

# A HIGH PRECISION PARTICLE-MOVING ALGORITHM FOR PARTICLE-IN-CELL SIMULATION OF PLASMA\*

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## Abstract

A new particle-moving algorithm for particle-in-cell simulation of plasma is developed based on the Linear Multistep Method. The conventional and the new algorithms are investigated by numerical experiments, which are conducted in three typical fashions of the electron motions in electromagnetic fields, that is, cyclotron in homogeneous magnetic field, drift in  $\mathbf{E} \times \mathbf{B}$  field and motions in inhomogeneous magnetic field. The new algorithm not only improves the accuracy but also relaxes the time step condition for the simulation. It can increase the computation efficiency.

## INTRODUCTION

One of the most important parts of the PIC plasma simulation process is the particles pusher [2, 3]. The typical method of the simulation uses the Boris leapfrog algorithm to push charged particles because of its simplicity [4]. When there is Lorentz Force, it will lead to the decline of the accuracy, since it has to use the velocity of integer points to estimate that of half integer points. A new particle-moving algorithm is developed based on the Linear Multistep Method [5]. The conventional and the new algorithms are investigated by numerical experiments [6].

## SIMULATION METHOD

We developed a new numerical scheme for particles movement which is as simple as the Leapfrog scheme but more accurate. In the Leapfrog method the particle velocity or the position is only calculated from the previous step. This is single step method. With the linear combinations of the velocity and acceleration on the former time steps which has been calculated, the new algorithm is multistep method that may has a high accuracy and takes the follow form:

$$\mathbf{r}_{n+1} = \alpha_0 \mathbf{r}_{n-1} + \alpha_1 \mathbf{r}_n + \Delta t (\beta_0 \mathbf{r}'_{n-1} + \beta_1 \mathbf{r}'_n) + \Delta t^2 (\gamma_0 \mathbf{r}''_{n-1} + \gamma_1 \mathbf{r}''_n) \quad (3)$$

where  $\mathbf{r}$  is the displacement,  $\alpha_0, \alpha_1, \beta_0, \beta_1, \gamma_0, \gamma_1$  are undetermined coefficients. As we know, the first-order derivative of  $\mathbf{r}$  is the velocity and the second-order derivative of  $\mathbf{r}$  is the acceleration. The Linear Multistep Method is using the Taylor series expansion method to construct the function. Assuming the value of  $\mathbf{r}$  at  $t_{n+1}$  is

$\mathbf{r}_{n+1}^-$ , expanding the fifth order approximation of Taylor

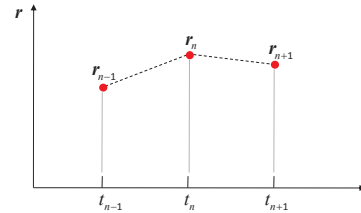


Figure 1: The linear multistep method.

expansion at  $t_n$ , as follows:

$$\begin{aligned} \mathbf{r}_{n+1}^- = \mathbf{r}(t_n + h) = & \mathbf{r}_n + \mathbf{r}'_n h + \frac{\mathbf{r}''_n}{2!} h^2 + \frac{\mathbf{r}^{(3)}_n}{3!} h^3 \\ & + \frac{\mathbf{r}^{(4)}_n}{4!} h^4 + \frac{\mathbf{r}^{(5)}_n}{5!} h^5 + O(h^6) \end{aligned} \quad (4)$$

Expanding the  $\mathbf{r}_{n-1}$  at  $t_n$  and taking it to the right of Eq.3:

$$\begin{aligned} \mathbf{r}_{n+1} = & (\alpha_0 + \alpha_1) \mathbf{r}_n + (-\alpha_0 + \beta_0 + \beta_1) \mathbf{r}'_n h + \\ & \left( \frac{\alpha_0}{2} - \beta_0 + \gamma_0 + \gamma_1 \right) \mathbf{r}''_n h^2 + \left( -\frac{\alpha_0}{6} + \frac{\beta_0}{2} - \gamma_0 \right) \mathbf{r}^{(3)}_n h^3 + \\ & \left( \frac{\alpha_0}{24} - \frac{\beta_0}{6} + \frac{\gamma_0}{2} \right) \mathbf{r}^{(4)}_n h^4 + \left( -\frac{\alpha_0}{120} + \frac{\beta_0}{24} - \frac{\gamma_0}{6} \right) \mathbf{r}^{(5)}_n h^5 + O(h^6) \end{aligned} \quad (5)$$

Compare the coefficients of the Eq. 4 and Eq. 5, we get the follow equations:

$$\left\{ \begin{array}{ll} \alpha_0 + \alpha_1 = 1 & : h^0 \\ -\alpha_0 + \beta_0 + \beta_1 = 1 & : h^1 \\ \frac{\alpha_0}{2} - \beta_0 + \gamma_0 + \gamma_1 = \frac{1}{2} & : h^2 \\ -\frac{\alpha_0}{6} + \frac{\beta_0}{2} - \gamma_0 = \frac{1}{6} & : h^3 \\ \frac{\alpha_0}{24} - \frac{\beta_0}{6} + \frac{\gamma_0}{2} = \frac{1}{24} & : h^4 \\ -\frac{\alpha_0}{120} + \frac{\beta_0}{24} - \frac{\gamma_0}{6} = \frac{1}{120} & : h^5 \end{array} \right. \quad (6)$$

All the coefficients can be get by solving the Eq. 6,

$$\alpha_0 = -31, \alpha_1 = 32, \beta_0 = -14, \beta_1 = -16, \gamma_0 = -2, \gamma_1 = 4$$

They are so large that can accumulate and amplify the errors. It will lead the instability of the algorithm. If we solve the first five equations and let  $\alpha_1$  be the variable, then the others can be expressed as:

$$\alpha_0 = 1 - \alpha_1, \beta_0 = 2 - \frac{\alpha_1}{2}, \beta_1 = -\frac{\alpha_1}{2}, \gamma_0 = \frac{2}{3} - \frac{\alpha_1}{12}, \gamma_1 = \frac{4}{3} + \frac{\alpha_1}{12}$$

The fourth order accuracy of the  $\mathbf{r}$  can be obtained when

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taking the value of  $\alpha_1$  from 0 to 1. If  $\alpha_1 = 1$ , the Eq. 3 is:

$$\mathbf{r}_{n+1} = \mathbf{r}_n + \frac{h}{2}(3\mathbf{r}'_{n-1} - \mathbf{r}'_n) + \frac{h^2}{12}(7\mathbf{r}''_{n-1} + 17\mathbf{r}''_n) \quad (7)$$

The truncation error is:

$$R_{n+1} = \frac{31}{720}h^5\mathbf{r}_n^{(5)} + O(h^6) \quad (8)$$

Using the same method, the formula of velocity has the form:

$$\mathbf{v}_{n+1} = \alpha_0\mathbf{v}_{n-1} + \alpha_1\mathbf{v}_n + h(\beta_{-1}\mathbf{v}'_{n+1} + \beta_0\mathbf{v}'_n + \beta_1\mathbf{v}'_{n-1}) \quad (9)$$

Eq. 9 is a two-step implicit scheme if  $\beta_{-1} \neq 0$ . We should predict the  $\mathbf{v}_{n+1}$  first for solve the  $\mathbf{v}'_{n+1}$  using the two-step explicit scheme:

$$\mathbf{v}_{n+1} = \alpha_0\mathbf{v}_{n-1} + \alpha_1\mathbf{v}_n + h(\beta_0\mathbf{v}'_n + \beta_1\mathbf{v}'_{n-1}) \quad (10)$$

Usually the implicit and the explicit scheme should have the same order, so the predictor- corrector function is:

$$\begin{cases} \bar{\mathbf{v}}_{n+1} = 5\mathbf{v}_{n-1} - 4\mathbf{v}_n + h(4\mathbf{v}'_n + 2\mathbf{v}'_{n-1}) & \text{predictor} \\ \mathbf{v}_{n+1} = \mathbf{v}_n + h(5\mathbf{v}'_{n+1} + 8\mathbf{v}'_n - \mathbf{v}'_{n-1})/12 & \text{corrector} \end{cases} \quad (11)$$

The Eq. 11 is a two-step scheme with three order accuracy.

Now the expression of the new algorithm is get. The precision of the displacement is the fourth order and the velocity is the third order that is very close to the fourth order Runge-Kutta method but more concise.

## RESULT COMPARISON

The comparison of the Linear Multistep Method with the leapfrog method is discussed through the numerical experiments, which are conducted in three typical fashions of the electron motions in electromagnetic fields, that is, cyclotron in homogeneous magnetic field, drift in  $\mathbf{E} \times \mathbf{B}$  field and motions in inhomogeneous magnetic field.

### Cyclotron in Homogeneous Magnetic Field

This test involves calculation of the electron trace under the effect of uniform magnetic field. The initial velocities  $v_x = 0$ ,  $v_y = 1.0 \times 10^6$  m/s,  $v_z = 0$  are applied to the electron.

The magnetic field with the constant value of 0.004T is installed in the system oriented in vertical z direction, when the electric field is set up to zero. The electron should perform the cyclotron motion with gyration radius  $r_L$  (in this test  $r_L = 0.00142$ m) and the cyclotron period  $T$  (in this test  $T = 8.93 \times 10^{-9}$ s). Figure 2(a) shows the cyclotron track of the electron in the magnetic field when the time step  $\Delta t = T/50$ . As we see, the trajectory calculated from the linear multistep method is almost equal to the analytical. That means the accuracy of electron orbits is very high. The energy of electron should be unaffected by the homogeneous magnetic field, while the energy increment should be zero, that is  $\Delta W / W_0 \approx 0$ . The accuracy in electron energy calculating when

$\Delta t = T/50$  has been compared in the two algorithms. The energy increment of the two algorithms as the function of amount of the time step is presented in Figure 2(c).

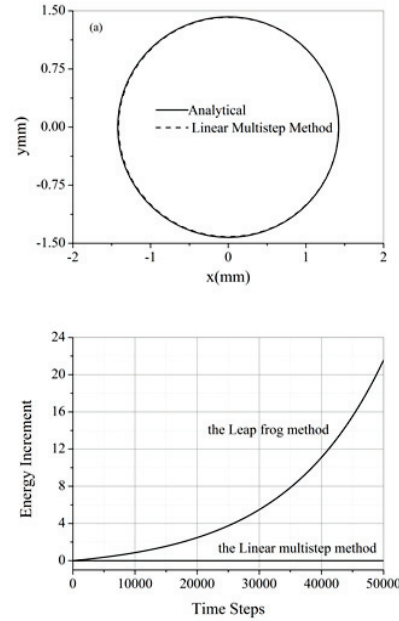


Figure 2: The comparison of the linear multistep method with the leapfrog method and the Runge-Kutta. (a) Cyclotron track of electron in magnetic field. (b) Energy increment as the function of amount of the time step.

At the end of the  $5 \times 10^4$  time step, the energy increment of the linear multistep method is under  $1 \times 10^{-4}$  and the Leap Frog method is about 25 times. That means the Linear Multistep Method can keep long time energy conservation, which is much better than the other two methods.

### Drift in Constant $\mathbf{E} \times \mathbf{B}$ Field

In the preceding section we have proved the correctness of the electron motion integrator in the presence of the constant magnetic field. The next step is to demonstrate accuracy of the electron trajectories in the electromagnetic field system. In this test the same constant magnetic field is used, while the constant electric field of  $1.0 \times 10^4$  V/m is set in -y direction. The velocity distribution of electron are also same. This velocity corresponds to the guiding centre drift velocity of the electron:

$$\mathbf{v}_{E \times B} = \frac{\mathbf{E} \times \mathbf{B}}{|\mathbf{B}|^2} \quad (12)$$

When the time step  $\Delta t = T/100$  the trajectory of the electron is shown in Figure 3(a). It is nearly the same with the analytical. The electron clearly execute  $\mathbf{E} \times \mathbf{B}$  drift and the guiding centre of the drift motion moves with the same velocity as expected. Figure 3(b) shows the position errors of the two methods. The position error of the linear multistep method is much lower than the Leap frog.

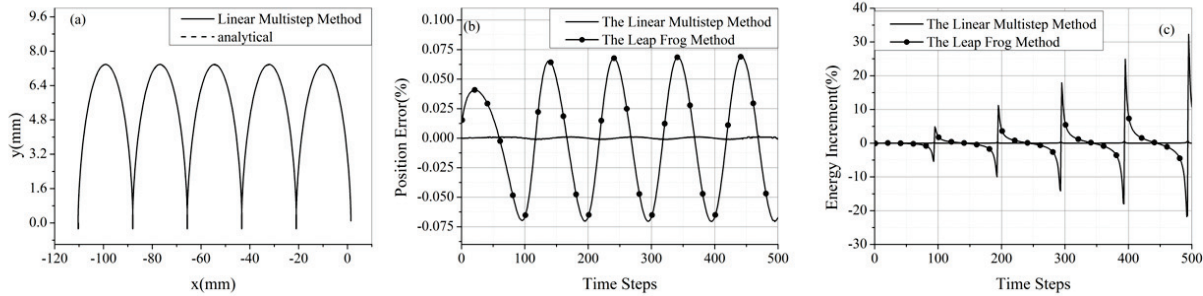


Figure 3: Test in constant  $E \times B$  field. (a) Drift track of electron in constant  $E \times B$  field. (b) Position errors of the three methods. (c) Energy increment of the three methods.

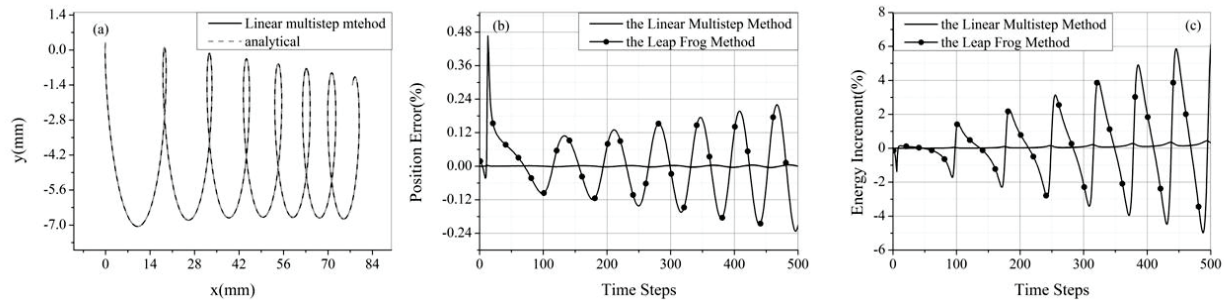


Figure 4: Test in inhomogeneous magnetic field. (a) Drift track of electron in inhomogeneous magnetic field. (b) Position errors of the three methods. (c) Energy increment of the three method

Figure 3(c) shows the Energy increment of the two methods that gives a same result.

### Motions in Inhomogeneous Magnetic Field

As the extension of the first two test, in this test the magnetic field is inhomogeneous in the  $z$  direction as a function of  $x$  is given as  $B_z(x) = 0.04x + 0.004$ (T), while the constant electric field of  $1.0 \times 10^4$  V/m is set in  $+y$  direction. The initial velocities is also same and the initial position is  $x_0 = y_0 = 0$ .  $T/100$  is set as time step, and  $T$  is the cyclotron period of the initial time. The guiding centre drift velocity of the electron is changed with the time and position (see Figure 4(a)). As can be see in Figure 4(b) and Figure 4(c), the Linear Multistep Method also has a much higher precision than the Leap frog method.

### CONCLUSION

From the comparison, the precision of the linear Multistep method is much better than the Leapfrog method in the same time step with a very simple format. But the precision of this method maybe a little worse than the fourth order Runge-Kutta method because the precision of the velocity is three order. Note that in the

beginning we should calculate the value on the second point with the fourth order Runge-Kutta method for starting this algorithm [7]. As its high precision and simply format it can be used in the particle-in-cell simulation of plasma directly.

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