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Why is Boris algorithm so good?

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Abstract

Due to its excellent long term accuracy, the Boris algorithm is the *de facto* standard for advancing a charged particle. Despite its popularity, up to now there has been no convincing explanation why the Boris algorithm has this advantageous feature. In this paper, we provide an answer to this question. We show that the Boris algorithm conserves phase space volume, even though it is not symplectic. The global bound on energy error typically associated with symplectic algorithms still holds for the Boris algorithm, making it an effective algorithm for the multi-scale dynamics of plasmas.

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In particle simulations of magnetized plasmas, the Boris algorithm [1–4] is the *de facto* standard for advancing a charged particle in an electromagnetic field in accordance with the equation of motion associated with the Lorentz force:

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}\,, \tag{1}$$

$$\frac{d\mathbf{v}}{dt} = \frac{q}{m}\left(\mathbf{E} + \frac{\mathbf{v}\times\mathbf{B}}{c}\right)\,. \tag{2}$$

Given the phase space coordinate $(\mathbf{x}_k, \mathbf{v}_k)$ at the k-th time-step $t_k = k\Delta t$, the Boris algorithm solves for the phase space coordinate of the particle $(\mathbf{x}_{k+1}, \mathbf{v}_{k+1})$ at the $(k+1)$-th time-step $t_{k+1} = (k+1)\Delta t$ from the discretized equation of motion:

$$\frac{\mathbf{x}_{k+1} - \mathbf{x}_k}{\Delta t} = \mathbf{v}_{k+1}\,, \tag{3}$$

$$\frac{\mathbf{v}_{k+1} - \mathbf{v}_k}{\Delta t} = \frac{q}{m}\left[\mathbf{E}_k + \frac{(\mathbf{v}_{k+1} + \mathbf{v}_k)\times\mathbf{B}_k}{2c}\right]\,, \tag{4}$$

where Δt is the step-size, and $\mathbf{x}_k \equiv \mathbf{x}(t_k)$, $\mathbf{v}_k \equiv \mathbf{v}(t_k - \Delta t/2)$, $t_k \equiv k\Delta t$, $\mathbf{E}_k \equiv \mathbf{E}(\mathbf{x}_k)$, and $\mathbf{B}_k \equiv \mathbf{B}(\mathbf{x}_k)$. At first glance, Eqs. (3) and (4) may imply that this scheme is implicit. However, the dependence on $\mathbf{v}_{k+1}$ is linear and $\mathbf{v}_{k+1}$ can be solved analytically in terms of $\mathbf{v}_k$. There are several equivalent ways to do so [1, 5]. The most commonly adopted method is to separate the electric and magnetic force as follows:

$$\mathbf{v}^- = \mathbf{v}_k + \frac{q}{m}\mathbf{E}_k\frac{\Delta t}{2}\,, \tag{5}$$

$$\frac{\mathbf{v}^+ - \mathbf{v}^-}{\Delta t} = \frac{q}{2mc}(\mathbf{v}^+ + \mathbf{v}^-)\times\mathbf{B}_k\,, \tag{6}$$

$$\mathbf{v}_{k+1} = \mathbf{v}^+ + \frac{q}{m}\mathbf{E}_k\frac{\Delta t}{2}\,. \tag{7}$$

Here, half of the electric impulse is added to $\mathbf{v}_k$ to first obtain $\mathbf{v}^-$. Then, $\mathbf{v}^+$ is calculated from Eq. (6) through a rotation of $\mathbf{v}^-$, and $\mathbf{v}_{k+1}$ is obtained by adding the remaining half of the electric impulse to $\mathbf{v}^+$. This method, defined by a one-step map $\psi_B : \mathbf{z}_k \equiv (\mathbf{x}_k, \mathbf{v}_k) \to \mathbf{z}_{k+1} \equiv (\mathbf{x}_{k+1}, \mathbf{v}_{k+1})$ according to Eqs. (3) and (5)-(7), was first used by Boris and was accordingly named the Boris algorithm. It has been successfully applied in simulation studies of magnetized plasmas for over forty years, mainly due to its excellent long term accuracy.

We emphasize that with the exciting development of groundbreaking petascale computing capability, we can now carry out large-scale, long term simulation studies of the complex plasma dynamics with higher physics fidelity than could even be imagined just a few years

ago. However, before we can fully utilize the enormous increasing power of high-performance computing, we need to ensure the accuracy and fidelity of our simulation algorithms extending to much greater temporal duration than ever before. For standard integrators of ordinary differential equations, numerical errors are estimated and controlled locally for each time-step. For instance, the standard 4th order Runge–Kutta (RK4) method carries a truncation error which is a 4th order quantity of the step-size for each time-step. Over many time-steps, the error of each time-step will add up coherently. Numerical error at later time is unbounded and can become significantly large. On the other hand, it has been discovered that the Boris algorithm is capable of solving particle's dynamics accurately for an arbitrarily large number of time-steps [3, 4]. This is of course much needed for simulation studies of plasma dynamics, which is intrinsically multi-scale, and long term accuracy is indispensable. Despite its popularity, there has been no convincing explanation as to why the Boris algorithm has this excellent capability of long term accuracy. We answer this question in this paper.

First, note that the Boris algorithm is explicit for fast computation and time-centered for second-order (local) accuracy. However, it is obvious that being explicit and time-centered has little to do with ensuring long term accuracy. Another often discussed feature of the Boris algorithm is that it conserves energy exactly when there is no electric field. For almost all applications, however, the electric field does not vanish. Hence, the energy is not conserved numerically, and a global bound on energy error would not be expected. Amazingly, we have found that the energy error for the Boris algorithm is bounded for all time-steps, as demonstrated by the numerical examples given below. This is indeed a pleasant surprise. Other similar global bounds on conserved quantities, such as the canonical momentum, have been observed as well [3, 4]. What is the reason of the existence of a global bound on numerical errors? One clue is that the Boris algorithm resembles a leapfrog scheme. In Eqs. (3) and (5)-(7), $\mathbf{v}_k$ is defined to be the velocity at $t = t_k - \Delta t/2$, a half time-step before t_k, where $\mathbf{x}_k$ is evaluated. This "staggered" time grid is the defining characteristic of a leapfrog scheme, whose property of global bound on energy error has long been recognized. Now it has been realized that this exceptional property is due to the fact that the leapfrog scheme is actually the simplest symplectic algorithm, which has been proven to be able to bound global errors in energy and other invariants of dynamics [6–9]. Unfortunately, the Boris algorithm is not a leapfrog method. This is because the acceleration force cannot

depend on velocity for the leapfrog scheme. One can insist on evaluating $\mathbf{v}_k$ at $t_k - \Delta t/2$ and $\mathbf{x}_k$ at t_k, even if the acceleration force depends on velocity. But the nice feature associated with leapfrog schemes may not hold up. Nevertheless, it is still appropriate to ask whether the Boris algorithm is symplectic. If so, then it is the reason for the existence of the global bound on energy error. If not, it is important to investigate whether the Boris algorithm possesses some characteristics of a symplectic algorithm that may contribute to it long term accuracy.

In this paper, we show that the Boris algorithm is not symplectic, but it does conserve phase space volume, *i.e.*, it is volume-preserving. An algorithm being volume-preserving is a necessary but not sufficient condition for it to be symplectic. In other words, we show that even though the Boris algorithm is not symplectic according to the standard definition, it does on the other hand possess the beneficial feature of sympletic algorithms, *i.e.*, the phase space volume is conserved, and this is the reason that the energy error is globally bounded for an arbitrarily large number of simulation time-steps. This revelation also suggests a new research direction for computational plasma physics, *i.e.*, exploring other kinds of volume-conserving algorithms for large-scale, long term simulations of multi-scale plasma physics phenomena.

We start from Eq. (4), which can be written as

$$\left(I + \hat{\Omega}_k\right) \begin{pmatrix} v^1_{k+1} \\ v^2_{k+1} \\ v^3_{k+1} \end{pmatrix} = \left(I - \hat{\Omega}_k\right) \begin{pmatrix} v^1_k \\ v^2_k \\ v^3_k \end{pmatrix} + \frac{q\Delta t}{m} \begin{pmatrix} E^1_k \\ E^2_k \\ E^3_k \end{pmatrix}. \tag{8}$$

Here, superscript $i = 1, 2, 3$ denotes the components of vectors in the three-dimensional configuration space, I is the 3×3 unit matrix. The 3×3 matrix

$$\hat{\Omega}_k = \frac{q\Delta t}{mc} \begin{pmatrix} 0 & -B^3_k & B^2_k \\ B^3_k & 0 & B^1_k \\ -B^2_k & -B^1_k & 0 \end{pmatrix} \tag{9}$$

is an anti-symmetric matrix associated with the vector $\Omega_k \equiv (B^1_k, B^2_k, B^3_k) q\Delta t/mc$. Such an association is the so-called hat map [10]. Then, the one-step map of the algorithm

$\psi_B : \mathbf{z}_k \equiv (\mathbf{x}_k, \mathbf{v}_k) \to \mathbf{z}_{k+1} \equiv (\mathbf{x}_{k+1}, \mathbf{v}_{k+1})$ is

$$\mathbf{v}_{k+1} = R\mathbf{v}_k + \left(I + \hat{\Omega}_k\right)^{-1} \frac{q\Delta t}{m}\mathbf{E}_k \,, \tag{10}$$

$$\mathbf{x}_{k+1} = \mathbf{x}_k + R\mathbf{v}_k\Delta t + \left(I + \hat{\Omega}_k\right)^{-1} \frac{q\Delta t^2}{m}\mathbf{E}_k \,, \tag{11}$$

where the matrix R is the Caylay transformation [11] of $\hat{\Omega}_k$, *i.e.*,

$$R \equiv \left(I + \hat{\Omega}_k\right)^{-1} \left(I - \hat{\Omega}_k\right). \tag{12}$$

From Eq. (12), it can be easily shown that $\hat{\Omega}_k \equiv (I + R)^{-1}(I - R)$, *i.e.*, $\hat{\Omega}_k$ is also the Caylay transformation of R. There is a theorem due to Weyl [7] which states that if P is the Caylay transformation of Q, then for an arbitrary matrix A the equation $P^T A P = A$ holds if and only if $Q^T A + AQ = 0$. For the matrices R and $\hat{\Omega}_k$ of interest, we have $\hat{\Omega}_k^T + \hat{\Omega}_k = 0$, and thus $R^T R = I$, *i.e.*, $R \in O(3)$. Since R is continuously connected to I as $\Delta t \to 0$, R must be a rotation in the 3D space, $R \in SO(3)$. The Jacobian matrix of the one-step map $\psi_B : \mathbf{z}_k \equiv (\mathbf{x}_k, \mathbf{v}_k) \to \mathbf{z}_{k+1} \equiv (\mathbf{x}_{k+1}, \mathbf{v}_{k+1})$ is simply

$$\frac{\partial \psi_B}{\partial \mathbf{z}_k} = \begin{pmatrix} I + \Delta t \dfrac{\partial \mathbf{v}_{k+1}}{\partial \mathbf{x}_k} & \Delta t R \\ \dfrac{\partial \mathbf{v}_{k+1}}{\partial \mathbf{x}_k} & R \end{pmatrix}, \tag{13}$$

where $\mathbf{v}_{k+1}$ depends on $\mathbf{x}_k$ through the inhomogeneity of the electromagnetic field.

We now prove that the Boris algorithm cannot be symplectic. The condition for a one-step map $\psi : \mathbf{z}_k \equiv (\mathbf{x}_k, \mathbf{v}_k) \to \mathbf{z}_{k+1} \equiv (\mathbf{x}_{k+1}, \mathbf{v}_{k+1})$ to be sympletic is that its Jacobian matrix is symplectic,

$$\left(\frac{\partial \psi}{\partial \mathbf{z}_k}\right)^T J \left(\frac{\partial \psi}{\partial \mathbf{z}_k}\right) = J \,, \tag{14}$$

where $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$ is the 6×6 unit symplectic matrix. If we write the Jacobian matrix in 3×3 blocks,

$$\frac{\partial \psi}{\partial \mathbf{z}_k} = \begin{pmatrix} S_1 & S_2 \\ S_3 & S_4 \end{pmatrix}, \tag{15}$$

then a set of sufficient and necessary conditions for it to be symplectic are

$$S_1 S_2^T = S_2 S_1^T \,, \tag{16}$$

$$S_3 S_4^T = S_4 S_3^T \,, \tag{17}$$

$$S_1 S_4^T - S_2 S_3^T = I \,. \tag{18}$$

These conditions are in general not satisfied by the Jacobian matrix of the Boris algorithm given by Eq. (13). To see this, consider the special case where the electric and magnetic fields are homogenous such that $\partial \mathbf{v}_{k+1}/\partial \mathbf{x}_k = 0$. In this case, $S_1 S_4^T - S_2 S_3^T = R^T \neq I$. Therefore, one-step map $\psi_B : \mathbf{z}_k \equiv (\mathbf{x}_k, \mathbf{v}_k) \to \mathbf{z}_{k+1} \equiv (\mathbf{x}_{k+1}, \mathbf{v}_{k+1})$ is not symplectic. For charged particle dynamics in an electromagnetic field, the canonical Hamiltonian structure is associated with the canonical momentum $\mathbf{p} \equiv m\mathbf{v} + e\mathbf{A}/c$. One may wonder whether the one-step map $(\mathbf{x}_k, \mathbf{p}_k) \to (\mathbf{x}_{k+1}, \mathbf{p}_{k+1})$ of the canonical momentum is symplectic. A straightforward calculation using the same method shows that the momentum map $(\mathbf{x}_k, \mathbf{p}_k) \to (\mathbf{x}_{k+1}, \mathbf{p}_{k+1})$ induced by $\psi_B : \mathbf{z}_k \equiv (\mathbf{x}_k, \mathbf{v}_k) \to \mathbf{z}_{k+1} \equiv (\mathbf{x}_{k+1}, \mathbf{v}_{k+1})$ is also not symplectic.

One of the merits of a symplectic algorithm is that the phase space volume is conserved. For a symplectic one-step map ψ, it is evident from Eq. (14) that the determinant of the Jacobian matrix is one, *i.e.*, $|\partial \psi/\partial \mathbf{z}_k| = 1$. Even though we have just proven that the Boris algorithm is not symplectic, it surprisingly does conserve the phase space volume. This fact is easily proven as follows.

$$\left|\frac{\partial \psi_B}{\partial \mathbf{z}_k}\right| = \begin{vmatrix} I + \Delta t \dfrac{\partial \mathbf{v}_{k+1}}{\partial \mathbf{x}_k} & \Delta t R \\ \dfrac{\partial \mathbf{v}_{k+1}}{\partial \mathbf{x}_k} & R \end{vmatrix} = \begin{vmatrix} I & 0 \\ \dfrac{\partial \mathbf{v}_{k+1}}{\partial \mathbf{x}_k} & R \end{vmatrix} = |R| = 1\,,$$

where the second row times Δt has been subtracted from the first row to obtain the second equal sign. The volume-preserving property is the reason that the Boris algorithm has the capability of long term accuracy.

We now proceed to demonstrate this property by several numerical examples. The first example is the 2D dynamics of a charged particle in a static electromagnetic field given by

$$\mathbf{B} = (x^2 + y^2)^{1/2}\mathbf{e}_z, \quad \phi = 10^{-2}(x^2 + y^2)^{-1/2}.$$

Physical quantities are normalized by the system size a, characteristic magnetic field B_0, and the gyro-frequency $\Omega_0 \equiv qB_0/mc$ of the particle. Plotted in Figs. 1 and 2 are the numerical solutions using the Boris algorithm and the RK4 method, respectively. Theoretical analysis shows that the particle's orbit is a spiraling circle with constant radius (see Fig. 1). The large circle corresponds to the ∇B drift and the $\mathbf{E} \times \mathbf{B}$ drift of the guiding center, and the small circle is the fast-scale gyromotion. The step-size for both calculations is $\pi/10$ (1/20 of the characteristic gyro-period). The Boris algorithm gives the correct orbit at the beginning and later stage of the numerical solution, whiles the RK4 method fails at the later

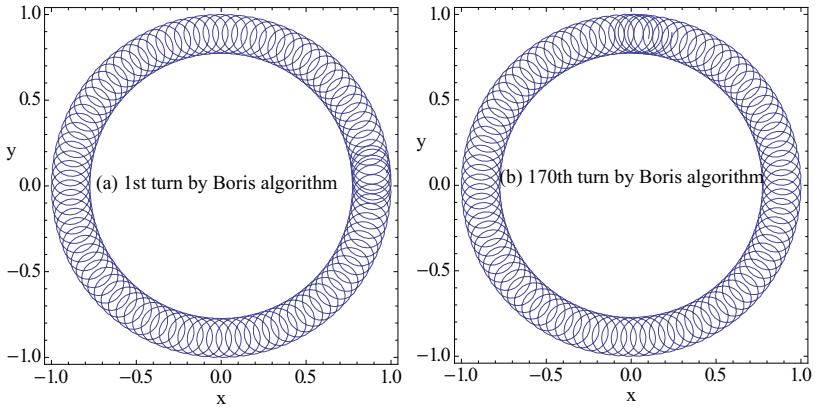

Figure 1: The Boris algorithm gives the correct orbit at the beginning (a) and later stage (b) of the numerical solution.

stage. For the result generated by the RK4 method, the gyromotion is numerically dissipated due to the numerical damping of energy. This is clearly demonstrated in Fig. 3, where the normalized energy for both methods are plotted as a function of time. The energy error for the Boris algorithm is not zero, but it is bounded for all simulation time-steps, which is the desirable feature associated with symplectic algorithms. As we have just proven, the Boris algorithm is not symplectic. However, it is volume-preserving, and it can be expected that the property of long term bound on energy error still holds. The RK4 algorithm fails because the problem investigated is multi-scale in nature. The fast gyromotion co-exists with the slow guiding center dynamics, and it is necessary to simulate the system for a large number of time-steps. The RK4 method, as a standard algorithm with local error control, is suitable for problems with only one time-scale. For multi-scale problems, it is essential to use symplectic or volume-preserving methods with global bound on numerical errors.

The next example considered is the banana orbit of a charged particle in an axi-symmetric tokamak geometry with and without an inductive electric field in the toroidal direction. Shown in Fig. 4 is the comparison of banana orbits calculated using the Boris algorithm and the RK4 algorithm when there is no toroidal electric field. Because of toroidal symmetry, the particle's guiding center should form a closed orbit that is superimposed on the fast time-scale gyromotion. This orbit is correctly obtained by the Boris algorithm. In contrast, the RK4 algorithm produces an erroneous orbit, where the banana orbit is not closed and gradually transformed into a circulating orbit due to the accumulation of numerical energy dissipation. The step-size for both methods is about 1/20 of the gyro-period. If an inductive

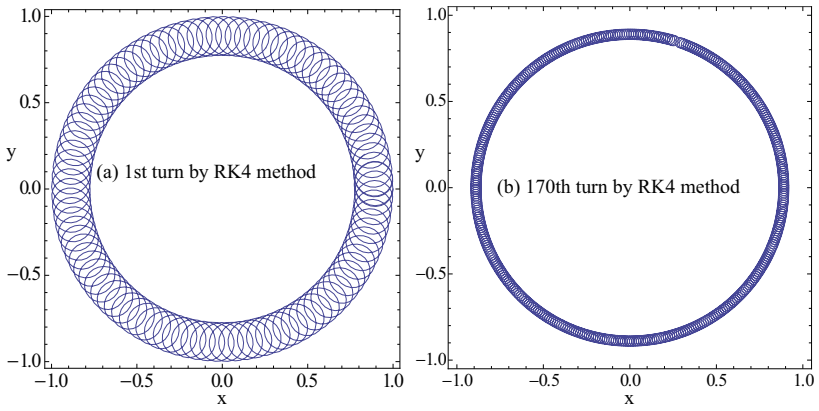

Figure 2: The RK4 method fails to generate the correct orbit at the later stage due to the accumulation of numerical error.

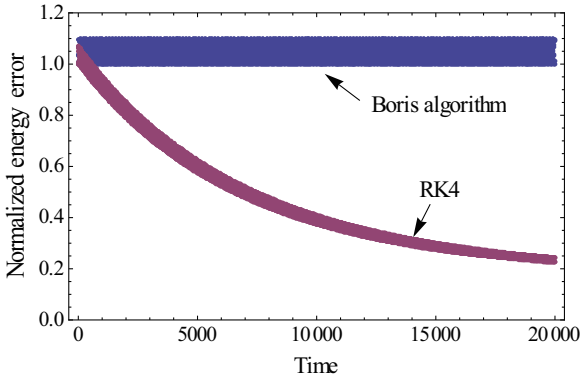

Figure 3: The energy error for the Boris algorithm is bounded for all time-steps, whiles that for the RK4 method increases without bound. The time axis has been normalized by the gyro-period.

electric field in the toroidal direction is imposed, the banana orbit will experience an inward pinch in the radial direction, which is known as the Ware pinch [12]. Simulation results are plotted in Fig. 5. The Boris algorithm captures the Ware pinch effect in great detail. For example, it is interesting to observe that in addition to the inward pinch, the up-down symmetry of the banana orbit (projected on a polodial plane) is broken due to the presence of an axi-symmetric toroidal electric field. As evident from Fig. 5(b), the RK4 method is unable to capture these important effects.

It is necessary to point out that even though the energy error is bounded for the Boris algorithm, there is no guarantee that the error in the phase of a periodic motion numerically calculated is bounded for all time. This is the case for all symplectic algorithms and volume-preserving algorithms. In some sense, this is not surprising because symplectic algrithms and

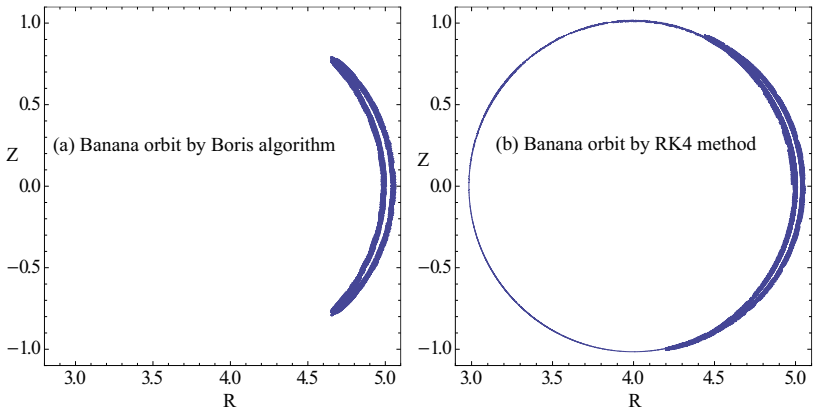

Figure 4: The banana orbit is correctly obtained by the Boris algorithm (a). The RK4 algorithm gives an erroneous orbit (b), where the banana orbits is not closed and is gradually transformed into a circulating orbit due to the accumulation of numerical energy dissipation. The orbit consists of a slow guiding center motion, superimposed on the fast time-scale gyromotion, which appears in the figure as a dense patch of dots along each point of the guiding center trajectory.

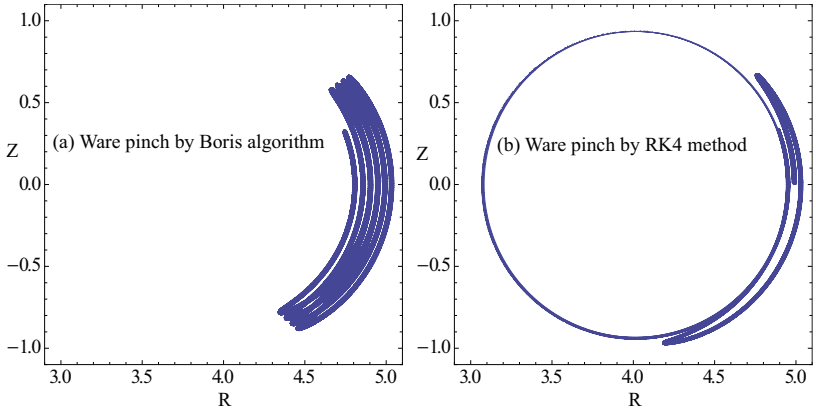

Figure 5: The Boris algorithm captures the Ware pinch effect in great detail (a). In contrast, the RK4 method fails dramatically for this case (b).

volume-preserving algorithms only bound the energy error for all time, but for most cases do not bound other invariants of the dynamics, such as the angular momentum for a system with angular symmetry. Nevertheless, conserving phase space volume and bounding energy error in general are beneficial. For systems with periodic orbits, such as the numerical examples studied in this paper, the phase error of the Boris algorithm will grow with time linearly, which indicates an error in the frequency of the periodic motion. Numerical calculations show that the error in frequency is always systematic rather than random, which suggests

that an algorithmic correction might be possible. This topic will be investigated in future studies.

In summary, we have proven that the widely adopted Boris algorithm for numerically solving for particle orbits in an electromagnetic field is not symplectic. However, it is volume-preserving, *i.e.*, it conserves the phase space volume. The global bound on energy error typically associated with symplectic algorithms still holds for the Boris algorithm. This is the reason why the Boris algorithm is an effective algorithm for charged particle dynamics in an electromagnetic field, which is intrinsically a multi-scale dynamic problem.

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