;) + 3A(\;) - 12A(\;)]\} \int_0^1 f(\xi z_1 + (1-\xi)z_0))d\xi, \qquad (4.12)$$

where $A(\tau) = A(\tau)(z_0)$ are coefficient matrices of $F = \int_0^1 f(\xi z_1 + (1-\xi)z_0))d\xi$. This method is of order five, but it can not preserve the Hamiltonian, because $\tilde{S}$ which is the corresponding total coefficient matrix of F turns out to be not skew-symmetric when expanding $F_f(\tau)(\xi z_1+(1-\xi)z_0)$ in a Taylor series about $z = z_0$.

Remark 4.2. Omitting the items containing h^5 in (4.10), the method

$$z_1 = z_0 + \left(hI - \frac{h^3}{12}A(\;)\right) \int_0^1 f(\xi z_1 + (1-\xi)z_0))d\xi$$

is the fourth order method (2.4), where $A(\;)$ is defined in (4.10).

Remark 4.3. We recall that a method $z_1 = \Phi_h(z_0)$ is symmetric if exchanging $z_0 \longleftrightarrow z_1$ and $h \longleftrightarrow -h$ leaves the method unaltered [17]. Letting $\eta = 1 - \xi$ in (4.10), we have

$$\int_0^1 f(\eta z_1 + (1-\eta) z_0) d\eta = \int_0^1 f(\xi z_0 + (1-\xi) z_1) d\xi. \tag{4.13}$$

It implies that the sixth order AVF method (4.10) is a symmetric method.

Remark 4.4. Considering the trees of order ≤ 4 (see [8, 9, 14]) in (4.10), the method is just the fourth order AVF method (2.4) (see [28]).

5. Numerical Simulations

We here report a few numerical experiments, in order to illustrate our results presented in the previous section.

The relative energy error at $t = t_j$ is defined as

$$RH_j = \frac{|H_j - H_0|}{|H_0|},$$

where H_j denotes the Hamiltonian at $t = t_j$, $j = 0, 1, \ldots, N$. The solution error at $t = t_N$ is defined as

$$error(h) = ||z_N - z(t_N)||_\infty,$$

where h is the time step. We define

$$order = \log_2 \left(\frac{error(h)}{error(h/2)} \right),$$

and recall that for a p-order accurate scheme

$$\frac{error(h)}{error(h/2)} \approx 2^p \ (h \to 0).$$

5.1. Numerical example 1

First, we consider a nonlinear Hamiltonian system

$$\dot{z} = J^{-1} \nabla H, \quad H(z) = \frac{1}{4}(p^2 + q^2)^2, \tag{5.1a}$$

$$z = \begin{pmatrix} p \\ q \end{pmatrix}, \quad z_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{5.1b}$$

which has the exact solution

$$p(t) = \cos(t), \quad q(t) = \sin(t).$$

We can obtain the sixth order AVF method of (5.1)

$$\begin{pmatrix} p_1 \\ q_1 \end{pmatrix} = \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} + \Big\{ hI - \frac{h^3}{12} A(\;) + \frac{h^5}{720} [6A(\;) - A(\;) + A(\;) - A(\;)$$

$$- \frac{3}{2} A(\;) - \frac{3}{2} A(\;) + 3A(\;) + 3A(\;)] \Big\} F,$$

Table 5.1: The convergence order of the sixth order AVF method with different time steps, $h_1 = 0.2, h_2 = 0.1, h_3 = 0.05, h_4 = 0.025, h_5 = 0.0125$.

Order	$\log_2\left(\frac{error(h_1)}{error(h_2)}\right)$	$\log_2\left(\frac{error(h_2)}{error(h_3)}\right)$	$\log_2\left(\frac{error(h_3)}{error(h_4)}\right)$	$\log_2\left(\frac{error(h_4)}{error(h_5)}\right)$
$t = 1$	5.9453	5.9864	5.9966	5.9987
$t = 2$	5.9453	5.9864	5.9966	5.9991
$t = 3$	5.9453	5.9864	5.9966	5.9984
$t = 4$	5.9452	5.9864	5.9966	5.9982
$t = 5$	5.9453	5.9864	5.9966	5.9985
$t = 200$	5.9459	5.9864	5.9985	5.9869
$t = 4000$	5.9436	5.9848	6.0295	5.9761

where $A(\tau) = A(\tau)(\frac{z_1+z_0}{2})$ are coefficient matrices of $F = \int_0^1 f(\xi z_1 + (1-\xi)z_0))d\xi$, and

$$F = \begin{pmatrix} F^1 \\ F^2 \end{pmatrix} = \begin{pmatrix} \int_0^1 f^1(\xi z_1 + (1-\xi)z_0))d\xi \\ \int_0^1 f^2(\xi z_1 + (1-\xi)z_0))d\xi \end{pmatrix}$$

$$= \begin{pmatrix} -\frac{1}{6}[H_q(z_1) + 4H_q(\frac{z_1+z_0}{2}) + H_q(z_0)] \\ \frac{1}{6}[H_p(z_1) + 4H_p(\frac{z_1+z_0}{2}) + H_p(z_0)] \end{pmatrix}.$$

To examine the performance of the proposed method in a long time computing, the problem is solved by the sixth order AVF method (AVF6) and a sixth order Runge-Kutta method with $\nu = 1/10$ (RK6) [23] till time $t = 4000$. Table 5.1 shows the convergence order of the AVF6 method with different time steps. We can conclude that the AVF6 method is order of six, supporting Theorem 4.3.

Figs. 5.1 and 5.2 provide the numerical solutions obtained by using the AVF6 method and the RK6 method from $t = 0$ to $t = 4000$, respectively. As can be seen from Figs. 5.1a and 5.2a, the solution errors of the AVF6 method grow linearly and are less than the errors of the RK6 method. The linear error growth and Table 5.1 indicate that there exist a positive constant C such that $||z_j - z(t_j)||_\infty \leq C t_j h^p$ for $j = 0, 1, \ldots, N$, where $p = 6$ is the order of the AVF6 method. Figs. 5.1b and 5.2b show the relative energy errors of the two methods respectively. Comparing with the RK6 method, the AVF6 method can conserve the Hamiltonian up to round-off error in long time, supporting Theorem 4.4. The relative energy errors look like to show slow linear increase because of the iteration errors.

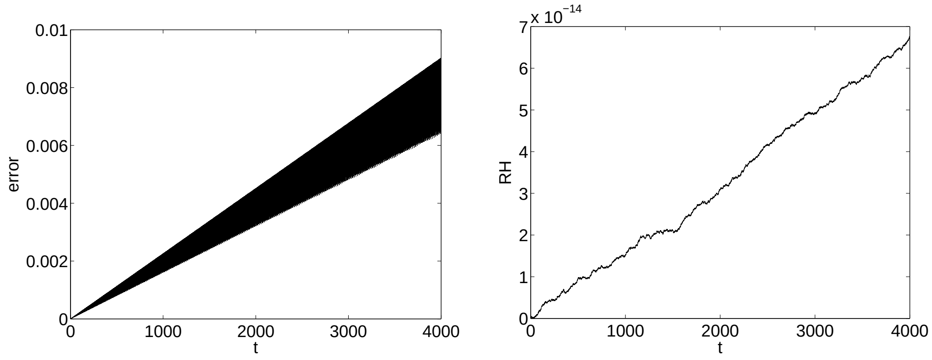
5.2. Numerical example 2

Second, we consider the Hénon-Heiles system

$$\dot{z} = J\nabla H, \quad H(z) = \frac{1}{2}(q_1^2 + q_2^2 + p_1^2 + p_2^2) + q_1^2 q_2 - \frac{1}{3}q_2^3, \tag{5.2a}$$

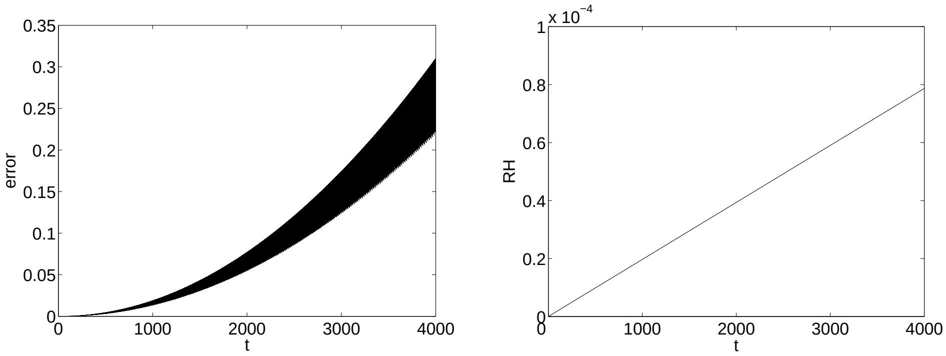
$$z = \begin{pmatrix} q_1 \\ q_2 \\ p_1 \\ p_2 \end{pmatrix}, \quad z_0 = \begin{pmatrix} 0.1 \\ -0.5 \\ 0 \\ 0 \end{pmatrix}, \quad J = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}. \tag{5.2b}$$

The Hénon-Heiles system has a critical energy value $E_c = 16$ at which the qualitative nature of the solution changes from bounded to unbounded orbits. In the experiment shown here, the



a Solution errors **b** Relative energy errors

Fig. 5.1. The numerical solution of the sixth order AVF method solving the example 1 with $h = 0.16$.



a Solution errors **b** Relative energy errors

Fig. 5.2. The numerical solution of the sixth order RK method solving the example 1 with $h = 0.16$.

energy of the system (5.3) is exactly E_c with initial spatial coordinates (q_1, q_2) at a point on the boundary of the critical triangular region (see [22, 28]).

We solve the system using the AVF6 method (see Fig. 5.3) and the RK6 method (see Fig. 5.4) with $h = 0.4$ respectively. From Fig. 5.3 we can see that the solution of the AVF6 method stays within the stable zone and conserves the energy E_c exactly in long time. Fig. 5.4 shows that the RK6 method can not preserve the energy and from $t = 1366$ the solution strays outside the stable zone and soon becomes completely unstable.

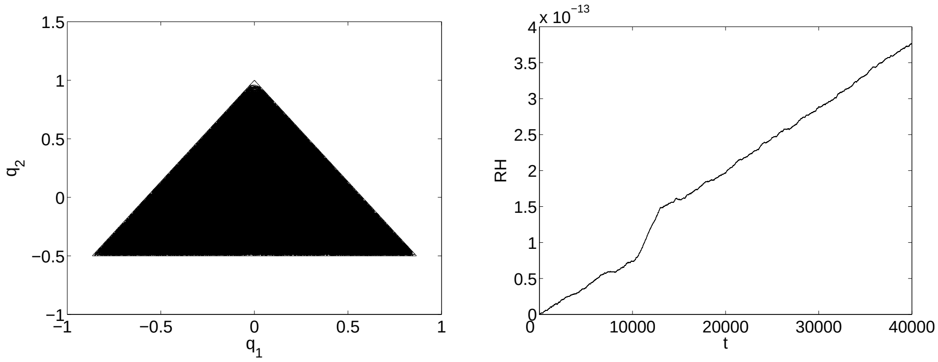
5.3. Numerical example 3

Finally, we consider the Kepler problem

$$\dot{z} = J^{-1}\nabla H, \quad H(z) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}}, \tag{5.3a}$$

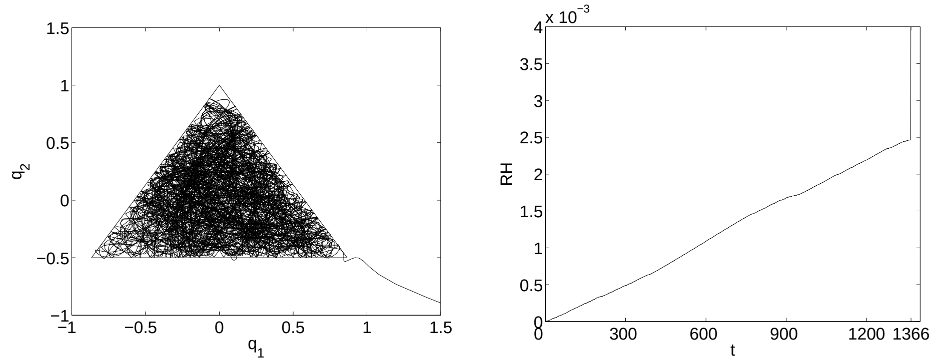
$$z = \begin{pmatrix} p_1 \\ p_2 \\ q_1 \\ q_2 \end{pmatrix}, \quad z_0 = \begin{pmatrix} 0 \\ 2 \\ 0.4 \\ 0 \end{pmatrix}, \quad J = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}. \tag{5.3b}$$

We solve the Kepler problem using the AVF6 method and the RK6 method from $t = 0$ to $t = 5000$ with $h = 0.1$ respectively. The integration $\int_0^1 f(\xi z_1 + (1-\xi)z_0))d\xi$ is calculated



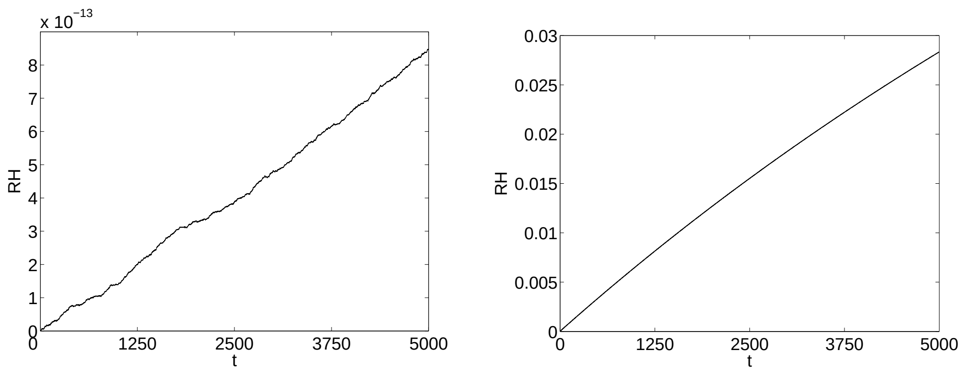
a Configuration space orbit **b** Relative energy errors

Fig. 5.3. The numerical solution of the sixth order AVF method solving the example 2 from $t = 0$ to $t = 40000$ with $h = 0.4$.



a Configuration space orbit **b** Relative energy errors

Fig. 5.4. The numerical solution of the sixth order RK method solving the example 2 from $t = 0$ to $t = 1366$ with $h = 0.4$.



a The AVF6 method **b** The RK6 method

Fig. 5.5. Relative energy errors of the numerical solution for solving the example 3 from $t = 0$ to $t = 5000$ with $h = 0.1$.

using the ninth order Gauss quadrature. Fig. 5.5 shows relative energy errors of the numerical solutions of the two methods. From Fig. 5.5a we can see that the errors in the integration is up to round-off error and the AVF6 method can conserve the energy exactly in longtime. We can conclude that, using the high order Gauss quadrature to the integration, the method can conserve the energy of non-polynomial Hamiltonian systems up to round-off error.

6. Conclusions

In this paper, we have proposed the concrete formulas of the substitution law for the trees of order = 5. Based on the new obtained substitution law, we have derived a B-series integrator extending the second order AVF method to sixth order. This approach that we expand a low order B-series integrator into a sixth order integrator can also be used in other geometric B-series integrators naturally, easily and automatically. We have proved that the new method is of order six and can preserve the energy of Hamiltonian systems. In [13], Faou et al have derived the conditions a B-series method must satisfy in order to be energy-preserving. This new method is a practical integrator of order six. We use the sixth order AVF method to solve linear and nonlinear Hamiltonian systems to test the accuracy and the energy-preserving ability of it. Numerical results confirm the theoretical results.

Acknowledgments. This work is supported by the Jiangsu Collaborative Innovation Center for Climate Change, the National Natural Science Foundation of China (Grant Nos. 11271195, 41231173) and the Priority Academic Program Development of Jiangsu Higher Education Institutions.

References

[1] L. Brugnano, F. Iavernaro and D. Trigiante, Hamiltonian boundary value methods (Energy preserving discrete line integral methods), *J. Numer. Anal. Ind. Appl. Math.*, **5** (2010), 17-37.

[2] T.J. Bridges, S. Reich, Numerical methods for Hamiltonian PDEs, *J. Phys. A: Math. Gen.*, **39** (2006), 5287-5320.

[3] J.C. Butcher, The numerical analysis of ordinary differential equations: Runge-Kutta and general linear methods, Wiley, New York, 1987.

[4] J.X. Cai, Y.S. Wang, Local structure-preserving algorithms for the "good" Boussinesq equation, *J. Comp. Phys.*, **239** (2013), 72-89.

[5] E. Celledoni, V. Grimm, R.I. McLachlan, D.I. McLaren, D. O'Neale, B. Owren and G.R.W. Quispel, Preserving energy resp. dissipation in numerical PDEs using the "Average Vector Field" method, *J. Comp. Phys.*, **231** (2012), 6770-6789.

[6] E. Celledoni, R.I. McLachlan, D.I. McLaren, B. Owren, G.R.W. Quispel and W.M. Wright, Energy-preserving Runge-Kutta methods, *Math. Model. Numer. Anal.*, **43** (2009), 645-649.

[7] P. Chartier, E. Faou and A. Murua, An algebraic approach to invariant preserving integators: the case of quadratic and Hamiltonian invariants, *Numer. Math.*, **103** (2006), 575-590.

[8] P. Chartier, E. Hairer and G. Vilmart, A substitution law for B-series vector fields, INRIA report, (2005), No. 5498.

[9] P. Chartier, E. Hairer and G. Vilmart, Numerical integration based on modified differential equation, *Math. Comp.*, **76** (2007), 1941-1953.

[10] P. Chartier, E. Lapôtre, Reversible B-series, INRIA report, (1988), No. 1221.

[11] Y. Chen, Y.J. Sun and Y.F. Tang, Energy-preserving numerical methods for Landau-Lifshitz equation, *J. Phys. A: Math. Theor.*, **44** (2011), 295207.

[12] K. Feng, Collected Works of Feng Kang II, National Defence Industry Press, Beijing, 1994.

[13] E. Faou, E. Hairer and T.-L. Pham, Energy conservation with non-Symplectic methods: examples and counter-examples, *BIT*, **44** (2004), 699-709.

[14] K. Feng, M.Z. Qin, Symplectic Geometric Algorithms for Hamiltonian Systems, Springer/Zhejiang Science and Technology Publishing House, Berlin/Hangzhou, 2010.

[15] O. Gonzalez, Time integration and discrete Hamiltonian systems, *J. Nonlinear Sci.*, **6** (1996), 449-467.

[16] E. Hairer, Energy-preserving variant of collocation methods, *J. Numer. Anal. Ind. Appl. Math.*, **5** (2010), 73-84.

[17] E. Hairer, C. Lubich and G. Wanner, Geometric Numerical Integration: Structure Preserving Algorithms for Ordinary Differential Equations, Springer, Berlin, 2002.

[18] E. Hairer, S.P. Norsett and G. Wanner, Solving Ordinary Differential Equations I, Nonstiff Problems (2nd ed.), Springer, Berlin, 1993.

[19] E. Hairer, G. Wanner, On the Butcher group and general multi-value methods, *Computing*, **13** (1974), 1-15.

[20] A. Iserles, A First Course in the Numerical Analysis of Differential Equations, 2nd ed., Cambridge University Press, Cambridge, 2008.

[21] F. Iavernaro, D. Trigiante, High-order symmetric schemes for the energy conservation of polynomial Hamiltonian problems, *J. Numer. Anal. Ind. Appl. Math.*, **4** (2009), 87-101.

[22] A.J. Lichtenberg and M.A. Liebermann, Regular and Chaotic Dynamics 2nd edn, Springer, New York, 1992.

[23] H.A. Luther, An explicit sixth-order Runge-Kutta formula, *Math. Comput.*, **22** (1968), 434-436.

[24] J.E. Marsden, G.W. Patrick and S. Shkoller, Multisymplectic geometry, variational integrators, and nonlinear PDEs, *Comm. Math. Phys.*, **199** (1998), 351-395.

[25] T. Matsuo, High-order schemes for conservative or dissipative systems, *J. Comput. Appl. Math.*, **152** (2003), 305-317.

[26] R.I. McLachlan, G.R.W. Quispel and N. Robidoux, Geometric integration using discrete gradients, *Phil. Trans. R. Soc. A.*, **357** (1999), 1021-1045.

[27] H. Qin, S.X. Zhang, J.Y. Xiao, J. Liu, Y.J. Sun and W.M. Tang, Why is Boris algorithm so good?, *Phys. Plasmas*, **20** (2013), 084503.

[28] G.R.W. Quispel, D.I. McLaren, A new class of energy-preserving numerical integration methods, *J. Phys. A: Math. Theor.*, **41** (2008), 045206.

[29] J.M. Sanz-Serna, Geometric integration, in: I.S. Duff, G.A. Watson (Eds.), The State of the Art in Numerical Analysis, Clarendon Press, Oxford, 1997, 121-143.

[30] J.M. Sanz-Serna, M.P. Calvo, Numerical Hamiltonian Problems, Chapman and Hall, London, 1994.

[31] J.Q. Sun, M.Z. Qin, Multi-symplectic methods for the coupled 1D nonlinear Schrödinger system, *Comp. Phys. Comm.*, **155** (2003), 221-235.

[32] Y.S. Wang, J.L. Hong, Multi-symplectic algorithms for Hamiltonian partial differential equations, *Comm. Appl. Math. Comput.*, **27** (2013), 163-230.

[33] S.D. Webb, Symplectic integration of magnetic systems, *J. Comput. Phys.*, **270** (2014), 570-576.