HIGH ORDER GAUSS-SEIDEL SCHEMES FOR CHARGED PARTICLE DYNAMICS

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(Communicated by Xiao-Ping Wang)

Abstract. Gauss-Seidel projection methods are designed for achieving desirable long-term computational efficiency and reliability in micromagnetics simulations. While conventional Gauss-Seidel schemes are explicit, easy to use and furnish a better stability as compared to Euler’s method, their order of accuracy is only one. This paper proposes an improved Gauss-Seidel methodology for particle simulations of magnetized plasmas. A novel new class of high order schemes are implemented via composition strategies. The new algorithms acquired are not only explicit and symmetric, but also volume-preserving together with their adjoint schemes. They are highly favorable for long-term computations. The new high order schemes are then utilized for simulating charged particle motions under the Lorentz force. Our experiments indicate a remarkable satisfaction of the energy preservation and angular momentum conservation of the numerical methods in multi-scale plasma dynamics computations.

1. Introduction. Plasma is a collection of charged particles interacting with electromagnetic fields, whose sources can be either external or internal [1]. The most fundamental physical process in collective dynamics of magnetized plasmas is the motion of charged particles under the influence of electromagnetic fields. Plasma characteristics can be understood and analyzed in terms of a single particle motion satisfying the Lorentz force equation. Efficient numerical methods for simulating such single particle models may significantly benefit the study of plasma dynamic behaviors. Discussions in the topic can be found in numerous recent publications (see [16, 22, 24, 9] and references therein, for example).

In the study of single particle motions and guiding center dynamics [12], highly stable integrations are necessary. Further, features to preserve certain geometric

2010 Mathematics Subject Classification. 60E10, 60J10, 60J27, 60J35.
Key words and phrases. Gauss-Seidel scheme, high order accuracy, long-time computation, volume-preserving, conservations.

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quantities, such as the symplecticity and time symmetry of the flow for Hamiltonian systems, are desirable \cite{8, 13}. To this end, several variational symplectic methods have been developed recently for the Lagrangian formalism of magnetic systems \cite{17, 15, 22, 24}. However, Lagrangian mechanics often lacks the canonical transformation formalism needed for deriving a symplectic integrator in general. Hamiltonian formulation is also applicable to single particle and other magnetized plasma models in special coordinates \cite{11}. Due to their implicit structures, however, symplectic methods are cumbersome for single particle motion equations that cannot be separated in terms of the canonical variables \((x, p)\) \cite{8, 4, 23}.

Volume-preserving integrators have gained increasing popularity for the explicit and conservations of the phase space volume of Lorenz force systems \cite{16, 9}. A Lorenz force system can be written in \((x, v)\), where \(x\) is the position variable and \(v\) is the velocity variable. In \((x, v)\) coordinates, a Lorenz force system is separable and source-free. A phase space volume is invariable along the solution flow of this system. On the other hand, the Boris algorithm \cite{3, 19, 2} can be applied readily for magnetized plasma simulations because of its remarkable long-term accuracy. Further, Qin et al. have shown that the Boris method is volume-preserving, although it is neither canonical nor non-canonically symplectic \cite{16}. The use of volume-preserving integrators for Lorenz force systems is in fact sensible. In 2015, utilizing a splitting approach, He et al. \cite{9} introduced a class of volume-preserving numerical methods in which the Boris scheme serves as a special case. Since a Boris algorithm can also be viewed as a conjugate of a symmetric method \(\tilde{G}_h^2\) of \cite{9}, the Boris and \(\tilde{G}_h^2\) methods share the same long-term behaviour (see p. 222 of \cite{8}).

The accumulative error of an explicit scheme, such as a fourth order explicit Runge-Kutta method, may become significant after a long-term execution. Direct implicit integrators, on the other hand, may be highly stable for long-term computations, but large numbers of calculations are often required. To improve the computational efficiency, Wang et al. \cite{21} proposed a Gauss-Seidel projection method for micromagnetics simulations. Their basic idea is to split the vector field of Landau-Lifshitz system into the gyromagnetic term and the heat flow of harmonic maps, which are then solved by a Gauss-Seidel implementation of a fractional step implicit scheme and the projection method \cite{5}, respectively. The Gauss-Seidel scheme for the gyromagnetic term is first order, easy to implement, and unconditionally stable. In this paper, we shall show that the Wang’s scheme is also volume-preserving, that is, its algorithm conserves the phase space volumes of a separable source-free system. To improve the accuracy, we shall propose a new class of high order Gauss-Seidel schemes. The high-order Gauss-Seidel schemes will be applied for charged particle motions under the Lorentz force. The new methods are explicit, symmetric and volume-preserving. Hence they are more appropriate for highly efficient long-term simulations of the multi-scale dynamics of plasmas. Numerical experiments will be presented to illustrate the satisfactory performance of the high order schemes as well as preservations of the energy and angular momentum conservations.

This paper is organized as follows: In Section 2, a brief review of several different formulations of the dynamics of charged particles involved is presented. The corresponding geometric and conservative properties are analyzed. In Section 3, the class of high order Gauss-Seidel methods is constructed for the Lorentz equation. Numerical experiments are presented in Section 4 to illustrate key properties of the proposed schemes in a long-term operations. We finally wrap up the study with our conclusions in Section 5.
2. The motion equation under Lorentz force. The dynamic motion of a charged particle in an electromagnetic field is governed by the Newton-Lorentz equation

\[ m\ddot{x} = q(E + \dot{x} \times B), \quad x \in \mathbb{R}^3, \tag{1} \]

where \( x \) is the position of the particle, \( m \) is the mass, and \( q \) denotes the electric charge. For the convenience, we may assume that \( B \) and \( E \) are static. Thus, \( B = \nabla \times A \) and \( E = -\nabla \varphi \) with \( A \) and \( \varphi \) being the potentials.

Eq. (1) is equivalent to an Euler-Lagrangian equation with

\[ L(x, \dot{x}) = \frac{1}{2} m \dot{x} \cdot \dot{x} + q \dot{x} \cdot A(x) - q \varphi(x). \tag{2} \]

Recall [17, 15, 22]. Let the conjugate momentum \( p = m \dot{x} + q A(x) \). Then the system (1) is with a Hamiltonian

\[ H(x, p) = \frac{1}{2m} (p - q A(x)) \cdot (p - q A(x)) + q \varphi(x), \tag{3} \]

which enables the use of canonical symplectic algorithms. Since (3) is not separable, that is, it cannot be split into the form \( H(x, p) = T(p) + U(x) \), a general symplectic method for solving (1) cannot be explicit [8, 4, 23]. However, note that Eq. (1) can be separated naturally to

\[
\begin{align*}
\dot{x} &= v, \\
\dot{v} &= \frac{q}{m} (E(x) + v \times B(x)),
\end{align*}
\tag{4}
\]

where the energy is \( H(x, v) = mv \cdot v/2 + q \varphi(x) \). Letting \( z = \begin{pmatrix} x \\ v \end{pmatrix} \), the system (4) can be rewritten as

\[ K(z) \dot{z} = \nabla_z H(z), \tag{5} \]

where \( K(z) = \begin{bmatrix} -q \hat{B}(x) & -mI \\ mI & 0 \end{bmatrix} \) is a skew-symmetric matrix with

\[ \hat{B}(x) = \begin{bmatrix} 0 & -B_3(x) & B_2(x) \\ B_3(x) & 0 & -B_1(x) \\ -B_2(x) & B_1(x) & 0 \end{bmatrix}, \]

and \( B(x) = [B_1(x), B_2(x), B_3(x)]^T \). There is a non-canonical symplectic structure (\( K \)-symplectic structure) preserved by the flow of (4) [9, 14]. It has been a difficult task to construct an explicit method that preserves the non-canonical structure \( K(z) \), and in the same time, is more efficient than symplectic method [10]. Denote \( f(x, v) = [v^T, q(E(x) + v \times B(x))]/m \). Then \( f \) is source-free, that is,

\[ \nabla \cdot f = \nabla_x \cdot v + \frac{q}{m} \nabla_v \cdot (E(x) + v \times B(x)) \equiv 0. \tag{6} \]

According to Liouville’s theorem, the corresponding volume is invariable along the solution flow of (4). A new class of volume-preserving methods was derived recently via splitting strategies [9].
3. Symmetric and volume-preserving methods. We consider a first order Gauss-Seidel scheme and its adjoint for (4). Based on them, a new class of explicit, symmetric and volume-preserving Gauss-Seidel schemes can be accomplished via compositions.

To this end, we rewrite (4) as

\[
\begin{cases}
\dot{x} = v, \\
\dot{v}_1 = \frac{a}{2} \left( E_1(x) + v_2 B_3(x) - v_3 B_2(x) \right), \\
\dot{v}_2 = \frac{a}{2} \left( E_2(x) + v_3 B_1(x) - v_1 B_3(x) \right), \\
\dot{v}_3 = \frac{a}{2} \left( E_3(x) + v_1 B_2(x) - v_2 B_1(x) \right).
\end{cases}
\]  

(7)

Based on the Gauss-Seidel scheme for Eq. (7), we have

\[
\Phi_h : \begin{cases}
x^{k+1} = x^k + hv^k, \\
v_1^{k+1} = v_1^k + \frac{h}{m} \left( E_1(x^{k+1}) + v_2^k B_3(x^{k+1}) - v_3^k B_2(x^{k+1}) \right), \\
v_2^{k+1} = v_2^k + \frac{h}{m} \left( E_2(x^{k+1}) + v_3^k B_1(x^{k+1}) - v_1^k B_3(x^{k+1}) \right), \\
v_3^{k+1} = v_3^k + \frac{h}{m} \left( E_3(x^{k+1}) + v_1^k B_2(x^{k+1}) - v_2^k B_1(x^{k+1}) \right).
\end{cases}
\]  

(8)

Its adjoint method \( \Phi_h^* \) can be comprised to

\[
\Phi_h^* : \begin{cases}
x^{k+1} = x^k + hv^{k+1}, \\
v_1^{k+1} = v_1^k + \frac{h}{m} \left( E_1(x^k) + v_2^{k+1} B_3(x^k) - v_3^{k+1} B_2(x^k) \right), \\
v_2^{k+1} = v_2^k + \frac{h}{m} \left( E_2(x^k) + v_3^{k+1} B_1(x^k) - v_1^{k+1} B_3(x^k) \right), \\
v_3^{k+1} = v_3^k + \frac{h}{m} \left( E_3(x^k) + v_1^{k+1} B_2(x^k) - v_2^{k+1} B_1(x^k) \right).
\end{cases}
\]  

(9)

Apparently, schemes (8) and (9) can be computed explicitly. Let us first show that (9) is volume-preserving. For this, we denote (9) as \( z^{k+1} = \Phi_h^*(z^k), z^k = [x^k; v^k] \).

**Theorem 3.1.** The scheme (9) is volume-preserving.

**Proof.** To see this, we only need to prove

\[
\det \left[ \frac{\partial \Phi_h^*(z^k)}{\partial z^k} \right] \equiv 1, \ k = 0, 1, 2, \ldots
\]  

(10)

According to properties of a determinant of a square matrix, we have

\[
\det \left[ \frac{\partial \Phi_h^*(z^k)}{\partial z^k} \right] = \det \left[ \begin{array}{cccc}
I & h \frac{\partial v^{k+1}}{\partial x^k} & h \frac{\partial v^{k+1}}{\partial x^k} & \vdots \\
0 & \frac{\partial v^{k+1}}{\partial v^k} & \frac{\partial v^{k+1}}{\partial v^k} & \vdots \\
0 & \frac{\partial v^{k+1}}{\partial v^k} & \frac{\partial v^{k+1}}{\partial v^k} & \vdots \\
\vdots & \vdots & \vdots & \ddots
\end{array} \right]
\]

\[
= \det \left[ \begin{array}{cc}
I & 0 \\
0 & \frac{\partial v^{k+1}}{\partial v^k}
\end{array} \right] = \det \left[ \frac{\partial v^{k+1}}{\partial v^k} \right],
\]

(11)

where

\[
\frac{\partial v^{k+1}}{\partial v^k} = \left[ \begin{array}{cccc}
1 + c^2 B_1 B_2 B_3 - c^2 B_3^2 - c^2 B_2^2 & c B_3 - c^3 B_2 B_3 + c^2 B_1 B_2 & c^2 B_1 B_3 - c B_2 & c B_3 \\
c^2 B_1 B_2 - c B_2 & 1 - c^2 B_2^2 & c B_1 & 0 \\
c B_2 & -c B_3 & 1 & 0
\end{array} \right]
\]

and \( c = \frac{hq}{m} \) and \( B_i = B_i(x^k), \ i = 1, 2, 3; \ k = 0, 1, 2, \ldots \) Therefore,

\[
\det \left[ \frac{\partial v^{k+1}}{\partial v^k} \right] = \det \left[ \begin{array}{ccc}
1 - c^2 B_2^2 & c B_3 & 0 \\
-c B_3 & 1 & 0 \\
c B_2 & -c B_1 & 1
\end{array} \right]
\]
This completes our proof. □

**Remark 1.** Similarly, we may show that

$$\det \left[ \frac{\partial \Phi_h^k(z^k)}{\partial z^k} \right] \equiv 1. \tag{12}$$

Therefore (8) is volume-preserving.

In fact, Gauss-Seidel methods of any order can be constructed through compositions of \( \Phi_h \) or \( \Phi_h^* \) [8]. Targeting at Lorentz force systems, the following result offers a simple and straightforward way to construct high order symmetric Gauss-Seidel methods.

**Theorem 3.2.** Based on first order Gauss-Seidel schemes (8) and (9), we have the following volume-preserving and symmetric formulas.

1. **Second order scheme:**

\[ GS_h^2 = \Phi_{h/2} \circ \Phi_{h/2}^*. \]

2. **2(1 + 1)th order scheme:**

\[ GS_h^{2(1+1)} = GS_{\alpha_1 h}^2 \circ GS_{\beta_1 h}^2 \circ GS_{\alpha_1 h}^2, \]

where \( h \) is the temporal step size, \( \alpha_1 = (2 - 2^{1/(2l+1)})^{-1} \) and \( \beta_1 = 1 - 2\alpha_1 < 0. \)

**Proof.**

a) It is firstly proved that the adjoint method has the same order as the original method, and, with a possible sign change, also the same leading error term. For the autonomous differential equations

\[ \dot{y} = f(y), \quad y(t_0) = y_0, \tag{13} \]

let \( \varphi_t \) be the exact flow and let \( \Psi_h \) be a one-step method of order \( p \) satisfying

\[ \Psi_h(y_0) = \varphi_h(y_0) + C(y_0)h^{p+1} + O(h^{p+2}). \tag{14} \]

Let \( e = y_0 - \Psi_{-h}(\varphi_h(y_0)) \). It follows (14) that

\[ e = (-1)^p C(\varphi_h(y_0))h^{p+1} + O(h^{p+2}). \tag{15} \]

The adjoint method \( \Psi_h^* \) of a method \( \Psi_h \) is defined as \( \Psi_h^* = \Psi_{-h}^{-1} \). Denote \( e^* \) the local error of \( \Psi_h^* \), i.e., \( e^* = \Psi_h^*(y_0) - \varphi_h(y_0) \). Using the Taylor expansion, we have

\[ y_0 = \Psi_{-h}(\varphi_h(y_0) + e^*) = \Psi_{-h}(\varphi_h(y_0)) + \frac{\partial}{\partial y} \Psi_{-h}(\varphi_h(y_0) + \theta e^*) \cdot e^*, \quad 0 \leq \theta \leq 1. \]

Due to \( \Psi_{-h}(y) = y + O(h) \), thus \( e = (I + O(h))e^* \). Since \( \varphi_h(y_0) = y_0 + O(h) \), it follows that

\[ e^* = (-1)^p C(y_0)h^{p+1} + O(h^{p+2}). \tag{16} \]

Furthermore, if the method is symmetric, its (maximal) order is even. Because \( \Psi_h = \Psi_h^* \) implies \( C(y_0) = (-1)^p C(y_0) \), and therefore \( C(y_0) \) can be different from zero only for even \( p \).

b) The adjoint method satisfies the usual properties such as \( (\Phi_h)^* = \Phi_h \) and \( (\Phi_h \circ \Psi_h)^* = \Psi_h^* \circ \Phi_h^* \). Thus, it is easily proved that the composition \( GS_h^2 = \Phi_{h/2} \circ \Phi_{h/2}^* \) is symmetric. Next, we prove that the method \( GS_h^2 \) is of order 2. Based
on part (a), we can assume that the first-order Gauss-Seidel method $\Phi_h$ and its adjoint method $\Phi_h^*$ satisfy

\[
\Phi_h(y_0) = \varphi_h(y_0) + C(y_0)h^2 + O(h^3), \quad (17)
\]
\[
\Phi_h^*(y_0) = \varphi_h(y_0) - C(y_0)h^2 + O(h^3). \quad (18)
\]

Let $y_1 = \Phi_{h/2}^*(y_0)$ and $Y_1 = \varphi_{h/2}(y_0)$. Since $y_1 = y_0 + O(h)$, it follows (17)-(18) that

\[
e_1 := y_1 - Y_1 = \Phi_{h/2}^*(y_0) - \varphi_{h/2}(y_0) = -\frac{1}{4}C(y_0)h^2 + O(h^3), \quad (19)
\]
\[
e_2 := \Phi_{h/2}(y_1) - \varphi_{h/2}(y_1) = \frac{1}{4}C(y_1)h^2 + O(h^3) = \frac{1}{4}C(y_0)h^2 + O(h^3). \quad (20)
\]

Similar to the proof of part (a), we have

\[
\varphi_{h/2}(y_1) - \varphi_{h/2}(Y_1) = (I + O(h))e_1. \quad (21)
\]

Therefore, we obtain

\[
GS_{h}^2(y_0) - \varphi_h(y_0) = \Phi_{h/2}(y_1) - \varphi_{h/2}(y_1) + \varphi_{h/2}(y_1) - \varphi_{h/2}(Y_1) = e_2 + (I + O(h))e_1 = O(h^5),
\]

which implies that the method $GS_h^2$ is of order 2.

c) The argument of order of the composition method $GS_{h}^{2(l+1)}$ proceeds in inductive way. Assume that $GS_h^{2l}$ is symmetric and of order $2l$. Now prove that $GS_{h}^{2(l+1)}$ is symmetric and of order $2(l+1)$. Since $GS_{h}^{2l}$ is symmetric, i.e., $GS_{h}^{2l} = GS_{h}^{2l}$, we have

\[
GS_{h}^{2(l+1)} = (GS_{h}^{2l} \circ GS_{h}^{2l} \circ GS_{h}^{2l}) = GS_{h}^{2l} \circ GS_{h}^{2l} \circ GS_{h}^{2l} = GS_{h}^{2(l+1)},
\]

which implies that $GS_{h}^{2(l+1)}$ is also symmetric. Assume that the $2l$-order method $GS_{h}^{2l}$ satisfies

\[
GS_{h}^{2l}(y_0) = \varphi_h(y_0) + C(y_0)h^{2l+1} + O(h^{2l+2}). \quad (22)
\]

Let $y_1 = GS_{h/2}^{2l}(y_0)$, $y_2 = GS_{h}^{2l}(y_1)$, $Y_1 = \varphi_{h}(y_0)$ and $Y_2 = \varphi_{h}(y_1)$. According to $y_i = y_0 + O(h)$ $(i = 1, 2)$, we obtain

\[
e_1 := y_1 - Y_1 = GS_{h/2}(y_0) - \varphi_{h}(y_0) = \alpha_{l+1}^{2l+1}C(y_0)h^{2l+1} + O(h^{2l+2}), \quad (23)
\]
\[
e_2 := y_2 - Y_2 = GS_{h/2}(y_1) - \varphi_{h}(y_1) = \beta_{l+1}^{2l+1}C(y_0)h^{2l+1} + O(h^{2l+2}), \quad (24)
\]
\[
e_3 := GS_{h/2}(y_2) - \varphi_{h}(y_2) = \alpha_{l+1}^{2l+1}C(y_0)h^{2l+1} + O(h^{2l+2}). \quad (25)
\]

In addition, we have

\[
\varphi_{h}(y_1) - \varphi_{h}(Y_1) = (I + O(h))e_1, \quad (26)
\]
\[
\varphi_{h}(y_2) - \varphi_{h}(Y_2) = (I + O(h))e_2. \quad (27)
\]

Notice that $2\alpha_{l+1} + \beta_{l+1} = 1$ and $2\alpha_{l+1}^2 + \beta_{l+1}^2 = 0$, we obtain

\[
GS_{h}^{2(l+1)}(y_0) - \varphi_h(y_0) = GS_{h/2}(y_2) - \varphi_{h}(y_2) + \varphi_{h}(y_2) - \varphi_{h}(Y_2) + \varphi_{h}(Y_2) - \varphi_{h}(Y_1) - \varphi_{h}(Y_1) = e_3 + (I + O(h))e_2 + (I + O(h))e_1
\]
\[
= (2\alpha_{l+1}^2 + \beta_{l+1}^2)C(y_0)h^{2l+1} + O(h^{2l+2}) = O(h^{2l+2})
\]
which implies that the method $GS_h^{2(l+1)}$ is at least of order $2l + 1$. Because the method $GS_h^{2(l+1)}$ is symmetric, so the order of $GS_h^{2(l+1)}$ is up to $2l + 2$.

Note that, since the methods $\Phi_h$ and $\Phi^*_h$ is volume-preserving, any composition method based on $\Phi_h$ and $\Phi^*_h$ is still volume-preserving. □

The aforementioned explicit methods can be effective and efficient for long-term simulations of the multi-scale dynamics of plasmas.

4. Numerical experiments. We consider two respective cases in this section.

4.1. 2D dynamics in a static electromagnetic field. Firstly, we consider the 2D dynamics of a charged particle in a static electromagnetic field

$$B = \nabla \times A = e_z, \quad E = -\nabla \varphi = \frac{10^{-2}}{R^3} (xe_x + ye_y), \quad (28)$$

where the potentials are chosen to be $A = [-y/2, x/2, 0]^T$, $\varphi = \frac{10^{-2}}{R}$ with $R = \sqrt{x^2 + y^2}$. In this example, the physical quantities are normalized by the system size $a$, the characteristic magnetic field $B_0$, and the gyro-frequency $\omega_0 \equiv qB_0/m$ of the particle. The Lagrangian is $L = (\dot{R}^2 + R^2\dot{\xi}^2 + \dot{z}^2)/2 + R^2\dot{\xi}/2 - \varphi$ in cylindrical coordinates $(R, \xi, z)$. Due to $\partial L/\partial \dot{\xi} \equiv 0$, the angular momentum

$$p_\xi = R^2\dot{\xi} + R^2/2$$

is invariant along the solution trajectory of system (4). It is known that the energy

$$H = \frac{1}{2} \mathbf{v} \cdot \mathbf{v} + \frac{10^{-2}}{R}$$

is a constant of motion.

Starting from the initial position $x_0 = [0, -1, 0]^T$ with the initial velocity $v_0 = [0.1, 0, 0.01, 0]^T$, the analytic orbit of the charged particle is a spiraling circle with constant radius. The large circle corresponds to the $\nabla \cdot B$ drift and the $E \times B$ drift of the guiding center, and the small circle is the fast-scale gyro-motion.

We first apply the Runge-Kutta method of order four denoted by $RK_4$ and the numerical results are shown in Fig. 1. The step size is $h = \pi/10$ which is the $1/20$ of the characteristic gyro-period. Though $RK_4$ has a fourth order of accuracy, the numerical error accumulation after $2.7 \times 10^5$ steps gives rise to a complete wrong solution orbit in Fig. 1(b), where the gyro-motion is numerically dissipated. The normalized errors of the invariants as a function of integration time are performed in Fig. 1(c) and (d). These figures show that the $RK_4$ cannot preserve the invariants inherited by this system.

Next, we test the symmetric and volume-preserving numerical methods. Fig. 2 shows the numerical orbits of the second order methods after $5 \times 10^5$ steps in (a), and that of the fourth order methods after $2.5 \times 10^5$ steps in (b). The volume-preserving methods provide a correct and stable gyro-motion over a very long integration time.

To test accuracy of the methods, the exact solution is computed by the $RK_4$ with a small step size $h = 0.0001$. In Fig. 3, the solution errors $|||x^n - v^n|||$ are computed at time $t = 30$. It is shown that the method $GS_h^2$ and the Boris method $G_h^4$ (Ref. [9]) have the convergence rate of order two; the method $GS_h^4$ and the splitting method $G_h^4$ (Ref. [9]) have the convergence rate of order four. It is also noticed that the method $GS_h^1$ (or $G_h^4$) is more accurate than the Boris method (or $GS_h^4$). In Fig. 4, we plot the relative errors of the invariants $H$ and $p_\xi$ as functions of the step size $h$. We observe that the invariant errors are about a scale of $h^2$ for
Figure 1. The fourth order explicit method $RK4$ is applied to the simple 2D dynamics with step size $h = \pi/10$. (a): The orbit in the first 2691 steps. (b): The orbit after $2.7 \times 10^5$ steps. (c): Energy error $H_n - H_0$. (d): Angular momentum error $p_\xi n - p_\xi 0$.

$GS_2^h$ and $\tilde{G}_2^h$, and a scale of $h^4$ for $GS_4^h$ and $G_4^h$. Among these methods, the method $G_4^h$ is best in preserving energy, while the method $GS_4^h$ is best in preserving angular momentum.

In Fig. 5, we illustrate the relative errors of the energy $H$ and the angular momentum $p_\xi$ computed by the four methods $GS_2^h$, $\tilde{G}_2^h$, $GS_4^h$ and $G_4^h$. It is observed that the errors are bounded over a long integration time. The errors of invariants become smaller when the higher order methods are used.

4.2. 2D dynamics in an axisymmetric tokamak geometry. In this subsection, we consider the motion of a charged particle in a 2-dimensional axisymmetric tokamak geometry without inductive electric field. The magnetic field in the toroidal coordinates $(r, \theta, \xi)$ is expressed as

$$\mathbf{B} = \frac{B_0 r}{q R} \mathbf{e}_\theta + \frac{B_0 R_0}{R} \mathbf{e}_\xi,$$

where $B_0 = 1$, $R_0 = 1$, and $q = 2$ are constant with their usual meanings. The corresponding vector potential $\mathbf{A}$ is chosen to be
Figure 2. Numerical orbits of the symmetric and volume-preserving methods with time step $h = \pi/10$. (a): The orbit after $5 \times 10^5$ steps by the second order method. (b): The orbit after $2.5 \times 10^5$ steps by the fourth order method.

Figure 3. Convergence rates of numerical solutions by the methods $GS^2_h$, $\tilde{G}^2_h$, $GS^4_h$ and $G^4_h$.

$$A = \frac{z}{2R}e_R + \frac{(1 - R)^2 + z^2}{4R}e_\xi - \frac{\ln R}{2}e_z. \quad (30)$$

To apply the proposed methods in Section 3, we transform $B$ (29) into the Cartesian coordinates $(x, y, z)$ which is

$$B = -\frac{2y + xz}{2R^2}e_x + \frac{2x - yz}{2R^2}e_y + \frac{R - 1}{2R}e_z. \quad (31)$$

In this example, the physical quantities are normalized by the system size $a$, characteristic magnetic field $B_0$, and the gyro-frequency $\omega_0 \equiv qB_0/m$. Here the Lagrangian is $L = (R^2 + R^2 \xi^2 + z^2)/2 + (Rz)/(2R) + ((R - 1)^2 + z^2)\xi/4 - \dot{z} \ln R/2$ in cylindrical coordinates $(R, \xi, z)$. Due to $\partial L/\partial \xi \equiv 0$, the angular momentum $p_\xi = R^2 \dot{\xi} + ((R - 1)^2 + z^2)/4$ is invariant along the solution trajectory of system (4). In the absence of electric field, the energy of the system is $H = \mathbf{v} \cdot \mathbf{v}/2$, which
is a constant of motion. With the conserved quantities, the solution orbit projected on \((R, z)\) space forms a closed orbit.

Starting with the initial position \(x_0 = [1.05, 0, 0]^T\) and the initial velocity \(v_0 = [0, 4.816e-4, -2.059e-3]^T\), the orbit projected on \((R, z)\) space is a banana orbit, and it will turn into a transit orbit when the initial velocity is changed to \(v_0 = [0, 2 \times 4.816e-4, -2.059e-3]^T\). Setting the step size \(h = \pi/10\) which is the 1/20 of the gyro-period, we adopt the RK4 and the volume-preserving methods developed above. The simulation over \(5 \times 10^5\) steps is shown in Fig. 6. For the results generated by the RK4 in Fig. 6(a) and (b), due to the numerical damping of energy the numerical orbits are not closed, and the gyro-motion is dissipated. The banana orbit gradually transformed into a circulating orbit and the transit orbit deviates to the right side. By comparison, in Fig. 6(c)-(d) the volume-preserving methods give correct and qualitatively better orbits over a very long integration.
time. We display the relative errors of the invariants $H$ and $p_\xi$ in Fig. 7, which show that the proposed methods conserve the invariants well.

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{banana_orbit.png} \quad \includegraphics[width=0.4\textwidth]{transit_orbit.png}
\caption{Numerical orbits. (a): Banana orbit by the RK4. (b): Transit orbit by the RK4. (c): Banana orbit by the volume-preserving methods. (d): Transit orbit by the volume-preserving methods. The step size is $h = \pi/10$, and the integration time interval is $[0, 5 \times 10^5 h]$.}
\end{figure}

5. **Concluding remarks.** In this paper, we prove that both the Gauss-Seidel scheme and its adjoint scheme for the Lorenz force system are volume-preserving schemes. Actually they can also be derived by splitting the original system into several source-free solvable subsystems [7]. The Gauss-Seidel scheme is explicit and volume-preserving, but it is only of order 1. To improve order of accuracy of the Gauss-Seidel scheme, a class of high-order Gauss-Seidel schemes are constructed by the theory of composition methods. These methods are explicit, symmetric and volume-preserving, and thus are very effective for the long-term simulation of the multi-scale dynamics of plasmas. By numerical experiments, we verify the order of accuracy of the proposed schemes, supporting Theorem 3.2. Numerical experiments also confirm that the high-order Gauss-Seidel methods could conserve conservative properties well and have excellent performance in a long time computing. It is noting that the proposed high-order methods are explicit when they are applied for the separable source-free system.

Another new second-order Gauss-Seidel scheme can be constructed by changing the combinational order of the Gauss-Seidel scheme and its adjoint method, i.e.,
Based on the second-order Gauss-Seidel scheme $\widetilde{GS}_h^2$, the fourth-order method can be obtained in terms of the Theorem 3.2

$$\widetilde{GS}_h^4 = \widetilde{GS}_h^{2\alpha_1} \circ \widetilde{GS}_h^{2\beta_1} \circ \widetilde{GS}_h^{2\alpha_1},$$

where $\alpha_1 = 1/(2 - 2^{1/3})$ and $\beta_1 = 1 - 2\alpha_1 < 0$. By numerical calculation, the schemes (32) and (33) perform the same good long-term simulation behaviour as the proposed methods in Section 3. Thus this paper provides a series of efficient schemes for long time simulation of charged particle motion under the Lorentz force. In addition, we can also apply other symmetric composition methods to develop new high-order methods (see II.4 and V.3.2 of [8]).

In order to compute efficiently in a long time, Wang et al. [21] developed a Gauss-Seidel projection method for micromagnetics simulations. Based on the first-order splitting model, they carried out a combination of a Gauss-Seidel implementation of a fractional step implicit solver for the gyromagnetic term and the projection method for the heat flow of harmonic maps. However, their method is only of order 1. In fact, we believe that a second-order Gauss-Seidel projection method can be constructed by the Strang splitting and combining the second-order Gauss-Seidel scheme and the second-order projection method of Ref. [5]. It will be discussed carefully in our future work.

Acknowledgments. Yuezheng Gong’s work is partially supported by the foundation of Jiangsu Key Laboratory for Numerical Simulation of Large Scale Complex Systems (201703). Jiaquan Gao’s work is partially supported by the National Natural Science Foundation of China (Grant No. 61379017) and the Qing Lan Project of Nanjing Normal University. Yushun Wang’s work is partially supported by the Jiangsu Collaborative Innovation Center for Climate Change, the National Natural Science Foundation of China (Grant Nos. 11271195, 41231173), the Priority Academic Program Development of Jiangsu Higher Education Institutions and the foundation of Jiangsu Key Laboratory for Numerical Simulation of Large Scale Complex Systems (115KJA110002).
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