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 Δt compared to the cyclotron period Ω^{-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

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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];

$$\boldsymbol{v}(t + \Delta t/2) - \boldsymbol{v}(t - \Delta t/2) = (q/m)[\boldsymbol{E}(t) + \boldsymbol{v}_0 \times \boldsymbol{B}(t)]\Delta t, \quad (1)$$

$$\boldsymbol{X}(t + \Delta t) - \boldsymbol{X}(t) = \boldsymbol{v}(t + \Delta t/2)\Delta t, \quad (2)$$

where $\boldsymbol{v}_0 = [\boldsymbol{v}(t + \Delta t/2) + \boldsymbol{v}(t - \Delta t/2)]/2$. Variables are the velocity $\boldsymbol{v}$, position $\boldsymbol{X}$, electric charge q, mass m, time t, and the time step Δt. The velocity and position are set differently each other with half-time-step separation. The electric field $\boldsymbol{E}(t)$ and magnetic field $\boldsymbol{B}(t)$ in Eq. (1) are chosen at the particle position $\boldsymbol{X}(t)$. One of notable merits of the LF method is to assure the energy conservation; $\boldsymbol{v}^2(t + \Delta t/2) - \boldsymbol{v}^2(t - \Delta t/2) = (2q\Delta t/m)\boldsymbol{E}(t) \cdot \boldsymbol{v}_0$. Due to the finiteness of Δt, the simulated cyclotron frequency $\Omega_{\rm LF}$ becomes smaller than real one, $\Omega = qB/m$, and the Larmor radius $\rho_{\rm LF}$ is larger than real one, $\rho = v_\perp/\Omega$ ($v_\perp$ is the speed perpendicular to $\boldsymbol{B}$);

$$\Omega_{\rm LF}\Delta t = 2\tan^{-1}(\Omega\Delta t/2), \quad \rho_{\rm LF} = \rho/\cos(\Omega_{\rm LF}\Delta t/2). \quad (3)$$

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

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In order to correct the gyro-phase delay, the Boris algorithm has been adopted [2, 3]. Removing the $\boldsymbol{E}$ effect, Eq. (1) of an implicit form is modified to an explicit form; $\boldsymbol{u}_{+\Delta t/2} - \boldsymbol{u}_{-\Delta t/2} = (\boldsymbol{u}_{-\Delta t/2} + \boldsymbol{u}_{-\Delta t/2} \times \boldsymbol{b}_*) \times 2\boldsymbol{b}_*/(1 + \boldsymbol{b}_*^2)$, where $\boldsymbol{b}_* = (\boldsymbol{B}/B)\tan(\Omega\Delta t/2)$, $\boldsymbol{u}_{-\Delta t/2} = \boldsymbol{v}_{-\Delta t/2} + (q\Delta t/2m)\boldsymbol{E}(t)$ and $\boldsymbol{v}_{+\Delta t/2} = \boldsymbol{u}_{+\Delta t/2} + (q\Delta t/2m)\boldsymbol{E}(t)$. Hereafter, we replace $\boldsymbol{v}(t \pm \Delta t/2)$ with $\boldsymbol{v}_{\pm\Delta t/2}$. The simulated cyclotron frequency is just the real frequency. In spite of the correct Ω, the Larmor radius is affected by the finite Δt as $\rho_{\rm Boris} = \rho \times |(\Omega\Delta t/2)/\sin(\Omega\Delta t/2)|$. When $\Omega\Delta t < 1$, the relative error, $\rho_{\rm Boris}/\rho - 1 = (\Omega\Delta t)^2/24$, is smaller than that of LF method. On the other hand, when $\Omega\Delta t \gg 1$, the radius is varied bizarrely; $\rho_{\rm Boris} = v_\perp\Delta t/2$ is similar to $\rho_{\rm LF}$ at $\Omega\Delta t = (2l + 1)\pi$, but it becomes infinitely large at $\Omega\Delta t = 2l\pi$ (l 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 ($\Omega_{\rm e}\Delta t \gg 1 > \Omega_{\rm i}\Delta t$), 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, $\Omega_{\rm LF}$ and $\rho_{\rm LF}$ 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, $\mu = mv_\perp^2/2B$, 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 $\boldsymbol{B}$ is realized, $\boldsymbol{F}_M = -\mu\nabla_\| B$. Here the characteristic length L_B is of the spatial variation of $\boldsymbol{B}$, and the characteristic time τ_B is of its temporal variation. This favorable property is based on a moment $M = m\rho_{LF}|v_{0\perp}|$ calculated from the r.h.s. of Eq. (1) being fully independent of $\Omega\Delta t$, $M = m\rho_{LF}v_\perp\cos(\Omega_{LF}\Delta t/2) = m\rho v_\perp$. As for the drift perpendicular to $\boldsymbol{B}$, (iv) the $E\times B$ drift, $\boldsymbol{V}_{E\times B} = (\boldsymbol{E}\times\boldsymbol{B})/B^2$, is correctly simulated, and (v) the polarization drift, $\boldsymbol{V}_{polar} = (\mathrm{d}\boldsymbol{E}/\mathrm{d}t)/B\Omega$, as well. Although $\rho_{LF} \approx v_\perp\Delta t/2 \gg \rho$ for $\Omega\Delta t \gg 1$, (vi) the curvature-∇B drift, $\boldsymbol{V}_{\nabla B} = (2v_\|^2 + v_\perp^2)(\boldsymbol{B}\times\nabla B)/2B^2\Omega$, can be simulated without worry ($v_\|$ is the speed parallel to $\boldsymbol{B}$).

The enlarged Larmor radius is a fatal demerit of the LF method if applied to $\Omega\Delta t \gg 1$. Strangely, the electron Larmor radius, $\rho_{e,LF} \sim v_e\Delta t/2$, becomes larger than that of deuterium ion, $\rho_{i,LF} \sim v_i/\Omega_i$, when $1 > \Omega_i\Delta t > 2v_i/v_e \sim 1/30$ (v_e and v_i are the thermal speed of electron and ion). Resultantly, the classical diffusion perpendicular to $\boldsymbol{B}$, $D_\perp \approx \rho_e^2/\tau_e$ (τ_e is the electron collision time), becomes abnormally larger by $(\Omega_e\Delta t)^2$.

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.

$$\boldsymbol{v}_{+\Delta t/2} - \boldsymbol{v}_{-\Delta t/2} = (q/m)[\boldsymbol{E}' + \boldsymbol{v}_0\times\boldsymbol{B}']\Delta t, \quad (4)$$

$$\boldsymbol{X}^\#(t+\Delta t) - \boldsymbol{X}'(t) = \boldsymbol{v}_{+\Delta t/2}\Delta t, \quad (5)$$

$$\boldsymbol{v}^\#_{+3\Delta t/2} - \boldsymbol{v}_{+\Delta t/2} = (q/m)[\boldsymbol{E}^\# + \boldsymbol{v}_1\times\boldsymbol{B}^\#]\Delta t, \quad (6)$$

$$\boldsymbol{X}(t+\Delta t) - \boldsymbol{X}(t) = \boldsymbol{w}_{+\Delta t/2}\Delta t, \quad (7)$$

$$\boldsymbol{w}_{+\Delta t/2} = (\alpha/2)(\boldsymbol{v}^\#_{+3\Delta t/2} + \boldsymbol{v}_{-\Delta t/2}) + (1-\alpha)\boldsymbol{v}_{+\Delta t/2}, \quad (8)$$

$$\boldsymbol{X}'(t+\Delta t) - \boldsymbol{X}(t+\Delta t) = (\alpha/2)(\boldsymbol{v}_{+\Delta t/2} - \boldsymbol{v}^\#_{+3\Delta t/2})\Delta t, \quad (9)$$

where $\boldsymbol{v}_1 = (\boldsymbol{v}^\#_{+3\Delta t/2} + \boldsymbol{v}_{+\Delta t/2})/2$. The virtual position $\boldsymbol{X}'$ (or $\boldsymbol{X}^\#$) moves along an enlarged gyration orbit with ρ_{LF}. To keep the real Larmor radius ρ, we use an averaged velocity $\boldsymbol{w}_{+\Delta t/2}$ to advance $\boldsymbol{X}$ in Eq. (7) with a coefficient $\alpha = [2 + 2\cos(\Omega_{LF}\Delta t/2)]^{-1}$. A simple reduction of the perpendicular movement, $\mathrm{d}\boldsymbol{X}_\perp = \boldsymbol{v}_{\perp,+\Delta t/2}\Delta t\times\cos(\Omega_{LF}\Delta t/2)$, cannot be applied because the $E\times B$ drift is also reduced. The gyration frequency Ω_{LF} is not corrected as it is, and the phase relation is the same as that of LF method; $\boldsymbol{X}_\perp \sim \exp(i\Omega_{LF}t)$ and $\boldsymbol{v}_\perp \sim i\exp(i\Omega_{LF}t)$. The virtual position $\boldsymbol{X}'(t+\Delta t)$ is reset in accordance with Eq. (9), so that its guiding center is not separating from that of $\boldsymbol{X}$ orbit. Using this Eq. (9), the initial value of $\boldsymbol{X}'(0)$ is determined from $\boldsymbol{X}(0)$ and $\boldsymbol{v}(-\Delta t/2)$; $\boldsymbol{X}'(0) - \boldsymbol{X}(0) = (\alpha/2)\,(\boldsymbol{v}_{-\Delta t/2} - \boldsymbol{v}^\#)\Delta t$ with $\boldsymbol{v}^\# - \boldsymbol{v}_{-\Delta t/2} = (q/m)\,[\boldsymbol{E}(\boldsymbol{X}(0)) + (\boldsymbol{v}^\# + \boldsymbol{v}_{-\Delta t/2})/2\times\boldsymbol{B}(\boldsymbol{X}(0))]\Delta t$. Tentative variables $\boldsymbol{X}^\#$ and $\boldsymbol{v}^\#$ do not continue to the next time-step calculation. Collisional change in $\boldsymbol{v}_{+\Delta t/2}$ [5] then can be given after the above DLF process. Gyration orbits of $\boldsymbol{X}$ (solid line) and $\boldsymbol{X}'$ (dashed line) are schematically shown in Fig. 1 for $\Omega\Delta t = 2.5$ ($\Omega_{LF}\Delta t = 1.79$ and $\rho_{LF} = 1.60\rho$).

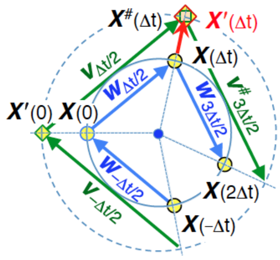

Fig. 1 Gyration orbit of $\boldsymbol{X}$ with correct Larmor radius ρ for $\Omega\Delta t = 2.5$. Velocity $\boldsymbol{v}$, averaged velocity $\boldsymbol{w}$, virtual orbit $\boldsymbol{X}'$ (or $\boldsymbol{X}^\#$) with larger $\rho_{LF} = 1.60\rho$ and resetting of $\boldsymbol{X}'(\Delta t)$ are schematically shown.

Electric and magnetic fields in Eqs. (4) and (6) are chosen at the virtual position; $\boldsymbol{E}'$ - $\boldsymbol{B}'$ at $\boldsymbol{X}'(t)$ and $\boldsymbol{E}^\#$ - $\boldsymbol{B}^\#$ at $\boldsymbol{X}^\#(t+\Delta t)$. By this setting, proper nature on the magnetic moment conservation and drift-velocity realization is safely inherited from the LF method. The electrostatic component $\boldsymbol{E}_s = -\nabla\phi$ (ϕ is the potential) could be chosen at the real position $\boldsymbol{X}(t)$. Since $\boldsymbol{X}(t+\Delta t)$ is still not determined before Eq. (6), how to self-consistently treat $\boldsymbol{E}^\#$ and $\boldsymbol{B}^\#$ is the future problem. The flux parallel to $\boldsymbol{B}$ is calculated at the real position, while the perpendicular flux including diamagnetic flow is calculated at the virtual position; $n\boldsymbol{V} = \Sigma_j\{S(\boldsymbol{X}-\boldsymbol{X}_j)\boldsymbol{v}_{0\|} + S(\boldsymbol{X}-\boldsymbol{X}'_j)\boldsymbol{v}_{0\perp}\}$, 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 ingenious model [6, 7] for large spatial-scale simulation. The DLF algorithm will be tested during our development of the PIXY code ($\Omega_e\Delta t \gg 1 > \Omega_i\Delta t$) [8] in the near future. The possibility of using this new modeling in kinetic simulations instead of using the gyrokinetic approach ($\Omega_i\Delta t \gg 1$) [9] will be examined in future studies.

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