Double Leap-Frog Method for Large-Time-Step Particle Simulation to Keep Larmor Radius Small

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A modified leap-frog (LF) scheme is presented that keeps the correct Larmor radius even in case of a large time step \( \Delta t \) compared to the cyclotron period \( \Omega^{-1} \), \( \Omega \Delta t \gg 1 \), for the particle simulation of a plasma in the strong magnetic field. The Larmor radius simulated by the conventional LF method becomes very large for \( \Omega \Delta t \gg 1 \), and such a numerical condition has been avoided in general. If the LF method is applicable to such situations, new particle simulation codes can be more easily developed for a wide area of plasma physics. By repeating the LF steps doubly and adopting the averaged velocity to advance the particle position, the Larmor radius is kept real independently of the \( \Omega \Delta t \) value. Proper nature on the energy conservation, magnetic moment conservation and drift-velocity realization is safely inherited from the LF method.

Keywords: particle simulation, leap-frog method, time step, Larmor radius

In first-principle particle-based simulation codes for plasma physics including cyclotron gyration effects, the leap-frog (LF) method has been widely used to integrate equations of motion of an individual numerical particle [1];

\[
\begin{align*}
\rho(t + \Delta t/2) - \rho(t - \Delta t/2) &= (q/m)[E(t) + v_0 \times B(t)]\Delta t, \\
X(t + \Delta t) - X(t) &= u(t + \Delta t/2)\Delta t, \\
\end{align*}
\]

where \( v_0 = [u(t + \Delta t/2) + u(t - \Delta t/2)]/2 \). Variables are the velocity \( u \), position \( X \), electric charge \( q \), mass \( m \), time \( t \), and the time step \( \Delta t \). The velocity and position are set differently each other with half-time-step separation. The electric field \( E(t) \) and magnetic field \( B(t) \) are chosen at the particle position \( X(t) \). One of notable merits of the LF method is to assure the energy conservation; \( u^2(t + \Delta t/2) - u^2(t - \Delta t/2) = (2q\Delta t/m)E(t) \cdot v_0 \). Due to the finiteness of \( \Delta t \), the simulated cyclotron frequency \( \Omega_{LF} \) becomes smaller than real one, \( \Omega = qB/m \), and the Larmor radius \( \rho_{LF} \) is larger than real one, \( \rho = v_\perp/\Omega \) (\( v_\perp \) is the speed perpendicular to \( B \));

\[
\begin{align*}
\Omega_{LF}\Delta t &= 2\tan^{-1}(\Omega\Delta t/2), \\
\rho_{LF} &= \rho/\cos(\Omega_{LF}\Delta t/2). \\
\end{align*}
\]

For \( \Omega \Delta t < 1 \), the relative errors are \( \Omega_{LF}/\Omega - 1 = -(\Omega\Delta t/2)^2/12 \) and \( \rho_{LF}/\rho - 1 = (\Omega\Delta t)^2/8 \). Note that the relation \( \rho_{LF} = v_\perp/\Omega_{LF} \) does not hold. When \( \Omega \Delta t \to \infty \), \( \Omega_{LF} \) and \( \rho_{LF} \) converge to \( \pi/\Delta t \) and \( v_\perp\Delta t/2 \), respectively. The perpendicular velocity is inversely changed every step, \( v_\perp(t + \Delta t/2) = -v_\perp(t - \Delta t/2) \). Here we consider the absolute value of \( \Omega \) for simplicity.

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In order to correct the gyro-phase delay, the Boris algorithm has been adopted [2, 3]. Removing the \( E \) effect, Eq. (1) of an implicit form is modified to an explicit form;

\[
\begin{align*}
u_\perp(t + \Delta t/2) - u_\perp(t - \Delta t/2) &= (2q\Delta t/m)E(t) \times b_\perp/(1 + b_\perp^2), \quad \text{where} \\
b_\perp = (B/B)\tan(\Omega\Delta t/2), \\
\end{align*}
\]

and \( \rho_{Belor} \sim 2, \rho_{Boris}/\rho - 1 = (\Omega\Delta t)^2/24 \), is smaller than that of LF method. On the other hand, when \( \Omega \Delta t \gg 1 \), the radius is varied bizarrely; \( \rho_{Boris} = v_\perp\Delta t/2 \) is similar to \( \rho_{LF} \) at \( \Omega \Delta t = (2I + 1)\pi \), but it becomes infinitely large at \( \Omega \Delta t = 2I\pi \) \( (I \) is an integer) .

Of course particle simulations with gyration motions have generally been carried out under the condition of \( \Omega \Delta t \ll 1 \). In an electrostatic particle-in-cell (PIC) simulation code for the edge plasma in the strong magnetic field (\( \Omega \Delta t \gg 1 > \Omega \Delta t_s \)), called PARASOL [4], the ion motion including gyration is solved by the LF method, while the motion of electron guiding center is solved by the predictor-corrector method. If the LF method is applicable to the large-time-step particle simulation of \( \Omega \Delta t \gg 1 \), new particle simulation codes can be more easily developed and simulation studies (longer time scale with the larger time step) can be promoted for a wide area of plasma physics.

First, we examine to which extent the LF method correctly simulates the charged particle motion in electric and magnetic fields when \( \Omega \Delta t \gg 1 \). As described above, \( \Omega_{LF} \) and \( \rho_{LF} \) converge to \( \pi/\Delta t \ll \Omega \) and \( v_\perp\Delta t/2 \gg \rho \), respectively. On the other hand, (i) the energy conservation
is assured, and (ii) the magnetic moment, $\mu = m v_0^2 / 2B$, is kept constant within the relative error $\sim O(\rho_{LF} / L_B)$ or $O(1/\Omega_{LF} \tau_B)$. Therefore, (iii) the mirror force parallel to $B$ is realized, $F_M = -\mu \nabla v_0$. Here the characteristic length $L_B$ is of the spatial variation of $B$, and the characteristic time $\tau_B$ is of its temporal variation. This favorable property is based on a moment $M = m \rho_{LF} |v_{01}|$ calculated from the r.h.s. of Eq. (1) being fully independent of $\Omega \Delta t$, $M = m \rho_{LF} (\cos(\Omega_{LF} \Delta t/2)) = m \rho_{L}$. As for the drift perpendicular to $B$, (iv) the $E \times B$ drift, $V_{EB} = (E \times B) / B^2$, is correctly simulated, and (v) the polarization drift, $V_{pol} = (dE/dt) / B \Omega$, as well. Although $\rho_{LF} \approx v_1 \Delta t/2 \gg \rho_\star \Omega \Delta t > 2 v_0 / v_e$, when $v_1 > v_e$, then $\Omega \Delta t \sim 1/30 (v_e$ and $v_i$ are the thermal speed of electron and ion). Resultantly, the classical diffusion perpendicular to $B$, $D_i \approx \rho_i^2 / \tau_e$ (where $\tau_e$ is the electron collision time), becomes abnormally larger by $(\Omega_{LF} \Delta t)^2$.

In order to keep the simulated Larmor radius small independently of the $\Omega \Delta t$ value, we propose a new scheme based on the LF method. The usual LF steps are repeated doubly as described below. We call this scheme, therefore, “double leap-frog (DLF)” method.

$$v_{+,3/2} - v_{-,3/2} = (q/m) (E' + v_{01} \times B') \Delta t,$$

$$X'^\ast(t + \Delta t) - X'(t) = v_{+,3/2} \Delta t,$$

$$v_{+,5/2} - v_{-,5/2} = (q/m) [E'' + v_1 \times B''] \Delta t,$$

$$X'(t + \Delta t) - X(t) = w_{+,5/2} \Delta t,$$

$$w_{-,5/2} = (\alpha/2) (v_{+,5/2} - v_{-,5/2}) + (1 - \alpha) w_{+,3/2},$$

$$X'(t + \Delta t) - X'(t + \Delta t) = (\alpha/2) (w_{+,5/2} - v_{-,3/2}) \Delta t,$$

where $v_1 = (v_{+,3/2} + v_{-,3/2}) / 2$. The virtual position $X'$ (or $X''$) moves along an enlarged gyration orbit with $\rho_{LF}$. To keep the real Larmor radius $\rho$, we use an averaged velocity $w_{+,3/2}$ to advance $X$ in Eq. (7) with a coefficient $\alpha = [2 + 2 \cos(\Omega_{LF} \Delta t/2)]^{-1}$. A simple reduction of the perpendicular movement, $dX_\perp = v_1 \Delta t / \Delta t \times \cos(\Omega_{LF} \Delta t/2)$, cannot be applied because the $E \times B$ drift is also reduced. The gyration frequency $\Omega_{LF}$ is not corrected as it is, and the phase relation is the same as that of LF method; $X_\perp \sim \exp(i \Delta t \Delta t)$ and $v_1 \sim i \exp(i \Delta t \Delta t)$. The virtual position $X'(t + \Delta t)$ is reset in accordance with Eq. (9), so that its guiding center is not separating from that of $X$ orbit. Using this Eq. (9), the initial value of $X'(0)$ is determined from $X(0)$ and $v'(-\Delta t/2)$: $X'(0) - X(0) = (\alpha/2) (v_{+,3/2} - v_{-,3/2}) \Delta t$ with $v' = v_{+,3/2} = (q/m) [E(X(0)) + (v_1 + v_{01}) \times 2 \times 2 \times B(X(0))] \Delta t$. Tentative variables $X''$ and $v''$ do not continue to the next time-step calculation. Collisional change in $v_{+,3/2}$ then can be given after the above DLF process. Gyration of $X$ (solid line) and $X'$ (dashed line) are schematically shown in Fig. 1 for $\Omega \Delta t = 2.5$ ($\Omega_{LF} \Delta t = 1.79$ and $\rho_{LF} = 1.60 \rho_\star$).

Electric and magnetic fields in Eqs. (4) and (6) are chosen at the virtual position; $E' - B'$ at $X'(t)$ and $E'' - B''$ at $X''(t + \Delta t)$. By this setting, proper nature on the magnetic moment conservation and drift-velocity realization is safely inherited from the LF method. The electrostatic component $E_x = -\nabla \phi$ (where $\phi$ is the potential) could be chosen at the real position $X(t)$. Since $X(t + \Delta t)$ is still not determined before Eq. (6), how to self-consistently treat $E''$ and $B''$ is the future problem. The flux parallel to $B$ is calculated at the real position, while the perpendicular flux including diamagnetic flow is calculated at the virtual position; $nV = \Sigma S(X - X_i) w_0 + S(X - X_i) w_0^1$, where $S$ is a shape function in a PIC simulation (j is the particle tag). Note that the diamagnetic flow cannot directly be obtained in the guiding-center system.

The DLF method for long temporal-scale particle simulation becomes more powerful when coupled with the in-vessel model [6,7] for large spatial-scale simulation. The DLF algorithm will be tested during our development of the PIXY code ([6,7] for large spatial-scale simulation). The DLF algorithm will be tested during our development of the PIXY code ([6,7] for large spatial-scale simulation). The DLF algorithm will be tested during our development of the PIXY code ([6,7] for large spatial-scale simulation). The DLF algorithm will be tested during our development of the PIXY code ([6,7] for large spatial-scale simulation). The DLF algorithm will be tested during our development of the PIXY code ([6,7] for large spatial-scale simulation).