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Higher order volume-preserving schemes for charged particle dynamics

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ABSTRACT

A class of higher order numerical methods for advancing the charged particles in a general electromagnetic field is developed based on processing technique. By taking the volume-preserving methods as the kernel, the processed methods are still volume-preserving, and preserve the conservative quantities for the Lorenz force system. Moreover, this class of numerical methods are explicit and are more efficient compared with other higher order composition methods. Linear stability analysis is given by applying the numerical methods to the test equation. It is shown that the newly constructed higher order methods have the better stability property. This allows the use of larger step sizes in their implementation.

1. Introduction

The motion of charged particles in an electromagnetic field is a basic process in the collective dynamics of magnetized plasmas [1]. Many important phenomena in plasmas can be understood and analyzed in terms of the single-particle motion. In the numerical simulation of this process, it is often necessary to carry out calculations on a large time scale due to the multi-scale nature of magnetized plasmas [2], such as the simulation of the plasma transport physics in a tokamak geometry. It is accordingly desirable for the applied algorithms to be able to maintain the long term accuracy and fidelity throughout the entire simulation. Some standard numerical methods, such as the classical fourth order Runge–Kutta method, can guarantee a small error at each time step. However, after a long-term simulation the global error of the numerical solution would become unacceptably large as a result of the error accumulation [3,4]. In comparison, numerical methods that inherit the intrinsic geometric properties of the given dynamical system, which are called the geometric integrators, often exhibit the superior properties in long-term numerical computation [5,6]. Classified by the geometric structure of the given system, geometric integrators include symplectic methods for Hamiltonian systems and volume-preserving methods for source-free systems etc. They have been successfully applied in simulating the charged particle dynamics and the simulation of magnetized plasmas (see [3,7–11] and references within).

In disregard of relativistic effects, the evolution of the charged particles in a given electromagnetic field **E** and **B** is simply described by Newton's equation under the Lorentz force law

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$$m\ddot{\mathbf{x}} = q\left(\mathbf{E} + \dot{\mathbf{x}} \times \mathbf{B}\right).$$

After setting the velocity $\mathbf{v}$ as a new variable, the Newton–Lorentz equation can be reexpressed in a non-canonical Hamiltonian system, which enables the application of non-canonical symplectic integrators. However, it is generally not trivial to construct the numerical methods which can preserve the non-canonical structure. We will study this in our other paper. In [8], the alternative explicit algorithms which intend to preserve the invariant volume form in phase space, are offered for the Lorentz force system. This class of methods are constructed based on the splitting technique through the following procedure: Split the original system as several subsystems possessing the volume-preserving property; Solve each subsystem exactly or approximately by a volume-preserving method; With a proper composition of exact (approximate) solutions, the resulting discretization is volume-preserving as a result of Lie group property. It is shown in [8] that this class of volume-preserving methods are symmetric, and can bound the errors of constants of motion for the Lorentz force system. This guarantees in some sense an accurate simulation of the motion of charged particles over long time.

Our purpose of this paper is to extend the idea presented in [8] and construct the volume-preserving methods with higher order of accuracy. One way to gain a higher-order volume-preserving method is by composing the lower-order methods. For instance, let Φ_h be a method of order p with h the time step. Using method Φ_h, it is possible to obtain higher order methods in the form

$$\tilde{\Phi}_h = \Phi_{a_1 h} \circ \cdots \circ \Phi_{a_s h},$$

where s is the stage number, and a_i are the composition coefficients. More details on composition methods can be found in [5,12–14]. Some of the higher order methods developed in this way have been successfully applied to the charged particle dynamics [8,9]. They usually provide numerical solutions with an improved high accuracy, and can be computed explicitly. However, it should be noticed that the higher the accuracy is demanded, the larger the stage number s is taken. The computation cost of the higher order numerical methods increases by times along with the increase of s. Therefore, in our study we adopt an alternative technique, the so-called processing technique [15,16] to derive the numerical methods of high order.

The processing technique was firstly introduced by Butcher [17] to improve the efficiency of Runge–Kutta methods. Then it was used in the last years for symplectic integrators [15]. Given a numerical method Φ_h, the processing approach [16] is to find a transformation χ_h such that the resulting method in the form

$$\tilde{\Phi}_h = \chi_h \circ \Phi_h \circ \chi_h^{-1}$$

is of higher order than Φ_h. Here $\tilde{\Phi}_h$ is called the processed method, Φ_h is called the kernel, and χ_h is called the processor. After N steps, we gain $\tilde{\Phi}_h^N = \chi_h \circ \Phi_h^N \circ \chi_h^{-1}$. It is clear that in this process χ_h and χ_h^{-1} are only evaluated once. Moreover, the processed numerical method maintains all the global properties of the kernel method. This allows one to construct more efficient high order integrators with good global properties by choosing the appropriate kernel method. For example, the processing technique has been shown very efficient in designing symplectic methods for some particular Hamiltonian systems, such as the integrable Hamiltonian systems, or separable Hamiltonian systems (a kind of systems which can be decomposed as several exactly solvable parts) [18]. In our study, the processing technique is extended to construct the efficient high order volume-preserving integrators for the charged particle dynamics.

The outline of this paper is as follows. In Section 2, we present the various splittings for the Lorentz force system, and construct four volume-preserving methods of second order based on the splittings. In Section 3, we review the processing technique presented in [18], and construct a fourth order numerical method for the Lorentz force system via this technique. In Section 4, we analyze the stability of the volume-preserving methods constructed in the previous section. In Section 5, we present the experiments for simulating the motion of charged particles in the uniform and nonuniform electromagnetic fields. We conclude this paper in Section 6.

2. Volume-preserving numerical methods

Consider the motion of a charged particle in a given electromagnetic field with $\mathbf{E}$ the electric field strength and $\mathbf{B}$ the magnetic flux density. Denote $\mathbf{x}$ as the position of the particle, m as the mass, and q as the electric charge. With the introduction of the velocity variable $\mathbf{v} = \dot{\mathbf{x}}$, the motion equation of the charged particle is

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{v}, \\ \dot{\mathbf{v}} &= \frac{q}{m}\mathbf{E} + \omega \mathbf{b} \times \mathbf{v}, \end{aligned} \tag{1}$$

where $\omega = -qB/m$ is the local cyclotron frequency, $B = \|\mathbf{B}\|$ is the magnitude of $\mathbf{B}$, and $\mathbf{b} = \mathbf{B}/\|\mathbf{B}\|$ is the unit vector in the direction of the magnetic field. It is known in [8,19] that system (1) is source-free, as the vector field of this system satisfies

$$\nabla_{\mathbf{x}} \cdot \mathbf{v} + \nabla_{\mathbf{v}} \cdot \left(\frac{q}{m}\mathbf{E} + \omega \mathbf{b} \times \mathbf{v}\right) = 0.$$

By Liouville's theorem, the volume form in phase space $(\mathbf{x}, \mathbf{v})$ is invariant along the exact trajectory.