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A discrete line integral method of order two for the Lorentz force system

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ABSTRACT

In this paper, we apply the Boole discrete line integral to solve the Lorentz force system which is written as a non-canonical Hamiltonian system. The method is exactly energy-conserving for polynomial Hamiltonians of degree $\nu \leq 4$. In any other case, the energy can also be conserved approximatively. With comparison to well-used Boris method, numerical experiments are presented to demonstrate the energy-preserving property of the method.

1. Introduction

With the fast development of computer, geometric methods become more and more powerful in scientific research. A numerical method is called geometric method if it can conserve the geometric properties of a system up to round-off error [1–4]. 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 [5–10].

Many important phenomena in plasmas can be understood and analyzed in terms of the single-particle motion which satisfies the Lorentz force equations [11]. The motion of charged particles in single particle model is governed by the Newton equation under the Lorentz force exerted by a given electromagnetic field. Hamiltonian formulation is available for the single particle model and other magnetized plasma models in special coordinates [12,13]. In long-term simulating the motion of charged particles, non-geometric methods such as the standard 4th order Runge–Kutta method may give rise to a complete wrong solution orbit, since the numerical errors of each time step will add up coherently and become significantly large over many time steps. In contrast, geometric methods show a good long-term accuracy, for instance, the volume-preserving algorithms [14,15], the Boris method which can also conserve phase space volume [16–19], the variational symplectic method [20–22] and so on. It is well-know that the most noticeable structure of a Hamiltonian system is the Hamiltonian function itself which is usually the energy of the system. The paper is devoted to constructing an energy-preserving method for the Lorenz force system.

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 since several decades. Many energy-preserving methods have been proposed [23–26]. The discrete gradient method is among the most popular methods for designing integral preserving schemes for ordinary differential equations, which was perhaps first discussed by Gonzalez [23]. Matsuo proposed a discrete variational method for nonlinear wave equation [24]. The averaged vector field method which is a B-series method

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has been proposed [25,26]. More recently, Brugnano and Iavernaro proposed the discrete line integral (DLI) methods [27,28], the Hamiltonian boundary value methods [29,30] and the line integral methods [31–33]. The key idea of the DLI methods is to exploit the relation between the method itself and the discrete line integral, i.e., the discrete counterpart of the line integral in conservative vector fields. This tool yields exact conservation for polynomial Hamiltonians of arbitrarily high-degree. Different quadrature formulas yield different DLI methods. Especially, if we choose Boole's rule which is the Newton–Cotes formula of degree 4, the so-called Boole discrete line integral (BDLI) method which is exactly energy-conserving for a polynomial Hamiltonian of degree $\nu \leq 4$ is obtained.

In this paper, the Lorentz force system is written as a non-canonical Hamiltonian form. We apply the BDLI method for the Hamiltonian system, and a new energy-preserving method is obtained. The new method is symmetric and can preserve the Hamiltonian up to round-off error.

The paper is organized as follows: In Section 2, the dynamics of charged particles in the electromagnetic field is shown and it is written as a non-canonical Hamiltonian system. In Section 3, we use the BDLI method to solve the Hamiltonian system. Based on Boole's rule, a new method for Lorentz force system is obtained. Numerical experiments are presented in Section 4 to confirm the theoretical results and the compare the efficiency of the new formula with the well-known Boris method [16]. We finish the paper with conclusions in Section 5.

2. Hamiltonian form of the Lorentz force system

In this section, we review the Hamiltonian form of the Lorentz force system [12–14]. For a charged particle in the electromagnetic field, its dynamics is governed by the Newton–Lorentz equation

$$m\ddot{\mathbf{x}} = q(\mathbf{E} + \dot{\mathbf{x}} \times \mathbf{B}), \quad x \in \mathbb{R}^3, \tag{2.1}$$

where $\mathbf{x}$ is the position of the charged particle, m is the mass, and q denotes the electric charge. For convenience, here we assume that $\mathbf{B}$ and $\mathbf{E}$ are static, thus $\mathbf{B} = \nabla \times \mathbf{A}$ and $\mathbf{E} = -\nabla\varphi$ with $\mathbf{A}$ and φ the potentials.

Let the conjugate momentum be $\mathbf{p} = m\dot{\mathbf{x}} + q\mathbf{A}(\mathbf{x})$, then the system (2.1) is Hamiltonian with

$$H(\mathbf{x}, \mathbf{p}) = \frac{1}{2m}(\mathbf{p} - q\mathbf{A}(\mathbf{x})) \cdot (\mathbf{p} - q\mathbf{A}(\mathbf{x})) + q\varphi(\mathbf{x}). \tag{2.2}$$

Exploiting the transformation $G : (\mathbf{x}, \mathbf{p}) \longrightarrow (\mathbf{x}, \mathbf{v}), \mathbf{x} = \mathbf{x}, \mathbf{v} = \mathbf{p}/m - q\mathbf{A}(\mathbf{x})/m$, system (2.1) is recast as

$$\dot{\mathbf{x}} = \mathbf{v}, \tag{2.3}$$

$$\dot{\mathbf{v}} = \frac{q}{m}(\mathbf{E}(\mathbf{x}) + \mathbf{v} \times \mathbf{B}(\mathbf{x})). \tag{2.4}$$

Denote $\mathbf{z} = [\mathbf{x}^T, \mathbf{v}^T]^T$. (2.3) and (2.4) can be written as the non-canonical Hamiltonian system

$$\dot{\mathbf{z}} = f(\mathbf{z}) = K(\mathbf{z})\nabla H(\mathbf{z}), \tag{2.5}$$

where $H(\mathbf{z}) = m\mathbf{v} \cdot \mathbf{v}/2 + q\varphi(\mathbf{x})$, and

$$K(\mathbf{z}) = \begin{pmatrix} 0 & \frac{1}{m}I \\ -\frac{1}{m}I & \frac{q}{m^2}\hat{\mathbf{B}}(\mathbf{x}) \end{pmatrix}$$

is a skew-symmetric matrix with

$$\hat{\mathbf{B}}(\mathbf{x}) = \begin{pmatrix} 0 & B_3(\mathbf{x}) & -B_2(\mathbf{x}) \\ -B_3(\mathbf{x}) & 0 & B_1(\mathbf{x}) \\ B_2(\mathbf{x}) & -B_1(\mathbf{x}) & 0 \end{pmatrix},$$

defined by $\mathbf{B}(\mathbf{x}) = [B_1(\mathbf{x}), B_2(\mathbf{x}), B_3(\mathbf{x})]^T$.

3. Boole discrete line integral method

It is well know that the flow of the system (2.5) preserves the energy which is usually the Hamiltonian $H(\mathbf{z})$ exactly. In this section, we derive a new energy-preserving scheme for the system (2.5) by using the BDLI method proposed in [27,28,33]. Starting from the initial condition $\mathbf{z}_0$ we want to produce a new approximation at $t = h$, say $\mathbf{z}_1$, such that the Hamiltonian is conserved. By considering the simplest possible path joining $\mathbf{z}_0$ and $\mathbf{z}_1$, i.e., the segment

$$\sigma(ch) = c\mathbf{z}_1 + (1-c)\mathbf{z}_0, \quad c \in [0, 1], \tag{3.1}$$

we obtain that

$$\begin{aligned} \frac{1}{h}(H(\mathbf{z}_1) - H(\mathbf{z}_0)) &= \frac{1}{h}(H(\sigma(h)) - H(\sigma(0))) \\ &= \frac{1}{h}\int_0^h \nabla H(\sigma(t))^T \sigma'(t)dt \end{aligned}$$